Lecture Notes in Quantum Mechanics

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These are the lecture notes ↗ of quantum mechanics courses ↗ that are given by DC at Ben-Gurion University. They cover textbook topics that are listed below, and also additional advanced topics (marked by *) at the same level of presentation.

Fundamentals I

- The classical description of a particle
- Hilbert space formalism
- A particle in an N site system
- The continuum limit ($N = \infty$)
- Translations and rotations

Fundamentals II

- Quantum states / EPR / Bell
- The 4 postulates of the theory
- The evolution operator
- The rate of change formula
- Finding the Hamiltonian for a physical system
- The non-relativistic Hamiltonian
- The "classical" equation of motion
- Symmetries and constants of motion

Fundamentals III

- Group theory, Lie algebra
- Representations of the rotation group
- Spin 1/2, spin 1 and $Y^{\ell,m}$
- Multiplying representations
- Addition of angular momentum (*)
- The Galilei group (*)
- Transformations and invariance (*)

Dynamics and driven systems

- Systems with driving
- The interaction picture
- The transition probability formula
- Fermi golden rule
- Markovian master equations
- Cross section / Born

- The adiabatic equation
- The Berry phase
- Theory of adiabatic transport (*)
- Linear response theory and Kubo (*)
- The Born-Oppenheimer picture (*)

The Green function approach (*)

- The evolution operator
- Feynman path integral
- The resolvent and the Green function

- Perturbation theory for the resolvent
- Perturbation theory for the propagator
- Complex poles from perturbation theory

Scattering theory (*)

- Scattering: T matrix formalism
- Scattering: S matrix formalism
- Scattering: R matrix formalism
- Cavity with leads 'mesoscopic' geometry
- Spherical geometry, phase shifts
- Cross section, optical theorem, resonances

Quantum mechanics in practice

- The dynamics of a two level system
- Fermions and Bosons in a few site system (*)
- Quasi 1D network systems (*)

- Approximation methods for H diagonalization
- Perturbation theory for $H = H_0 + V$
- Wigner decay, LDOS, scattering resonances

- The Aharonov-Bohm effect
- Magnetic field (Landau levels, Hall effect)
- Motion in a central potential, Zeeman
- The Hamiltonian of spin 1/2 particle, implications

Special Topics (*)

- Quantization of the EM field
- Fock space formalism

- The Wigner Weyl formalism
- Theory of quantum measurements
- Theory of quantum computation
- The foundations of Statistical Mechanics

Opening remarks

These lecture notes are based on 3 courses in non-relativistic quantum mechanics that are given at BGU: "Quantum 2" (undergraduates), "Quantum 3" (graduates), and "Selected topics in Quantum and Statistical Mechanics" (graduates). The lecture notes are self contained, and give the *road map* to quantum mechanics. However, they do not intend to come instead of the standard textbooks. In particular I recommend:

[1] L.E.Ballentine, Quantum Mechanics (library code: QC 174.12.B35).

[2] J.J. Sakurai, Modern Quantum mechanics (library code: QC 174.12.S25).

[3] Feynman Lectures Volume III.

[4] A. Messiah, Quantum Mechanics. [for the graduates]

The major attempt in this set of lectures was to give a self contained presentation of quantum mechanics, *which is not based on the historical "quantization" approach.* The main inspiration comes from Ref.[3] and Ref.[1]. The challenge was to find a compromise between the over-heuristic approach of Ref.[3] and the too formal approach of Ref.[1].

Another challenge was to give a presentation of scattering theory that goes well beyond the common undergraduate level, but still not as intimidating as in Ref.[4]. A major issue was to *avoid the over emphasis on spherical geometry.* The language that I use is much more suitable for research with "mesoscopic" orientation.

Some *highlights* for those who look for original or advanced pedagogical pieces: The EPR paradox, Bell's inequality, and the notion of quantum state; The 4 postulates of quantum mechanics; Berry phase and adiabatic processes; Linear response theory and the Kubo formula; Wigner-Weyl formalism; Quantum measurements; Quantum computation; The foundations of Statistical mechanics. Note also the following example problems: Analysis of systems with 2 or 3 or more sites; Analysis of the Landau-Zener transition; The Bose-Hubbard Hamiltonian; Quasi 1D networks; Aharonov-Bohm rings; Various problems in scattering theory.

Additional topics are covered by:

[5] D. Cohen, *Lecture Notes in Statistical Mechanics and Mesoscopic*, arXiv:1107.0568

Credits

The first drafts of these lecture notes were prepared and submitted by students on a weekly basis during 2005. Undergraduate students were requested to use HTML with ITEX formulas. Typically the text was written in Hebrew. Graduates were requested to use Latex. The drafts were corrected, integrated, and in many cases completely re-written by the lecturer. The English translation of the undergraduate sections has been prepared by my former student *Gilad Rosenberg*. He has also prepared most of the illustrations. The current version includes further contributions by my PhD students *Maya Chuchem* and *Itamar Sela*. I also thank my colleague Prof. *Yehuda Band* for some comments on the text. The arXiv versions are quite remote from the original (submitted) drafts, but still I find it appropriate to list the names of the students who have participated: Natalia Antin, Roy Azulai, Dotan Babai, Shlomi Batsri, Ynon Ben-Haim, Avi Ben Simon, Asaf Bibi, Lior Blockstein, Lior Boker, Shay Cohen, Liora Damari, Anat Daniel, Ziv Danon, Barukh Dolgin, Anat Dolman, Lior Eligal, Yoav Etzioni, Zeev Freidin, Eyal Gal, Ilya Gurwich, David Hirshfeld, Daniel Hurowitz, Eyal Hush, Liran Israel, Avi Lamzy, Roi Levi, Danny Levy, Asaf Kidron, Ilana Kogen, Roy Liraz, Arik Maman, Rottem Manor, Nitzan Mayorkas, Vadim Milavsky, Igor Mishkin, Dudi Morbachik, Ariel Naos, Yonatan Natan, Idan Oren, David Papish, Smadar Reick Goldschmidt, Alex Rozenberg, Chen Sarig, Adi Shay, Dan Shenkar, Idan Shilon, Asaf Shimoni, Raya Shindmas, Ramy Shneiderman, Elad Shtilerman, Eli S. Shutorov, Ziv Sobol, Jenny Sokolevsky, Alon Soloshenski, Tomer Tal, Oren Tal, Amir Tzvieli, Dima Vingurt, Tal Yard, Uzi Zecharia, Dany Zemsky, Stanislav Zlatopolsky.

Contents

Fundamentals (part I)

Fundamentals (part II)

Fundamentals (part III)

Dynamics and Driven Systems

The Green function approach

Scattering Theory

QM in Practice (part I)

QM in Practice (part II)

QM in Practice (part III)

Special Topics

Fundamentals (part I)

[1] Introduction

━━━━ [1.1] The building blocks of the universe

The universe consists of a variety of particles which are described by the "standard model". The known particles are divided into two groups:

- Quarks: constituents of the proton and the neutron, which form the ~ 100 nuclei known to us.
- Leptons: include the electrons, muons, taus, and the neutrinos.

The interaction between the particles is via fields (direct interaction between particles is contrary to the principles of the special theory of relativity). These interactions are responsible for the way material is "organized". We shall consider in this course the electromagnetic interaction. The electromagnetic field is described by the Maxwell equations. Within the framework of the "standard model" there are additional gauge fields that can be treated on equal footing. In contrast the gravity field has yet to be incorporated into quantum theory.

━━━━ [1.2] A particle in an electromagnetic field

This section is inteted for 3rd year BSc Physics students: its purpose is to place this course in the context of classical analytical mechanics. Those who do not have this eduction can skip sections [1.2]-[1.3]-[1.4]. A terse summary of classical mechanics is provided in lecture [2], and can be skipped as well.

Within the framework of classical electromagnetism, the electromagnetic field is described by the scalar potential $V(x)$ and the vector potential $\vec{A}(x)$. In addition one defines:

$$
\begin{aligned}
\mathcal{B} &= \nabla \times \vec{A} \\
\mathcal{E} &= -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} - \nabla V
\end{aligned}
\tag{1.1}
$$

We will not be working with natural units in this course, but from now on we are going to absorb the constants c and e in the definition of the scalar and vector potentials:

$$
\begin{aligned}
\frac{e}{c}A &\to A, & eV &\to V \\
\frac{e}{c}\mathcal{B} &\to \mathcal{B}, & e\mathcal{E} &\to \mathcal{E}
\end{aligned}
\tag{1.2}
$$

In classical mechanics, the effect of the electromagnetic field is described by Newton's second law with the Lorentz force. Using the above units convention we write:

$$
\ddot{x} = \frac{1}{\mathsf{m}}\left(\mathcal{E} - \mathcal{B} \times v\right)
\tag{1.3}
$$

The Lorentz force dependents on the velocity of the particle. This seems arbitrary and counter intuitive, but we shall see in the future how it can be derived from general and fairly simple considerations.

In analytical mechanics it is customary to derive the above equation from a Lagrangian. Alternatively, one can use a Legendre transform and derive the equations of motion from a Hamiltonian:

$$
\begin{aligned}
\dot{x} &= \frac{\partial \mathcal{H}}{\partial p} \\
\dot{p} &= -\frac{\partial \mathcal{H}}{\partial x}
\end{aligned}
\tag{1.4}
$$

where the Hamiltonian is:

$$\mathcal{H}(x,p) = \frac{1}{2m}(p - A(x))^2 + V(x) \tag{1.5}$$

The Hamiltonian that describes a system of several charged particles in 3 dimensional space, including the electromagnetic field in the Coulomb gauge, can be written as follows:

$$\mathcal{H}(\mathbf{r}, \mathbf{p}, A, \mathcal{E}) \;\; = \;\; \sum_i \frac{1}{2m_i}(\mathbf{p}_i - e_i A(\mathbf{r}_i))^2 + \sum_{\langle ij \rangle} \frac{e_i e_j}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{1}{8\pi} \int (\mathcal{E}_\perp^2 + c^2 (\nabla \times A)^2) d^3 x \tag{1.6}$$

The canonical coordinates of the particles are $(\mathbf{r}_i, \mathbf{p}_i)$, and the canonical coordinates of the radiations field are $(A, \mathcal{E}_\perp)$. The magnetic field is defined as $\mathcal{B} = \nabla \times A$. One can define an electrostatic electric field $\mathcal{E}_\parallel$, and express the second term as an integral over $\mathcal{E}_\parallel^2 / (8\pi)$.

The units of $\mathcal{E}$ as well as the prefactor $1/(8\pi)$ are determined via Coulomb law as in the Gaussian CGI convention. The units of A are determined as in the SI convention, namely, we do not make here the replacement $A \mapsto (1/c)A$, and therefore the equations of motion for the radiation field imply that $\mathcal{E}_\perp = -\dot{A}$. Accordingly $\mathcal{B}$ and $\mathcal{E}$ do not have the same units, and the Lorentz force formula does not included $(1/c)$ prefactor.

In the absence of particles the radiation term of the Hamiltonian describes waves that have a dispersion relation $\omega = c|k|$. The strength of the interaction is determined by the coupling constants e_i. Assuming that all the particles have elementary charge $e_i = \pm e$, it follows that after canonical quantization (see below) the above Hamiltonian is characterized by a single dimensionless coupling constant $e^2/(\hbar c)$, which is knows as the "fine-structure constant".

======= [1.3] Canonical quantization

The historical method of deriving the quantum description of a system is canonical quantization. In this method we assume that the particle is described by a "wave function" that obeys the equation:

$$\frac{\partial \Psi(x)}{\partial t} = -\frac{i}{\hbar} \mathcal{H}\left(x, -i\hbar \frac{\partial}{\partial x}\right) \Psi(x) \tag{1.7}$$

This seems arbitrary and counter-intuitive. In this course we shall abandon the historical approach. Instead we shall construct quantum mechanics using simple heuristic considerations. Later we shall see that classical mechanics can be obtained as a special limit of the quantum theory.

======= [1.4] Second quantization

The method for quantizing the electromagnetic radiation field is to write its Hamiltonian as a sum of harmonic oscillators (normal modes) and then to quantize the oscillators. It is exactly the same as finding the normal modes of spheres connected with springs. Every normal mode has a characteristic frequency. The ground state of the field (all the oscillators are in the ground state) is called the "vacuum state". If a specific oscillator is excited to level n, we say that there are n photons with frequency ω in the system.

A similar formalism is used to describe a many particle system. A vacuum state and occupation states are defined. This formalism is called "second quantization". A better name would be "formalism of quantum field theory". One important ingredient of this formulation is the distinction between fermions and bosons.

In the first part of this course we regard the electromagnetic field as a classical entity, where $V(x), A(x)$ are given as an input. The distinction between fermions and bosons will be obtained using the somewhat unnatural language of "first quantization".

═══════ [1.5] Definition of mass

The "gravitational mass" is defined using a weighting apparatus. Since gravitational theory is not includes in this course, we shall not use that definition. Another possibility is to define "inertial mass". This type of mass is determined by considering the collision of two bodies:

$$m_1 v_1 + m_2 v_2 = m_1 u_1 + m_2 u_2 \tag{1.8}$$

Accordingly one can extract the mass ratio of the two bodies:

$$\frac{m_1}{m_2} = -\frac{u_2 - v_2}{u_1 - v_1} \tag{1.9}$$

In order to give information on the inertial mass of an object, we have to agree on some reference mass, say the "kg", to set the units. (less arbitrary would be to take the mass of the proton as the reference). Anyway, within the framework of quantum mechanics the above Newtonian definition of inertial mass will not be used. Rather we define mass in an absolute way, that does not require to fix a reference mass. We shall define mass as a parameter in the "dispersion relation".

The dispersion relation.– It is possible to prepare a "monochromatic" beam of particles (say electrons) that all have the same velocity, and the same De-Broglie wavelength. The velocity of the particles can be measured by using a pair of rotating circular plates (discs). The wavelength of the beam can be measured using a diffraction grating. We define the momentum of the moving particles ("wave number") as:

$$p = 2\pi/\text{wavelength} \tag{1.10}$$

It is possible to find (say by an experiment) the relation between the velocity of the particle and its momentum. This relation is called the "dispersion relation". Here is a plot of what we expect to observe:
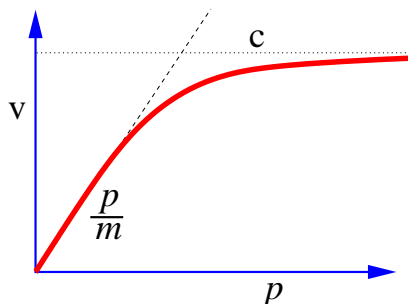
For low (non relativistic) velocities the relation is approximately linear:

$$v = \frac{cp}{\sqrt{(mc^2)^2 + (cp)^2}} c \approx \frac{1}{m} p \tag{1.11}$$

This relation defines the "mass" parameter. The implied units of mass are

$$[m] = \frac{T}{L^2} \tag{1.12}$$

If we use arbitrary units for measuring mass, say "kg", then the conversion prescription is:

$$m[\text{kg}] = \hbar \, m \left[\frac{\text{second}}{\text{meter}^2} \right], \qquad \hbar = \frac{h}{2\pi} \tag{1.13}$$

where $\hbar$ is known as the Planck constant.

======= [1.6] Semiclassical perspective

Within the semi-classical picture we specify the state of a particle using two dynamical variables (x, p). It is a phenomenological observation that the momentum (as defined in the previous section) can be increased by applying "force". In fact we can define the term force in a semi-Newtonian way:

$$\frac{d}{dt}\boldsymbol{p} \;=\; F \;\equiv\; -\frac{\partial V(\boldsymbol{x})}{\partial \boldsymbol{x}} \tag{1.14}$$

where $V(x)$ is a function that describes the field of force. Similarly we can define kinetic-energy-function $K(p)$ from which the dispersion relation is derived:

$$\frac{d}{dt}\boldsymbol{x} \;=\; v(\boldsymbol{p}) \;\equiv\; \frac{\partial K(\boldsymbol{p})}{\partial \boldsymbol{p}} \tag{1.15}$$

The standard dispersion relation is

$$K(p) \;=\; \sqrt{(\mathsf{m}c^2)^2 + (cp)^2} \;\approx\; mc^2 + \frac{p^2}{2\mathsf{m}} \tag{1.16}$$

The latter expression is the non-relativistic approximation. We can define Hamiltonian formally as follows

$$H(\boldsymbol{x}, \boldsymbol{p}) \;=\; K(\boldsymbol{p}) + V(\boldsymbol{x}) \tag{1.17}$$

and derive from it the equations of motion. We define the energy as

$$E \;=\; H(\boldsymbol{x}, \boldsymbol{p}) \tag{1.18}$$

It is easily verified that E is a constant of motion ($dE/dt = 0$). The energy has units of *frequency*. The conversion to SI units is:

$$E\left[\frac{\text{kg} \cdot \text{meter}^2}{\text{second}^2}\right] \;=\; \hbar\, E\left[\frac{1}{\text{second}}\right] \tag{1.19}$$

======= [1.7] Spin

Apart from the degrees of freedom of being in space, the particles also have an inner degree of freedom called "spin". We say that a particle has spin s if its inner degree of freedom is described by a representation of the rotations group of dimension $2s+1$. For example, "spin $\frac{1}{2}$" can be described by a representation of dimension 2, and "spin 1" can be described by a representation of dimension 3. In order to make this abstract statement clearer we will look at several examples.

- Electrons have spin $\frac{1}{2}$, hence 180° difference in polarization ("up" and "down") means orthogonality.

- Photons have spin 1, hence 90° difference in linear polarizations means orthogonality.

If we position two polarizers one after the other in the angles that were noted above, no particles will pass through. We see that an abstract mathematical consideration (representations of the rotational group) has very realistic consequences.

[2] Digression: The classical description of nature

═══════ [2.1] The electromagnetic field

The electric field $\mathcal{E}$ and the magnetic field $\mathcal{B}$ can be derived from the vector potential A and the electric potential V:

$$\begin{aligned}
\mathcal{E} &= -\nabla V - \frac{1}{c}\frac{\partial \vec{A}}{\partial t} \\
\mathcal{B} &= \nabla \times \vec{A}
\end{aligned}$$
(2.1)

The electric potential and the vector potential are not uniquely determined, since the electric and the magnetic fields are not affected by the following changes:

$$\begin{aligned}
V &\mapsto \tilde{V} = V - \frac{1}{c}\frac{\partial \Lambda}{\partial t} \\
A &\mapsto \tilde{A} = A + \nabla \Lambda
\end{aligned}$$
(2.2)

where $\Lambda(x,t)$ is an arbitrary scalar function. Such a transformation of the potentials is called "gauge". A special case of "gauge" is changing the potential V by an addition of a constant.

Gauge transformations do not affect the classical motion of the particle since the equations of motion contain only the derived fields $\mathcal{E}, \mathcal{B}$.

$$\frac{d^2 x}{dt^2} = \frac{1}{\mathsf{m}}\left[e\mathcal{E} - \frac{e}{c}\mathcal{B} \times \dot{x} \right]$$
(2.3)

This equation of motion can be derived from the Lagrangian:

$$\mathcal{L}(x, \dot{x}) = \frac{1}{2}\mathsf{m}\dot{x}^2 + \frac{e}{c}\dot{x}A(x,t) - eV(x,t)$$
(2.4)

Or, alternatively, from the Hamiltonian:

$$\mathcal{H}(x,p) = \frac{1}{2\mathsf{m}}(p - \frac{e}{c}A)^2 + eV$$
(2.5)

═══════ [2.2] The Lorentz Transformation

The Lorentz transformation takes us from one reference frame to the other. A Lorentz boost can be written in matrix form as:

$$S = \begin{pmatrix} \gamma & -\gamma\beta & 0 & 0 \\ -\gamma\beta & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$
(2.6)

where β is the velocity of our reference frame relative to the reference frame of the lab, and

$$\gamma = \frac{1}{\sqrt{1 - \beta^2}}$$
(2.7)

We use units such that the speed of light is $c = 1$. The position of the particle in space is:

$$\mathbf{x} = \begin{pmatrix} t \\ x \\ y \\ z \end{pmatrix} \tag{2.8}$$

and we write the transformations as:

$$\mathbf{x}' = S\mathbf{x} \tag{2.9}$$

We shall see that it is convenient to write the electromagnetic field as:

$$F = \begin{pmatrix} 0 & \mathcal{E}_1 & \mathcal{E}_2 & \mathcal{E}_3 \\ \mathcal{E}_1 & 0 & \mathcal{B}_3 & -\mathcal{B}_2 \\ \mathcal{E}_2 & -\mathcal{B}_3 & 0 & \mathcal{B}_1 \\ \mathcal{E}_3 & \mathcal{B}_2 & -\mathcal{B}_1 & 0 \end{pmatrix} \tag{2.10}$$

We shall argue that this transforms as:

$$F' = SFS^{-1} \tag{2.11}$$

or in terms of components:

$$
\begin{array}{ll}
\mathcal{E}_1' = \mathcal{E}_1 & \mathcal{B}_1' = \mathcal{B}_1 \\
\mathcal{E}_2' = \gamma(\mathcal{E}_2 - \beta\mathcal{B}_3) & \mathcal{B}_2' = \gamma(\mathcal{B}_2 + \beta\mathcal{E}_3) \\
\mathcal{E}_3' = \gamma(\mathcal{E}_3 + \beta\mathcal{B}_2) & \mathcal{B}_3' = \gamma(\mathcal{B}_3 - \beta\mathcal{E}_2)
\end{array}
$$

===== [2.3] Momentum and energy of a particle

Let us write the displacement of the particle as:

$$d\mathbf{x} = \begin{pmatrix} dt \\ dx \\ dy \\ dz \end{pmatrix} \tag{2.12}$$

We also define the proper time (as measured in the particle frame) as:

$$d\tau^2 = dt^2 - dx^2 - dy^2 - dz^2 = (1 - v_x{}^2 - v_y{}^2 - v_z{}^2)dt^2 \tag{2.13}$$

or:

$$d\tau = \sqrt{1 - v^2}\, dt \tag{2.14}$$

The relativistic velocity vector is:

$$\mathbf{u} = \frac{d\mathbf{x}}{d\tau}, \qquad [u_t^2 - u_x^2 - u_y^2 - u_z^2 = 1] \tag{2.15}$$

It is customary to define the *non-canonical* momentum as

$$\mathbf{p} = \mathbf{m}\mathbf{u} = \begin{pmatrix} \epsilon \\ \mathbf{p}_x \\ \mathbf{p}_y \\ \mathbf{p}_z \end{pmatrix} \tag{2.16}$$

According to the above equations we have:

$$\epsilon^2 - \mathbf{p}_x^2 - \mathbf{p}_y^2 - \mathbf{p}_z^2 = \mathbf{m}^2 \tag{2.17}$$

and write the dispersion relation:

$$\begin{aligned} \epsilon &= \sqrt{\mathbf{m}^2 + \mathbf{p}^2} \\ v &= \frac{p}{\sqrt{\mathbf{m}^2 + \mathbf{p}^2}} \end{aligned} \tag{2.18}$$

We note that for non-relativistic velocities $\mathbf{p}_i \approx \mathbf{m}v_i$ for $i = 1, 2, 3$ while:

$$\epsilon = \mathbf{m}\frac{dt}{d\tau} = \frac{\mathbf{m}}{\sqrt{1 - v^2}} \approx \mathbf{m} + \frac{1}{2}\mathbf{m}v^2 + \ldots \tag{2.19}$$

[2.4] Equations of motion for a particle

The non-relativistic equations of motion for a particle in an electromagnetic field are:

$$\mathbf{m}\frac{d\vec{v}}{dt} = e\mathcal{E} - e\mathcal{B} \times \vec{v} \tag{2.20}$$

The right hand side is the so-called Lorentz force $\vec{f}$. It gives the rate of change of the *non-canonical* momentum. The rate of change of the associated non-canonical energy E is

$$\frac{d\epsilon}{dt} = \vec{f} \cdot \vec{v} = e\mathcal{E} \cdot \vec{v} \tag{2.21}$$

The electromagnetic field has equations of motion of its own: the Maxwell equations. We shall see shortly that Maxwell equations are Lorentz invariant. But what Newton's second law as written above is not Lorentz invariant. In order for the Newtonian equations of motion to be Lorentz invariant we have to adjust them. It is not difficult to see that the obvious required revision is:

$$\mathbf{m}\frac{d\mathbf{u}}{d\tau} = eF\mathbf{u} \tag{2.22}$$

To prove the invariance under the Lorentz transformation we write:

$$\frac{du'}{d\tau} = \frac{d}{d\tau}(Su) = S\frac{d}{d\tau}u = S\frac{e}{\mathbf{m}}F\mathbf{u} = \frac{e}{\mathbf{m}}SFS^{-1}(S\mathbf{u}) = \frac{e}{\mathbf{m}}F'\mathbf{u}' \tag{2.23}$$

Hence we have deduced the transformation $F' = SFS^{-1}$ of the electromagnetic field.

═══════ [2.5] Equations of motion of the field

Back to the Maxwell equations. A simple way of writing them is

$$\partial^{\dagger} F = 4\pi J^{\dagger} \tag{2.24}$$

where the derivative operator ∂, and the four-current J, are defined as:

$$\partial = \begin{pmatrix} \frac{\partial}{\partial t} \\ -\frac{\partial}{\partial x} \\ -\frac{\partial}{\partial y} \\ -\frac{\partial}{\partial z} \end{pmatrix} \qquad\qquad \partial^{\dagger} = \left(\frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \tag{2.25}$$

and:

$$\mathbf{J} = \begin{pmatrix} \rho \\ J_x \\ J_y \\ J_z \end{pmatrix} \qquad\qquad \mathbf{J}^{\dagger} = (\rho, -J_x, -J_y, -J_z) \tag{2.26}$$

The Maxwell equations are invariant because $\mathbf{J}$ and ∂ transform as vectors. For more details see Jackson. An important note about notations: in this section we have used what is called a "contravariant" representation for the column vectors. For example $u = \text{column}(u_t, u_x, u_y, u_z)$. For the "adjoint" we use the "covariant" representation $u = \text{row}(u_t, -u_x, -u_y, -u_z)$. Note that $u^{\dagger} u = (u_t)^2 - (u_x)^2 - (u_y)^2 - (u_z)^2$ is a Lorentz scalar.

[3] Hilbert space

══════ [3.1] Linear algebra

In Euclidean geometry, three dimensional vectors can be written as:

$$\vec{u} = u_1\vec{e}_1 + u_2\vec{e}_2 + u_3\vec{e}_3 \tag{3.1}$$

Using Dirac notation we can write the same as:

$$|u\rangle = u_1|e_1\rangle + u_2|e_2\rangle + u_3|e_3\rangle \tag{3.2}$$

We say that the vector has the representation:

$$|u\rangle \mapsto u_i = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} \tag{3.3}$$

The operation of a linear operator A is written as $|v\rangle = A|u\rangle$ which is represented by:

$$\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} \tag{3.4}$$

or shortly as $v_i = A_{ij}u_j$. Thus a linear operator is represented by a matrix:

$$A \mapsto A_{ij} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \tag{3.5}$$

══════ [3.2] Orthonormal basis

We assume that an inner product $\langle u|v\rangle$ has been defined. From now on we assume that the basis has been chosen to be orthonormal:

$$\langle e_i|e_j\rangle = \delta_{ij} \tag{3.6}$$

In such a basis the inner product (by linearity) can be calculated as follows:

$$\langle u|v\rangle = u_1^* v_1 + u_2^* v_2 + u_3^* v_3 \tag{3.7}$$

It can also be easily proved that the elements of the representation vector can be calculated as follows:

$$u_j = \langle e_j|u\rangle \tag{3.8}$$

And for the matrix elements we can prove:

$$A_{ij} = \langle e_i|A|e_j\rangle \tag{3.9}$$

═══════ [3.3] Completeness of the basis

In Dirac notation the expansion of a vector is written as:

$$|u\rangle \;=\; |e_1\rangle\langle e_1|u\rangle + |e_2\rangle\langle e_2|u\rangle + |e_3\rangle\langle e_3|u\rangle \tag{3.10}$$

which implies

$$\mathbf{1} \;=\; |e_1\rangle\langle e_1| + |e_2\rangle\langle e_2| + |e_3\rangle\langle e_3| \tag{3.11}$$

Above $\mathbf{1} \mapsto \delta_{ij}$ stands for the identity operator, and $P^j = |e_j\rangle\langle e_j|$ are called "projector operators",

$$\mathbf{1} \mapsto \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad P^1 \mapsto \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad P^2 \mapsto \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad P^3 \mapsto \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{3.12}$$

Now we can define the "completeness of the basis" as the requirement

$$\sum_j P^j \;=\; \sum_j |e_j\rangle\langle e_j| \;=\; \mathbf{1} \tag{3.13}$$

From the completeness of the basis it follows e.g. that for any operator

$$A \;=\; \left[\sum_i P^i\right] A \left[\sum_j P^j\right] \;=\; \sum_{i,j} |e_i\rangle\langle e_i|A|e_j\rangle\langle e_j| \;=\; \sum_{i,j} |e_i\rangle A_{ij}\langle e_j| \tag{3.14}$$

═══════ [3.4] Operators

In what follows we are interested in "normal" operators that are diagonal in some orthonormal basis. Say that we have an operator A. By definition, if it is normal, there exists an orthonormal basis $\{|a\rangle\}$ such that A is diagonal. Hence we write

$$A \;=\; \sum_a |a\rangle a \langle a| \;=\; \sum_a a P^a \tag{3.15}$$

In matrix representation it means:

$$\begin{pmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{pmatrix} = a_1 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + a_2 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + a_3 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{3.16}$$

It is useful to define what is meant by $\hat{B} = f(\hat{A})$ where $f()$ is an arbitrary function. Assuming that $\hat{A} = \sum |a\rangle a \langle a|$, it follows by definition that $\hat{B} = \sum |a\rangle f(a) \langle a|$. Another useful rule to remember is that if $A|k\rangle = B|k\rangle$ for some complete basis k, then it follows by linearity that $A|\psi\rangle = B|\psi\rangle$ for any vector, and therefore $A = B$.

With any operator A, we can associate an "adjoint operator" $A^\dagger$. By definition it is an operator that satisfies the following relation:

$$\langle u|Av\rangle = \langle A^\dagger u|v\rangle \tag{3.17}$$

If we substitute the basis vectors in the above relation we get the equivalent matrix-style definition

$$(A^\dagger)_{ij} = A_{ji}^* \tag{3.18}$$

If A is normal then it is diagonal in some orthonormal basis, and then also $A^\dagger$ is diagonal in the same basis. It follows that a normal operator has to satisfy the *necessary* condition $A^\dagger A = AA^\dagger$. As we show below this is also a *sufficient* condition for "normality".

We first consider Hermitian operators, and show that they are "normal". By definition they satisfy $A^\dagger = A$. If we write this relation in the eigenstate basis we deduce after one line of algebra that $(a^* - b)\langle a|b\rangle = 0$, where a and b are any two eigenvalues. If follows (considering $a = b$) that the eigenvalues are *real*, and furthermore (considering $a \neq b$) that eigenvectors that are associate with different eigenvalues are orthogonal. This is called the *spectral theorem*: one can find an orthonormal basis in which A is diagonal.

We now consider a general operator Q. Always we can write it as

$$Q = A + iB, \quad \text{with } A = \frac{1}{2}(Q + Q^\dagger), \quad \text{and } B = \frac{1}{2i}(Q - Q^\dagger) \tag{3.19}$$

One observes that A and B are Hermitian operators. It is easily verified that $Q^\dagger Q = QQ^\dagger$ iff $AB = BA$. It follows that there is an orthonormal basis in which both A and B are diagonal, and therefore Q is a normal operator.

We see that an operator is normal iff it satisfies the commutation $Q^\dagger Q = QQ^\dagger$ and iff it can be written as a function $f(H)$ of an Hermitian operator H. We can regard any H with non-degenerate spectrum as providing a specification of a basis, and hence any other operator that is diagonal in that basis can be expressed as a function of this H.

Of particular interest are unitary operators. By definition they satisfy $U^\dagger U = \mathbf{1}$, and hence they are "normal" and can be diagonalized in an orthonormal basis. Hence their eigenvalues satisfy $\lambda_r^* \lambda_r = 1$, which means that they can be written as:

$$U = \sum_r |r\rangle e^{i\varphi_r} \langle r| = e^{iH} \tag{3.20}$$

where H is Hermitian. This is an example for the general statement that any normal operator can be written as a function of some Hermitian operator H.

▭▭▭▭ [3.5] Generators

Later we are going to discuss unitary operations that depend on some parameter. For example: $\boldsymbol{D}(a)$ is distance a displacement; $\boldsymbol{R}(\Phi)$ is angle Φ rotation; and $\boldsymbol{U}(t)$ is evolution during time t. Note that $\boldsymbol{D}(0) = \boldsymbol{R}(0) = \boldsymbol{U}(0) = \mathbf{1}$. We shall define generators for those operations. For example, for evolution we define $\boldsymbol{U}(t) = \exp(-it\boldsymbol{H})$.

Proof: We assume that the operation, say the evolution, has the so-called group property

$$U(t_2 + t_1) = U(t_2)\, U(t_1) \tag{3.21}$$

It follows that

$$U(t) = [U(t/N)]^N \tag{3.22}$$

where N can be as large as we want. The evolution during an infinitesimal time interval can be written as:

$$U(dt) = \hat{1} + Gdt + \mathcal{O}(dt^2) \equiv \hat{1} - idt\mathcal{H} + \mathcal{O}(dt^2) \tag{3.23}$$

The first equality is a Taylor expansion, or one may say that G is the derivative of $U(t)$. Loosely speaking G is the "evolution per unit of time". From $U^\dagger U = 1$ it follows that $G^\dagger = -G$. The physics community does not like

anti-hermitian operators, and therefore we define $\mathcal{H} \equiv iG$, that satisfies $\mathcal{H}^\dagger = \mathcal{H}$. By multiplying many infinitesimal time steps we get:

$$\hat{U} \;=\; (1 - idt\mathcal{H}) \cdots (1 - idt\mathcal{H})(1 - idt\mathcal{H}) \;=\; \left(1 - i\frac{t}{N}\mathcal{H}\right)^N \;=\; e^{-it\mathcal{H}} \tag{3.24}$$

In the last step we have taken the $N \to \infty$ limit, and used the definition of the exponential function, Namely, $\exp(t) = \lim(1 + t/N)^N$, that follows from the assumed multiplicative property $\exp(t_1)\exp(t_2) = \exp(t_1 + t_2)$.

========= [3.6] Conventions regarding notations

In Mathematica there is a clear distinction between dummy indexes and fixed values. For example $f(x_-) = 8$ means that $f(x) = 8$ for any x, hence x is a dummy index. But if $x = 4$ then $f(x) = 8$ means that only one element of the vector $f(x)$ is specified. Unfortunately in the printed mathematical literature there are no clear conventions. However the tradition is to use notations such as $f(x)$ and $f(x')$ where x and x' are dummy indexes, while $f(x_0)$ and $f(x_1)$ where x_0 and x_1 are fixed values. Thus

$$A_{ij} \;=\; \begin{pmatrix} 2 & 3 \\ 5 & 7 \end{pmatrix} \tag{3.25}$$
$$A_{i_0 j_0} \;=\; 5 \qquad \text{for } i_0 = 2 \text{ and } j_0 = 1$$

Another typical example is

$$T_{x,k} \;=\; \langle x|k\rangle \;=\; \text{matrix} \tag{3.26}$$
$$\Psi(x) \;=\; \langle x|k_0\rangle \;=\; \text{column} \tag{3.27}$$

In the first equality we regard $\langle x|k\rangle$ as a matrix: it is the transformation matrix form the position to the momentum basis. In the second equality we regard the same object (with fixed k_0) as a column, or as a "wave-function".

We shall keep the following extra convention: The "bra" indexes would appear as subscripts (used for representation), while the "ket" indexes would appear as superscripts (reserved for the specification of the state). For example:

$$Y^{\ell m}(\theta, \varphi) \;=\; \langle \theta, \varphi|\ell m\rangle \quad = \text{ spherical harmonics} \tag{3.28}$$
$$\varphi^n(x) \;=\; \langle x|n\rangle \quad = \text{ harmonic oscillator eigenfunctions} \tag{3.29}$$
$$\psi_n \;=\; \langle n|\psi\rangle \quad = \text{ representation of wavefunction in the } n \text{ basis} \tag{3.30}$$

Sometime it is convenient to use the Einstein summation convention, where summation over repeated dummy indexes is implicit. For example:

$$f(\theta, \varphi) \;=\; \sum_{\ell m} \langle \theta, \varphi|\ell m\rangle\langle \ell m|f\rangle \;=\; f_{\ell m} Y^{\ell m}(\theta, \varphi) \tag{3.31}$$

In any case of ambiguity it is best to translate everything into Dirac notations.

========= [3.7] Change of basis

Definition of T:

Assume we have an "old" basis and a "new" basis for a given vector space. In Dirac notation:

$$\text{old basis} \;=\; \{\, |i = 1\rangle, \; |i = 2\rangle, \; |i = 3\rangle, \; \dots \} \tag{3.32}$$
$$\text{new basis} \;=\; \{\, |n = 1\rangle, \; |n = 2\rangle, \; |n = 3\rangle, \; \dots \}$$

The matrix $T_{i,n}$ whose columns represent the vectors of the new basis in the old basis is called the "transformation matrix from the old basis to the new basis". In Dirac notation this may be written as:

$$|n\rangle \;=\; \sum_i T_{i,\alpha} \,|i\rangle \tag{3.33}$$

In general, the bases do not have to be orthonormal. However, if they are orthonormal then $\boldsymbol{T}$ must be unitary and we have

$$T_{i,n} \;=\; \langle i|n\rangle \tag{3.34}$$

In this section we will discuss the general case, not assuming orthonormal basis, but in the future we will always work with orthonormal bases.

Definition of S:

If we have a vector-state then we can represent it in the old basis or in the new basis:

$$|\psi\rangle \;=\; \sum_i \psi_i \,|i\rangle \tag{3.35}$$
$$|\psi\rangle \;=\; \sum_n \tilde{\psi}_n \,|n\rangle$$

So, the change of representation can be written as:

$$\tilde{\psi}_n \;=\; \sum_i S_{n,i} \psi_i \tag{3.36}$$

Or, written abstractly:

$$\tilde{\psi} \;=\; \boldsymbol{S}\psi \tag{3.37}$$

The transformation matrix $\boldsymbol{S} = \boldsymbol{T}^{-1}$ reflects that change of basis can be regarded as an active operation on the state of the system. For example, if $\boldsymbol{T}$ represents forward translation of the axes (change of basis, passive point of view), then $\boldsymbol{S}$ represents a backward translation of the system (operation, active point of view).

Similarity Transformation:

A unitary operation can be represented in either the new basis or the old basis:

$$\varphi_i \;=\; \sum_i A_{i,j} \psi_j \tag{3.38}$$
$$\tilde{\varphi}_n \;=\; \sum_n \tilde{A}_{n,m} \tilde{\psi}_m$$

The implied transformation between the representations is:

$$\tilde{A} \;=\; \boldsymbol{S}\boldsymbol{A}\boldsymbol{S}^{-1} \;=\; \boldsymbol{T}^{-1}\boldsymbol{A}\boldsymbol{T} \tag{3.39}$$

This is called a similarity transformation.

━━━━━ [3.8] Non-orthonormal basis and the dual basis

Given an arbitrary basis that is not necessarily orthonormal, we define a metric $g_{ij} = \langle i|j \rangle$ such that the inner product can be calculated as follows

$$\langle u|v \rangle = \sum_{ij} g_{ij} u_i^* v_j \tag{3.40}$$

A dual basis $\big|\tilde{j}\big\rangle$ is defined such that

$$\big\langle i\big|\tilde{j}\big\rangle = \delta_{i,j} \tag{3.41}$$

On the technical level the representation of the j-th dual state is found from the equation $\sum_k g_{i,k} \psi_k = \delta_{i,j}$. Accordingly, the transformation matrix $\boldsymbol{G}$ from the original basis to the dual basis is the inverse of the metric $\boldsymbol{g}$. For the coefficients of $|u\rangle = \sum_i u_i |i\rangle$ we get $u_i = \big\langle \tilde{i}\big|u\big\rangle$. The completeness relation is

$$\sum_i |i\rangle \big\langle \tilde{i}\big| = \mathbf{1} \tag{3.42}$$

If we change basis from $|i\rangle$ to $|n\rangle$ the transformation matrix is $T_{i,n} = \big\langle \tilde{i}\big|n\big\rangle$. The inverse transformation is with $S_{n,j} = \big\langle \tilde{n}\big|j\big\rangle$. Note that $\boldsymbol{TS} = \mathbf{1}$. It also follows that change of representation of an operator is a similarity transformation, in agreement with the simpler presentation of the previous section.

━━━━━ [3.9] Generalized spectral decompositions

Not any operator is normal: that means that not any matrix can be diagonalized by a unitary transformation. In particular we have sometime to deal with non-Hermitian Hamiltonian that appear in the reduced description of open systems. For this reason and others it is important to know how the spectral decomposition can be generalized. The generalization has a price: either we have to work with non-orthonormal basis or else we have to work with two unrelated orthonormal sets. The latter procedure is known as singular value decomposition (SVD).

Given a matrix A we can find its eigenvalues λ_r, which we assume below to be non degenerate. without making any other assumption we can always define a set $|r\rangle$ of right eigenstates that satisfy $A|r\rangle = \lambda_r |r\rangle$. We can also define a set $|\tilde{r}\rangle$ of left eigenstates that satisfy $A^\dagger |\tilde{r}\rangle = \lambda_r^* |\tilde{r}\rangle$. Unless A is normal, the r basis is not orthogonal, and therefore $\langle r|A|s \rangle$ is not diagonal. But by considering $\langle \tilde{r}|A|s \rangle$ we can prove that $\langle \tilde{r}|s \rangle = 0$ if $r \neq s$. Hence we have dual basis sets, and without loss of generality we adopt a normalization convention such that

$$\langle \tilde{r}|s \rangle = \delta_{r,s} \tag{3.43}$$

so as to have the generalized spectral decomposition:

$$A = \sum_r |r\rangle \lambda_r \langle \tilde{r}| = T\,[\text{diag}\{\lambda_r\}]\,T^{-1} \tag{3.44}$$

where T is the transformation matrix whose columns are the right eigenvectors, while the rows of T^{-1} are the left eigenvectors. In the standard decomposition method A is regarded as describing stretching/squeezing in some principal directions, where T is the transformation matrix. The SVD procedure provides a different type of decompositions. Within the SVD framework A is regarded as a sequence of 3 operations: a generalized "rotation" followed by stretching/squeezing, and another generalized "rotation". Namely:

$$A = \sum_r |U_r\rangle \sqrt{p_r} \langle V_r| = U\,\sqrt{\text{diag}\{p_r\}}\,V^\dagger \tag{3.45}$$

Here the positive numbers p_r are called singular values, and U_r and V_r are not dual bases but unrelated orthonormal sets. The corresponding unitary transformation matrices are U and V.

===== [3.10] The separation of variables theorem

Assume that the operator $\mathcal{H}$ commutes with an Hermitian operator A. It follows that if $|a, \nu\rangle$ is a basis in which A is diagonalized, then the operator $\mathcal{H}$ is block diagonal in that basis:

$$\langle a, \nu | A | a', \nu' \rangle \;\; = \;\; a \delta_{aa'} \delta_{\nu\nu'} \tag{3.46}$$

$$\langle a, \nu | \mathcal{H} | a', \nu' \rangle \;\; = \;\; \delta_{aa'} \mathcal{H}^{(a)}_{\nu\nu'} \tag{3.47}$$

where the top index indicates which is the block that belongs to the eigenvalue a.
To make the notations clear consider the following example:

$$A = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 9 & 0 & 0 \\ 0 & 0 & 0 & 9 & 0 \\ 0 & 0 & 0 & 0 & 9 \end{pmatrix} \qquad H = \begin{pmatrix} 5 & 3 & 0 & 0 & 0 \\ 3 & 6 & 0 & 0 & 0 \\ 0 & 0 & 4 & 2 & 8 \\ 0 & 0 & 2 & 5 & 9 \\ 0 & 0 & 8 & 9 & 7 \end{pmatrix} \qquad H^{(2)} = \begin{pmatrix} 5 & 3 \\ 3 & 6 \end{pmatrix} \qquad H^{(9)} = \begin{pmatrix} 4 & 2 & 8 \\ 2 & 5 & 9 \\ 8 & 9 & 7 \end{pmatrix} \tag{3.48}$$

Proof: $[\mathcal{H}, A] = 0$ $\hspace{6cm}$ (3.49)

$\langle a, \nu | \mathcal{H} A - A \mathcal{H} | a', \nu' \rangle = 0$

$a' \langle a, \nu | \mathcal{H} | a', \nu' \rangle - a \langle a, \nu | \mathcal{H} | a', \nu' \rangle = 0$

$(a - a') \mathcal{H}_{a\nu, a'\nu'} = 0$

$a \neq a' \;\; \Rightarrow \;\; \mathcal{H}_{a\nu, a'\nu'} = 0$

$\langle a, \nu | \mathcal{H} | a', \nu' \rangle \;\; = \;\; \delta_{aa'} \, \mathcal{H}^{(a)}_{\nu\nu'}$

It follows that there is a basis in which both A and $\mathcal{H}$ are diagonalized. This is because we can diagonalize the matrix H block by block (the diagonalizing of a specific block does not affect the rest of the matrix).

===== [3.11] Separation of variables - examples

A trivial example for "separation of variables" concerns Hamiltonian that is "separable" by construction. Consider a system with two degrees-of-freedom $|x, y\rangle \equiv |x\rangle \otimes |y\rangle$. The x can be a spatial coordinate of a particle, and the y can be a transverse coordinate, or an up/down spin degree of freedom. If there is no coupling between the two freedoms, the Hamiltonian is the sum of two commuting terms, namely $\mathcal{H} = \boldsymbol{H}^{(x)} \otimes \boldsymbol{1} + \boldsymbol{1} \otimes \boldsymbol{H}^{(y)}$. The corresponding eigenstates have a factorized form $|n, m\rangle = |n\rangle \otimes |m\rangle$, with eigenvalues $E_{n,m} = \varepsilon^{(x)}_n + \varepsilon^{(y)}_m$.

A less trivial standard example for "separation of variables" is for the Hamiltonian of a particle in a centrally symmetric field in 2D or in 3D. In the first case L_z is constant of motion while in the second case both L^2 and L_z are constants of motion. The separation of the Hamiltonian into blocks is as follows:

Central symmetry in 2D:

$$\text{standard basis} \;\; = \;\; |x, y\rangle \;\; = \;\; |r, \varphi\rangle \tag{3.50}$$

$$\text{constant of motion} \;\; = \;\; L_z \tag{3.51}$$

$$\text{basis for separation} \;\; = \;\; |m, r\rangle \tag{3.52}$$

$$\langle m, r | \mathcal{H} | m', r' \rangle \;\; = \;\; \delta_{m,m'} \, \mathcal{H}^{(m)}_{r,r'} \tag{3.53}$$

The original Hamiltonian and its blocks:

$$\mathcal{H} \quad = \quad \frac{1}{2}\boldsymbol{p}^2 + V(r) \quad = \quad \frac{1}{2}\left(p_r^2 + \frac{1}{r^2}L_z^2\right) + V(r) \tag{3.54}$$

$$\mathcal{H}^{(m)} \quad = \quad \frac{1}{2}p_r^2 + \frac{m^2}{2r^2} + V(r) \qquad\qquad \text{where } p_r^2 \mapsto -\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) \tag{3.55}$$

Central symmetry in 3D:

$$\text{standard basis} \quad = \quad |x, y, z\rangle \quad = \quad |r, \theta, \varphi\rangle \tag{3.56}$$

$$\text{constants of motion} \quad = \quad L^2, \ L_z \tag{3.57}$$

$$\text{basis for separation} \quad = \quad |\ell m, r\rangle \tag{3.58}$$

$$\langle \ell m, r|\mathcal{H}|\ell' m', r'\rangle \quad = \quad \delta_{\ell,\ell'}\ \delta_{m,m'}\ \mathcal{H}^{(\ell m)}_{r,r'} \tag{3.59}$$

The original Hamiltonian and its blocks:

$$\mathcal{H} \quad = \quad \frac{1}{2}\boldsymbol{p}^2 + V(r) \quad = \quad \frac{1}{2}\left(p_r^2 + \frac{1}{r^2}L^2\right) + V(r) \tag{3.60}$$

$$\mathcal{H}^{(\ell m)} \quad = \quad \frac{1}{2}p_r^2 + \frac{\ell(\ell+1)}{2r^2} + V(r) \qquad\qquad \text{where } p_r^2 \mapsto -\frac{1}{r}\frac{\partial^2}{\partial r^2}r \tag{3.61}$$

[4]   A particle in an N site system

════════   ## [4.1]   N site system

A site is a location where a particle can be positioned. If we have $N = 5$ sites it means that we have a 5-dimensional Hilbert space of quantum states. Later we shall assume that the particle can "jump" between sites. For mathematical reasons it is conveneint to assume torus topology. This means that the next site after $x = 5$ is $x = 1$. This is also called periodic boundary conditions.

The standard basis is the position basis. For example: $|x\rangle$ with $x = 1, 2, 3, 4, 5$. So we can define the position operator as follows:

$$\hat{x}|x\rangle = x|x\rangle \tag{4.1}$$

In this example we get:

$$\hat{x} \mapsto \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 5 \end{pmatrix} \tag{4.2}$$

The operation of this operator on a state vector is for example:

$$|\psi\rangle = 7|3\rangle + 5|2\rangle$$
$$\hat{x}|\psi\rangle = 21|3\rangle + 10|2\rangle \tag{4.3}$$

════════   ## [4.2]   Translation operators

The one-step translation operator is defined as follows:

$$\hat{D}|x\rangle = |x+1\rangle \tag{4.4}$$

For example:

$$D \mapsto \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \tag{4.5}$$

and hence $D|1\rangle = |2\rangle$ and $D|2\rangle = |3\rangle$ and $D|5\rangle = |1\rangle$. Let us consider the superposition:

$$|\psi\rangle = \frac{1}{\sqrt{5}}[|1\rangle + |2\rangle + |3\rangle + |4\rangle + |5\rangle] \tag{4.6}$$

It is clear that $D|\psi\rangle = |\psi\rangle$. This means that ψ is an eigenstate of the translation operator (with eigenvalue e^{i0}). The translation operator has other eigenstates that we will discuss in the next section.

[4.3] Momentum states

The momentum states are defined as follows:

$$|k\rangle \to \frac{1}{\sqrt{N}}e^{ikx} \tag{4.7}$$

$$k = \frac{2\pi}{N}n, \quad n = \text{integer} \mod (N)$$

In the previous section we have encountered the $k = 0$ momentum state. In Dirac notation this is written as:

$$|k\rangle = \sum_x \frac{1}{\sqrt{N}}e^{ikx}|x\rangle \tag{4.8}$$

or equivalently as:

$$\langle x|k\rangle = \frac{1}{\sqrt{N}}e^{ikx} \tag{4.9}$$

while in old fashioned notation it is written as:

$$\psi_x^k = \langle x|k\rangle \tag{4.10}$$

where the upper index k identifies the state, and the lower index x is the representation index. Note that if x were continuous then it would be written as $\psi^k(x)$.

The k states are eigenstates of the translation operator. This can be proved as follows:

$$D|k\rangle = \sum_x D|x\rangle\langle x|k\rangle = \sum_x |x+1\rangle\frac{1}{\sqrt{N}}e^{ikx} = \sum_{x'} |x'\rangle\frac{1}{\sqrt{N}}e^{ik(x'-1)} = e^{-ik}\sum_{x'}|x'\rangle\frac{1}{\sqrt{N}}e^{ikx'} = e^{-ik}|k\rangle \tag{4.11}$$

Hence we get the result:

$$D|k\rangle = e^{-ik}|k\rangle \tag{4.12}$$

and conclude that $|k\rangle$ is an eigenstate of $\hat{D}$ with an eigenvalue e^{-ik}. Note that the number of independent eigenstates is N. For exmaple for a 5-site system we have $e^{ik_6} = e^{ik_1}$.

[4.4] Momentum operator

The momentum operator is defined as follows:

$$\hat{p}|k\rangle \equiv k|k\rangle \tag{4.13}$$

From the relation $\hat{D}|k\rangle = e^{-ik}|k\rangle$ it follows that $\hat{D}|k\rangle = e^{-i\hat{p}}|k\rangle$. Therefore we deduce the operator identity:

$$\hat{D} = e^{-i\hat{p}} \tag{4.14}$$

We can also define 2-step, 3-step, and a-step translation operators as follows:

$$\hat{D}(2) = (\hat{D})^2 = e^{-i2\hat{p}} \tag{4.15}$$
$$\hat{D}(3) = (\hat{D})^3 = e^{-i3\hat{p}}$$
$$\hat{D}(a) = (\hat{D})^a = e^{-ia\hat{p}}$$

[5] The continuum limit

════════ [5.1] Definition of the Wave Function

Below we will consider a site system in the continuum limit. $\epsilon \to 0$ is the distance between the sites, and L is the length of the system. So, the number of sites is $N = L/\epsilon \to \infty$. The eigenvalues of the position operator are $x_i = \epsilon \times$ integer. We use the following recipe for changing a sum into an integral:

$$\sum_i \mapsto \int \frac{dx}{\epsilon} \tag{5.1}$$
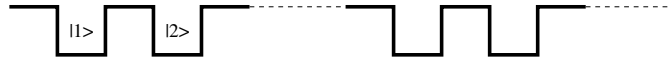
The definition of the position operator is:

$$\hat{x}|x_i\rangle = x_i|x_i\rangle \tag{5.2}$$

The completeness of the basis can be written as follows

$$\mathbf{1} = \sum |x_i\rangle\langle x_i| = \int |x\rangle dx\langle x| \tag{5.3}$$

In order to get rid of the ϵ in the integration measure we have re-defined the normalization of the basis states as follows:

$$|x\rangle = \frac{1}{\sqrt{\epsilon}}|x_i\rangle \qquad \text{[infinite norm!]} \tag{5.4}$$

Accordingly the orthonormality relation takes the following form,

$$\langle x|x'\rangle = \delta(x - x') \tag{5.5}$$

where the Dirac delta function is defined as $\delta(0) = 1/\epsilon$ and zero otherwise. Consequently the representation of a quantum state is:

$$|\psi\rangle = \sum_i \psi_i|x_i\rangle = \int dx\, \psi(x)|x\rangle \tag{5.6}$$

where

$$\psi(x) \equiv \langle x|\psi\rangle = \frac{1}{\sqrt{\epsilon}}\psi_x \tag{5.7}$$

Note the normalization of the "wave function" is:

$$\langle \psi|\psi\rangle = \sum_x |\psi_x|^2 = \int \frac{dx}{\epsilon}|\psi_x|^2 = \int dx|\psi(x)|^2 = 1 \tag{5.8}$$

══════ [5.2] Momentum States

The definition of the momentum states using this normalization convention is:

$$\psi^k(x) = \frac{1}{\sqrt{L}}\mathrm{e}^{ikx} \tag{5.9}$$

where the eigenvalues are:

$$k = \frac{2\pi}{L} \times \text{integer} \tag{5.10}$$

We use the following recipe for changing a sum into an integral:

$$\sum_k \mapsto \int \frac{dk}{2\pi/L} \tag{5.11}$$

We can verify the orthogonality of the momentum states:

$$\langle k_2 | k_1 \rangle = \sum_x \langle k_2 | x \rangle \langle x | k_1 \rangle = \sum_x \psi_x^{k_2 *} \psi_x^{k_1} = \int dx \psi^{k_2}(x)^* \psi^{k_1}(x) = \frac{1}{L} \int dx \mathrm{e}^{i(k_1 - k_2)x} = \delta_{k_2, k_1} \tag{5.12}$$

The transformation from the position basis to the momentum basis is:

$$\Psi_k = \langle k | \psi \rangle = \sum_x \langle k | x \rangle \langle x | \psi \rangle = \int \psi^k(x)^* \psi(x) dx = \frac{1}{\sqrt{L}} \int \psi(x) \mathrm{e}^{-ikx} dx \tag{5.13}$$

For convenience we will define:

$$\Psi(k) = \sqrt{L} \Psi_k \tag{5.14}$$

Now we can write the above relation as a Fourier transform:

$$\Psi(k) = \int \psi(x) \mathrm{e}^{-ikx} dx \tag{5.15}$$

Or, in the reverse direction:

$$\psi(x) = \int \frac{dk}{2\pi} \Psi(k) \mathrm{e}^{ikx} \tag{5.16}$$

══════ [5.3] Translations

We define the translation operator:

$$D(a)|x\rangle = |x + a\rangle \tag{5.17}$$

We now proof the following:

$$\begin{array}{lll} \text{Given that:} & |\psi\rangle \mapsto \psi(x) & \tag{5.18} \\ \text{It follows that:} & D(a)|\psi\rangle \mapsto \psi(x - a) & \tag{5.19} \end{array}$$

In Dirac notation we may write:

$$\langle x|D(a)|\psi\rangle = \langle x-a|\psi\rangle \tag{5.20}$$

This can obviously be proved easily by operating $D^\dagger$ on the "bra". However, for pedagogical reasons we will also present a longer proof: Given

$$|\psi\rangle = \sum_x \psi(x)|x\rangle \tag{5.21}$$

Then

$$D(a)|\psi\rangle = \sum_x \psi(x)|x+a\rangle = \sum_{x'} \psi(x'-a)|x'\rangle = \sum_x \psi(x-a)|x\rangle \tag{5.22}$$

══════ [5.4] The Momentum Operator

The momentum states are eigenstates of the translation operators:

$$D(a)|k\rangle = \mathrm{e}^{-iak}|k\rangle \tag{5.23}$$

The momentum operator is defined the same as in the discrete case:

$$\hat{p}|k\rangle = k|k\rangle \tag{5.24}$$

Therefore the following operator identity emerges:

$$\hat{D}(a) = \mathrm{e}^{-ia\hat{p}} \tag{5.25}$$

For an infinitesimal translation:

$$D(\delta a) = 1 - i\delta a\hat{p} \tag{5.26}$$

We see that the momentum operator is the generator of the translations.

══════ [5.5] The differential representation

The matrix elements of the translation operator are:

$$\langle x|D(a)|x'\rangle \;\; = \;\; \delta((x-x')-a) \tag{5.27}$$

For an infinitesimal translation we write:

$$\langle x|(\hat{1} - i\delta a\hat{p})|x'\rangle \;\; = \;\; \delta(x-x') - \delta a\delta'(x-x') \tag{5.28}$$

Hence we deduce:

$$\langle x|\hat{p}|x'\rangle \;\; = \;\; -i\delta'(x-x') \tag{5.29}$$

We notice that the delta function is symmetric, so its derivative is anti-symmetric. In analogy to multiplying a matrix with a column vector we write: $\hat{A}|\Psi\rangle \mapsto \sum_j A_{ij}\Psi_j$. Let us examine how the momentum opertor operates on a "wavefunction":

$$\hat{p}|\Psi\rangle \quad \mapsto \quad \sum_{x'} \hat{p}_{xx'}\Psi_{x'} \quad = \quad \int \langle x|\hat{p}|x'\rangle \Psi(x')dx' \quad = \tag{5.30}$$

$$= \quad -i\int \delta'(x-x')\Psi(x')dx' \quad = \quad -i\frac{\partial}{\partial x}\int \delta(x-x')\Psi(x')dx' \quad = \quad -i\frac{\partial}{\partial x}\Psi(x)$$

Therefore:

$$\hat{p}|\Psi\rangle \quad \mapsto \quad -i\frac{\partial}{\partial x}\Psi(x) \tag{5.31}$$

We see that in the continuum limit the operation of p can be realized by a differential operator. Let us perform a consistency check. We have already proved in a previous section that:

$$D(a)|\psi\rangle \quad \mapsto \quad \psi(x-a) \tag{5.32}$$

For an infinitesimal translation we have:

$$\left(1 - i\delta a\hat{p}\right)|\psi\rangle \quad \mapsto \quad \psi(x) - \delta a\frac{d}{dx}\psi(x) \tag{5.33}$$

From here it follows that

$$\langle x|p|\psi\rangle \quad = \quad -i\frac{d}{dx}\psi(x) \tag{5.34}$$

This means: the operation of p on a wavefunction is realized by the differential operator $-i(d/dx)$.

▬▬▬ [5.6] Algebraic characterization of translations

If $|x\rangle$ is an eigenstate of $\hat{x}$ with eigenvalue x, then $D|x\rangle$ is an eigenstate of $\hat{x}$ with eigenvalue $x+a$. In Dirac notations:

$$\hat{x}\Big[D|x\rangle\Big] \quad = \quad (x+a)\Big[D|x\rangle\Big] \qquad \text{for any } x \tag{5.35}$$

We have $(x+a)D = D(x+a)$, and $x|x\rangle = \hat{x}|x\rangle$. Therefore the above equality can be re-written as

$$\hat{x}D|x\rangle \quad = \quad D\left(\hat{x}+a\right)|x\rangle \qquad \text{for any } x \tag{5.36}$$

Therefore the following operator identity is implied:

$$\hat{x}\,D \quad = \quad D\,(\hat{x}+a) \tag{5.37}$$

Which can also be written as

$$[\hat{x}, D] \quad = \quad aD \tag{5.38}$$

The opposite is correct too: if an operator D fulfills the above relation with another operator x, then the former is a translation operator with respect to the latter, where a is the translation distance.

The above characterization applies to any type of translation operators, include "raising/lowering" operators which are not necessarily unitary. A nicer variation of the algebraic relation that characterizes a translation operator is obtained if D is unitary:

$$D^{-1}\hat{x}D \;=\; \hat{x} + a \tag{5.39}$$

If we write the infinitesimal version of this operator relation, by substituting $D(\delta a) = 1 - i\delta a\hat{p}$ and expanding to the first order, then we get the following commutation relation:

$$[\hat{x},\hat{p}] \;=\; i \tag{5.40}$$

The commutation relations allow us to understand the operation of operators without having to actually use them on wave functions.

===== [5.7] Particle in a 3D space

Up to now we have discussed the representation of a a particle which is confined to move in a one dimensional geometry. The generalization to a system with three geometrical dimensions is straightforward:

$$\begin{aligned}
|x,y,z\rangle &\;=\; |x\rangle \otimes |y\rangle \otimes |z\rangle \\
\hat{x}|x,y,z\rangle &\;=\; x|x,y,z\rangle \\
\hat{y}|x,y,z\rangle &\;=\; y|x,y,z\rangle \\
\hat{z}|x,y,z\rangle &\;=\; z|x,y,z\rangle
\end{aligned} \tag{5.41}$$

We define a "vector operator" which is actually a "package" of three operators:

$$\hat{\mathbf{r}} = (\hat{x},\hat{y},\hat{z}) \tag{5.42}$$

And similarly:

$$\begin{aligned}
\hat{\mathbf{p}} &\;=\; (\hat{p}_x,\hat{p}_y,\hat{p}_z) \\
\hat{\mathbf{v}} &\;=\; (\hat{v}_x,\hat{v}_y,\hat{v}_z) \\
\hat{\mathbf{A}} &\;=\; (\hat{A}_x,\hat{A}_y,\hat{A}_z)
\end{aligned} \tag{5.43}$$

Sometimes an operator is defined as a function of other operators:

$$\hat{\mathbf{A}} = \mathbf{A}(\hat{\mathbf{r}}) = (A_x(\hat{x},\hat{y},\hat{z}), A_y(\hat{x},\hat{y},\hat{z}), A_z(\hat{x},\hat{y},\hat{z})) \tag{5.44}$$

For example $\hat{\mathbf{A}} = \hat{\mathbf{r}}/|\hat{\mathbf{r}}|^3$. We also note that the following notation is commonly used:

$$\hat{\mathbf{p}}^2 = \hat{\mathbf{p}} \cdot \hat{\mathbf{p}} = \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2 \tag{5.45}$$

===== [5.8] Translations in 3D space

The translation operator in 3-D is defined as:

$$\hat{D}(\mathbf{a})|\mathbf{r}\rangle \;=\; |\mathbf{r} + \mathbf{a}\rangle \tag{5.46}$$

An infinitesimal translation can be written as:

$$
\begin{aligned}
\hat{D}(\delta\mathbf{a}) &= \mathrm{e}^{-i\delta a_x \hat{p}_x}\mathrm{e}^{-i\delta a_y \hat{p}_y}\mathrm{e}^{-i\delta a_z \hat{p}_z} \\
&= \hat{1} - i\delta a_x \hat{p}_x - i\delta a_y \hat{p}_y - i\delta a_z \hat{p}_z = \hat{1} - i\delta\mathbf{a}\cdot\hat{\mathbf{p}}
\end{aligned}
\tag{5.47}
$$

The matrix elements of the translation operator are:

$$
\langle\mathbf{r}|D(\mathbf{a})|\mathbf{r}'\rangle = \delta^3(\mathbf{r}-(\mathbf{r}'+\mathbf{a}))
\tag{5.48}
$$

Consequently, the differential representation of the momentum operator is:

$$
\hat{\mathbf{p}}|\Psi\rangle \;\mapsto\; \left(-i\frac{\partial}{\partial x}\Psi, -i\frac{\partial}{\partial y}\Psi, -i\frac{\partial}{\partial z}\Psi\right)
\tag{5.49}
$$

or in simpler notation $\hat{\mathbf{p}}|\Psi\rangle \mapsto -i\nabla\Psi$. We also notice that $\mathbf{p}^2|\Psi\rangle \mapsto -\nabla^2\Psi$.

[6] Rotations

══════ [6.1] The Euclidean Rotation Matrix

The Euclidean Rotation Matrix $R^E(\vec{\Phi})$ is a 3×3 matrix that rotates the vector $\mathbf{r}$.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} ROTATION \\ MATRIX \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \tag{6.1}$$

The Euclidean matrices constitute a representation of dimension 3 of the rotation group. The parametrization of a rotation is requires three numbers that are kept in a vector $\vec{\Phi}$. These are the rotation axis orientation (θ, φ), and the rotation angle Φ. Namely,

$$\vec{\Phi} \;=\; \Phi \vec{n} \;=\; \Phi(\sin\theta\cos\phi, \; \sin\theta\sin\phi, \; \cos\theta) \tag{6.2}$$

An infinitesimal rotation $\delta\vec{\Phi}$ can be written as:

$$R^E \mathbf{r} \;=\; \mathbf{r} + \delta\vec{\Phi} \times \mathbf{r} \tag{6.3}$$

Recalling the definition of a cross product we write this formula using matrix notations:

$$\sum_j R^E_{ij} \mathbf{r}_j \;=\; \sum_j \left[\delta_{ij} + \sum_k \delta\Phi_k \, \epsilon_{kji} \right] \mathbf{r}_j \tag{6.4}$$

Hence we deduce that the matrix that represents an arbitrary *infinitesimal* rotations is

$$R^E_{ij} \;=\; \delta_{ij} + \sum_k \delta\Phi_k \, \epsilon_{kji} \tag{6.5}$$

To find the matrix representation for a *finite* rotation is more complicated. In the future we shall learn a simple recipe how to construct a matrix that represents an arbitrary large rotation around an arbitrary axis. For now we shall be satisfied in writing the matrix that represents an arbitrary large rotation around the Z axis:

$$R(\Phi\vec{e}_z) \;=\; \begin{pmatrix} \cos(\Phi) & -\sin(\Phi) & 0 \\ \sin(\Phi) & \cos(\Phi) & 0 \\ 0 & 0 & 1 \end{pmatrix} \;\equiv\; R^z(\Phi) \tag{6.6}$$

Similar expressions hold for X axis and Y axis rotations. We note that $\vec{\Phi} = R^z(\varphi)R^y(\theta)\vec{e}_z$, hence by similarity transformation it follows that

$$R(\vec{\Phi}) \;=\; R^z(\varphi)R^y(\theta)R^z(\Phi)R^y(-\theta)R^z(-\varphi) \tag{6.7}$$

This shows that it is enough to know the rotations matrices around Y and Z to construct any other rotation matrix. However, this is not an efficient way to construct rotation matrices. Optionally a rotation matrice can be parameterized by its so-called "Euler angles"

$$R(\vec{\Phi}) \;=\; R^z(\alpha) \, R^x(\beta) \, R^z(\gamma) \tag{6.8}$$

This reflects the same idea (here we use the common ZXZ convention). To find the Euler angles can be complicated, and the advantage is not clear.

═══════ [6.2] The Rotation Operator Over the Hilbert Space

The rotation operator over the Hilbert space is defined (in analogy to the translation operator) as:

$$\hat{R}(\vec{\Phi})|\mathbf{r}\rangle \;\equiv\; |R^E(\vec{\Phi})\mathbf{r}\rangle \tag{6.9}$$

This operator operates over an infinite dimension Hilbert space (the standard basis is an infinite number of "sites" in the three-dimensional physical space). Therefore, it is represented by an infinite dimension matrix:

$$R_{r'r} \;=\; \langle r'|\hat{R}|r\rangle \;=\; \langle r'|R^E r\rangle \;=\; \delta(r' - R^E r) \tag{6.10}$$

That is in direct analogy to the translation operator which is represented by the matrix:

$$D_{r'r} \;=\; \langle r'|\hat{D}|r\rangle \;=\; \langle r'|r + a\rangle \;=\; \delta(r' - (r + a)) \tag{6.11}$$

Both operators $\hat{R}$ and $\hat{D}$ can be regarded as "permutation operators". When they act on some superposition (represented by a "wavefunction") their effect is to shift it somewhere else. As discussed in a previous section if a wavefunction $\psi(\mathbf{r})$ is translated by $D(a)$ then it becomes $\psi(\mathbf{r} - a)$. In complete analogy,

$$\text{Given that:} \qquad |\psi\rangle \;\mapsto\; \psi(r) \tag{6.12}$$
$$\text{It follows that:} \qquad \hat{R}(\Phi)|\psi\rangle \;\mapsto\; \psi(R^E(-\Phi)r) \tag{6.13}$$

═══════ [6.3] Which Operator is the Generator of Rotations?

The generator of rotations (the "angular momentum operator") is defined in analogy to the definition of the generator of translations (the "linear momentum operator"). In order to define the generator of rotations around the axis n we will look at an infinitesimal rotation of an angle $\delta\Phi\vec{n}$. An infinitesimal rotation is written as:

$$R(\delta\Phi\vec{n}) \;=\; \mathbf{1} - i\delta\Phi L_n \tag{6.14}$$

Below we will prove that the generator of rotations around the axis n is:

$$L_n = \vec{n} \cdot (\mathbf{r} \times \mathbf{p}) \tag{6.15}$$

where:

$$\hat{\mathbf{r}} \;=\; (\hat{x}, \hat{y}, \hat{z}) \tag{6.16}$$
$$\hat{\mathbf{p}} \;=\; (\hat{p}_x, \hat{p}_y, \hat{p}_z)$$

Proof: We shall show that both sides of the equation give the same result if they operate on any basis state $|\mathbf{r}\rangle$. This means that we have an operator identity.

$$R(\delta\vec{\Phi})|\mathbf{r}\rangle \;=\; |R^E(\delta\vec{\Phi})\mathbf{r}\rangle = |\mathbf{r} + \delta\vec{\Phi} \times \mathbf{r}\rangle = D(\delta\vec{\Phi} \times \mathbf{r})|\mathbf{r}\rangle \tag{6.17}$$
$$=\; [\hat{1} - i(\delta\vec{\Phi} \times \mathbf{r}) \cdot \hat{\mathbf{p}}]|\mathbf{r}\rangle = [\hat{1} - i\hat{\mathbf{p}} \cdot \delta\vec{\Phi} \times \mathbf{r}]|\mathbf{r}\rangle = [\hat{1} - i\hat{\mathbf{p}} \cdot \delta\vec{\Phi} \times \hat{\mathbf{r}}]|\mathbf{r}\rangle$$

So we get the following operator identity:

$$R(\delta\vec{\Phi}) = \hat{1} - i\hat{\mathbf{p}} \cdot \delta\vec{\Phi} \times \hat{\mathbf{r}} \tag{6.18}$$

Which can also be written (by exploiting the cyclic property of the triple vectorial multiplication):

$$R(\delta\vec{\Phi}) = \hat{1} - i\delta\vec{\Phi} \cdot (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) \tag{6.19}$$

From here we get the desired result. Note: The more common procedure to derive this identity is based on expanding the rotated wavefunction $\psi(R^E(-\delta\Phi)\mathbf{r}) = \psi(r - \delta\Phi \times \mathbf{r})$, and exploiting the association $p \mapsto -i\nabla$.

====== [6.4] Algebraic characterization of rotations

A unitary operator $\hat{D}$ realizes a translation a in the basis which is determined by an observable $\hat{x}$ if we have the equality $\hat{D}^{-1}\hat{x}\hat{D} = \hat{x} + a$. Let us prove the analogous statement for rotations: A unitary operator $\hat{R}$ realizes rotation Φ in the basis which is determined by an observable $\hat{r}$ if we have the equality

$$\hat{R}^{-1}\hat{r}_i\hat{R} \;\;=\;\; \sum_j R_{ij}^E \hat{r}_j \tag{6.20}$$

where R^E is the Euclidean rotation matrix. This relation constitutes an algebraic characterization of the rotation operator. As a particular example we write the characterization of an operator that induce 90° rotation around the Z axis:

$$\hat{R}^{-1}\hat{x}\hat{R} = -\hat{y}, \qquad \hat{R}^{-1}\hat{y}\hat{R} = \hat{x}, \qquad \hat{R}^{-1}\hat{z}\hat{R} = \hat{z} \tag{6.21}$$

This should be contrasted, say, with the characterization of translation in the X direction:

$$\hat{D}^{-1}\hat{x}\hat{D} = \hat{x} + a, \qquad \hat{D}^{-1}\hat{y}\hat{D} = \hat{y}, \qquad \hat{D}^{-1}\hat{z}\hat{D} = \hat{z} \tag{6.22}$$

Proof: The proof of the general statement with regard to the algebraic characterization of the rotation operator is totally analogous to that in the case of translations. We first argue that $\hat{R}$ is a rotation operator iff

$$\hat{R}|\boldsymbol{r}\rangle \;\;=\;\; |R^E\boldsymbol{r}\rangle \quad \text{for any } \boldsymbol{r} \tag{6.23}$$

This implies that

$$\hat{r}_i\left[\hat{R}|r\rangle\right] \;\;=\;\; \left(\sum_j R_{ij}^E r_j\right)\left[\hat{R}|r\rangle\right] \qquad \text{for any } r \tag{6.24}$$

By the same manipulation as in the case of translations we deduce that

$$\hat{r}_i\,\hat{R}\,|r\rangle \;\;=\;\; \sum_j R_{ij}^E\,\hat{R}\,\hat{r}_j\,|r\rangle \qquad \text{for any } r \tag{6.25}$$

From here, operating on both sides with $\hat{R}^{-1}$, we get the identity that we wanted to prove.

════ [6.5] The algebra of the generators of rotations

Going on in complete analogy with the case of translations we write the above algebraic characterization for an *infinitesimal* rotation:

$$[1 + i\delta\Phi_j L_j]\, \hat{r}_i\, [1 - i\delta\Phi_j L_j] \quad = \quad \hat{r}_i + \epsilon_{ijk}\,\delta\Phi_j\,\hat{r}_k \tag{6.26}$$

where we used the Einstein summation convention. We deduce that

$$[L_j, \hat{r}_i] \quad = \quad -i\,\epsilon_{ijk}\,\hat{r}_k \tag{6.27}$$

Thus we deduce that in order to know if a set of operators (J_x, J_y, J_z) generate rotations of eigenstates of a 3-component observable A, we have to check whether the following algebraic relation is satisfied:

$$[\hat{J}_i, \hat{A}_j] \quad = \quad i\,\epsilon_{ijk}\,\hat{A}_k \tag{6.28}$$

Note that for a stylistic convenience we have interchanged the order of the indexes. In particular we deduce that the algebra that characterized the generators of rotations is

$$[\hat{J}_i, \hat{J}_j] \quad = \quad i\,\epsilon_{ijk}\,\hat{J}_k \tag{6.29}$$

This is going to be the starting point for constructing other representations of the rotation group.

════ [6.6] Scalars, Vectors, and Tensor Operators

We can classify operators according to the way that they transform under rotations. The simplest possibility is a scalar operator C. It has the defining property

$$\hat{R}^{-1}\hat{C}\hat{R} \quad = \quad \hat{C}, \qquad \text{for any rotation} \tag{6.30}$$

which means that

$$[J_i, \hat{C}] \quad = \quad 0 \tag{6.31}$$

Similarly the defining property of a vector is

$$\hat{R}^{-1}\hat{A}_i\hat{R} \quad = \quad R^E_{ij}\hat{A}_j \qquad \text{for any rotation} \tag{6.32}$$

or equivalently

$$[\hat{J}_i, \hat{A}_j] \quad = \quad i\epsilon_{ijk}\hat{A}_k \tag{6.33}$$

The generalization of this idea leads to the notion of a tensor. A multi-component observer is a tensor of rank ℓ, if it transforms according to the R^ℓ_{ij} representation of rotations. Hence a tensor of rank ℓ should have $2\ell + 1$ components. In the special case of a 3-component "vector", as discussed above, the transformation is done using the Euclidean matrices R^E_{ij}.

It is easy to prove that if A and B are vector operators, then $C = A \cdot B$ is a scalar operator. We can prove it either directly, or by using the commutation relations. The generalization of this idea to tensors leads to the notion of "contraction of indices".

══════ [6.7] Wigner-Eckart Theorem

If we know the transformation properties of an operator, it has implications on its matrix elements. This section assumes that the student is already familiar with the representations of the rotation group.

Let us assume that the representation of the rotations over our Hilbert (sub)space is irreducible of dimension dim=$2j+1$. The basis states are $|m\rangle$ with $m = -j... + j$. Let us see what are the implications with regard to scalar and vector operators.

The representation of a scalar operator C should be trivial, i.e. proportional to the identity, i.e. a "constant":

$$C_{m'm} \;=\; c\,\delta_{m'm} \qquad \text{within a given } j \text{ irreducible subspace} \tag{6.34}$$

else it would follow from the "separation of variables theorem" that all the generators (J_i) are block-diagonal in the same basis. Note that within the pre-specified subspace we can write $c = \langle C\rangle$, where the expectation value can be taken with any state.

A similar theorem applies to a vector operator A. Namely,

$$[A_k]_{m'm} \;=\; g \times [J_k]_{m'm} \qquad \text{within a given } j \text{ irreducible subspace} \tag{6.35}$$

How can we determine the coefficient g? We simply observe that from the last equation it follows that

$$[A \cdot J]_{m'm} \;=\; g\,[J^2]_{m'm} \;=\; g\,j(j+1)\,\delta_{m'm} \tag{6.36}$$

in agreement with what we had claimed regarding scalars in general. Therefore we get the formula

$$g \;=\; \frac{\langle J \cdot A\rangle}{j(j+1)} \tag{6.37}$$

where the expectation value of the scalar can be calculated with any state.

The direct proof of the Wigner-Eckart theorem, as e.g. in Cohen-Tannoudji, is extremely lengthy. Here we propose a very short proof that can be regarded as a variation on what we call the "separation of variable theorem".

Proof step (1): From $[A_x, J_x] = 0$ we deduce that A_x is diagonal in the J_x basis, so we can write this relation as $A_x = f(J_x)$. The rotational invariance implies that the same function $f()$ related A_y to J_y and A_z to J_z. This invariance is implied by a similarity transformation and using the defining algebraic property of vector operators.

Proof step (2): Next we realize that for a vector operator $[J_z, A_+] = A_+$ where $A_+ = A_x + iA_y$. It follows that A_+ is a raising operator in the J_z basis, and therefore must be expressible as $A_+ = g(J_z)[J_x + iJ_y]$, where $g()$ is some function.

Proof step (3): It is clear that the only way to satisfy the equality $f(J_x) + if(J_y) = g(J_z)[J_x + iJ_y]$, is to have $f(X) = gX$ and $g(X) = g$, where g is a constant. Hence the Wigner-Eckart theorem is proved.

Fundamentals (part II)

[7] Quantum states / EPR / Bell / postulates

═══════ [7.1] The two slit experiment

If we have a beam of electrons, that have been prepared with a well defined velocity, and we direct it to a screen through two slits, then we get an interference pattern from which we can determine the "de-Broglie wavelength" of the electrons. I will assume that the student is familiar with the discussion of this experiment from introductory courses. The bottom line is that the *individual* electrons behave *like wave* and can be characterized by a wavefunction $\psi(x)$. This by itself does not mean that our world in not classical. We still can speculate that $\psi(x)$ has a classical interpenetration. Maybe our modeling of the system is not detailed enough. Maybe the two slits, if they are both open, deform the space in a special way that makes the electrons likely to move only in specific directions? Maybe, if we had better experimental control, we could *predict with certainty* where each electron will hit the screen.

The modern interpenetration of the two slit experiment is not classical. The so called "quantum picture" is that the electron can be at the same time at two different places: it goes via both slits and interferes with itself. This sounds strange.

Whether the quantum interpenetration is correct we cannot establish: maybe in the future we will have a different theory. What we *can* establish is that a classical interpretation of reality is *not* possible. This statement is based on a different type of an experiment that we discuss below.

═══════ [7.2] Is the world classical? (EPR, Bell)

We would like to examine whether the world we live in is "classical" or not. The notion of classical world includes mainly two ingredients: (i) realism (ii) determinism. By realism we means that any quantity that can be measured is well defined even if we do not measure it in practice. By determinism we mean that the result of a measurement is determined in a definite way by the state of the system and by the measurement setup. We shall see later that quantum mechanics is not classical in both respects: In the case of spin $1/2$ we cannot associate a definite value of $\hat{\sigma}_y$ for a spin which has been polarized in the $\hat{\sigma}_x$ direction. Moreover, if we measure the $\hat{\sigma}_y$ of a $\hat{\sigma}_x$ polarized spin, we get with equal probability ± 1 as the result.

In this section we would like to assume that our world is "classical". Also we would like to assume that interactions cannot travel faster than light. In some textbooks the latter is called "locality of the interactions" or "causality". It has been found by Bell that the two assumptions lead to an inequality that can be tested experimentally. It turns out from actual experiments that Bell's inequality are violated. This means that our world is either non-classical or else we have to assume that interactions can travel faster than light.

If the world is classical it follows that for any set of initial conditions a given measurement would yield a definite result. Whether or not we know how to predict or calculate the outcome of a possible measurement is not assumed. To be specific let us consider a particle of zero spin, which disintegrates into two particles going in opposite directions, each with spin $1/2$. Let us assume that each spin is described by a set of state variables.

$$
\begin{aligned}
\text{state of particle A} &= x_1^A, x_2^A, ... \\
\text{state of particle B} &= x_1^B, x_2^B, ...
\end{aligned}
\tag{7.1}
$$

The number of state variables might be very big, but it is assumed to be a finite set. Possibly we are not aware or not able to measure some of these "hidden" variables.

Since we possibly do not have total control over the disintegration, the emerging state of the two particles is described by a joint probability function $\rho\left(x_1^A, ..., x_1^B, ...\right)$. We assume that the particles do not affect each other after the disintegration ("causality" assumption). We measure the spin of each of the particles using a Stern-Gerlach apparatus. The measurement can yield either 1 or -1. For the first particle the measurement outcome will be denoted as a,

and for the second particle it will be denoted as b. It is assumed that the outcomes a and b are determined in a deterministic fashion. Namely, given the state variables of the particle and the orientation θ of the apparatus we have

$$
\begin{aligned}
a &= f(\theta_A, x_1^A, x_2^A, ...) = \pm 1 \\
b &= f(\theta_B, x_1^B, x_2^B, ...) = \pm 1
\end{aligned}
\tag{7.2}
$$

where the function $f()$ is possibly very complicated. If we put the Stern-Gerlach machine in a different orientation then we will get different results:

$$
\begin{aligned}
a' &= f\left(\theta_A', x_1^A, x_2^A, ...\right) = \pm 1 \\
b' &= f\left(\theta_B', x_1^B, x_2^B, ...\right) = \pm 1
\end{aligned}
\tag{7.3}
$$

We have the following innocent identity:

$$
ab + ab' + a'b - a'b' = \pm 2
\tag{7.4}
$$

The proof is as follows: if $b = b'$ the sum is $\pm 2a$, while if $b = -b'$ the sum is $\pm 2a'$. Though this identity looks innocent, it is completely non trivial. It assumes both "reality" and "causality". The realism is reflected by the assumption that both a and a' have definite values, as implied by the function $f()$, even if we do not measure them. In the classical context it is not an issue whether there is a practical possibility to measure both a and a' at a single run of the experiment. As for the causality: it is reflected by assuming that a depends on θ_A but not on the distant setup parameter θ_B.

Let us assume that we have conducted this experiment many times. Since we have a joint probability distribution ρ, we can calculate average values, for instance:

$$
\langle ab \rangle = \int \rho \left(x_1^A, ..., x_1^B, ...\right) f\left(\theta_A, x_1^A, ...\right) f\left(\theta_B, x_1^B, ...\right)
\tag{7.5}
$$

Thus we get that the following inequality should hold:

$$
|\langle ab \rangle + \langle ab' \rangle + \langle a'b \rangle - \langle a'b' \rangle| \leq 2
\tag{7.6}
$$

This is called Bell's inequality (in fact it is a variation of the original version). Let us see whether it is consistent with quantum mechanics. We assume that all the pairs are generated in a singlet (zero angular momentum) state. It is not difficult to calculate the expectation values. The result is

$$
\langle ab \rangle = -\cos(\theta_A - \theta_B) \equiv C(\theta_A - \theta_B)
\tag{7.7}
$$

we have for example

$$
C(0^o) = -1, \qquad C(45^o) = -\frac{1}{\sqrt{2}}, \qquad C(90^o) = 0, \qquad C(180^o) = +1.
\tag{7.8}
$$

If the world were classical the Bell's inequality would imply

$$
|C(\theta_A - \theta_B) + C(\theta_A - \theta_B') + C(\theta_A' - \theta_B) - C(\theta_A' - \theta_B')| \leq 2
\tag{7.9}
$$

Let us take $\theta_A = 0^o$ and $\theta_B = 45^o$ and $\theta_A' = 90^o$ and $\theta_B' = -45^o$. Assuming that quantum mechanics holds we get

$$
\left| \left(-\frac{1}{\sqrt{2}}\right) + \left(-\frac{1}{\sqrt{2}}\right) + \left(-\frac{1}{\sqrt{2}}\right) - \left(+\frac{1}{\sqrt{2}}\right) \right| = 2\sqrt{2} > 2
\tag{7.10}
$$

It turns out, on the basis of celebrated experiments that Nature has chosen to violate Bell's inequality. Furthermore it seems that the results of the experiments are consistent with the predictions of quantum mechanics. Assuming that we do not want to admit that interactions can travel faster than light it follows that our world is not classical.

In order to generalize the Bell inequality for other systems, it is worth noting that it is a variation of $\langle F \rangle < \sqrt{\langle F^2 \rangle}$. Above $F = (ab + ab' + a'b - a'b')$. The issue is that $\langle F^2 \rangle_{cl}$ provides a lower bound, while $\langle F^2 \rangle_{qm}$ is larger.

═══════ [7.3] Optional tests of realism

Mermin and Greenberger-Horne-Zeilinger have proposed optional tests for realism. The idea is to show that the *feasibility* of preparing some quantum states cannot be explained within the framework of a *classical* theory. We provide below two simple examples. The spin 1/2 mathematics that is required to understand these examples will be discussed in later lecture. What we need below is merely the following identities that express polarizations in the X and Y directions as a superposition of polarizations in the Z direction:

$$|x\rangle = \frac{1}{\sqrt{2}} (|z\rangle + |\bar{z}\rangle) \tag{7.11}$$

$$|\bar{x}\rangle = \frac{1}{\sqrt{2}} (|z\rangle - |\bar{z}\rangle) \tag{7.12}$$

$$|y\rangle = \frac{1}{\sqrt{2}} (|z\rangle + i|\bar{z}\rangle) \tag{7.13}$$

$$|\bar{y}\rangle = \frac{1}{\sqrt{2}} (|z\rangle - i|\bar{z}\rangle) \tag{7.14}$$

We use the notations $|z\rangle$ and $|\bar{z}\rangle$ for denoting "spin up" and "spin down" in Z polarization measurement, and similar convection for polarization measurement in the other optional directions X and Y.

Three spin example.– Consider 3 spins that are prepared in the following superposition state:

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\uparrow\rangle - |\downarrow\downarrow\downarrow\rangle) \equiv \frac{1}{\sqrt{2}} (|zzz\rangle - |\bar{z}\bar{z}\bar{z}\rangle) \tag{7.15}$$

If we measure the polarization of 3 spins we get $a = \pm 1$ and $b = \pm 1$ and $c = \pm 1$, and the product would be $C = abc = \pm 1$. If the the measurement is in the ZZZ basis the result might be either $C_{ZZZ} = +1$ or $C_{ZZZ} = -1$ with equal probabilities. But optionally we can perform an XXX measurement or XYY, or YXY, or YYX measurement. If for example we perform XYY measurement it is useful to write the state in the XYY basis:

$$|\psi\rangle = \frac{1}{2} (|\bar{x}y\bar{y}\rangle + |\bar{x}\bar{y}y\rangle + |x\bar{y}\bar{y}\rangle + |xyy\rangle) \tag{7.16}$$

We see that the product of polarization is always $C_{XYY} = +1$. Similarly one can show that $C_{YXY} = +1$ and $C_{YYX} = +1$. If the world were classical we could predict the result of an XXX measurement:

$$C_{XXX} = a_x b_x c_x = a_x\, b_x\, c_x\, a_y^2\, b_y^2\, c_y^2 = C_{XYY} C_{YXY} C_{YYX} = 1 \tag{7.17}$$

But quantum theory predicts a contradicting result. To see what is the expected result we write the state in the XXX basis:

$$|\psi\rangle = \frac{1}{2} (|\bar{x}xx\rangle + |x\bar{x}x\rangle + |xx\bar{x}\rangle + |\bar{x}\bar{x}\bar{x}\rangle) \tag{7.18}$$

We see that the product of polarization is always $C_{XXX} = -1$. Thus, the experimental feasibility of preparing such quantum state contradicts classical realism.

Two spin example.– Consider 2 spins that are prepared in the following superposition state:

$$|\psi\rangle \quad = \quad \frac{1}{\sqrt{3}} \left(|z\bar{z}\rangle + |\bar{z}z\rangle - |\bar{z}\bar{z}\rangle \right) \tag{7.19}$$

$$= \quad \frac{1}{\sqrt{6}} \left(|zx\rangle - |z\bar{x}\rangle + 2|\bar{z}\bar{x}\rangle \right) \tag{7.20}$$

$$= \quad \frac{1}{\sqrt{6}} \left(|xz\rangle - |\bar{x}z\rangle + 2|\bar{x}\bar{z}\rangle \right) \tag{7.21}$$

$$= \quad \frac{1}{\sqrt{12}} \left(|xx\rangle + |x\bar{x}\rangle + |\bar{x}x\rangle - 3|\bar{x}\bar{x}\rangle \right) \tag{7.22}$$

Above we wrote the state in the optional bases ZZ and ZX and XZ and XX. By inspection we see the following:

(1) The ZZ measurement result $|zz\rangle$ is impossible.
(2) The ZX measurement result $|\bar{z}x\rangle$ is impossible.
(3) The XZ measurement result $|x\bar{z}\rangle$ is impossible.
(4) All XX measurement results are possible with finite probability.

We now realize that in a classical reality observation (4) is in contradiction with observations (1-3). The argument is as follow: in each run of the experiment the state $\vec{a} = (a_x, a_z)$ of the first particle is determined by some set of hidden variables. The same applies with regard to the $\vec{b} = (b_x, b_z)$ of the second particle. We can define a *joint* probability function $f\left(\vec{a}, \vec{b}\right)$ that gives the probabilities to have any of the 4×4 possibilities (irrespective of what we measure in practice). It is useful to draw a 4×4 truth table and to indicate all the possibilities that are not compatible with (1-3). Then it turns out that the remaining possibilities are all characterized by having $a_x = -1$ or $b_x = -1$. This means that in a classical reality the probability to measure $|xx\rangle$ is zero. This contradicts the quantum prediction (4). Thus, the experimental feasibility of preparing such quantum state contradicts classical realism.

====== [7.4] The notion of quantum state

A-priori we can classify the possible "statistical states" of a prepared system as follows:

- Classical state: any measurement gives a definite value.

- Pure state: there is a complete set of measurements that give definite value, while any other measurement gives an uncertain value.

- Mixture: it is not possible to find a complete set of measurements that give a definite value.

When we go to Nature we find that classical states do not exist. The best we can get are "pure states". For example:

(1) The best we can have with the spin of an electron is 100% polarization (say) in the X direction, but then any measurement in any different direction gives an uncertain result, except the $-X$ direction which we call the "orthogonal" direction. Consequently we are inclined to postulate that polarization (say) in the non-orthogonal Z direction is a superposition of the orthogonal X and $-X$ states.

(2) With photons we are inclined to postulate that linear polarization in the 45° direction is a superposition of the orthogonal X polarization and Y polarization states. Note however that contrary to the electronic spin, here the superposition of linear polarized states can optionally give *different type* of polarization (circular / elliptic).

(3) With the same reasoning, and on the basis of the "two slit experiment" phenomenology, we postulate that a particle can be in a superposition state of two different locations. The subtlety here is that superposition of different locations is not another location but rather (say) a momentum state, while superposition of different polarizations states is still another polarization state.

Having postulated that all possible pure states can be regarded as forming an Hilbert space, it still does not help us to define the notion of quantum state in the statistical sense. We need a second postulate that would imply the following: If a full set of measurements is performed (in the statistical sense), then one should be able to predict (in the statistical sense) the result of any other measurement.

Example: In the case of spins 1/2, say that one measures the average polarization M_i in the $i = X, Y, Z$ directions. Can one predict the result for M_n, where $\boldsymbol{n}$ is a unit vector pointing in an arbitrary direction? According to the second postulate of quantum mechanics (see next section) the answer is positive. Indeed experiments reveal that $M_n = \boldsymbol{n} \cdot M$. Taking together the above two postulates, our objective would be to derive and predict such linear relations from our conception of Hilbert space. In the spin 1/2 example we would like to view $M_n = \boldsymbol{n} \cdot M$ as arising from the dim=2 representation of the rotation group. Furthermore, we would like to derive more complicated relations that would apply to other representations (higher spins).

====== [7.5] The four Postulates of Quantum Mechanics

The 18th century version of classical mechanics can be derived from three postulates: The three laws of Newton. The better formulated 19th century version of classical mechanics can be derived from three postulates: (1) The state of classical particles is determined by the specification of their positions and its velocities; (2) The trajectories are determined by an "action principle", hence derived from a Lagrangian. (3) The form of the Lagrangian of the theory is determined by symmetry considerations, namely Galilei invariance in the non-relativistic case. See the Mechanics book of Landau and Lifshitz for details.

Quantum mechanics requires four postulates: two postulates define the notion of quantum state, while the other two postulates, in analogy with classical mechanics, are about the laws that govern the evolution of quantum mechanical systems. The four postulates are:

(1) The collection of "pure" states is a linear space (Hilbert).

(2) The expectation values of observables obey linearity: $\langle \alpha \hat{X} + \beta \hat{Y} \rangle = \alpha \langle \hat{X} \rangle + \beta \langle \hat{Y} \rangle$

(3) The evolution in time obey the superposition principle: $\alpha |\Psi^0\rangle + \beta |\Phi^0\rangle \rightarrow \alpha |\Psi^t\rangle + \beta |\Phi^t\rangle$

(4) The dynamics of a system is invariant under specific transformations ("gauge", "Galilei").

The first postulate refers to "pure states". These are states that have been filtered. The filtering is called "preparation". For example: we take a beam of electrons. Without "filtering" the beam is not polarized. If we measure the spin we will find (in any orientation of the measurement apparatus) that the polarization is zero. On the other hand, if we "filter" the beam (e.g. in the left direction) then there is a direction for which we will get a definite result (in the above example, in the right/left direction). In that case we say that there is full polarization - a pure state. The "uncertainty principle" tells us that if in a specific measurement we get a definite result (in the above example, in the right/left direction), then there are different measurements (in the above example, in the up/down direction) for which the result is uncertain. The uncertainty principle is implied by the first postulate.

The second postulate use the notion of "expectation value" that refers to "quantum measurement". In contrast with classical mechanics, the measurement has meaning only in a statistical sense. We measure "states" in the following way: we prepare a collection of systems that were all prepared in the same way. We make the measurement on all the "copies". The outcome of the measurement is an event $\hat{x} = x$ that can be characterized by a distribution function. The single event can show that a particular outcome has a non-zero probability, but cannot provide full information on the state of the system. For example, if we measured the spin of a single electron and get $\hat{\sigma}_z = 1$, it does not mean that the state is polarized "up". In order to know whether the electron is polarized we must measure a large number of electrons that were prepared in an identical way. If only 50% of the events give $\hat{\sigma}_z = 1$ we should conclude that there is no definite polarization in the direction we measured.

====== [7.6] Observables as random variables

Observable is a random variable that can have upon measurement a real numerical value. In other words $\hat{x} = x$ is an *event*. Let us assume, for example, that we have a particle that can be in one of five sites: $x = 1, 2, 3, 4, 5$. An experimentalist could measure $\text{Prob}(\hat{x} = 3)$ or $\text{Prob}(\hat{p} = 3(2\pi/5))$. Another example is a measurement of the probability $\text{Prob}(\hat{\sigma}_z = 1)$ that the particle will have spin up.

The collection of values of x is called the spectrum of values of the observable. We make the distinction between random variables with a discrete spectrum, and random variables with a continuous spectrum. The probability

function for a random variable with a discrete spectrum is defined as:

$$f(x) = \text{Prob}(\hat{x} = x) \tag{7.23}$$

The probability density function for a random variable with a continuous spectrum is defined as:

$$f(x)dx = \text{Prob}(x < \hat{x} < x + dx) \tag{7.24}$$

The expectation value of a variable is defined as:

$$\langle \hat{x} \rangle = \sum_x f(x)x \tag{7.25}$$

where the sum should be understood as an integral $\int dx$ in the case the x has a continuous spectrum. Of particular importance is the random variable

$$\hat{P}^x = \delta_{\hat{x},x} \tag{7.26}$$

This random variable equals 1 if $\hat{x} = x$ and zero otherwise. Its expectation value is the probability to get 1, namely

$$f(x) = \langle \hat{P}^x \rangle \tag{7.27}$$

Note that $\hat{x}$ can be expressed as the linear combination $\sum_x x\hat{P}^x$.

===== [7.7] Quantum Versus Statistical Mechanics

Quantum mechanics stands opposite classical statistical mechanics. A particle is described in classical statistical mechanics by a probability function:

$$\rho(x,p)dxdp = \text{Prob}(x < \hat{x} < x + dx, p < \hat{p} < p + dp) \tag{7.28}$$

Optionally this definition can be expressed as the expectation value of a phase space projector

$$\rho(x,p) = \langle \delta(\hat{x} - x)\delta(\hat{p} - p) \rangle \tag{7.29}$$

The expectation value of a random variable $\hat{A} = A(\hat{x}, \hat{p})$ is implied:

$$\langle \hat{A} \rangle = \int A(x,p)\rho(x,p)dxdp \tag{7.30}$$

From this follows the linear relation:

$$\langle \alpha\hat{A} + \beta\hat{B} \rangle = \alpha\langle \hat{A} \rangle + \beta\langle \hat{B} \rangle \tag{7.31}$$

We see that the linear relation of the expectation values is a trivial result of classical probability theory. It assumes that a *joint probability function* can be defined. But in quantum mechanics we cannot define a "quantum state" using a joint probability function, as implied by the observation that our world is not "classical". For example we cannot have both the location and the momentum well defined simultaneously: a momentum state, by definition, is spread all over space. For this reason, we have to use a more sophisticated definition of ρ. The more sophisticated definition

regards ρ as set of expectation values, from which all other expectation values can be deduced, taking the linearity of the expectation value as a postulate.

===== [7.8] Observables as operators

In the quantum mechanical treatment we regard an observable $\hat{x}$ as an operator. Namely we *define* its operation on the basis states as $\hat{x}|x\rangle = x|x\rangle$, and by linearity its operation is defined on any other state. We can associate with the basis states projectors $\hat{P}^x$. For example

$$\hat{x} \mapsto \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}; \qquad \hat{P}^1 \mapsto \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \qquad \hat{P}^2 \mapsto \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \qquad \hat{P}^3 \mapsto \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \qquad (7.32)$$

In order to further discuss the implications of the first two postulates of quantum mechanics it is useful to consider the simplest example, which is spin 1/2. Motivated by the experimental context, we make the following associations between random variables and operators:

$$\hat{\sigma}_n \;\; \mapsto \;\; \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_{\text{in the } n \text{ basis}} \qquad\qquad n = x, y, z \text{ or any other direction} \qquad\qquad (7.33)$$

Optionally we can define the projectors

$$\hat{P}^n \;\; \mapsto \;\; \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}_{\text{in the } n \text{ basis}} \qquad\qquad n = x, y, z \text{ or any other direction} \qquad\qquad (7.34)$$

Note that

$$\hat{\sigma}_n \;\; = \;\; 2\hat{P}^n - \hat{1} \qquad\qquad (7.35)$$

It follows from the first postulate that the polarization state $|n\rangle$ can be expressed as a linear combination of, say, "up" and "down" polarizations. We shall see that the mathematical theory of the rotation group representation, implies that in the standard (up/down) basis the operators $\hat{\sigma}_x$, $\hat{\sigma}_y$, and $\hat{\sigma}_z$ are represented by the Pauli matrices σ_x, σ_y, and σ_z. We use the notations:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad\qquad (7.36)$$

Furthermore, the mathematical theory of the rotation group representation, allows us to write any σ_n as a linear combination of $(\sigma_x, \sigma_y, \sigma_z)$, namely $\sigma_n = \vec{n} \cdot \vec{\sigma} = n_x \sigma_x + n_y \sigma_y + n_z \sigma_z$.

Taking a more abstract viewpoint we point out that any spin operator is represented by a 2×2 matrix, that can be written as a linear combination of standard basis matrices as follows:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \;\; = \;\; a \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + b \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + c \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + d \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \;\; = \;\; \sum_{nm} A_{nm} \mathbb{P}^{mn} \qquad\qquad (7.37)$$

In the example above we denote the basis matrices as $\{P^z, S^+, S^-, P^{-z}\}$. In general we use the notation $\mathbb{P}^{mn} = |n\rangle\langle m|$. Note that $P^n = \mathbb{P}^{nn}$ are projectors, while the $n \neq m$ operators are not even hermitian, and therefore cannot be interpreted as representing observables.

Instead of using the standard basis $\{P^z, S^+, S^-, P^{-z}\}$ it is possibly more physically illuminating to take $\{\mathbf{1}, \hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\}$ as the basis set. Optionally one can take $\{\mathbf{1}, \hat{P}^x, \hat{P}^y, \hat{P}^z\}$ or $\{\hat{P}^z, \hat{P}^{-z}, \hat{P}^x, \hat{P}^y\}$ as the basis set.

The bottom line is that the operators that act on an N dimensional Hilbert space form an N^2 dimensional space. We can span this space in the standard basis, but physically it is more illuminating, and always possible, to pick a basis set of N^2 hermitian operators. Optionally we can pick a complete set of N^2 linearly independent projectors. The linear relations between sets of states (as implied by the first postulate of quantum mechanics) translate into linear relations between sets of operators. One should be careful not to abuse the latter statement: in the above example the projectors $\{P^x, P^y, P^z\}$ are linearly independent, while the associated states $\{|x\rangle, |y\rangle, |z\rangle\}$ are not.

===== [7.9] The tomography of quantum states

The first postulate of Quantum Mechanics implies that with any *observable* we can associate an Hermitian operator that belongs to the N^2-dimensional space of operators. We can span the whole space of observables by any set of N^2 independent operators $\hat{P}^r$. The standard basis is not physically illuminating, because the matrices $\mathbb{P}^{mn}$ are not hermitian, and therefore cannot be associated with random variables. But without loss of generality we can always assume an optional basis of hermitian matrices, possibly N^2 independent projectors.

From the second postulate of Quantum mechanics it follows that if $\hat{A} = \sum_r a_r \hat{P}^r$ then

$$\langle \hat{A} \rangle \;=\; \sum_r a_r \rho_r \qquad \text{where } \rho_r \equiv \langle \hat{P}^r \rangle \tag{7.38}$$

The set of N^2 expectation values fully characterizes the quantum state. Hence we can say the ρ represents the quantum state, in the same sense that a probability function represent a statistical state in classical mechanics. The determination of the state ρ on the basis of a set of measurements is called "quantum tomography". It should be clear that if we know ρ we can predict the expectation value of any other measurement.

In the dim$= 2$ spin case any operator can be written as a linear combination of the Pauli matrices:

$$\hat{A} \;=\; a_0 \hat{1} + a_x \sigma_x + a_y \sigma_y + a_z \sigma_z \;=\; a_0 + \boldsymbol{a} \cdot \boldsymbol{\sigma} \tag{7.39}$$

It is implied by the second postulate of quantum mechanics that

$$\langle \hat{A} \rangle \;=\; a_0 + a_x \langle \sigma_x \rangle + a_y \langle \sigma_y \rangle + a_z \langle \sigma_z \rangle \;=\; a_0 + \boldsymbol{a} \cdot \boldsymbol{M} \tag{7.40}$$

where the polarization vector is defined as follows:

$$\boldsymbol{M} \;=\; \Big(\langle \hat{\sigma}_x \rangle, \langle \hat{\sigma}_y \rangle, \langle \hat{\sigma}_z \rangle \Big) \tag{7.41}$$

In the general case, to be discussed below, we define a package $\rho = \{\rho_r\}$ of expectation values that we call *probability matrix*. The polarization vector $\boldsymbol{M}$ can be regarded as the simplest example for such matrix. The term "matrix" is used because in general the label r that distinguishes the N^2 basis operators is composed of two indexes. We note that a measurement of a non-degenerate *observable* provides $N-1$ independent expectation values (the probabilities to get any of the possible outcomes). Accordingly quantum tomography requires the measurement of $N+1$ non-commuting observables.

===== [7.10] Definition of the probability matrix

The definition of ρ in quantum mechanics is based on the trivial observation that any observable A can be written as a linear combination of N^2-1 independent projectors. If we know the associated N^2-1 independent probabilities, or any other set of N^2-1 independent expectation values, then we can predict the result of any other measurement (in the statistical sense). The possibility to make a prediction is based on taking the linearity of the expectation value as a postulate. The above statement is explained below, but the best is to consider the $N = 2$ example that comes later.

Any Hermitian operator can be written as a combination of N^2 operators as follows:

$$\hat{A} \;=\; \sum_{n,m} |n\rangle \langle n|A|m\rangle \langle m| \;=\; \sum_{n,m} A_{nm} \hat{\mathbb{P}}^{mn} \tag{7.42}$$

where $\hat{\mathbb{P}}^{mn} = |n\rangle\langle m|$. These N^2 operators are not all hermitians, and therefore, strictly speaking, they do not represent a set of observables. However we can easily express them using a set of N^2 hermitian observables as follows:

$$\mathbb{P}^{nn} \;=\; P^n \tag{7.43}$$

$$\mathbb{P}^{mn} \;=\; \frac{1}{2}(X^r + iY^r) \qquad \text{for } m{>}n \tag{7.44}$$

$$\mathbb{P}^{mn} \;=\; \frac{1}{2}(X^r - iY^r) \qquad \text{for } m{<}n \tag{7.45}$$

where $r = (nm) = (mn)$ is a composite index that runs over the $[N(N-1)/2]$ possible combinations of n and m. The definitions of X^r and Y^r are implied by the above expressions: in the dim$=2$ case X and Y are called Pauli matrices, while here we shall call them generalized Pauli matrices. It is useful to notice that the generalized Pauli matrices can be expressed as combinations of elementary Projectors. Define Q^r as a projector on the state $|n\rangle + |m\rangle$ and R^r as a projector on the state $|n\rangle + i|m\rangle$. Then we have:

$$X^{(nm)} \;=\; 2Q^{(nm)} - P^n - P^m \tag{7.46}$$

$$Y^{(nm)} \;=\; 2R^{(nm)} - P^n - P^m \tag{7.47}$$

Accordingly the set of generalized projectors $\mathbb{P}^{mn}$, is in fact equivalent to a set of N^2 proper projectors (P^n, Q^r, R^r). If one can extract from measurements the associated probabilities, it becomes possible to predict the result of any other expectation value according to the equation:

$$\langle A \rangle \;=\; \sum_{n,m} A_{nm}\,\rho_{mn} \;=\; \text{trace}(A\rho) \tag{7.48}$$

where ρ is named *the probability matrix*. Each entry in the probability matrix is a linear combination of expectation values of projectors. Note that the expectation value of a projector $P = |\psi\rangle\langle\psi|$ is the probability to find the systems in the state $|\psi\rangle$, while the expectation values of a generalized projector $\mathbb{P}^r$ is defined as $(\langle X^r \rangle \pm i\langle Y^r \rangle)/2$, as implied by the definitions above.

======== [7.11] Example: probability matrix for spin

Let us relate the two common ways in which one can specify the quantum state of a spin $1/2$ entity. On possibility is to specify the polarization vector, as discussed in previous section. The other way is to define a 2×2 probability matrix as follows. The generalized projectors are

$$\mathbb{P}^{\uparrow\uparrow} = |\uparrow\rangle\langle\uparrow| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}(1 + \sigma_z) = P^z \tag{7.49}$$

$$\mathbb{P}^{\downarrow\downarrow} = |\downarrow\rangle\langle\downarrow| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}(1 - \sigma_z) = 1 - P^z$$

$$\mathbb{P}^{\downarrow\uparrow} = |\uparrow\rangle\langle\downarrow| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}(\sigma_x + i\sigma_y) = \frac{1}{2}(2P^x - 1) + \frac{i}{2}(2P^y - 1)$$

$$\mathbb{P}^{\uparrow\downarrow} = |\downarrow\rangle\langle\uparrow| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}(\sigma_x - i\sigma_y) = \frac{1}{2}(2P^x - 1) - \frac{i}{2}(2P^y - 1)$$

The elements of the probability matrix are the expectation values of the above generalized projectors. Consequently we deduce the following relation between the probability matrix and the polarization vector:

$$\rho \;=\; \langle P^{ji} \rangle \;=\; \begin{pmatrix} \frac{1}{2}(1 + M_3) & \frac{1}{2}(M_1 - iM_2) \\ \frac{1}{2}(M_1 + iM_2) & \frac{1}{2}(1 - M_3) \end{pmatrix} \;=\; \frac{1}{2}(\hat{1} + \vec{M}\cdot\vec{\sigma}) \tag{7.50}$$

═══════ [7.12] Pure states as opposed to mixed states

After diagonalization, the probability matrix can be written as:

$$\rho \;\rightarrow\; \begin{pmatrix} p_1 & 0 & 0 & . \\ 0 & p_2 & 0 & . \\ 0 & 0 & p_3 & . \\ . & . & . & . \\ & & & & . \\ & & & & & . \end{pmatrix} \tag{7.51}$$

The convention is to order the diagonal elements in descending order. Using the common jargon we say that the state represented by ρ is a mixture of $|1\rangle, |2\rangle, |3\rangle, \ldots$ with weights $p_1, p_2, p_3, \ldots$. The most well known mixed state is the canonical state:

$$p_r = \frac{1}{Z} e^{-\beta E_r}, \qquad \beta \equiv 1/T, \quad Z \equiv \sum_r e^{-\beta E_r} \tag{7.52}$$

A "pure state" is the special case where the probability matrix after diagonalization is of the form:

$$\rho \;\rightarrow\; \begin{pmatrix} 1 & 0 & 0 & . \\ 0 & 0 & 0 & . \\ 0 & 0 & 0 & . \\ . & . & . & . \\ & & & & . \\ & & & & & . \end{pmatrix} \tag{7.53}$$

This may be written in a more compact way as $\rho = |1\rangle\langle 1| = |\psi\rangle\langle\psi| = P^\psi$. Note that $\langle P^\psi \rangle = 1$. This means a definite outcome for a measurement that is aimed in checking whether the particle is in state "1". That is why we say that the state is pure.

═══════ [7.13] Various versions of the expectation value formula

[1] The standard version of the expectation value formula:

$$\langle A \rangle \;=\; tr(A\rho) \tag{7.54}$$

[2] The "mixture" formula:

$$\langle A \rangle \;=\; \sum_r p_r \langle r|A|r \rangle \tag{7.55}$$

[3] The "sandwich" formula:

$$\langle A \rangle_\psi \;=\; \langle \psi|A|\psi \rangle \tag{7.56}$$

[4] The "projection" formula:

$$\text{Prob}(\phi|\psi) \;=\; |\langle\phi|\psi\rangle|^2 \tag{7.57}$$

The equivalence of statements 1-4 can be proved. In particular let us see how we go from the fourth statement to the third:

$$\langle A \rangle_\psi \;=\; \sum_a \text{Prob}(a|\psi)a \;=\; \sum_a |\langle a|\psi\rangle|^2 a \;=\; \langle\psi|A|\psi\rangle \tag{7.58}$$

[8] The evolution of quantum mechanical states

▬▬▬▬ [8.1] The Evolution Operator and the Hamiltonian

Consider a particle in an N site system. If we redefine the first basis state as $|\tilde{1}\rangle = -8|1\rangle$ we get a non-orthonormal basis, and therefore not convenient for practical mathematical calculations. *Explanation:* if we represent the state $|\psi\rangle$ as a linear combination of normalized basis vectors $|\psi\rangle = \sum_j \psi_j|j\rangle$, then we can find the coefficients of the combination by using the formula $\psi_i = \langle i|\psi\rangle$.

Even if we decide to work with a set of orthonormal states, still there is some freedom left which is called "gauge freedom" or "phase freedom": multiplying a state with a phase factor does not imply a different state, ρ stays the same, and hence all physical expectation values remain the same too. *Example:* The spin states $|\uparrow\rangle$ and $e^{\frac{\pi}{8}i}|\uparrow\rangle$ are represented by the same polarization vector, or optionally by the same ρ.

From the superposition principle, and from the above remarks regarding the normalization, it follows that the evolution in quantum mechanics is described by a unitary operator:

$$
\begin{aligned}
|\psi^{t=0}\rangle &\rightarrow |\psi^t\rangle \\
|\psi^t\rangle &= U|\psi^{t=0}\rangle
\end{aligned}
\tag{8.1}
$$

It is assumed here that the system is *isolated.* In order to simplify the discussion below we further assume that the external fields are constant in time. In such a case, the evolution operator must fulfill the following "group property":

$$
U(t_2 + t_1) = U(t_2)\, U(t_1)
\tag{8.2}
$$

It follows that the evolution operator can be written as

$$
U(t) = e^{-it\mathcal{H}}
\tag{8.3}
$$

where $\mathcal{H}$ is called the Hamiltonian or "generator" of the evolution.

Proof: The constructive way of proving the last formula is as follows: In order to know the evolution of a system from t_1 to t_2 we divide the time into many small intervals of equal size $dt = (t_2 - t_1)/N$. This means that:

$$
U(t_2, t_1) = U(t_2, t_2 - dt) \cdots U(t_1 + 2dt, t_1 + dt)\, U(t_1 + dt, t_1)
\tag{8.4}
$$

The evolution during an infinitesimal time interval can be written as:

$$
U(dt) \equiv \hat{1} - idt\mathcal{H}
\tag{8.5}
$$

where the Hamiltonian can be regarded as the "evolution per unit of time". Or we may say that $\mathcal{H}$ is the log derivative of U with respect to time. By multiplying many infinitesimal time steps we get:

$$
\hat{U} = (1 - idt\mathcal{H}) \cdots (1 - idt\mathcal{H})(1 - idt\mathcal{H}) = \left(1 - i\frac{t}{\#steps}\mathcal{H}\right)^{\#steps} = e^{-it\mathcal{H}}
\tag{8.6}
$$

where we have assumed that the Hamiltonian does not change in time, so that the multiplication of exponents can be changed into a single exponent with a sum of powers. We have used above the definition of the exponential function in mathematics: $\exp(t) = \lim(1 + t/N)^N$, that follows from the assumed multiplicative property $\exp(t_1)\exp(t_2) = \exp(t_1 + t_2)$.

══════ [8.2] The Schrödinger Equation

Consider the evolution of a pure state:

$$\psi^t = U\psi^{t=0} \tag{8.7}$$

From the rerlation $\psi^{t+dt} = (1 - idt\mathcal{H})\psi^t$ it follows that

$$\frac{d\psi}{dt} = -i\mathcal{H}\psi \tag{8.8}$$

This is the Schrödinger equation. We have allowed ourselves above to use sloppy notations (the "ket" has been omitted). One should realize that the Schrödinger equation reflects the definition of the Hamiltonian as the generator of the evolution.

We now consider the evolution of a general mixture:

$$\rho = \sum_r |r\rangle p_r \langle r| \tag{8.9}$$

we have $|r\rangle \rightarrow U|r\rangle$ and $\langle r| \rightarrow \langle r|U^\dagger$, therefore the evolution of ρ in time is:

$$\rho^t = U\rho^{t=0}U^\dagger \tag{8.10}$$

$$\frac{d\rho}{dt} = -i[\mathcal{H}, \rho] \tag{8.11}$$

This is the Liouville von-Neumann equation. One of its advantages is that the correspondence between the formalism of statistical mechanics and quantum mechanics becomes explicit. The difference is that in quantum mechanics we deal with a probability matrix whereas in statistical mechanics we deal with a probability function.

══════ [8.3] Stationary States (the "Energy Basis")

We can find the eigenstates $|n\rangle$ and the eigenvalues E_n of a Hamiltonian, which is called diagonalization:

$$\mathcal{H}|n\rangle = E_n|n\rangle \tag{8.12}$$

$$U|n\rangle = \mathrm{e}^{-iE_nt}|n\rangle \tag{8.13}$$

$$U \rightarrow \delta_{n,m}\mathrm{e}^{-iE_nt} \tag{8.14}$$

Using Dirac notations:

$$\langle n|U|m\rangle = \delta_{nm}\mathrm{e}^{-iE_nt} \tag{8.15}$$

If we prepare a superposition of basis states:

$$|\psi^{t=0}\rangle = \sum_n \psi_n |n\rangle \tag{8.16}$$

we get after time t

$$|\psi(t)\rangle = \sum_n \mathrm{e}^{-iE_nt}\psi_n |n\rangle \tag{8.17}$$

[8.4] How do we construct the Hamiltonian?

We construct the Hamiltonian from "symmetry" considerations. In the next lecture our object will be to show that the Hamiltonian of a non-relativistic particle is of the form:

$$\mathcal{H} \;=\; \frac{1}{2\mathsf{m}}(p - A(x))^2 + V(x) \tag{8.18}$$

In this lecture we discuss a simpler case: the Hamiltonian of a particle in a two-site system. We make the following assumptions about the two-site dynamics:

● The system is symmetric with respect to reflection.
● The particle can move from site to site.
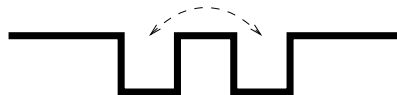
These two assumptions determine the form of the Hamiltonian. In addition, we will see how "gauge" considerations can make the Hamiltonian simpler, without loss of generality.

In advance we note that because of gauge considerations, the Hamiltonian can only be determined up to a constant.

$$\mathcal{H} \;\to\; \mathcal{H} + \epsilon_0 \hat{1} \tag{8.19}$$

Namely, if we add a constant to a Hamiltonian, then the evolution operator only changes by a global phase factor:

$$U(t) \;\to\; \mathrm{e}^{-it(\mathcal{H}+\epsilon_0 \hat{1})} \;=\; \mathrm{e}^{-i\epsilon_0 t}\,\mathrm{e}^{-it\mathcal{H}} \tag{8.20}$$

This global phase factor can be gauged away by means of time dependent gauge transformation. We shall discuss gauge transformations in the next sections.

[8.5] The Hamiltonian of a two-site system

It would seem that the most general Hamiltonian for a particle in a two-site system includes 4 parameters:

$$\mathcal{H} \;=\; \begin{pmatrix} \epsilon_1 & c\mathrm{e}^{-i\phi} \\ c\mathrm{e}^{i\phi} & \epsilon_2 \end{pmatrix} \tag{8.21}$$

The first observation is that thanks to gauge freedom we can define a new basis such that $\phi = 0$. The new basis is

$$\begin{aligned} |\tilde{1}\rangle &= |1\rangle \\ |\tilde{2}\rangle &= \mathrm{e}^{i\phi}|2\rangle \end{aligned} \tag{8.22}$$

and we see that:

$$\langle \tilde{2}|\mathcal{H}|\tilde{1}\rangle \;=\; \mathrm{e}^{-i\phi}\langle 2|\mathcal{H}|1\rangle \;=\; \mathrm{e}^{-i\phi}c\mathrm{e}^{i\phi} \;=\; c \tag{8.23}$$

Next we can make change the Hamiltonian by a constant ϵ_0. This can be regarded as gauge transformation in time. This means that the basis in time t is identified as $|\tilde{1}\rangle = \exp(-i\epsilon_0 t)|1\rangle$ and $|\tilde{2}\rangle = \exp(-i\epsilon_0 t)|2\rangle$. In this time dependent basis the diagonal matrix elements of the Hamiltonian becomes $\tilde{\epsilon}_1 = \epsilon_1 - \epsilon_0$ and $\tilde{\epsilon}_2 = \epsilon_2 - \epsilon_0$. It should be emphasized

that on physical grounds one cannot say whether the old or new basis is "really" time dependent. All we can say is that the new basis is time dependent relative to the old basis. This is just another example of the relativity principle.

The bottom line is that, without loss of generality, we can set $\phi = 0$ and write the most general Hamiltonian of a two site systems with just two physical parameters:

$$\mathcal{H} = \begin{pmatrix} \epsilon & c \\ c & 0 \end{pmatrix} = c\boldsymbol{\sigma}_1 + (\epsilon/2)\boldsymbol{\sigma}_3 + \text{const} = \vec{h} \cdot \vec{\boldsymbol{\sigma}} + \text{const} = h\boldsymbol{\sigma}_n + \text{const} \tag{8.24}$$

where $\vec{h} = (c, 0, \epsilon/2)$, and $h = \sqrt{c^2 + (\epsilon/2)^2}$, such that $\vec{h} = h\vec{n}$, and $\boldsymbol{\sigma}_n = \vec{n} \cdot \vec{\boldsymbol{\sigma}}$. The matrices $\boldsymbol{\sigma}_1$ and $\boldsymbol{\sigma}_3$ and in general $\boldsymbol{\sigma}_n$ are known as the Pauli matrices. They satisfy $\boldsymbol{\sigma}_n^2 = 1$, and therefore have eigenvalues ± 1. It follows that the eigenvalues of $\mathcal{H}$ are $\pm h + \text{const}$.

===== [8.6] The evolution of a two-site system

For the purpose of demonstration we further assume the the two-site system has a reflection symmetry. This implies $\epsilon = 0$. We are left with a single parameter Hamiltonian: In a future lecture we will see that the hopping frequency c is just a different (optional) was to specify the *inertial mass* of the particle. The eigenstates of the mirror symmetric Hamiltonian are the states that are symmetric or anti-symmetric with respect to reflection:

$$|+\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) \tag{8.25}$$

$$|-\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle) \tag{8.26}$$

The Hamiltonian in the new basis is:

$$\mathcal{H} = \begin{pmatrix} c & 0 \\ 0 & -c \end{pmatrix} \equiv \begin{pmatrix} E_+ & 0 \\ 0 & E_- \end{pmatrix} \tag{8.27}$$

Let us assume that we have prepared the particle in the first site:

$$|\psi^{t=0}\rangle = |1\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle) \tag{8.28}$$

The state of the particle, after time t will be:

$$|\psi^t\rangle = \frac{1}{\sqrt{2}}(\mathrm{e}^{-ict}|+\rangle + \mathrm{e}^{-i(-c)t}|-\rangle) = \cos(ct)|1\rangle - i\sin(ct)|2\rangle \tag{8.29}$$

We see that a particle in a two-site system makes coherent oscillations between the two sites. In particular the probability to find it in the initial site is:

$$P(t) = |\cos(ct)|^2 = \frac{1}{2}[1 + \cos(\Omega t)] \tag{8.30}$$

where the frequency of oscillations is $\Omega = 2c$. This result should be contrasted with classical stochastic evolution where the probability to be in each site (if we wait long enough time) would become equal. We can repeat the procedure for a non-symmetric two site system, with the result

$$\Omega = E_+ - E_- = \sqrt{(2c)^2 + \epsilon^2} \tag{8.31}$$

Here $\pm$ signifies arbitrary indexing of the two eigenstates, namely, $|+\rangle$ is the upper orbital and $|-\rangle$ is the lower orbital.

[9] The non-relativistic Hamiltonian

══════ [9.1] N Site system in the continuum Limit

In the last lecture we deduced the Hamiltonian $\hat{\mathcal{H}}$ that describes a two-site system using gauge and symmetry considerations. Now we are going to generalize this deduction for an N-site system. We start with 1D modeling, where the distance between two adjacent sites is a. The assumption is that the particle is able to move from site to site. We want to write an expression for the generator $\hat{\mathcal{H}}$ of the particle movement, such that

$$U_{ij}(dt) \;=\; \delta_{ij} - idt\mathcal{H}_{ij} \tag{9.1}$$
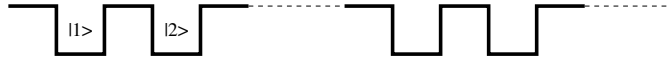
The Hamiltonian should reflect the possibility that the particle can either stay in its place or move one step right or one step left. Say that $N = 4$. Taking into account that $\hat{\mathcal{H}}$ should be Hermitian it has to be of the form

$$\mathcal{H}_{ij} \;=\; \begin{pmatrix} v & c^* & 0 & c \\ c & v & c^* & 0 \\ 0 & c & v & c^* \\ c^* & 0 & c & v \end{pmatrix} \;\equiv\; K(\text{so called kinetic part}) + V(\text{so called potential part}) \tag{9.2}$$

For a moment we assume that all the diagonal elements ("on sites energies") are the same, and that also all the hopping amplitudes are the same. Thus for general N we can write

$$\hat{\mathcal{H}} \;=\; cD + c^*D^{-1} + \text{Const} \;=\; ce^{-ia\hat{p}} + c^*e^{ia\hat{p}} + \text{Const} \tag{9.3}$$

We define $c = c_0e^{i\phi}$, where c_0 is real, and get:

$$\hat{\mathcal{H}} \;=\; c_0e^{-i(a\hat{p}-\phi)} + c_0e^{i(a\hat{p}-\phi)} + \text{Const} \tag{9.4}$$

We define $A = \phi/a$ (phase per unit distance) and get:

$$\hat{\mathcal{H}} \;=\; c_0e^{-ia(\hat{p}-A)} + c_0e^{ia(\hat{p}-A)} + \text{Const} \tag{9.5}$$

By using the identity $e^{ix} \approx 1 + ix - (1/2)x^2$ we get:

$$\hat{\mathcal{H}} \;=\; \frac{1}{2\mathsf{m}}(\hat{p}-A)^2 + V, \qquad \frac{1}{2\mathsf{m}} \equiv -c_0a^2, \quad V \equiv \text{Const} + 2c_0 \tag{9.6}$$

The above expression for $\mathcal{H}$ has three constants: m, A, V. If we assume that the space is homogeneous then the constants are the same all over space. But, in general, it does not have to be so, therefore:

$$\hat{\mathcal{H}} \;=\; \frac{1}{2\mathsf{m}}(\hat{p}-A(\hat{x}))^2 + V(\hat{x}) \tag{9.7}$$

If A and V depend on x we say that there is a field in space. In fact also m can be a function of x, but then one should be careful to keep $\hat{\mathcal{H}}$ hermitian, caring for appropriate "symmetrization". A mass that changes from place to place could perhaps describe an electron in a non-uniform metal. Here we discuss a particle whose mass m is the same all over space, for a reason that will be explained in the next section.

[9.2] The Hamiltonian of a Particle in 3-D Space

In 3D we can adopt the same steps in order to deduce the Hamiltonian. We write:

$$
\begin{aligned}
\mathcal{H} &= cD_x + c^* D_x^{-1} + cD_y + c^* D_y^{-1} + cD_z + c^* D_z^{-1} \\
&= ce^{-ia\hat{p}_x} + c^* e^{ia\hat{p}_x} + ce^{-ia\hat{p}_y} + c^* e^{ia\hat{p}_y} + ce^{-ia\hat{p}_z} + c^* e^{ia\hat{p}_z}
\end{aligned} \tag{9.8}
$$

After expanding to second order and allowing space dependence we get:

$$
\begin{aligned}
\mathcal{H} &= \frac{1}{2\mathsf{m}}(\hat{p}_x - A_x(\hat{x},\hat{y},\hat{z}))^2 + \frac{1}{2\mathsf{m}}(\hat{p}_y - A_y(\hat{x},\hat{y},\hat{z}))^2 + \frac{1}{2\mathsf{m}}(\hat{p}_z - A_z(\hat{x},\hat{y},\hat{z}))^2 + V(\hat{x},\hat{y},\hat{z}) \\
&= \frac{1}{2\mathsf{m}}(\hat{\mathbf{p}} - \mathbf{A}(\hat{\mathbf{r}}))^2 + V(\hat{\mathbf{r}}) \quad = \quad \frac{1}{2\mathsf{m}}(\hat{\mathbf{p}} - \hat{\mathbf{A}})^2 + \hat{V}
\end{aligned} \tag{9.9}
$$

This is the most general Hamiltonian that is invariant under Galilein transformations. Note that having a mass that is both isotropic and position-independent is required by this invariance requirement. The Galilein group includes translations, rotations and boosts. The relativistic version of the Galilein group is the Lorentz group (not included in the syllabus of this course). In addition, we expect the Hamiltonian to be invariant under gauge transformations, which is indeed the case as further discussed below.

[9.3] The dynamical phase, electric field

Consider the case where there is no hopping between sites ($c_0 = 0$). Accordingly the Hamiltonian $\mathcal{H} = V(x)$ does not include a kinetic part, and the evolution operator is $\hat{U}(t) = \exp[-itV(\hat{x})]$. A particle that is located in a given point in space will accumulate so called a dynamical phase:

$$
\hat{U}(t)|x_0\rangle = e^{-itV(x_0)}|x_0\rangle \tag{9.10}
$$

The potential V is the "dynamical phase" that the particle accumulates per unit time. The V in a specific site is called "binding energy" or "on site energy" or "potential energy" depending on the physical context. A $V(x)$ that changes from site to site reflects the non-homogeneity of the space, or the presence of an "external field". To further clarify the significance of V let us consider a simple prototype example. Let us assume that $V(x) = -\mathcal{E}x$. If the particle is initially prepared in a momentum eigenstate we get after some time

$$
\hat{U}(t)|p_0\rangle = e^{-itV}|p_0\rangle = e^{i\mathcal{E}t\hat{x}}|p_0\rangle = |p_0 + \mathcal{E}t\rangle \tag{9.11}
$$

This means that the momentum changes with time. The rate of momentum increase equals $\mathcal{E}$. We shall see later that this can be interpreted as the "second law of Newton".

[9.4] The geometric phase, magnetic field

Once we assume that the particle can move from site to site we have a hopping amplitude which we write as $c = c_0 e^{i\phi}$. It includes both a *geometric* phase ϕ and an *inertial* parameter c_0. The latter tells us what is the tendency of the particle to "leak" from site to site. In order to have a Galileo invariant Hamiltonian we assume that c_0 is isotropic and the same all over space, hence we can characterize the particle by its inertial mass m.

Still, in general the hopping amplitudes might be complex numbers $c_{i\to j} \propto e^{i\phi_{i\to j}}$. These phases do not threaten Galileo invariance. Accordingly, as the particle moves from site to site, it accumulates in each jump an additional phase $\phi_{i\to j}$ that can vary along its path. This is called "geometric phase". By definition the vector potential A is the "geometric phase" that the particle accumulates per unit distance. It is defined via the following formula:

$$
\phi_{i\to j} \equiv \vec{A} \cdot (\mathbf{r}_j - \mathbf{r}_i) = A_x dx + A_y dy + A_z dz \tag{9.12}
$$

The three components of $\vec{A}$ give the accumulated phase per distance for motion in the X, Y, and Z directions respectively. An infinitesimal jump in a diagonal direction is regarded as a sum of infinitesimal jumps in the X, Y, and Z directions, hence the scalar product.

In the following section we shall clarify that using gauge freedom we can describe the same system by a different $\vec{A}$. However, the circulation of $\vec{A}$, which gives the total phase that is accumulated along a closed trajectory, is gauge invariant. Consequently we can define the circulation per unit area:

$$\mathcal{B} \;=\; \nabla \times A \tag{9.13}$$

We shall see later that this can be interpreted as "magnetic field". This field characterizes $\vec{A}$ in a gauge invariant way.

══════ [9.5] What determines $V(x)$ and $A(x)$

We have defined $V(x)$ and $A(x)$ as the phase that is accumulated by a particle per time or per distance, respectively. In the next section we shall see that the presence of $V(x)$ and $A(x)$ in the Hamiltonian are required in order to ensure *gauge invariance*: the Hamiltonian should have the same form irrespective of the way we gauge the "phases" of the position basis states. Next comes the *physical* question: what determines $V(x)$ and $A(x)$ in reality. A-priori the particle can accumulate phase either due to a non-trivial *geometry* of space-time, or due to the presence of *fields*. The former effect is called *Gravitation*, while the latter are implied by the *standard model*. For our purpose it is enough to consider the electromagnetic (EM) field. It is reasonable to postulate that different particles have different couplings to the EM field. Hence we characterize a particle by its charge (e) and write in CGS units:

$$V(x) \;=\; V(x) \;+\; eV^{\mathrm{EM}}(x) \tag{9.14}$$
$$A(x) \;=\; A(x) \;+\; (e/c)A^{\mathrm{EM}}(x) \tag{9.15}$$

With regard to the gravitation we note that on the surface of Earth we have $V = \mathsf{m}gh$, where h is the vertical height of the particle, and $\nabla \times A = 2\mathsf{m}\Omega$ which is responsible for the Coriolis force. Note that by the *equivalence principle*, so-called fictitious forces are merely a simple example of a gravitational effect, i.e. they reflect a non-trivial metric tensor that describes the space-time geometry in a given coordinate system.

From now on, unless stated otherwise, $V(x)$ and $A(x)$ refer to the electromagnetic field. We note that in the Feynman path-integral formalism, which we describe in a different lecture, the probability amplitude of a particle to get form point 1 to point 2, namely $\langle x_2|U(t_2,t_1)|x_1\rangle$, is expressed as a sum over amplitudes $\exp[i\phi[x(t)]]$. The sum extends over all possible paths. The contribution of the electromagnetic field to the accumulated phase along a given path is

$$\phi[x(t)] \;=\; -\mathsf{m}\int_1^2 d\tau \;-\; e\int_1^2 V\,dt \;+\; e\int_1^2 A \cdot dx \tag{9.16}$$

This is the so-called "action" in classical mechanics. The proper time along the trajectory is an integral over $d\tau = [g_{\mu\nu}dx^\mu dx^\nu]^{1/2}$. Accordingly, the first term can be written as an integral over $\mathcal{L}_0(\boldsymbol{x},\dot{\boldsymbol{x}})dt$. The $\mathcal{L}_0$ function can be expanded in $\dot{\boldsymbol{x}}$ in order to get the non-relativistic Lagrangian. The two other terms are due to the electromagnetic field, and can be written compactly as a line integral over $-eA_\mu dx^\mu$.

══════ [9.6] Invariance under Gauge Transformation

Let us define a new basis:

$$|\tilde{x}\rangle \;=\; \mathrm{e}^{-i\Lambda(x)}|x\rangle \tag{9.17}$$

The hopping amplitudes from $|\tilde{x}_1\rangle = \mathrm{e}^{-i\Lambda_1}|x_1\rangle$ to $|\tilde{x}_2\rangle = \mathrm{e}^{-i\Lambda_2}|x_2\rangle$ is

$$\tilde{c}_{1\to 2} \;=\; \langle \tilde{x}_2|\hat{\mathcal{H}}|\tilde{x}_1\rangle \;=\; \mathrm{e}^{i(\Lambda_2-\Lambda_1)}\langle x_2|\hat{\mathcal{H}}|x_1\rangle \;=\; \mathrm{e}^{i(\Lambda_2-\Lambda_1)}c_{1\to 2} \tag{9.18}$$

We can rewrite this as:

$$\tilde{\phi}_{1\to2} \quad = \quad \phi_{1\to2} + (\Lambda_2 - \Lambda_1) \tag{9.19}$$

Dividing by the size of the step and taking the continuum limit we get:

$$\tilde{A}(x) \quad = \quad A(x) + \frac{d}{dx}\Lambda(x) \tag{9.20}$$

Or, in three dimensions:

$$\tilde{A}(x) \quad = \quad A(x) + \nabla\Lambda(x) \tag{9.21}$$
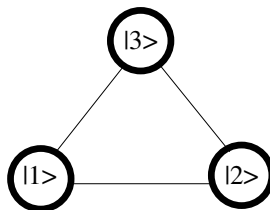
We see that the Hamiltonian is invariant (keeps its form) under gauge. As we have said, there is also invariance for all the Galilei transformations (notably boosts). This means that it is possible to find transformation laws that connect the fields in the "new" reference frame with the fields in the "laboratory" reference frame.

══════ [9.7] Is it possible to simplify the Hamiltonian further?

Is it possible to find a gauge transformation of the basis so that A will disappear? We have seen that for a two-site system the answer is yes: by choosing $\Lambda(x)$ correctly, we can eliminate A and simplify the Hamiltonian. On the other hand, if there is more than one route that connects two points, the answer becomes no. The reason is that in any gauge we may choose, the following expression will always be gauge invariant:

$$\oint \tilde{A} \cdot dl \quad = \quad \oint A \cdot dl \quad = \quad \text{gauge invariant} \tag{9.22}$$

In other words: it is possible to change each of the phases separately, but the sum of phases along a closed loop will always stay the same. We shall demonstrate this with a three-site system:

$$
\begin{aligned}
|\tilde{1}\rangle &= e^{-i\Lambda_1}|1\rangle \\
|\tilde{2}\rangle &= e^{-i\Lambda_2}|2\rangle \\
|\tilde{3}\rangle &= e^{-i\Lambda_3}|3\rangle \\
\tilde{\phi}_{1\to2} &= \phi_{1\to2} + (\Lambda_2 - \Lambda_1) \\
\tilde{\phi}_{2\to3} &= \phi_{2\to3} + (\Lambda_3 - \Lambda_2) \\
\tilde{\phi}_{3\to1} &= \phi_{3\to1} + (\Lambda_1 - \Lambda_3) \\
\tilde{\phi}_{1\to2} + \tilde{\phi}_{2\to3} + \tilde{\phi}_{3\to1} &= \phi_{1\to2} + \phi_{2\to3} + \phi_{3\to1}
\end{aligned}
$$

If the system had three sites but with an open topology, then we could have gotten rid of A like in the two-site system. That is also generally true of all the one dimensional problems, if the boundary conditions are "zero" at infinity. Once the one-dimensional topology is closed ("ring" boundary conditions) such a gauge transformation cannot be made. Furthermore, when the motion is in two or three dimensional space, there is always more than one route that connects

any two points, without regard to the boundary conditions. Consequently we can define the gauge invariant field $\mathcal{B}$ that characterizes A. It follows that in general one cannot eliminate A from the Hamiltonian.

════════ [9.8] Gauging away the $V(x)$ potential

We have concluded that in general it is impossible to gauge away the $A(x)$. But we can ask the opposite question, whether it is possible to gauge away the $V(x)$. The answer here is trivially positive, but the "price" is getting time dependent hopping amplitudes. The gauge transformation that does the job is

$$|\tilde{x}\rangle = \mathrm{e}^{-i\Lambda(x,t)}|x\rangle \quad \text{with} \quad \Lambda(x,t) = V(x)\,t \tag{9.23}$$

This is a temporal gauge of the basis. It is analogous to a transforming into a moving frame (in both cases the new basis is time dependent relative to the lab frame). In the new frame we have

$$\tilde{V}(x;t) \;=\; V - \frac{\partial\Lambda}{\partial t} \;=\; 0 \tag{9.24}$$

$$\tilde{A}(x;t) \;=\; A + \frac{\partial\Lambda}{\partial x} \;=\; A(x) + t\nabla V(x) \tag{9.25}$$

Hence we get the same magnetic and electric fields, but now both derived from a time dependent $A(x;t)$. In practical terms: we can always generate electric fields by time dependent fluxes.

════════ [9.9] Invariance of the Hamiltonian

The definition of "invariance" is as follows: Given that $\mathcal{H} = h(x,p;V,A)$ is the Hamiltonian of a system in the laboratory reference frame, there exist $\tilde{V}$ and $\tilde{A}$ such that the Hamiltonian in the "new" reference frame is $\tilde{\mathcal{H}} = h(x,p;\tilde{V},\tilde{A})$. The most general Hamiltonian that is invariant under translations, rotations and boosts is:

$$\hat{\mathcal{H}} \;=\; h(\hat{x},\hat{p};V,A) \;=\; \frac{1}{2\mathsf{m}}(\hat{p} - A(\hat{x}))^2 + V(\hat{x}) \tag{9.26}$$

Let us demonstrate the invariance of the Hamiltonian under translations: in the original basis $|x\rangle$ we have the fields $V(x)$ and $A(x)$. In the translated reference frame the new basis is $|\tilde{x}\rangle \equiv |x+a\rangle$, hence $\langle \tilde{x}|\mathcal{H}|\tilde{x}'\rangle = \langle x|\tilde{\mathcal{H}}|x'\rangle$ with $\tilde{\mathcal{H}} = D^\dagger \mathcal{H} D$. Hence we deduce that the Hamiltonian is "invariant" (keeps its form) with

$$\tilde{V}(x) \;=\; V(x+a) \tag{9.27}$$
$$\tilde{A}(x) \;=\; A(x+a) \tag{9.28}$$

In order to verify that we are not confused with the signs, let us consider the potential $V(x) = \delta(x)$. If we make a translation with $a = 7$, then the basis in the new reference frame will be $|\tilde{x}\rangle = |x+7\rangle$, and we get $\tilde{V}(x) = \delta(x+7)$ which means a delta at $x = -7$.

For completeness we cite how the Hamiltonian transform under Galilean transformation T to a moving frame whose velocity is v_0. This transformation is composed of a translation $\mathrm{e}^{-iv_0 t\hat{p}}$ and a boost $\mathrm{e}^{i\mathsf{m}v_0\hat{x}}$. The following result is derived in a dedicated lecture:

$$\tilde{\mathcal{H}} \;=\; T^\dagger\,\mathcal{H}\,T \;-\; v_0 \cdot \hat{\mathbf{p}} \;=\; h(\hat{\mathbf{x}},\hat{\mathbf{p}};\tilde{V},\tilde{A}) \tag{9.29}$$

where

$$\tilde{V}(x) \;=\; V(x+v_0 t) \;-\; v_0 \cdot A(x+v_0 t) \tag{9.30}$$
$$\tilde{A}(x) \;=\; A(x+v_0 t) \tag{9.31}$$

From here follows the well know no-relativistic transformation $\tilde{\mathcal{E}} = \mathcal{E} + v_0 \times \mathcal{B}$, and $\tilde{\mathcal{B}} = \mathcal{B}$.

[10] Getting the equations of motion

═══════ [10.1] Rate of change of the expectation value

Given an Hamiltonian, with any operator $\hat{A}$ we can associate an operator $\hat{B}$,

$$\hat{B} \;=\; i[\hat{\mathcal{H}}, \hat{A}] + \frac{\partial A}{\partial t} \tag{10.1}$$

such that

$$\frac{d\langle\hat{A}\rangle}{dt} \;=\; \langle\hat{B}\rangle \tag{10.2}$$

proof: From the expectation value formula:

$$\langle\hat{A}\rangle_t = \mathsf{trace}(\hat{A}\rho(t)) \tag{10.3}$$

Using the Liouville equation and the cyclic property of the trace, we get:

$$\begin{aligned}
\frac{d}{dt}\langle\hat{A}\rangle_t &= \mathsf{trace}\left(\frac{\partial A}{\partial t}\rho(t)\right) + \mathsf{trace}\left(\hat{A}\frac{d\rho(t)}{dt}\right) \\[2mm]
&= \mathsf{trace}\left(\frac{\partial A}{\partial t}\rho(t)\right) - i\,\mathsf{trace}\left(A[\mathcal{H},\rho(t)]\right) \\[2mm]
&= \mathsf{trace}\left(\frac{\partial A}{\partial t}\rho(t)\right) + i\,\mathsf{trace}\left([\mathcal{H},A]\rho(t)\right) \\[2mm]
&= \left\langle\frac{\partial A}{\partial t}\right\rangle + i\left\langle[\mathcal{H},A]\right\rangle
\end{aligned} \tag{10.4}$$

Optionally, if the state is pure, we can write:

$$\langle\hat{A}\rangle_t \;=\; \langle\psi(t)|\hat{A}|\psi(t)\rangle \tag{10.5}$$

Using the Schrödinger equation, we get

$$\begin{aligned}
\frac{d}{dt}\left\langle\hat{A}\right\rangle &= \left\langle\frac{d}{dt}\psi\Big|\hat{A}\Big|\psi\right\rangle + \left\langle\psi\Big|A\frac{d}{dt}\psi\right\rangle + \left\langle\psi\Big|\frac{\partial A}{\partial t}\Big|\psi\right\rangle \\[2mm]
&= i\left\langle\psi\Big|\mathcal{H}A\Big|\psi\right\rangle - i\left\langle\psi\Big|A\mathcal{H}\Big|\psi\right\rangle + \left\langle\psi\Big|\frac{\partial A}{\partial t}\Big|\psi\right\rangle \;=\; \ldots
\end{aligned} \tag{10.6}$$

We would like to highlight the distinction between a full derivative and a partial derivative. Let us assume that there is an operator that perhaps represents a field that depends on the time t, for example $\hat{A} = \hat{x}^2 + t\hat{x}^8$. Then the partial derivative with respect to t is: $\partial A/\partial t = \hat{x}^8$, while the total derivative of $\langle\hat{A}\rangle$ takes into account the change in the quantum state too.

Useful identities:
Commutation by parts: $[A, BC] = [A, B]C + B[A, C]$
Poisson brackets: $[f(x), p] = if'(x)$ and $[x, g(p)] = ig'(p)$
Jacobi identity: $[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$
Heisenberg picture: $A(t) \equiv U(t)^{\dagger}AU(t)$,   hence $\langle\hat{A}\rangle_t = \langle\Psi|A(t)|\Psi\rangle$.
To calculate $A(t)$ one can use the identity:

$$e^{A}Be^{-A} \;=\; B + [A, B] + \frac{1}{2!}[A, [A, B]] + \frac{1}{3!}[A, [A, [A, B]]] + \cdots \;=\; e^{[A,\cdot]}B \tag{10.7}$$

═══ [10.2] The classical equations of motion

If $\hat{x}$ is the location of a particle, then its rate of change is called velocity. By the rate of change formula we identify the velocity operator v as follows:

$$\hat{v} = i[\hat{\mathcal{H}}, \hat{x}] = i\left[\frac{1}{2\mathsf{m}}(\hat{p} - A(\hat{x}))^2, \hat{x}\right] = \frac{1}{\mathsf{m}}(\hat{p} - A(x)) \tag{10.8}$$

and we have:

$$\frac{d\langle\hat{x}\rangle}{dt} = \langle\hat{v}\rangle, \qquad\qquad \text{3D:} \quad \hat{x} := (\hat{x}, \hat{y}, \hat{z}), \quad \hat{v} := (\hat{v}_x, \hat{v}_y, \hat{v}_z) \tag{10.9}$$

It is useful to relaize that the kinetic part of the Hamiltonian can be written as $(1/2)\mathsf{m}\hat{v}^2$. The commutaion relations of the velocity components are

$$[\mathsf{m}\hat{v}_i, \mathsf{m}\hat{v}_j] = i(\partial_i A_j - \partial_j A_i) = i\epsilon_{ijk}B_k \tag{10.10}$$
$$[V(\hat{x}), \mathsf{m}\hat{v}_j] = i\,\partial_j V(\hat{x}) \tag{10.11}$$

The rate of change of the velocity $\hat{v}$ is called acceleration. By the rate of change formula

$$\frac{d\langle\hat{v}\rangle}{dt} = \left\langle i\left[\frac{1}{2}\mathsf{m}\hat{v}^2 + V(\hat{x}),\ \hat{v}\right] + \frac{\partial\hat{v}}{\partial t}\right\rangle = \frac{1}{\mathsf{m}}\left\langle\frac{1}{2}(v \times \mathcal{B} - \mathcal{B} \times v) + \mathcal{E}\right\rangle \tag{10.12}$$

Note that this is dense vector-style writing of 3 equations, for the rate of change of $\langle\hat{v}_x\rangle$ and $\langle\hat{v}_y\rangle$ and $\langle\hat{v}_z\rangle$. Above we have used the follwing notations:

$$\mathcal{B} = \nabla \times A \tag{10.13}$$
$$\mathcal{E} = -\frac{\partial A}{\partial t} - \nabla V$$

We would like to emphasize that the Hamiltonian is the "generator" of the evolution of the system, and therefore all the equations of motion can be derived from it. From the above it follows that in case of a "minimal" wavepacket the expectation values of $\hat{x}$ and $\hat{v}$ obey the classical equations approximately. The classical Lorentz force equation becomes exact if the $\mathcal{B}$ and $\mathcal{E}$ are *constants* in the region where the motion takes place:

$$\frac{d\langle\hat{v}\rangle}{dt} = \frac{1}{\mathsf{m}}\left[-\mathcal{B}_0 \times \langle v\rangle + \mathcal{E}_0\right] \tag{10.14}$$

═══ [10.3] Heuristic interpretation

In the expression for the acceleration we have two terms: the "electric" force and the "magnetic" (Lorentz) force. These forces bend the trajectory of the particle. It is important to realize that the bending of trajectories has to do with *interference* and has a very intuitive heuristic explanation. This heuristic explanation is due to Huygens: We should regard each front of the propagating beam as a point-like source of waves. The next front (after time dt) is determined by interference of waves that come from all the points of the previous front. For presentation purpose it is easier to consider first the interference of $N = 2$ points, then to generalize to N points, and then to take the continuum limit of plane-wave front. The case $N = 2$ is formally equivalent to a two slit experiment. The main peak of constructive interference is in the forward direction. We want to explain why the presence of an electric or a magnetic field can shift the main peak. A straightforward generalization of the argument explains why a trajectory of a plane-wave is bent.

The Huygens deflection formula: Consider a beam with wavenumber k that propagates in the x direction. It goes through two slits that are located on the y axis. The transverse distance between the slits is d. A detector is positioned at some angle θ very far away from the slits. The phase difference between the oscillations that arrive to the detector from the two slits is

$$\phi_2 - \phi_1 \;\; = \;\; \Delta\phi \;\; - \;\; k \cdot d \cdot \theta \tag{10.15}$$

In this formula it is assumed that after the slits there is a "scattering region" of length Δx where fields may be applied. We define $\Delta\phi$ as the phase difference after this "scattering region", while $\phi_2 - \phi_1$ is the phase difference at the very distant detector. The ray propagation direction is defined by the requirement $\phi_2 - \phi_1 = 0$, leading to the optical deflection formula $\theta = \Delta\phi/(kd)$. Changing notations $k \mapsto p_x$ and $d \mapsto \Delta y$ we write the deflection formula as follows:

$$\theta \;\; = \;\; \frac{\Delta p_y}{p_x} \;\; = \;\; \text{Deflection angle} \tag{10.16}$$

$$\Delta p_y \;\; \equiv \;\; \frac{\Delta\phi}{\Delta y} \;\; = \;\; \text{Optical Impulse} \tag{10.17}$$

From the definition of the dynamical and the geometrical phases it follows that if there are electric and magnetic fields in the scattering region then

$$\Delta\phi \;\; = \;\; (V_2 - V_1)\Delta t \;\; + \;\; \Phi_B \tag{10.18}$$

where $\Phi_B = \mathcal{B}\Delta x \Delta y$ is the magnetic flux that is enclosed by the interfering rays, and $V_2 - V_1 = \mathcal{E}\Delta y$ is the potential difference between the two slits, and $\Delta t = \Delta x/v$ is the travel time via the scattering region. From here follows that the optical impulse is

$$\Delta p_y \;\; = \;\; \frac{\Delta\phi}{\Delta y} \;\; = \;\; \mathcal{E}\Delta t \;\; + \;\; \mathcal{B}\Delta x \tag{10.19}$$

The Newtonian deflection formula: In the Newtonian perspective the deflection of a beam of particles is

$$\theta \;\; = \;\; \frac{\Delta p_y}{p_x} \;\; = \;\; \text{Deflection angle} \tag{10.20}$$

$$\Delta p_y \;\; \equiv \;\; F\Delta t \;\; = \;\; \text{Newtonian Impulse} \tag{10.21}$$

where F is called the "Newtonian force". By comparison with the Huygens analysis we deduce that the "force" on the particles is

$$F \;\; = \;\; \frac{\Delta p_y}{\Delta t} \;\; = \;\; \mathcal{E} + \mathcal{B}v \;\; = \;\; \text{Lorentz force} \tag{10.22}$$

It is important to realize that the deflection is due to an interference effect: The trajectory is bending either due to a gradient in $V(x)$, or due to the presence of an enclosed magnetic flux. Unlike the classical point of view, it is not $\mathcal{B}(x)$ that matters but rather $A(x)$, which describes the geometric accumulation of the phase along the interfering rays. We further discuss this interference under the headline "The Aharonov Bohm effect":

═══════ [10.4] Semiclassical perspective

Consider Hamiltonian $\mathcal{H} = H(x,p)$, with conjugate operators $[x,p] = i$. Commutators can be approximated by Poisson Brackets, namely, $[f,g] \approx i[f,g]_{\mathrm{PB}}$. Therefore the quantum equations of motion for $\dot{x}$ and $\dot{p}$ can be approximated by the classical Hamilton equations. For that we have to assume that we are dealing with a "minimal" wavepacket such that $\langle f(x,p) \rangle \approx f(\langle x \rangle, \langle p \rangle)$ holds for any reasonable smooth function f. If quantum dynamics can be approximated by classical dynamics we say that there is Quantum-to-Classical Correspondence (QCC). There are more refined statements regarding QCC, that do not involve assumption regarding the wavepacket preparation, but we shall not get into it here...

Irrespective of QCC, we can play with the units of x and p, and also with the units of the time t. Let us define scaled units such that $x = \alpha X$ and $p = \beta P$ and $t = \gamma T$. Let us define a classical Hamiltonian

$$\tilde{H}_{cl}(X,P) \;\;=\;\; [\gamma/(\alpha\beta)]\; H(\alpha X, \beta P) \tag{10.23}$$

Note that $[X,P] = i\hbar$, with $\hbar = 1/(\alpha\beta)$. One can easily verify that $U = \exp[-it\mathcal{H}] = \exp[-i(T/\hbar)\tilde{H}_{cl}(X,P)]$. Furthermore, one can easily verify that the correct equations of motion are obtained for $\dot{X}$ and $\dot{P}$ using Hamilton's equations.

Using this procedure we can bring the original Hamiltonian into a scaled form, that determines the classical dynamics, while in the quantum version we have an additional dimensionless parameter $\hbar$ that has no effect on the classical dynamics. For example, consider the Hamiltonian $H = B^2 p^2 + A^2(x^2 + y^2) + C^2 x^2 y^2$. If we choose $\alpha = A/C$ and $\beta = A^2/(BC)$ and $\gamma = 1/(AB)$ we get $\tilde{H}_{cl} = P^2 + X^2 + Y^2 + X^2 Y^2$, with $\hbar = BC^2/A^3$. Now we can test how QCC is affected as $\hbar$ becomes smaller...

Let us discuss an additional example, that better illuminates the meaning of the scaled $\hbar$. Consider a particle of mass M is a one-dimensional box of length L and depth V. In a classical scaling procedure it is natural to choose units such that $L = 1$, and the units of momentum such that $2\sqrt{2MV} = 1$, and the units of time such that $(2/L)\sqrt{2V/M} = 1$. With such units the phase-space area is unity, and $2\pi\hbar$ is the so called Planck cell area, measured in phase-space units. Clearly we can place a particle in this box only if the QCC condition $2\pi\hbar \ll 1$ is satisfied. Essentially the same example, in a somewhat different presentation, refers to a particle of mass M and kinetic energy E is a box of length L. Here the we can choose units such that $\sqrt{2ME} = 1$. Then it follows that the the dimensionless $\hbar$ is the ratio between between its De-Broglie wavelength and the length L of the box.

We can also go in reverse. Say we are given classical Hamiltonian $\tilde{H}_{cl}(X,P)$ with conjugate coordinates $[X,P] = i\hbar$. From a quantum perspective it is then more natural to define coordinates $X = x$ and $P = \hbar p$, such that $[x,p] = i$. The evolution $U = \exp[-i\mathcal{H}t]$ is generated by the quantum Hamiltonian

$$\mathcal{H} \;\;=\;\; \frac{1}{\hbar}\tilde{H}_{cl}(x, \hbar p) \;\;=\;\; \hbar\frac{p^2}{2M} + \frac{1}{\hbar}V(x) \tag{10.24}$$

One has to realize that different values of $\hbar$ are classically equivalent (up to choice of units) but it is not so quantum-mechanically.

QCC for eigenstates.– Using the Wigner-Weyl formalism (see special topics lecture) it can be established that eigenstates correspond to classical microcanonical states that are supported by energy shells $H(X,P) = \mathrm{const}$. This statement strictly holds for fully chaotic systems. The analogous statement for single degree of freedom system is implied by the WKB formalism (see dedicated lecture), while the generalization to integrable systems with more degrees of freedom is known as EBK.

Quasi periodicity.– In general the quantum dynamics is always quasi-periodic on the so-called Heisenberg time scale $t_H = 2\pi/\Delta$ where Δ is the mean level spacing. But breakdown of QCC can happen much before. On the technical level the breakdown is related to higher $\hbar$ orders in the expansion of $[f,g]$, and also to the failure to factorize expectation values, namely, in general $\langle fg \rangle \neq \langle f \rangle \langle g \rangle$. In a semiclassical perspective $\hbar$ sets a limit for the resolution of structures in phase space, and non-classical features may arise in the dynamical evolution.

Recurrences.– Of special interest are simple systems such as oscillator or particle-in-a-box where the spectrum is $E_n = \Omega n + \Lambda n^2$. Observables oscillates with frequencies $\Omega_{nm} = (E_n - E_m)$. There are two periods involved here: $2\pi/\Omega$ and $2\pi/\Lambda$. Recurrences happens whenever the time t is multiple of those periods, aka Talbot effect.

====== **[10.5] The continuity Equation (conservation of probability)**

The Schrodinger equation is traditionally written as follows:

$$
\begin{aligned}
\hat{\mathcal{H}} &= \mathcal{H}(\hat{x}, \hat{p}) \\
\frac{\partial |\Psi\rangle}{\partial t} &= -i\hat{\mathcal{H}} |\Psi\rangle \\
\frac{\partial \Psi}{\partial t} &= -i\mathcal{H}\left(x, -i\frac{\partial}{\partial x}\right)\Psi \\
\frac{\partial \Psi}{\partial t} &= -i\left[\frac{1}{2\mathsf{m}}(-i\nabla - A(x))^2 + V(x)\right]\Psi(x)
\end{aligned}
\tag{10.25}
$$

Using the "rate of change formula" for the probability density we can obtain a continuity equation:

$$
\frac{\partial \rho(x)}{\partial t} = -\nabla \cdot J(x)
\tag{10.26}
$$

In this formula the probability density and probability current are defined as the expectation values of the following operators:

$$
\hat{\rho}(x) = \delta(\hat{x} - x)
\tag{10.27}
$$

$$
\hat{J}(x) = \frac{1}{2}(\hat{v}\delta(\hat{x} - x) + \delta(\hat{x} - x)\hat{v})
\tag{10.28}
$$

leading to

$$
\rho(x) = \langle\Psi|\hat{\rho}(x)|\Psi\rangle = |\Psi(x)|^2
\tag{10.29}
$$

$$
J(x) = \langle\Psi|\hat{\mathbf{J}}(x)|\Psi\rangle = \mathrm{Re}\left[\Psi^*(x)\frac{1}{\mathsf{m}}(-i\nabla - A(x))\Psi(x)\right]
\tag{10.30}
$$

The procedure to get this result can be optionally applied to a particle in an N-site system.

====== **[10.6] Definition of generalized forces**

We would like to know how the system energy changes when we change a parameters X on which the Hamiltonian $\mathcal{H}$ depends. We define the generalized force $\mathcal{F}$ as

$$
\mathcal{F} = -\frac{\partial \mathcal{H}}{\partial X}
\tag{10.31}
$$

We recall that the rate of change formula for an operator A is:

$$
\frac{d\langle \hat{A}\rangle}{dt} = \left\langle i[\hat{\mathcal{H}}, \hat{A}] + \frac{\partial \hat{A}}{\partial t}\right\rangle
\tag{10.32}
$$

In particular, the rate of change of the energy is:

$$
\frac{dE}{dt} = \frac{d\langle \hat{\mathcal{H}}\rangle}{dt} = \left\langle i[\hat{\mathcal{H}}, \hat{\mathcal{H}}] + \frac{\partial \mathcal{H}}{\partial t}\right\rangle = \left\langle \frac{\partial \mathcal{H}}{\partial t}\right\rangle = \dot{X}\left\langle \frac{\partial \mathcal{H}}{\partial X}\right\rangle = -\dot{X}\langle\mathcal{F}\rangle
\tag{10.33}
$$

If $E(0)$ is the energy at time $t = 0$ we can calculate the energy $E(t)$ at a later time. Using standard phrasing we say that an external work $E(t) - E(0)$ is involved in the process. Hence it is customary to define the work W which is done by the system as:

$$W \;\; = \;\; -(E(t) - E(0)) \;\; = \;\; \int \langle \mathcal{F} \rangle \, \dot{X} dt \;\; = \;\; \int \langle \mathcal{F} \rangle \, dX \tag{10.34}$$

A "Newtonian force" is associated with the displacement of a piston. A generalized force called "pressure" is associated with the change of the volume of a box. A generalized force called "polarization" is associated with the change in an electric field. A generalized force called "magnetization" is associated with the change in a magnetic field.

═══════ [10.7] Definition of currents

There are two ways to define "current" operators. The "probability current" is defined via the rate of change of the occupation operator (see discussion of the "continuity equation"). The "electrical current" is defined as the generalized force associated with the change in a magnetic flux. Namely, let us assume that at a moment t the flux is Φ, and that at the moment $t + dt$ the flux is $\Phi + d\Phi$. The electromotive force (measured in volts) is according to Faraday's law:

$$\text{EMF} \;\; = \;\; -\frac{d\Phi}{dt} \tag{10.35}$$

If the electrical current is I then the amount of charge that has been displaced is:

$$dQ \;\; = \;\; I dt \tag{10.36}$$

The ("external") work which is done by the electric field on the displaced charge, is

$$-dW \;\; = \;\; \text{EMF} \times dQ \;\; = \;\; -I d\Phi \tag{10.37}$$

This formula implies that the generalized force which is associated with the change of magnetic flux is in fact the electrical current. Note the analogy between flux and magnetic field, and hence between current and magnetization. In fact one can regard the current in the ring as the "magnetization" of a spinning charge.

===== [10.8] The Concept of Symmetry

Symmetry and invariance are two different concepts. Invariance means that the laws of physics and hence the form of the Hamiltonian do not change. But the fields in the Hamiltonian may change. In contrast to that in case of a symmetry we requite $\tilde{\mathcal{H}} = \mathcal{H}$, meaning that the fields look the literally same. As an example consider a particle that moves in the periodic potential $V(x; R) = \cos(2\pi(x - R)/L)$. The Hamiltonian is invariant under translations: If we make translation a then the new Hamiltonian will be the same but with $R = R - a$. But in the special case that R/L is an integer we have symmetry, because then $V(x; R)$ stays the same.

Pedagogical remark.– In order to motivate and to clarify the abstract discussion in this section it is recommended to consider the problem of finding the Landau levels in Hall geometry, where the system is invariant to x translations and hence p_x is a constant of motion. Later the ideas are extended to discuss motion in centrally symmetrical potentials.

Significance of Commutation.– Let us assume for example that $[\mathcal{H}, p_x] = 0$. We say in such case that the Hamiltonian commutes with the generator of translations. What are the implication of this statement? The answer is that in such case:

- The Hamiltonian is symmetric under translations
- The Hamiltonian is block diagonal in the momentum basis
- The momentum is a constant of motion
- There might be systematic degeneracies in the spectrum

The second statement follows from the "separation of variables" theorem. The third statement follows from the expectation value rate of change formula:

$$\frac{d\langle p_x \rangle}{dt} \;=\; \langle i[\mathcal{H}, p_x] \rangle \;=\; 0 \tag{10.38}$$

The first and the fourth statements are further discussed below.

Conservation of Momentum.– Consider a collision between two particles. Assuming that they have an interaction $V(x_1 - x_2)$ that depends on their distance, the Hamiltonian has symmetry under translations, and hence the total momentum $P = p_1 + p_2$ is constant of motion. This observations implies that the quantum definition of mass (as parameter in the dispersion relation) is consistent with the Newtonian definition of inertial mass (where mass ratio is determined via a collision experiment).

Conservation of Energy.– For time independent Hamiltonians $E = \langle \mathcal{H} \rangle$ is a constant of the motion because $[\mathcal{H}, \mathcal{H}] = 0$. Thus $\langle \mathcal{H} \rangle = $ const is associated with symmetry with respect to "translations" in time, while $\langle p \rangle = $ const is associated with symmetry with respect to translations in space, and $\langle L \rangle = $ const is associated with symmetry with respect to rotations.

===== [10.9] Symmetry under translations and rotations

We would like to clarify the algebraic characterization of symmetry. For simplicity of presentation we consider translations. We claim that the Hamiltonian is symmetric under translations iff

$$[\mathcal{H}, p_i] = 0 \;\; \text{for } i = x, y, z \tag{10.39}$$

This implies that

$$[\mathcal{H}, D(a)] = 0, \;\;\; \text{for any } a \tag{10.40}$$

which can be written as $\mathcal{H}D - D\mathcal{H} = 0$, or optionally as

$$D^{-1}\mathcal{H}D \;=\; \mathcal{H} \tag{10.41}$$

If we change to a translated frame of reference, then we have a new basis which is defined as follows:

$$|\tilde{x}\rangle \;=\; |x+a\rangle \;=\; D|x\rangle \tag{10.42}$$

The transformation matrix is

$$T_{x_1,x_2} \;\equiv\; \langle x_1|\tilde{x}_2\rangle \;=\; \Big[D(a)\Big]_{x_1,x_2} \tag{10.43}$$

and the Hamiltonian matrix in the new basis is

$$\tilde{\mathcal{H}}_{x_1,x_2} \;\equiv\; \langle \tilde{x}_1|\mathcal{H}|\tilde{x}_2\rangle \;=\; \Big[T^{-1}\mathcal{H}T\Big]_{x_1,x_2} \tag{10.44}$$

The commutation of $\mathcal{H}$ with D implies that the transformed Hamiltonian $\tilde{\mathcal{H}}$ is the same in the translated frame of reference. An analogous statement holds for rotations. The algebraic characterization of symmetry in this case is

$$[\mathcal{H}, L_i] = 0 \;\; \text{for } i = x, y, z \tag{10.45}$$

which implies $[\mathcal{H}, R(\vec{\Phi})] = 0$ for any $\vec{\Phi}$, leading as before to the conclusion that the Hamiltonian remains the same if we transform it to a rotated frame of reference.

======= [10.10] Momentum for particle-and-field system

We have clarified above, for a system that is symmetric under translation, that the momentum operator is a constant of motion. Let us find the explicit expression for the (total) momentum operator in the less trivial case of particle-and-field system. In what follows we are going to explain that it can be expressed as $\boldsymbol{P} = \boldsymbol{p} + \sum_k k\boldsymbol{n}_k$, where bold letters indicate operators. The operator $\boldsymbol{p}$ is the generator of particle translations. The modes of the field are distinguished by the wavenumber index k. The $\boldsymbol{n}_k$ are the respective occupation operators.

In order to have a tangible model of field in mind, let us assume that in each point x of space we have an harmonic oscillator whose dynamics is described by the complex coordinate $\boldsymbol{A}_x = (\boldsymbol{Q}_x + i\boldsymbol{P}_x)/\sqrt{2}$. The Hamiltonian $\mathcal{H}_A$ of the free field contains interaction between the oscillators. If we assume that $\mathcal{H}_A$ is invariant under translation, the normal modes are denoted $\boldsymbol{a}_k$, such that $\boldsymbol{A}_x = L^{-1/2}\sum_k e^{ikx}\boldsymbol{a}_k$, where L is the length of the system. The dynamics of a normal modes is generated by $(\Omega_k/2)[\boldsymbol{P}_k^2 + \boldsymbol{Q}_k^2]$ or equivalently $\Omega_k \boldsymbol{a}_k^\dagger \boldsymbol{a}_k$. Accordingly, the free field Hamiltonian takes the form $\mathcal{H}_A = \sum_k \Omega_k \boldsymbol{n}_k$, where the occupation operators are defined as $\boldsymbol{n}_k = \boldsymbol{a}_k^\dagger \boldsymbol{a}_k$. For the free particle let us assume $\mathcal{H}_P \propto \boldsymbol{p}^2$, where $\boldsymbol{p}$ generates translations in $\boldsymbol{r}$. For the particle-field system let us consider

$$\mathcal{H} \;=\; \mathcal{H}_P + \mathcal{H}_A + \sum_x u(\boldsymbol{r} - x)\,\boldsymbol{A}_x^\dagger \boldsymbol{A}_x \tag{10.46}$$

where $\mathcal{H}_A$ is invariant under translation, namely, $\delta\mathcal{H}_A = 0$ for $\boldsymbol{A}_x \mapsto \boldsymbol{A}_x - \delta x \partial_x \boldsymbol{A}_x$. If we treat this Hamiltonian classically, the dynamics is generate by the Hamilton's equations of motion:

$$\dot{\boldsymbol{p}} \;=\; -\sum_x u'(\boldsymbol{r} - x)\,\boldsymbol{A}_x^\dagger \boldsymbol{A}_x \tag{10.47}$$

$$\dot{\boldsymbol{A}}_x \;=\; -i\frac{\partial \mathcal{H}_A}{\partial \boldsymbol{A}_x^\dagger} - i\,u(\boldsymbol{r} - x)\,\boldsymbol{A}_x \tag{10.48}$$

By direct substitution one can verify that there are two constants of motions $\boldsymbol{N}$ and $\boldsymbol{P}$ that we defined below, such that $(d/dt)\boldsymbol{N} = (d/dt)\boldsymbol{P} = 0$. These constants of motion are related to symmetries of $\mathcal{H}$ for $\boldsymbol{A}$-gauge and for

translations. The respective generators are

$$N \;\; = \;\; \sum_x \boldsymbol{A}_x^\dagger \boldsymbol{A}_x \;\; = \;\; \sum_k \boldsymbol{n}_k \tag{10.49}$$

$$P \;\; = \;\; \boldsymbol{p} - i \sum_x \boldsymbol{A}_x^\dagger \partial_x \boldsymbol{A}_x \;\; = \;\; \boldsymbol{p} \; + \; \sum_k k \, \boldsymbol{n}_k \tag{10.50}$$

The respective transformations are $\boldsymbol{R} = \exp(-i\phi\boldsymbol{N})$ and $\boldsymbol{D} = \exp(-i\ell\boldsymbol{P})$. Clearly $\boldsymbol{R}$ "rotates" the phase of the field operators, namely, $\boldsymbol{R}^\dagger \boldsymbol{A}_x \boldsymbol{R} = e^{-i\phi} \boldsymbol{A}_x$. It is also clear that $\boldsymbol{D}$ translates the particle, namely $\boldsymbol{D}^\dagger \boldsymbol{r} \boldsymbol{D} = r + \ell$. In order to prove that $\boldsymbol{D}$ also translates the field we note that $\boldsymbol{D}^\dagger \boldsymbol{a}_k \boldsymbol{D} = e^{-ik\ell} \boldsymbol{a}_k$. Then it follows that $\boldsymbol{D}^\dagger \boldsymbol{A}_x \boldsymbol{D} = \boldsymbol{A}_{x-\ell}$, which is the algebraic characterization of field translations. Recall that this algebraic characterization implies that a Fock-occupation state $|\Psi\rangle = [...(\boldsymbol{A}_2^\dagger)^{n_2}(\boldsymbol{A}_1^\dagger)^{n_1}] |0, 0, ...\rangle$ is displaced if we operate on it with $\boldsymbol{D}$.

===== [10.11] Symmetry implied degeneracies

Let us assume that $\mathcal{H}$ is symmetric under translations D. Then if $|\psi\rangle$ is an eigenstate of $\mathcal{H}$ then also $|\varphi\rangle = D|\psi\rangle$ is an eigenstate with the same eigenvalue. This is because

$$\mathcal{H}|\varphi\rangle = \mathcal{H}D|\psi\rangle = D\mathcal{H}|\psi\rangle = E|\varphi\rangle \tag{10.51}$$

Now there are two possibilities. One possibility is that $|\psi\rangle$ is an eigenstate of D, and hence $|\varphi\rangle$ is the same state as $|\psi\rangle$. In such case we say that the symmetry of $|\psi\rangle$ is the same as of $\mathcal{H}$, and a degeneracy is not implied. The other possibility is that $|\psi\rangle$ has lower symmetry compared with $\mathcal{H}$. Then it is implied that $|\psi\rangle$ and $|\varphi\rangle$ span a subspace of degenerate states. If we have two symmetry operations A and B, then we might suspect that some eigenstates would have both symmetries: that means both $A|\psi\rangle \propto |\psi\rangle$ and $B|\psi\rangle \propto |\psi\rangle$. If both symmetries hold for all the eigenstates, then it follows that $[A, B] = 0$, because both are diagonal in the same basis.

In order to argue a symmetry implied degeneracy the Hamiltonian should *commute with a non-commutative group of operators*. It is simplest to explain this statement by considering an example. Let us consider particle on a clean ring. The Hamiltonian has symmetry under translations (generated by $\hat{p}$) and also under reflections (R). We can take the k_n states as a basis. They are eigenstates of the Hamiltonian, and they are also eigenstates of $\hat{p}$. The ground state $n = 0$ has the same symmetries as that of the Hamiltonian and therefore there is no implied degeneracy. But $|k_n\rangle$ with $n \neq 0$ has lower symmetry compared with $\mathcal{H}$, and therefore there is an implied degeneracy with its mirror image $|k_{-n}\rangle$. These degeneracies are unavoidable. If all the states were non-degenerated it would imply that both $\hat{p}$ and R are diagonal in the same basis. This cannot be the case because the group of translations together with reflection is non-commutative.

The dimensions of a degenerate subspaces.– These are determined by the dimensions of the *irreducible* representations of the symmetry group. The jargon will be better clarified in a future lecture. In simple language it is implied by the following argument: One can regard $\mathcal{H}$ as a mutual constant of motion for all the group operators; therefore, by the "separation of variables theorem", it induces a block-decomposition of the group representation. The dimensions of the blocks are the dimensions of the degenerate subspaces, and at the same time they must be compatible with the dimensions of the irreducible representations of the group.

Accidental degeneracies.– Above we were discussing only the systematic degeneracies that are implied by the symmetry group of the Hamiltonian. In principle we can have also "accidental" degeneracies which are not implied by symmetries. The way to "cook" such symmetry is as follows: pick two neighboring levels, and change some parameters in the Hamiltonian so as to make them degenerate. It can be easily argued that in general we have to adjust 3 parameters in order to cook a degeneracy. If the system has time reversal symmetry, then the Hamiltonian can be represented by a real matrix. In such case it is enough to adjust 2 parameters in order to cook a degeneracy.

Avoided crossings.– A more common scenario that leads to accidental degeneracies, assumes that the Hamiltonian is block diagonal due to some symmetry, for *any* value of a control parameter. The control parameter is likely to affect *differently* the blocks. As the control parameter is varied, the levels that are associated with one block cross the levels that are associated with the other blocks. This typically lead to multiple crossing points. These crossings become *avoided crossings* if a perturbation that does not respect the symmetry is added to the Hamiltonian.

Fundamentals (part III)

[11] Group representation theory

═══════ [11.1] Groups

A group is a set of elements with a binary operation:

- The operation is defined by a multiplication table for $\tau * \tau'$.
- There is a unique identity element $\mathbf{1}$.
- Every element has an inverse element such that $\tau\tau^{-1} = \mathbf{1}$
- Associativity: $\tau * (\tau' * \tau'') = (\tau * \tau') * \tau''$

Commutativity does not have to be obeyed: this means that in general $\tau * \tau' \neq \tau' * \tau$. In practice, a group that has a finite number of elements, can be defined via a *multiplication table*. But this is strategy is not practical if we are dealing with a group that has infinite number of elements. Such is the group of rotations SO(3).

For a Lie group, we assume that each element τ of the group is labeled by a set of parameters that serve as coordinates. Therefore we can regard the set of elements as a set of points that form a *manifold*. By convention we label the identity $\mathbf{1}$ as $\tau = (0, 0, ..., 0)$, and refer to it as the origin of the manifold. For SO(3) the standard labeling of rotations is $\vec{\Phi} = (\Phi_x, \Phi_y, \Phi_z)$, and the manifold is a ball of radius π.

In order to provide a tangible definition for the group operation, each element of the group is regarded as a *transformation* over some space:

$$
\begin{array}{rcll}
\text{element of the group} & = & \boldsymbol{\tau} = (\tau_1, \tau_2, ..., \tau_d) & (11.1) \\
\text{corresponding transformation} & = & U(\boldsymbol{\tau}) & (11.2) \\
\text{the "group property"} & = & U(\boldsymbol{\tau})U(\boldsymbol{\tau}') = U(\boldsymbol{\tau} * \boldsymbol{\tau}') & (11.3)
\end{array}
$$

The association $\boldsymbol{\tau} \mapsto U(\boldsymbol{\tau})$ is called a *realization*. We use the notations $\tau * \tau * ... * \tau \equiv n\tau$, where n is the number of repetitions. Accordingly $U(0) = \mathbf{1}$, and $U(n\tau) = U(\tau)U(\tau)...U(\tau) = U(\tau)^n$. The crucial observation for a Lie group is that we can generate large transformations from infinitesimal transformations. Thus it is meaningful to define a *ray* of elements as $U(\alpha\tau)$ where α is a real number. For SO(3) a ray of elements includes all the rotations around the same axis.

═══════ [11.2] Realization using linear transformations

As defined above, a realization means that we regard each element of the group as an operation over a space. We treat the elements as transformations. Below we discuss the possibility of finding a realization that consists of *linear* transformations.

First we will discuss the concept of linear transformation, in order to clarify it. Consider a function that can be regarded as a realization for a translation, namely, $f(x) = x + 5$. Is it a linear function? A linear function must fulfill the condition:

$$f(\alpha X_1 + \beta X_2) = \alpha f(X_1) + \beta f(X_2) \tag{11.4}$$

Checking $f(x)$:

$$
\begin{aligned}
& f(3) = 8, f(5) = 10, f(8) = 13 \\
& f(3 + 5) \neq f(3) + f(5)
\end{aligned}
\tag{11.5}
$$

Hence we realize that $f(x)$ is not linear.

In the defining realization of the Galilein group over phase space, rotations are linear transformations, but translations and boosts are not. If we want to realize the Galilein group using linear transformations, the most natural way would be to define a realization over the function space. For example, the translation of a function is defined as:

$$\tau_{\mathbf{a}} : \quad \tilde{\Psi}(x) = \Psi(x - a) \tag{11.6}$$

The translation of a function is a linear operation. In other words, if we translate the function $\alpha\psi(x) + \beta\varphi(x)$ a spatial distance a, then we get the appropriate linear combination of the translated functions $\alpha\psi^a(x - a) + \beta\varphi(x - a)$.

Linear transformations are represented by matrices. This leads us to the concept of a "representation", which we discuss in the next section.

===== [11.3] Representation of a group using matrices

A *representation* associates with each element $\boldsymbol{\tau}$ of the group a matrix $U_{ij}(\boldsymbol{\tau})$. The "multiplication table" of the matrices is required to be be in one-to-one correspondence to the multiplication table of the elements of the group. Below we "soften" this requirement, being satisfied with having a "multiplication table" that is the same "up to a phase factor":

$$U(\tau' * \tau'') \;=\; e^{i(\text{phase})} U(\tau') U(\tau'') \tag{11.7}$$

It is natural to consider realizations that consist of orthogonal transformations over a real space, or unitary transformations over a complex space. Any realization using a linear transformations provides a "representation" once a basis is chosen: linear transformations are represented by matrices. For example, we may consider the realization of translations over the function space. Any function can be written as a combination of delta functions:

$$\Psi(x) = \int \Psi(x') \delta(x - x') dx \tag{11.8}$$

In Dirac notation this can be written as:

$$|\Psi\rangle = \sum_x \Psi_x |x\rangle \tag{11.9}$$

In this basis, each translation is represented by a matrix:

$$D_{x,x'} \;=\; \langle x|D(a)|x'\rangle \;=\; \delta(x - (x' + a)) \tag{11.10}$$

Finding a "representation" for a group is very useful: the operative meaning of "multiplying group elements" becomes "multiplying matrices". This means that we can deal with groups using Linear Algebra tools.

===== [11.4] Some algebraic observations

Given two matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ that do not commute we have in general

$$e^{\boldsymbol{A}} e^{\boldsymbol{B}} \;\neq\; e^{\boldsymbol{B}} e^{\boldsymbol{A}} \;\neq\; e^{\boldsymbol{A}+\boldsymbol{B}} \tag{11.11}$$

But if the matrices are infinitesimal then:

$$e^{\epsilon\boldsymbol{A}+\epsilon\boldsymbol{B}} \;=\; e^{\epsilon\boldsymbol{A}} e^{\epsilon\boldsymbol{B}} \;=\; e^{\epsilon\boldsymbol{B}} e^{\epsilon\boldsymbol{A}} \;=\; \mathbf{1} + \epsilon\boldsymbol{A} + \epsilon\boldsymbol{B} + \mathcal{O}(\epsilon^2) \tag{11.12}$$

If the small parameter ϵ is absent, we can still do the exponentiation in small steps, leading to the so called *Trotter formula*, namely,

$$e^{\boldsymbol{A}+\boldsymbol{B}} \quad = \quad \lim_{N\to\infty} \left[e^{(1/N)\boldsymbol{A}}\, e^{(1/N)\boldsymbol{B}} \right]^N \tag{11.13}$$

Above the small parameter is $\epsilon = 1/N$, and the re-ordering of the multiplication involves $\mathcal{O}(N)$ transpositions, each with error ϵ^2. To get $e^{\boldsymbol{A}}e^{\boldsymbol{B}}$ using further re-ordering is not possible because the number of required transpositions exceeds $\mathcal{O}(N^2)$, leading to and error that does not vanish in the $N \to \infty$ limit.

A similar reasoning leads to the following *Commutator formula*

$$e^{[\boldsymbol{A},\boldsymbol{B}]} \quad = \quad \left[e^{-i\sqrt{\epsilon}\boldsymbol{B}}\, e^{-i\sqrt{\epsilon}\boldsymbol{A}}\, e^{i\sqrt{\epsilon}\boldsymbol{B}}\, e^{i\sqrt{\epsilon}\boldsymbol{A}} \right]^N \tag{11.14}$$

where $\epsilon = 1/N$, and we used the leading-order identity

$$1 + \epsilon\,(\boldsymbol{AB} - \boldsymbol{BA}) \;=\; \left(1 - i\sqrt{\epsilon}\boldsymbol{B} - \frac{1}{2}\epsilon\boldsymbol{B}^2\right)\left(1 - i\sqrt{\epsilon}\boldsymbol{A} - \frac{1}{2}\epsilon\boldsymbol{A}^2\right)\left(1 + i\sqrt{\epsilon}\boldsymbol{B} - \frac{1}{2}\epsilon\boldsymbol{B}^2\right)\left(1 + i\sqrt{\epsilon}\boldsymbol{A} - \frac{1}{2}\epsilon\boldsymbol{A}^2\right)$$

Finally we mention the *Baker-Campbell-Hausdorff formula* that allows to express the result of multiplication in terms of commutators:

$$e^{\boldsymbol{A}}e^{\boldsymbol{B}} \quad = \quad e^{\boldsymbol{A}+\boldsymbol{B}+\boldsymbol{C}} \tag{11.15}$$

Here $\boldsymbol{C}$ is an expression that includes linear combination of matrices and their commutators. The explicit expression for $\boldsymbol{C}$ requires a Taylor expansion

$$\boldsymbol{C} \quad = \quad \log(e^{\boldsymbol{A}}e^{\boldsymbol{B}}) - \boldsymbol{A} - \boldsymbol{B} \quad = \quad \frac{1}{2}[\boldsymbol{A},\boldsymbol{B}] + \frac{1}{12}[(\boldsymbol{A}-\boldsymbol{B}),[\boldsymbol{A},\boldsymbol{B}]] + ... \tag{11.16}$$

It is possible to find an explicit expression up to any desired accuracy. For details see Wikipedia, or a paper by Wilcox (1967).

══════ [11.5] Generators and their Algebra

For a given *ray* of elements we can defined a generator, say we call it G_1. Then we can define a parameter τ_1 that labels the elements along this ray. Namely,

$$U(\delta\tau_1) \quad \equiv \quad \boldsymbol{1} - i\delta\tau_1 G_1 \tag{11.17}$$

Such that

$$U(\tau_1) \quad = \quad e^{-i\tau_1 G_1} \tag{11.18}$$

There are infinitely many rays, so there are infinitely many generators. But the set of generators form a linear space. This means that if G_1 and G_2 are generators, then also $G = \alpha_1 G_1 + \alpha_2 G_2$ is a generator. The argument is as follows: We have to show that $U = \exp[itG]$ is an element of the group. Using the Trotter formula we can express it as a multiplication of $\exp[-i\delta\tau_1 G_1]$ and $\exp[-i\delta\tau_2 G_2]$ operations. The latter represent elements of the group, hence also their product represents an element of the group.

In fact the set of generators form an Algebra that is known as *Lie Algebra*. Namely, we also have an operation such that if G_1 and G_2 are generators, then also $G = i[G_1, G_2]$ is a generator. It should be clear that if $G_1 = A$ and $G_2 = B$

generate (say) rotations, it does not imply (say) that the hermitian operator $H = A^3B^2 + B^2A^3$ is a generator of a rotation. On the other hand, it does imply that $G = i[A, B]$ is a generator of a group element. The argument for that proceeds as in the previous paragraph, using the *Commutator formula*.

===== [11.6] Generating a representation

The linear space of generators obviously has a finite dimension because the generators are represented by matrices that have finite dimension. Note that the dimension of this linear-space is the dimension of the group-manifold. For example, in the standard representations of SO(3) and SU(3) the generators are 3×3 matrices, and the dimension of the manifold is $d=3$ and $d=8$ respectively. Consequently we can choose a basis G_μ, such that a general generator is written as a linear combination

$$G \;=\; \sum_\mu \alpha_\mu G_\mu \;\equiv\; \boldsymbol{\alpha} \cdot \boldsymbol{G} \tag{11.19}$$

Then, using G, we can generate matrices that represent a *ray* of group elements:

$$U(t) \;=\; \exp[-itG] \;\equiv\; \exp[-i\boldsymbol{\tau} \cdot \boldsymbol{G}] \;\equiv\; U(\tau_1, \tau_2, ...) \tag{11.20}$$

The bottom line is that any element of the group can be represented by a matrix $U(\boldsymbol{\tau})$, where $\boldsymbol{\tau}$ is a set of coordinates that label points of the group-manifold. The Trotter formula can be used in order to express any such U as a composition of infinitesimal transformations as follows:

$$\begin{aligned} U(\boldsymbol{\tau}) &= [U(\delta\boldsymbol{\tau})]^N \\ &= [\, U(\delta\tau_1)\, U(\delta\tau_2)\cdots]^N = \\ &= [\, e^{-i\delta\tau_1 G_1}\, e^{-i\delta\tau_2 G_2}\cdots]^N \end{aligned} \tag{11.21}$$

===== [11.7] Structure constants

We have argued that $i[G_\mu, G_\nu]$ is a generator. Therefore, it must be a linear combination of the basic generators. In other words, there exit constants $c_{\mu\nu}^\lambda$ such that the following closure relation is satisfied:

$$[G_\mu, G_\nu] \;=\; i\sum_\lambda c_{\mu\nu}^\lambda G_\lambda \tag{11.22}$$

The constants $c_{\mu\nu}^\lambda$ are called the *structure constants* of the group. Every *Lie group* has its own structure coefficients. If we know the structure constants, we can reconstruct the group *multiplication table*. This observation is based on the *Baker-Campbell-Hausdorff formula*. Form this formula it follows that

$$e^{-i\boldsymbol{\alpha}\cdot\boldsymbol{G}}\, e^{-i\boldsymbol{\beta}\cdot\boldsymbol{G}} \;=\; e^{-i\boldsymbol{\gamma}\cdot\boldsymbol{G}} \tag{11.23}$$

where

$$\gamma_\lambda \;=\; \alpha_\lambda + \beta_\lambda + \frac{1}{2}c_{\mu\nu}^\lambda \alpha_\mu \beta_\nu - \frac{1}{12}c_{\kappa\sigma}^\lambda c_{\mu\nu}^\kappa (\alpha - \beta)_\sigma \alpha_\mu \beta_\nu + ... \tag{11.24}$$

In the next lecture we shall deduce the structure constants of the rotation group from its defining representation, and then we shall learn how to build up all its other representations, just from our knowledge of the structure constants.

═══════ [11.8] The group of rotations

In the next lecture we are going to concentrate of the group of rotations. More precisely we consider on equal footing the groups SO(3) and SU(2). Both are characterized by the same Lie algebra, and consequently share the same multiplication table up to phase factors. The difference between the two groups is the topology of their manifold. The manifold of SO(3) is a ball of radius π, where apposite points on its boundary are identified as the same point. The manifold of SU(2) is simpler. It is a ball of radius 2π, where all the points on its boundary are identified as the same point. This gives as expected a sphere (S^3). We say "as expected", because any SU(2) matrix can be parameterized trivially as follows:

$$R = \begin{pmatrix} x_1 + ix_2 & x_3 + ix_4 \\ -x_3 + ix_4 & x_1 - ix_2 \end{pmatrix} \tag{11.25}$$

with $x_1^2 + x_2^2 + x_3^2 + x_4^2 = 1$.

═══════ [11.9] The Galilein Group

The Galilein group includes translations, rotations, and boosts. A translation is specified uniquely by three parameters $\mathbf{a} = (a_1, a_2, a_3)$. Rotations are specified by (θ, φ, Φ), from which $\mathbf{\Phi}$ is constructed. A boost is parametrized by the relative velocity $\mathbf{u} = (u_1, u_2, u_3)$. A general element is any translation, rotation, boost, or any combination of them. The Galilein group is a Lie group with 9 parameters. The rotation group is a Lie group with 3 parameters. The realization that defines the Galilein group is over the six dimensional phase space $(\mathbf{x}, \mathbf{v})$. The realization of a translation is

$$\tau_{\mathbf{a}} : \begin{cases} \tilde{\mathbf{x}} = \mathbf{x} + \mathbf{a} \\ \tilde{\mathbf{v}} = \mathbf{v} \end{cases} \tag{11.26}$$

The realization of a boost is

$$\tau_{\mathbf{u}} : \begin{cases} \tilde{\mathbf{x}} = \mathbf{x} \\ \tilde{\mathbf{v}} = \mathbf{v} + \mathbf{u} \end{cases} \tag{11.27}$$

and the realization of a rotation is

$$\tau_{\mathbf{\Phi}} : \begin{cases} \tilde{\mathbf{x}} = R^E(\Phi)\mathbf{x} \\ \tilde{\mathbf{v}} = R^E(\Phi)\mathbf{v} \end{cases} \tag{11.28}$$

A translation by $\mathbf{b}$, and afterward a translation by $\mathbf{a}$, gives a translation by $\mathbf{b} + \mathbf{a}$. This composition rule is simple. More generally the "multiplication" of group elements $\tau = \tau' * \tau''$ implies a very complicated function

$$(\mathbf{a}, \mathbf{\Phi}, \mathbf{u}) = f(\mathbf{a}', \mathbf{\Phi}', \mathbf{u}'; \mathbf{a}'', \mathbf{\Phi}'', \mathbf{u}'') \tag{11.29}$$

We notice that this function requires 18 input parameters, and outputs 9 parameters. It is not practical to construct this function explicitly. Rather, in order to "multiply" elements we compose transformations.

The number of independent generators is the same as the number of parameters that specify the elements of the group, e.g. 3 generators for the rotation group. In the case of the Galieli we have 9 generators, but since we allow arbitrary phase factor in the multiplaication table, we have in fact 10 generators:

$$\hat{P}_x, \hat{P}_y, \hat{P}_z, \hat{J}_x, \hat{J}_y, \hat{J}_z, \hat{Q}_x, \hat{Q}_y, \hat{Q}_z, \quad \text{and} \quad \hat{\mathbf{1}}. \tag{11.30}$$

Consider the standard representation over wavefunctions. It follows from the commutation relation $[\hat{x}, \hat{p}] = i$ that $-\hat{x}$ is the generator of translations in $\hat{p}$. Hence it follows that he generators of the boosts are $\hat{Q}_x = -\mathsf{m}\hat{x}$, where m is the mass.

══════ [11.10] The Heisenberg group

In the present section we relate to the group of translations and boosts. Without loss of generality we assume a one-dimensional geometrical space. One option is to define this group is via a realization over an (x, v) phase space. If we adopt this definition we get a Abelian group whose elements commute with each other. Let us call it the "Galilein version" of the group.

Optionally we can consider a realization of translations and boosts over complex wavefunctions $\Psi(x)$. In the standard representation the space of wavefunctions is spanned by the eigenstates of the $\hat{x}$ operator, and the translations are generated by $P = \hat{p}$. It follows from $[\hat{x}, \hat{p}] = i$ that the generator of boosts is $Q = -\hat{x}$. Hence the group is non-Abelian and characterized by the Lie algebra $[P, Q] = i$. It is known as the "Heisenberg group". It has the same multiplication table as the Abelian "Galilein version", up to phase factors.

If we believe (following the two slit experiment) that the state of particle is described by a wavefunction, it follows, as argued above, that boost and translations do not commute. Let us illuminate this point using an intuitive physics language. Say we have a particle in the laboratory reference frame that is described by a wavefunction $\Psi(x)$ that is an eigenstate of the translation operators. In other words, we are talking about a momentum eigenstate that has a well defined wavenumber k. Let us transform to a moving reference frame. Assuming that boosts were commuting with translations, if follows that boost is a symmetry operation, and hence the transformed state $\tilde{\Psi}(x)$ is still a momentum eigenstate with the same k. From this we would come to the absurd conclusion that the particle has the same momentum in all reference frames.

It is interesting to look for a *realization* of the Heisenberg group over a finite-dimensional "phase-space". For this purpose we have to assume that phase space has a third coordinate: instead of (x, v) we need (a, b, c). The way to come to this conclusion is based on the observation that any element of the Heisenberg group can be written in the standard representation as

$$U(a, b, c) \quad = \quad \exp\left(iaQ + ibP + ic\right) \tag{11.31}$$

Hence the multiplication $U(a_1, b_1, c_1) \, U(a_2, b_2, c_c)$ is realized by the composition law

$$\left(a_1, b_1, c_1\right) \star \left(a_2, b_2, c_2\right) \quad = \quad \left(a_1 + a_2, \ b_1 + b_2, \ c_1 + c_2, + \frac{1}{2}(a_1 b_2 - b_1 a_2)\right) \tag{11.32}$$

Here a is position displacement, and b is momentum displacement, and c is an additional coordinate. If the order of a translation and a boost is reversed the new result is different by a phase factor $\exp(iC)$, where C equals the symplectic area of the encircled phase-space cell. This non-commutativity is reflected in the c coordinate.

[12] The group of rotations

======= [12.1] The rotation group SO(3)

The multiplication table of the rotation group $SO(3)$ is defined by its "natural" representaion, namely, the set of 3×3 orthogonal matrices that has +1 determinant. It is a non-commutative group: the order of rotations is important. Despite this, it is important to remember that infinitesimal rotations commute. We have already pointed out this statement in general, but let us demonstrate it once again for the specific case of rotations, using elemntary vector notations:

$$R(\delta\mathbf{\Phi})\mathbf{r} = \mathbf{r} + \delta\mathbf{\Phi} \times \mathbf{r} \tag{12.1}$$

Therefore, in the first-order approximation,

$$\begin{aligned} R(\delta\mathbf{\Phi}^2)R(\delta\mathbf{\Phi}^1)\mathbf{r} &= (\mathbf{r} + \delta\mathbf{\Phi}^1 \times \mathbf{r}) + \delta\mathbf{\Phi}^2 \times (\mathbf{r} + \delta\mathbf{\Phi}^1 \times \mathbf{r}) = \\ &= \mathbf{r} + (\delta\mathbf{\Phi}^1 + \delta\mathbf{\Phi}^2) \times \mathbf{r} = R(\delta\mathbf{\Phi})\mathbf{r} \end{aligned} \tag{12.2}$$

Obviously, this is not correct for finite non-infinitesimal rotations:

$$R(\vec{\Phi}^1)R(\vec{\Phi}^2) \neq R(\vec{\Phi}^1 + \vec{\Phi}^2) \neq R(\vec{\Phi}^2)R(\vec{\Phi}^1) \tag{12.3}$$

We can construct any infinitesimal rotation from small rotations around the major axes:

$$R(\delta\vec{\Phi}) = R(\delta\Phi_x\vec{e}_x + \delta\Phi_y\vec{e}_y + \delta\Phi_z\vec{e}_z) = R(\delta\Phi_x\vec{e}_x)R(\delta\Phi_y\vec{e}_y)R(\delta\Phi_z\vec{e}_z) \tag{12.4}$$

Using the vector notation $\vec{M} = (M_x, M_y, M_z)$, we conclude that a finite rotation around any axis can be written as:

$$\begin{aligned} R(\Phi\vec{n}) &= R(\vec{\Phi}) = R(\delta\vec{\Phi})^N = (R(\delta\Phi_x)R(\delta\Phi_y)R(\delta\Phi_z))^N \\ &= (e^{-i\delta\vec{\Phi}\cdot\vec{M}})^N = e^{-i\vec{\Phi}\cdot\vec{M}} = e^{-i\Phi M_n} \end{aligned} \tag{12.5}$$

Hence we conclude that $M_n = \vec{n} \cdot \vec{M}$ is the generator of the rotations around the axis $\vec{n}$.

======= [12.2] Structure constants of the rotation group

We would like to find the structure constants of the rotation group $SO(3)$, using its defining representation. The $SO(3)$ matrices induce rotations without performing reflections and all their elements are real. The matrix representation of a rotation around the z axis is:

$$R(\Phi\vec{e}_z) = \begin{pmatrix} \cos(\Phi) & -\sin(\Phi) & 0 \\ \sin(\Phi) & \cos(\Phi) & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{12.6}$$

For a small rotation:

$$R(\delta\Phi\vec{e}_z) = \begin{pmatrix} 1 & -\delta\Phi & 0 \\ \delta\Phi & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \hat{1} + \delta\Phi \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \hat{1} - i\delta\Phi M_z \tag{12.7}$$

where:

$$M_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{12.8}$$

We can find the other generators in the same way:

$$M_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \qquad M_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \tag{12.9}$$

In compact notation the 3 generators are

$$\left[M_k \right]_{ij} = -i\epsilon_{ijk} \tag{12.10}$$

Now we can calculate the structure constants. For example $[M_x, M_y] = iM_z$, and in general:

$$[M_i, M_j] = i\epsilon_{ijk}M_k \tag{12.11}$$

We could of course use a different representation of the rotation group in order to deduce this Lie algebra. In particular we could use the differential representation of the L_i over the infinite-dimensional Hilbert space of wavefunctions.

═════ [12.3] The "rotation" group SU(2)

We have defined the rotation group by the Euclidean realization over 3D space. Obviously, this representation can be used to make calculations ("to multiply rotations"). The advantage is that it is intuitive, and there is no need for complex numbers. The disadvantage is that they are 3×3 matrices with inconvenient algebraic properties, so a calculation could take hours. It would be convenient if we could "multiply rotations" with simple 2×2 matrices. In other words, we are interested in a dim=2 representation of the rotation group. The mission is to find three simple 2×2 matrices that fulfill:

$$[J_x, J_y] = iJ_z \quad \text{etc.} \tag{12.12}$$

In the next lecture we will learn a systematic approach to building all the representations of the rotation group. In the present lecture, we will simply find the requested representation by guessing. It is easy to verify that the matrices

$$S_x = \frac{1}{2}\sigma_x, \quad S_y = \frac{1}{2}\sigma_y, \quad S_z = \frac{1}{2}\sigma_z \tag{12.13}$$

fulfill the above commutation relations. So, we can use them to create a dim=2 representation of the rotation group. We construct the rotation matrices using the formula:

$$R(\vec{\Phi}) = e^{-i\vec{\Phi}\cdot\vec{S}} \tag{12.14}$$

The matrices that are generated necessarily satisfy the group multiplication table.

In fact the dim=2 representation that we have found is not a representation of SO(3) but a representation of SU(2). The two groups have in a sense the same multiplication table, but there is a twist. For SO(3) the generated $R(\Phi\vec{n})$ matrices are duplicated modulo 2π, while for SU(2) they are duplicated modulo 4π. In the latter case $R(\Phi\vec{n}) = -1$ for a $\Phi=2\pi$ rotation. We can say that the radius of the SU(2) manifold is twice compared to that of SO(3). Namely, it is $|\Phi| < 2\pi$ instead of $|\Phi| < \pi$.

═══════ [12.4] Algebraic perspective on SU(2), SU(3) and SO(3)

Let us forget about rotations, and ask what is the Lie Algebra of SU(2). Any unitary matrix can be written as $U = \exp(-iH)$ where H is hermitain. Any hermitain 2×2 matrix can be written a linear combination $H = c\mathbf{1} + \alpha_1 \boldsymbol{\sigma}_1 + \alpha_2 \boldsymbol{\sigma}_2 + \alpha_3 \boldsymbol{\sigma}_3$, with real coefficients $(c, \alpha_1, \alpha_2, \alpha_3)$. If we require $\det(U) = 1$, we have to impose $c = 0$. So we reach again the conclusion that SU(2) has a 3-dimensional manifold. The Lie algebra is $[\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2] = i2\boldsymbol{\sigma}_3$, etc. But then we realize that upon the definition of the generators S_1, S_2, S_3 we get exactly the same Lie algebra as that of SO(3). Hence we conclude that the two groups have the same multiplication table, disregarding the different "periodic boundary conditions" that are satisfied by their respective manifolds.

The same algebraic approach can be used for SU(3). Any unitary matrix can be writtenb as $U = \exp(-iH)$ where H is hermitain. Any hermitian 3×3 matrix can be written a linear combination of 9 generators. Imposing the requirement $\det(U) = 1$, we conclude that SU(3) has 8 generators, meaning that the Lie algebra of SU(3) is much richer than that of the rotation group.

The same algebraic approach can be used for SO(3). The group elements can be regarded as sub-set of SU(3). The additional requirement is to have real matrices. Writing $U = \exp(A)$ with $A = -iH$, the generator A has to be a real antisymmetric matrix

$$A \;=\; \begin{pmatrix} 0 & -\alpha_3 & \alpha_2 \\ \alpha_3 & 0 & -\alpha_1 \\ -\alpha_2 & \alpha_1 & 0 \end{pmatrix} \;=\; \alpha_1[-iM_1] + \alpha_2[-iM_2] + \alpha_3[-iM_3] \tag{12.15}$$

Thus we find that we have 3 generators, that upon *realization* we can identify as generating rotations.

We should remember the distinction between a *realization* and a *representation*: in a realization it matters what we are rotating. In a representation it only matters to us that the correct multiplication table is satisfied. Is it possible to regard any representation as a realization? Is it possible to say what the rotation matrices rotate? When there is a dim=3 Euclidean rotation matrix we can use it on real vectors that represent points in space. If the matrix operates on complex vectors, then we must look for another interpretation for the vectors. This will lead us to the definition of the concept of spin (spin 1). When we are talking about a dim=2 representation it is possible to give the vectors an interpretation. The interpretation will be another type of spin (spin 1/2).

═══════ [12.5] How to calculate a general rotation matrix

The calculation of a 2×2 rotation matrix is extremely simple. All the even powers of a given Pauli matrix are equal to the identity matrix, while all the odd powers are equal to the original matrix. From this (using Taylor expansion and separating into two partial sums), we get the result:

$$R(\Phi) \;=\; R(\Phi\vec{n}) = \mathrm{e}^{-i\Phi S_n} \;=\; \cos(\Phi/2)\hat{\mathbf{1}} - i\sin(\Phi/2)\sigma_n \tag{12.16}$$

where $\sigma_n = \vec{n} \cdot \vec{\sigma}$, and $S_n = (1/2)\sigma_n$ is the generator of a rotation around the $\vec{n}$ axis.

The analogous formula for constructing a 3×3 rotation matrix is:

$$R(\vec{\Phi}) \;=\; R(\Phi\vec{n}) = \mathrm{e}^{-i\Phi M_n} \;=\; 1 + (\cos(\Phi) - 1)M_n^2 - i\sin(\Phi)M_n \tag{12.17}$$

where $M_n = \vec{n} \cdot \vec{M}$ is the generator of a rotation around the $\vec{n}$ axis. The proof is based on a Taylor expansion. We notice that $M_z^3 = M_z$, from this it follows that for all the odd powers $M_z^k = M_z$, while for all the even powers $M_z^k = M_z^2$ where $k > 0$. The same properties apply to any M_n, because all the rotations are "similar" one to the other (moving to another reference frame is done by means of a similarity transformation that represents a change of basis).

══════ [12.6] An example for multiplication of rotations

Let us make a 90° rotation $R(90^0 e_z)$ around the Z axis, followed by a 90° rotation $R(90^0 e_y)$ around the Y axis. We would like to know what this sequence gives. Using the Euclidean representation

$$R = 1 - i \sin \Phi M_n - (1 - \cos \Phi) M_n^2 \tag{12.18}$$

we get

$$R(90^0 e_z) = 1 - i M_z - M_z^2$$
$$R(90^0 e_y) = 1 - i M_y - M_y^2 \tag{12.19}$$

We do not wish to open the parentheses, and add up 9 terms which include multiplications of 3×3 matrices. Therefore we abandon the Euclidean representation and try and do the same thing with a dim=2 representation, working with the 2×2 Pauli matrices.

$$R(\Phi) = \cos(\Phi/2)\hat{1} - i \sin(\Phi/2)\sigma_n \tag{12.20}$$
$$R(90^0 e_z) = \frac{1}{\sqrt{2}}(\hat{1} - i\sigma_z)$$
$$R(90^0 e_y) = \frac{1}{\sqrt{2}}(\hat{1} - i\sigma_y)$$

Hence

$$R = R(90^0 e_y) R(90^0 e_z) = \frac{1}{2}(1 - i\sigma_x - i\sigma_y - i\sigma_z) \tag{12.21}$$

where we have used the fact that $\sigma_y \sigma_z = i\sigma_x$. We can write this result as:

$$R = \cos \frac{120^o}{2} - i \sin \frac{120^o}{2} \vec{n} \cdot \vec{\sigma} \tag{12.22}$$

where $n = \frac{1}{\sqrt{3}}(1, 1, 1)$. This defines the equivalent rotation which is obtained by combining the two 90° rotations.

[13] Building the representations of rotations

════════ [13.1] Irreducible representations

A reducible representation is a representation for which a basis can be found such that each matrix in the group decomposes into the same block structure. In this basis the set of single-block sub-matrices obeys the same multiplication table as that of the full matrices, hence we say that the representation is the sum of smaller representations. For a commutative group a basis can be found in which all the matrices are diagonal. In the latter case we can say that the representation decomposes into one-dimensional representations.

The rotation group is not a commutative group. We are interested in finding all its irreducible representations. Let us assume that someone hands us an irreducible representation. We can find its generators, written as matrices in some "standard basis", and we can verify that they satisfy the desired Lie algebra. We shall see that it is enough to know the *dimension* of the irreducible representation in order to figure out what are the matrices that we have in hand (up to a choice of basis). In this way we establish that there is one, and only one, irreducible representation for each dimension.

════════ [13.2] First Stage - determination of basis

If we have a representation of the rotation group, we can look at infinitesimal rotations and define generators. For a small rotation around the X axis, we can write:

$$R(\delta\Phi\vec{e}_x) \;\;=\;\; \hat{1} - i\delta\Phi\hat{J}_x \tag{13.1}$$

In the same way we can write rotations round the Z and Y axes. So, we can find the matrices $\hat{J}_x, \hat{J}_y, \hat{J}_z$. How can we check that the representation that we have is indeed a representation of the rotation group? All we have to do is check that the following equation is obeyed:

$$[\hat{J}_i, \hat{J}_j] \;\;=\;\; i\epsilon_{ijk}\hat{J}_k \tag{13.2}$$

We define:

$$\hat{J}_\pm \;\;=\;\; \hat{J}_x \pm i\hat{J}_y \tag{13.3}$$
$$\hat{J}^2 \;\;=\;\; \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 = \frac{1}{2}(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+) + \hat{J}_z^2$$

We notice that the operator $\hat{J}^2$ commutes with all the generators, and therefore also with all the rotation matrices. From the "separation of variable" theorems it follows that if $\hat{J}^2$ has (say) two different eigenvalues, then it induces a decomposition of all the rotation matrices into two blocks. So in such case the representation is reducible. Without loss of generality our interest is focused on irreducible representations for which we necessarily have $\hat{J}^2 = \lambda\mathbf{1}$, where λ is a constant. Later we shall argue that λ is uniquely determined by the *dimension* of the irreducible representation.

If we have a representation, we still have the freedom to decide in which basis to write it. Without loss of generality, we can decide on a basis that is determined by the operator $\hat{J}_z$:

$$\hat{J}_z|m\rangle \;\;=\;\; m|m\rangle \tag{13.4}$$

Obviously, the other generators, or a general rotation matrix will not be diagonal in this basis, so we have

$$\langle m|\hat{J}^2|m'\rangle \;\;=\;\; \lambda\delta_{mm'} \tag{13.5}$$
$$\langle m|\hat{J}_z|m'\rangle \;\;=\;\; m\delta_{mm'}$$
$$\langle m|R|m'\rangle \;\;=\;\; R_{mm'}^\lambda$$

===== [13.3] Reminder: Ladder Operators

Given an operator $\hat{D}$, which does not have to be unitary or Hermitian, and an observable $\hat{x}$ that obeys the commutation relation

$$[\hat{x}, \hat{D}] \quad = \quad a\hat{D} \tag{13.6}$$

we prove that $\hat{D}$ is a "ladder" operator that shifts between eigenstates of $\hat{x}$.

$$
\begin{aligned}
\hat{x}\hat{D} - \hat{D}\hat{x} &= a\hat{D} \\
\hat{x}\hat{D} &= \hat{D}(\hat{x} + a) \\
\hat{x}\hat{D}|x\rangle &= \hat{D}(\hat{x} + a)|x\rangle \\
\hat{x}\hat{D}|x\rangle &= \hat{D}(x + a)|x\rangle \\
\hat{x}[\hat{D}|x\rangle] &= (x + a)[\hat{D}|x\rangle]
\end{aligned}
\tag{13.7}
$$

So the state $|\Psi\rangle = \hat{D}|x\rangle$ is an eigenstate of $\hat{x}$ with eigenvalue $(x + a)$. The normalization of $|\Psi\rangle$ is determined by:

$$||\Psi|| \quad = \quad \sqrt{\langle\Psi|\Psi\rangle} \quad = \quad \sqrt{\langle x|\hat{D}^\dagger\hat{D}|x\rangle} \tag{13.8}$$

===== [13.4] Second stage: identification of ladder operators

It follows from the commutation relations of the generators that:

$$[\hat{J}_z, \hat{J}_\pm] \quad = \quad \pm\hat{J}_\pm \tag{13.9}$$

So $\hat{J}_\pm$ are ladder operators in the basis that we have chosen. Using them we can shift from a given eigenstate $|m\rangle$ to other eigenstates: $..., |m-2\rangle, |m-1\rangle, |m+1\rangle, |m+2\rangle, |m+3\rangle, ...$

From the commutation relations of the generators

$$(\hat{J}_+\hat{J}_-) - (\hat{J}_-\hat{J}_+) \quad = \quad [\hat{J}_+, \hat{J}_-] = 2\hat{J}_z \tag{13.10}$$

From the definition of $\hat{J}^2$

$$(\hat{J}_+\hat{J}_-) + (\hat{J}_-\hat{J}_+) \quad = \quad 2(\hat{J}^2 - (\hat{J}_z)^2) \tag{13.11}$$

By adding and subtracting these two identities we get respectively:

$$
\begin{aligned}
\hat{J}_-\hat{J}_+ &= \hat{J}^2 - \hat{J}_z(\hat{J}_z + 1) \\
\hat{J}_+\hat{J}_- &= \hat{J}^2 - \hat{J}_z(\hat{J}_z - 1)
\end{aligned}
\tag{13.12}
$$

Now we can find the normalization of the states that are found by using the ladder operators:

$$||\hat{J}_+|m\rangle||^2 \quad = \quad \langle m|\hat{J}_-\hat{J}_+|m\rangle \quad = \quad \langle m|\hat{J}^2|m\rangle - \langle m|\hat{J}_z(\hat{J}_z + 1)|m\rangle \quad = \quad \lambda - m(m+1) \tag{13.13}$$

$$||\hat{J}_-|m\rangle||^2 \quad = \quad \langle m|\hat{J}_+\hat{J}_-|m\rangle \quad = \quad \langle m|\hat{J}^2|m\rangle - \langle m|\hat{J}_z(\hat{J}_z - 1)|m\rangle \quad = \quad \lambda - m(m-1) \tag{13.14}$$

It will be convenient from now on to write the eigenvalue of $\hat{J}^2$ as $\lambda = j(j+1)$. Therefore:

$$\hat{J}_+|m\rangle = \sqrt{j(j+1) - m(m+1)} \, |m+1\rangle \tag{13.15}$$
$$\hat{J}_-|m\rangle = \sqrt{j(j+1) - m(m-1)} \, |m-1\rangle \tag{13.16}$$

Mathematical Comment.– Define $j \equiv N/2$ and an observable $\boldsymbol{n}$ such that $J_z = -(N/2) + \boldsymbol{n}$. The ladder operators perform translations in the range $n = 0, 1, 2, ..., N$. Define a unitary translation operator such that $\boldsymbol{D}\,|n\rangle \equiv |n+1\rangle$. Then it follows from the above that $\hat{J}_+\,|n\rangle = \sqrt{(n+1)(N-n)}\,|n+1\rangle$, and therefore we can write

$$\hat{J}_+ = \boldsymbol{D}\sqrt{(\boldsymbol{n}+1)(N-\boldsymbol{n})} = \sqrt{\boldsymbol{n}}\,\boldsymbol{D}\,\sqrt{N-\boldsymbol{n}} \tag{13.17}$$

A related trick is known as the Holstein-Primakoff transformation. Define $\boldsymbol{n} = \boldsymbol{a}^\dagger \boldsymbol{a}$ as for harmonic oscillator, then it follows that $\hat{J}_+ = \boldsymbol{a}^\dagger\sqrt{(N - \boldsymbol{a}^\dagger\boldsymbol{a})}$, where we used $\boldsymbol{a}^\dagger = \sqrt{\boldsymbol{n}}\boldsymbol{D}$.

═══════ [13.5] Third stage - deducing the representation

Since the representation is of a finite dimension, the shift process of raising or lowering cannot go on forever. By looking at the results of the last section we may conclude that there is only one way that the raising process could stop: at some stage we should get $m = +j$. Similarly, there is only one way that the lowering process could stop: at some stage we should get $m = -j$. Hence from the raising/lowering process we get a ladder that includes $\dim = 2j + 1$ basis states. This number must be an integer number. Therefore j must be either an integer or half integer number.

For a given j the matrix representation of the generators is determined uniquely. This is based on the formulas of the previous section, from which we conclude:

$$[\hat{J}_+]_{m'm} = \sqrt{j(j+1) - m(m+1)} \, \delta_{m',m+1} \tag{13.18}$$
$$[\hat{J}_-]_{m'm} = \sqrt{j(j+1) - m(m-1)} \, \delta_{m',m-1}$$

And all that is left to do is to write:

$$[\hat{J}_x]_{m'm} = \frac{1}{2}\left[(\hat{J}_+)_{m'm} + (\hat{J}_-)_{m'm}\right] \tag{13.19}$$
$$[\hat{J}_y]_{m'm} = \frac{1}{2i}\left[(\hat{J}_+)_{m'm} - (\hat{J}_-)_{m'm}\right]$$
$$[\hat{J}_z]_{m'm} = m\,\delta_{m'm}$$

And then we get every rotation matrix in the representation by:

$$R_{m'm} = \mathrm{e}^{-i\vec{\Phi}\cdot\vec{J}} \tag{13.20}$$

A technical note: In the raising/lowering process described above we get a "multiplet" of m states. Can we get several independent multiplets? Without loss of generality we had assumed that we are dealing with an irreducible representation, and therefore there is only one multiplet.

[14] Rotations of spins and of wavefunctions

━━━━━━━ ## [14.1] Building the dim=2 representation (spin $1/2$)

Let us find the $j = 1/2$ representation. This representation can be interpreted as a realization of spin 1/2. We therefore use from now on the notation S instead on J.

$$S^2|m\rangle \;\; = \;\; \frac{1}{2}\left(\frac{1}{2}+1\right)|m\rangle \tag{14.1}$$

$$S_z \;\; = \;\; \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} \tag{14.2}$$

Using formulas of the previous section we find S_+ and S_- and hence S_x and S_y

$$S_+ \;\; = \;\; \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{14.3}$$

$$S_- \;\; = \;\; \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{14.4}$$

$$S_x \;\; = \;\; \frac{1}{2}\left(\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\right) \;\; = \;\; \frac{1}{2}\sigma_x \tag{14.5}$$

$$S_y \;\; = \;\; \frac{1}{2i}\left(\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\right) \;\; = \;\; \frac{1}{2}\sigma_y \tag{14.6}$$

We recall that

$$R(\Phi) \;\; = \;\; R(\Phi\vec{n}) \;\; = \;\; \mathrm{e}^{-i\Phi S_n} \;\; = \;\; \cos(\Phi/2)\hat{1} - i\sin(\Phi/2)\sigma_n \tag{14.7}$$

where

$$\vec{n} \;\; = \;\; (\sin\theta\cos\varphi,\ \sin\theta\sin\varphi,\ \cos\theta) \tag{14.8}$$

$$\sigma_n \;\; = \;\; \vec{n}\cdot\vec{\sigma} \;\; = \;\; \begin{pmatrix} \cos\theta & \mathrm{e}^{-i\varphi}\sin\theta \\ \mathrm{e}^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix} \tag{14.9}$$

Hence

$$R(\vec{\Phi}) \;\; = \;\; \begin{pmatrix} \cos(\Phi/2) - i\cos(\theta)\sin(\Phi/2) & -i\mathrm{e}^{-i\varphi}\sin(\theta)\sin(\Phi/2) \\ -i\mathrm{e}^{i\varphi}\sin(\theta)\sin(\Phi/2) & \cos(\Phi/2) + i\cos(\theta)\sin(\Phi/2) \end{pmatrix} \tag{14.10}$$

In particular a rotation around the Z axis is given by:

$$R \;\; = \;\; \mathrm{e}^{-i\Phi S_z} \;\; = \;\; \begin{pmatrix} \mathrm{e}^{-i\Phi/2} & 0 \\ 0 & \mathrm{e}^{i\Phi/2} \end{pmatrix} \tag{14.11}$$

And a rotation round the Y axis is given by:

$$R \;\; = \;\; \mathrm{e}^{-i\Phi S_y} \;\; = \;\; \begin{pmatrix} \cos(\Phi/2) & -\sin(\Phi/2) \\ \sin(\Phi/2) & \cos(\Phi/2) \end{pmatrix} \tag{14.12}$$

═══════ [14.2] Polarization states of Spin $1/2$

We now discuss the physical interpretation of the "states" that the $s = 1/2$ matrices rotate. Any state of "spin 1/2" is represented by a vector with two complex number. That means we have 4 parameters. After gauge and normalization, we are left with 2 physical parameters which can be associated with the polarization direction (θ, φ). Thus it makes sense to represent the state of spin 1/2 by an arrow that points to some direction in space.

The eigenstates of S_z do not change when we rotate them around the Z axis (aside from a phase factor). Therefore the following interpretation comes to mind:

$$\left| m = +\frac{1}{2} \right\rangle = |\vec{z}\rangle = |\uparrow\rangle \mapsto \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{14.13}$$

$$\left| m = -\frac{1}{2} \right\rangle = |\overleftarrow{z}\rangle = |\downarrow\rangle \mapsto \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{14.14}$$

This interpretation is confirmed by rotating the "up" state by 180 degrees, and getting the "down" state.

$$R = e^{-i\pi S_y} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{14.15}$$

We see that:

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \rightsquigarrow 180^0 \rightsquigarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} \rightsquigarrow 180^0 \rightsquigarrow -\begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{14.16}$$

With two rotations of 180° we get back the "up" state, with a minus sign. Optionally one observes that

$$e^{-i2\pi S_z} = e^{-i\pi \sigma_z} = -1 \tag{14.17}$$

and hence by similarity this holds for any 2π rotation. We see that the representation that we found is not a one-to-one representation of the rotation group. It does not obey the multiplication table in a one-to-one fashion! In fact, we have found a representation of $SU(2)$ and not $SO(3)$. The minus sign has a physical significance. In a two slit experiment it is possible to turn destructive interference into constructive interference by placing a magnetic field in one of the paths. The magnetic field rotates the spin of the electrons. If we induce 360° rotation, then the relative phase of the interference change sign, and hence constructive interference becomes destructive and vice versa. The relative phase is important! Therefore, we must not ignore the minus sign.

It is important to emphasize that the physical degree of freedom that is called "spin 1/2" cannot be visualized as a arising from the spinning of small rigid body around some axis like a top. If it were possible, then we could say that the spin can be described by a wave function. In this case, if we would rotate it by 360° we would get the same state, with the same sign. But in the representation we are discussing we get minus the same state. That is in contradiction with the definition of a (wave) function as a single valued object.

We can get from the "up" state all the other possible states merely by using the appropriate rotation matrix. In particular we can get any spin polarization state by combining a rotation round the Y axis and a rotation round the Z axis. The result is:

$$|\vec{n}_{\theta,\varphi}\rangle = R(\varphi)R(\theta)|\uparrow\rangle = e^{-i\varphi S_z}e^{-i\theta S_y}|\uparrow\rangle \mapsto \begin{pmatrix} e^{-i\varphi/2}\cos(\theta/2) \\ e^{i\varphi/2}\sin(\theta/2) \end{pmatrix} \tag{14.18}$$

════ [14.3] Building the dim=3 representation (spin 1)

Let us find the $j = 1$ representation. This representation can be interpreted as a realization of spin 1, and hence we use the notation S instead of J as in the previous section.

$$S^2|m\rangle \quad = \quad 1(1+1)|m\rangle \tag{14.19}$$

$$S_z \quad = \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{14.20}$$

$$S_+ \quad = \quad \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \tag{14.21}$$

The standard representation of the generators is:

$$S \quad \rightarrow \quad \left[\frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \right] \tag{14.22}$$

We remember that the Euclidean representation is:

$$M \quad \rightarrow \quad \left[\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right] \tag{14.23}$$

Now we have two different dim=3 representations that represent the rotation group. They are actually the same representation in a different basis. By changing bases (diagonalizing M_z) it is possible to move from the Euclidean representation to the standard representation. It is obvious that diagonalizing M_z is only possible over the complex field. In the defining realization, the matrices of the Euclidean representation rotate points in the real space. But it is possible also to use them on complex vectors. In the latter case it is a realization for spin 1.

For future use we list some useful matrices:

$$S_x^2 = \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}, \quad S_y^2 = \frac{1}{2} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix}, \quad S_z^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{14.24}$$

As expected for the $s = 1$ representation we have

$$S^2 \quad = \quad S_x^2 + S_y^2 + S_z^2 \quad = \quad \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad = \quad s(s+1)\delta_{m,m'} \tag{14.25}$$

We note that one can define a projector $P^z = 1 - S_z^2$ on the $m = 0$ state. Similarly we can define projectors $P^x = 1 - S_x^2$ and $P^y = 1 - S_y^2$. We see that this set is complete $P^x + P^y + P^z = \mathbf{1}$, and one can verify that these projectors are orthogonal. In the next section we shall see that they define the Euclidean basis that consist of so-called linearly polarized states. In this basis the generators are represented by the matrices M_x, M_y, M_z.

Having found the generators we can construct any rotation of spin 1. We notice the following equation:

$$S_i^3 \quad = \quad S_i^2 S_i \quad = \quad S_i \quad \text{for } i = x, y, z \tag{14.26}$$

From this equation we conclude that all the odd powers $(1, 3, 5, ...)$ are the same and are equal to S_i, and all the even powers $(2, 4, 6, ...)$ are the same and equal to S_i^2. It follows (by way of a Taylor expansion) that:

$$U(\vec{\Phi}) \quad = \quad e^{-i\vec{\Phi}\cdot\vec{S}} \quad = \quad \hat{1} - i\sin(\Phi)S_n - (1 - \cos(\Phi))S_n^2 \tag{14.27}$$

where:

$$S_n = \vec{n} \cdot \vec{S} \tag{14.28}$$

Any rotation can be given by a combination of a rotation round the z axis and a rotation round the y axis. We mark the rotation angle around the y axis by θ, and the rotation angle around the z axis by φ, and get:

$$U(\varphi \vec{n}_z) = e^{-i\varphi S_z} = \begin{pmatrix} e^{-i\varphi} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\varphi} \end{pmatrix} \tag{14.29}$$

$$U(\theta \vec{n}_y) = e^{-i\theta S_y} = \begin{pmatrix} \frac{1}{2}(1+\cos\theta) & -\frac{1}{\sqrt{2}}\sin\theta & \frac{1}{2}(1-\cos\theta) \\ \frac{1}{\sqrt{2}}\sin\theta & \cos\theta & -\frac{1}{\sqrt{2}}\sin\theta \\ \frac{1}{2}(1-\cos\theta) & \frac{1}{\sqrt{2}}\sin\theta & \frac{1}{2}(1+\cos\theta) \end{pmatrix} \tag{14.30}$$

===== [14.4] Polarization states of a spin 1

The states of "Spin 1" cannot be represented by simple arrows. This should be obvious in advance because it is represented by a vector that has three complex components. That means we have 6 parameters. After gauge and normalization, we still have 4 physical parameters. Hence it is not possible to find all the possible states of spin 1 by using only rotations. Below we further discuss the physical interpretation of spin 1 states. This discussion suggest to use the following notations for the basis states of the standard representation:

$$|m=1\rangle = |\vec{z}\rangle = |\Uparrow\rangle \mapsto \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \tag{14.31}$$

$$|m=0\rangle = |\overset{\leftrightarrow}{z}\rangle = |\Updownarrow\rangle \mapsto \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \tag{14.32}$$

$$|m=-1\rangle = |\overset{\leftarrow}{z}\rangle = |\Downarrow\rangle \mapsto \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{14.33}$$

The first and the last states represent circular polarizations. By rotating the first state by 180° around the Y axis we get the third state. This means that we have 180° degree orthogonality. However, the middle state is different: it describes linear polarization. Rotating the middle state by 180° degrees around the Y axis gives the same state again! This explains the reason for marking this state with a double headed arrow.

If we rotate the linear polarization state $|\Updownarrow\rangle$ by 90°, once around the Y axis and once around the X axis, we get an orthogonal set of states:

$$|\overset{\leftrightarrow}{x}\rangle = \frac{1}{\sqrt{2}}(-|\Uparrow\rangle + |\Downarrow\rangle) \mapsto \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} \tag{14.34}$$

$$|\overset{\leftrightarrow}{y}\rangle = \frac{i}{\sqrt{2}}(|\Uparrow\rangle + |\Downarrow\rangle) \mapsto \frac{1}{\sqrt{2}}\begin{pmatrix} i \\ 0 \\ i \end{pmatrix} \tag{14.35}$$

$$|\overset{\leftrightarrow}{z}\rangle = |\Updownarrow\rangle \mapsto \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \tag{14.36}$$

This basis is called the linear basis. States of "spin 1" can be written either in the standard basis or in the basis

of linear polarizations. The latter option, where we have 90° orthogonality of the basis vectors, corresponds to the Euclidean representation.

We can rotate the state $|\Uparrow\rangle$ in order to get other circularly polarized states:

$$|\vec{n}_{\theta,\varphi}\rangle \quad = \quad U(\varphi\vec{n}_z)U(\theta\vec{n}_y)|\Uparrow\rangle \quad = \quad \begin{pmatrix} \frac{1}{2}(1+\cos\theta)\mathrm{e}^{-i\varphi} \\ \frac{1}{\sqrt{2}}\sin\theta \\ \frac{1}{2}(1-\cos\theta)\mathrm{e}^{i\varphi} \end{pmatrix} \tag{14.37}$$

Similarly, we can rotate the state $|\Updownarrow\rangle$ in order to get other linearly polarized states:

$$|\overleftrightarrow{n}_{\theta,\varphi}\rangle \quad = \quad U(\varphi\vec{n}_z)U(\theta\vec{n}_y)|\Updownarrow\rangle \quad = \quad \begin{pmatrix} -\frac{1}{\sqrt{2}}\sin\theta\mathrm{e}^{-i\varphi} \\ \cos\theta \\ \frac{1}{\sqrt{2}}\sin\theta\mathrm{e}^{i\varphi} \end{pmatrix} \tag{14.38}$$

In particular we note that linearly polarized states in the XY plane can be written as follows:

$$|\overleftrightarrow{n}_{\varphi}\rangle \quad = \quad \frac{1}{\sqrt{2}}(-\mathrm{e}^{-i\varphi}|\Uparrow\rangle + \mathrm{e}^{i\varphi}|\Downarrow\rangle) \quad = \quad \cos(\varphi)|\overleftrightarrow{x}\rangle + \sin(\varphi)|\overleftrightarrow{y}\rangle \tag{14.39}$$

As defined above the circularly polarized states are obtained by rotating the $|\Uparrow\rangle$ state, while the linearly polarized states are obtained by rotating the $|\Updownarrow\rangle$ state. But a general polarization state will not necessarily be circularly polarized, neither linearly polarized. We shall argue below that any polarization state of spin 1 can be obtained by rotation of so-called elliptically polarized state

$$|\text{elliptic}\rangle \quad \equiv \quad \frac{1}{\sqrt{2}}\left(\sqrt{1+q}|\Uparrow\rangle - \sqrt{1-q}|\Downarrow\rangle\right) \tag{14.40}$$

where $0 < q < 1$. This is an interpolation between $q = 1$ circular polarization in the Z direction, and $q = 0$ linear polarization in the X direction. The states that are obtained by rotation of the $q = 1$ state are the circularly polarized states, while the states that are obtained by rotation of the $q = 0$ state are the linearly polarized states. From this follows that a general spin 1 state is characterized by 4 parameters: q and the 3 angles that define rotation. This is consistent with the discussion in the opening of this section.

In order to establish that the most general polarization state is elliptic we define the following procedure. Given an arbitrary state vector (ψ_+, ψ_0, ψ_-) we can re-orient the z axis in a (θ, φ) direction such that $\psi_0 = 0$. We say that this (θ, φ) direction defines a "polarization plane". Using ϕ rotation around the new Z axis, and taking gauge freedom into account, we can arrange that the amplitudes (ψ_+, ψ_-) would be real with opposite sign (representing X polarization). Hence we have establish that after suitable rotation we get what we called elliptic polarization that can be characterized by a number $0 < q < 1$. Thus we see that indeed an arbitrary state is characterized by the four parameters $(\theta, \varphi, \phi, q)$. We can represent the state by an ellipse as follows: The angles (θ, φ) define the plane of the ellipse, while ϕ describes the angle of major axes in this plane, and q describes the ratio of the major radii. Note that 180° rotation in the polarization plane leads to the same state (with minus sign). The special case $q = 0$ is called circular polarization because any rotation in the polarization plane leads to the same state (up to a phase). The special case $q = 0$ is called linear polarization: the ellipse becomes a double headed arrow.

It follows from the above procedure that is possible to find one-to-one relation between polarization states of spin 1 and ellipses. The direction of the polarization is the orientation of the ellipse. When the ellipse is a circle, the spin is circularly polarized, and when the ellipse shrinks down to a line, the spin is linearly polarized. In the latter case the orientation of the polarization plane is ill defined.

═══════ [14.5] Translations and rotations of wavefunctions

We first consider in this section the space of functions that live on a torus (bagel). We shall see that the representation of *translations* over this space decomposes into one-dimensional irreducible representations, as expected in the case of a commutative group. Then we consider the space of functions that live on the surface of a sphere. We shall see that the representation of *rotations* over this space decomposes as $1 \oplus 3 \oplus 5 \oplus \ldots$. The basis in which this decomposition becomes apparent consists of the spherical harmonics.

Consider the space of functions that live on a torus (bagel). This functions can represent the motion of a particle in a 2-D box of size $L_x \times L_y$ with periodic boundary conditions. Without loss of generality we assume that the dimensions of the surface are $L_x = L_y = 2\pi$, and use $\boldsymbol{x} = (\theta, \varphi)$ as the coordinates. The representation of the state of a particle in the standard basis is:

$$|\Psi\rangle \;=\; \sum_{\theta,\varphi} \psi(\theta,\varphi)|\theta,\varphi\rangle \tag{14.41}$$

The momentum states are labeled as $\boldsymbol{k} = (n,m)$. The representation of a wavefunction in this basis is:

$$|\Psi\rangle \;=\; \sum_{n,m} \Psi_{n,m}|n,m\rangle \tag{14.42}$$

where the transformation matrix is:

$$\langle\theta,\varphi|n,m\rangle \;=\; \frac{1}{2\pi}\mathrm{e}^{i(n\theta+m\varphi)} \tag{14.43}$$

The displacement operators in the standard basis are not diagonal:

$$D_{\boldsymbol{x},\boldsymbol{x}'} \;=\; \delta(\theta-(\theta'+a))\delta(\varphi-(\varphi'+b)) \tag{14.44}$$

However, in the momentum basis we get diagonal matrices:

$$D_{\boldsymbol{k},\boldsymbol{k}'} \;=\; \delta_{n,n'}\delta_{m,m'}\,\mathrm{e}^{-i(an+bm)} \tag{14.45}$$

In other words, we have decomposed the translations group into 1-D representations. This is possible because the group is commutative. If a group is not commutative it is not possible to find a basis in which all the matrices of the group are diagonal simultaneously.

Now we consider the space of functions that live on the surface of a sphere. This functions can represent the motion of a particle in a 2-D spherical shell. Without loss of generality we assume that the radius of the sphere is unity. In full analogy with the case of a torus, the standard representation of the states of a particle that moves on the surface of a sphere is:

$$|\Psi\rangle \;=\; \sum_{\theta,\varphi} \psi(\theta,\varphi)|\theta,\varphi\rangle \tag{14.46}$$

Alternatively, we can work with a different basis:

$$|\Psi\rangle \;=\; \sum_{\ell m} \Psi_{\ell m}|\ell,m\rangle \tag{14.47}$$

where the transformation matrix is:

$$\langle\theta,\varphi|\ell,m\rangle \;=\; Y^{\ell m}(\theta,\varphi) \tag{14.48}$$

The "displacement" matrices are actually "rotation" matrices. They are not diagonal in the standard basis:

$$R_{\mathbf{x},\mathbf{x'}} \;=\; \delta(\theta - f(\theta', \varphi'))\delta(\varphi - g(\theta', \varphi')) \tag{14.49}$$

where $f()$ and $g()$ are complicated functions. But if we take $Y^{\ell m}(\theta, \varphi)$ to be the spherical harmonics then in the new basis the representation of rotations becomes simpler:

$$R_{\ell m, \ell' m'} \;=\; \begin{pmatrix} 1 \times 1 & 0 & 0 & 0 \\ 0 & 3 \times 3 & 0 & 0 \\ 0 & 0 & 5 \times 5 & 0 \\ 0 & 0 & 0 & \ldots \end{pmatrix} \;=\; \text{block diagonal} \tag{14.50}$$

When we rotate a function, each block stays "within itself". The rotation does not mix states that have different ℓ. In other words: in the basis $|\ell, m\rangle$ the representation of rotations decomposes into a sum of irreducible representations of finite dimension:

$$1 \oplus 3 \oplus 5 \oplus \ldots \tag{14.51}$$

In the next section we show how the general procedure that we have learned for decomposing representations, does indeed help us to find the $Y^{\ell m}(\theta, \varphi)$ functions.

════ [14.6] The spherical harmonics

We have already found the representation of the generators of rotations over the 3D space of wavefunctions. Namely we have proved that $\vec{L} = \vec{r} \times \vec{p}$. If we write the differential representation of L is spherical coordinates we find as expected that the radial coordinate r is not involved:

$$L_z \;\rightarrow\; -i\frac{\partial}{\partial \varphi} \tag{14.52}$$

$$L_{\pm} \;\rightarrow\; e^{\pm i\varphi}\left(\pm\frac{\partial}{\partial\theta} + i\cot(\theta)\frac{\partial}{\partial\varphi}\right) \tag{14.53}$$

$$L^2 \;\rightarrow\; -\left[\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}(\sin(\theta)\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] \tag{14.54}$$

Thus the representation trivially decompose with respect to r, and without loss of generality we can focus on the subspace of wavefunctions $\Psi(\theta, \varphi)$ that live on a spherical shell of a given radius. We would like to find the basis in which the representation decomposes, as defined by

$$L^2\Psi = \ell(\ell+1)\Psi \tag{14.55}$$
$$L_z\Psi = m\Psi \tag{14.56}$$

The solution is:

$$Y^{\ell m}(\theta, \phi) \;=\; \left[\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}\right]^{1/2} [(-1)^m P_{\ell m}(\cos(\theta))]\, e^{im\varphi} \tag{14.57}$$

It is customary in quantum textbooks to absorb the factor $(-1)^m$ in the definition of the Legendre polynomials. We note that it is convenient to start with

$$Y^{\ell\ell}(\theta, \phi) \;\propto\; (\sin(\theta))^\ell\, e^{i\ell\varphi} \tag{14.58}$$

and then to find the rest of the functions using the lowering operator:

$$|\ell, m\rangle \; \propto \; L_-^{(\ell-m)} \, |\ell, \ell\rangle \tag{14.59}$$

Let us give some examples for Spherical Functions. The simplest function is spread uniformly over the surface of the sphere, while a linear polarization state along the Z axis is concentrated mostly at the poles:

$$Y^{0,0} = \frac{1}{\sqrt{4\pi}}, \qquad\qquad Y^{1,0} = \sqrt{\frac{3}{4\pi}} \cos(\theta) \tag{14.60}$$
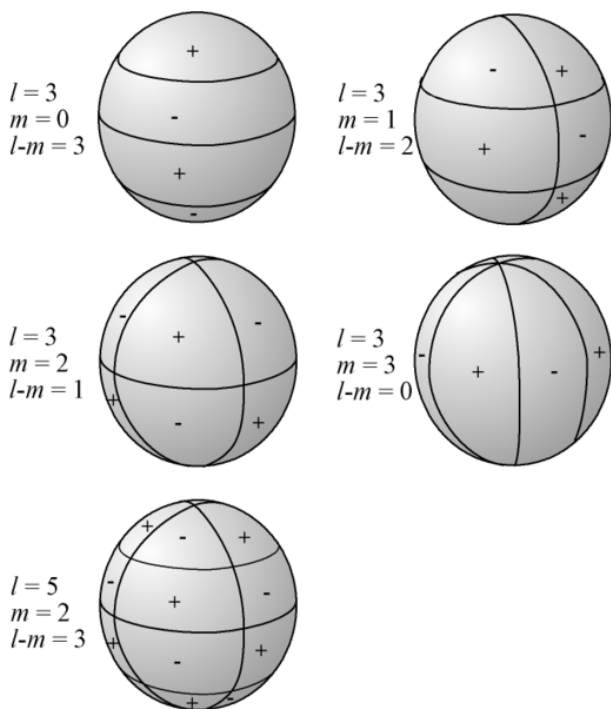
If we rotate the polar wave function by 90 degrees we get:

$$Y^{1,x} = \sqrt{\frac{3}{4\pi}} \sin(\theta) \cos(\varphi), \qquad\qquad Y^{1,y} = \sqrt{\frac{3}{4\pi}} \sin(\theta) \sin(\varphi) \tag{14.61}$$

While according to the standard "recipe" the circular polarizations are:

$$Y^{1,1} = -\sqrt{\frac{3}{8\pi}} \sin(\theta) e^{i\varphi}, \qquad\qquad Y^{1,-1} = \sqrt{\frac{3}{8\pi}} \sin(\theta) e^{-i\varphi} \tag{14.62}$$

The Y^{lm} can be visualized as a free-wave with m periods in the azimuthal φ direction, and $\ell-m$ nodal circles in the θ direction. Here is an illustration that is taken from Wikipedia:

[15] Multiplying representations

════════ [15.1] Product space

Let us assume that we have two Hilbert spaces. One is spanned by the basis $|i\rangle$ and the other is spanned by the basis $|\alpha\rangle$. We can multiply the two spaces "externally" and get a space with a basis defined by:

$$|i, \alpha\rangle \ = \ |i\rangle \otimes |\alpha\rangle \tag{15.1}$$

The dimension of the Hilbert space that we obtain is the multiplication of the dimensions. For example, we can multiply the "position" space x by the spin space m. We assume that the space contains three sites $x = 1, 2, 3$, and that the particle has spin $1/2$ with $m = \pm 1/2$. The dimension of the space that we get from the external multiplication is $2 \times 3 = 6$. The basis states are

$$|x, m\rangle \ = \ |x\rangle \otimes |m\rangle \tag{15.2}$$

A general state is represented by a column vector:

$$|\Psi\rangle \ \rightarrow \ \begin{pmatrix} \Psi_{1\uparrow} \\ \Psi_{1\downarrow} \\ \Psi_{2\uparrow} \\ \Psi_{2\downarrow} \\ \Psi_{3\uparrow} \\ \Psi_{3\downarrow} \end{pmatrix} \tag{15.3}$$

Or, in Dirac notation:

$$|\Psi\rangle \ = \ \sum_{x,m} \Psi_{x,m} |x, m\rangle \tag{15.4}$$

If x has a continuous spectrum then the common notational style is

$$|\Psi\rangle \ = \ \sum_{x,m} \Psi_m(x) |x, m\rangle \ \mapsto \ \Psi_m(x) = \begin{pmatrix} \Psi_\uparrow(x) \\ \Psi_\downarrow(x) \end{pmatrix} \tag{15.5}$$

If we prepare separately the position wavefunction as ψ_x and the spin polarization as χ_m, then the state of the particle is:

$$|\Psi\rangle \ = \ |\psi\rangle \otimes |\chi\rangle \ \longmapsto \ \Psi_{x,m} \ = \ \psi_x \chi_m \ = \ \begin{pmatrix} \psi_1 \chi_\uparrow \\ \psi_1 \chi_\downarrow \\ \psi_2 \chi_\uparrow \\ \psi_2 \chi_\downarrow \\ \psi_3 \chi_\uparrow \\ \psi_3 \chi_\downarrow \end{pmatrix} \tag{15.6}$$

It should be clear that in general an arbitrary $|\Psi\rangle$ of a particle cannot be written as a product of some $|\psi\rangle$ with some $|\chi\rangle$. In other words: the space and spin degrees of freedom of the particle might be *entangled*. More generally, one observes that different subsystems might be *entangled*: this is typically the case after the subsystems interact with each other.

════════ [15.2] External multiplication of operators

Let us assume that in the Hilbert space that is spanned by the basis $|\alpha\rangle$, an operator is defined, with the representation $\hat{A} \rightarrow A_{\alpha,\beta}$. This definition has a natural extension over the product space $|i, \alpha\rangle$, namely $\hat{A} \rightarrow \delta_{i,j} A_{\alpha,\beta}$. Similarly for

an operator that acts over the second Hilbert space $\hat{B} \to B_{i,j}\delta_{\alpha,\beta}$. Formally if we have operators A and B that are defined over the respective Hilbert spaces, we can use the notations $\hat{1} \otimes \hat{A}$ and $\hat{B} \otimes \hat{1}$ for their extension over the product space, and define their external product as
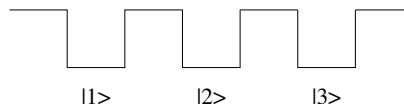
$$\hat{C} \;\equiv\; \hat{B} \otimes \hat{A} \;\equiv\; (\hat{B} \otimes \hat{1})(\hat{1} \otimes \hat{A}), \qquad\qquad C_{i\alpha,j\beta} \;\to\; B_{i,j}\,A_{\alpha,\beta} \tag{15.7}$$

In Dirac notation:

$$\langle i\alpha|\hat{C}|j\beta\rangle \;=\; \langle i|\hat{B}|j\rangle \langle\alpha|\hat{A}|\beta\rangle \tag{15.8}$$

For example, let us assume that we have a particle in a three-site system:

$$\hat{x} \;=\; \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix} \tag{15.9}$$

$$|1\rangle \qquad |2\rangle \qquad |3\rangle$$

If the particle has spin $1/2$ we must define the position operator as:

$$\hat{x} \;=\; \hat{x} \otimes \hat{1} \tag{15.10}$$

That means that:

$$\hat{x}|x,m\rangle \;=\; x|x,m\rangle \tag{15.11}$$

And the matrix representation is:

$$\hat{x} \;=\; \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \;=\; \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \end{pmatrix} \tag{15.12}$$

The system has a 6 dimensional basis. We notice that in physics textbooks there is no distinction between the notation of the operator in the original space and the operator in the space that includes the spin. We must understand the "dimension" of the operator representation by the context. A less trivial example of an external multiplication of operators:

$$\begin{pmatrix} 1 & 0 & 4 \\ 0 & 2 & 0 \\ 4 & 0 & 3 \end{pmatrix} \otimes \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \;=\; \begin{pmatrix} 2 & 1 & 0 & 0 & 8 & 4 \\ 1 & 2 & 0 & 0 & 4 & 8 \\ 0 & 0 & 4 & 2 & 0 & 0 \\ 0 & 0 & 2 & 4 & 0 & 0 \\ 8 & 4 & 0 & 0 & 6 & 3 \\ 4 & 8 & 0 & 0 & 3 & 6 \end{pmatrix} \tag{15.13}$$

Specifically, we see that if the operator that we are multiplying externally is diagonal, then we get a block diagonal matrix.

══════ [15.3] External multiplication of spin spaces

Let us consider two operators in different Hilbert spaces $\hat{L}$ and $\hat{S}$. The bases of the spaces are $|m_\ell\rangle, |m_s\rangle$. The eigenvalues are $m_\ell = 0, \pm 1$ and $m_s = \pm 1/2$. We label the new states as follows: $|\Uparrow\uparrow\rangle$, $|\Uparrow\downarrow\rangle$, $|\Updownarrow\uparrow\rangle$, $|\Updownarrow\downarrow\rangle$, $|\Downarrow\uparrow\rangle$, $|\Downarrow\downarrow\rangle$ This basis consists of 6 states. Therefore, each operator is represented by a 6×6 matrix. For example:

$$\hat{J}_x \;=\; \hat{S}_x + \hat{L}_x \tag{15.14}$$

A mathematician would write it as follows:

$$\hat{J}_x \;=\; \hat{1} \otimes \hat{S}_x + \hat{L}_x \otimes \hat{1} \tag{15.15}$$

Let us consider for example the case $\ell = 1$ and $s = 1/2$. In the natural basis we have

$$S_z \;\to\; \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix} \otimes \tfrac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \;=\; \frac{1}{2} \begin{pmatrix} 1 & 0 & & & & \\ 0 & -1 & & & & \\ & & 1 & 0 & & \\ & & 0 & -1 & & \\ & & & & 1 & 0 \\ & & & & 0 & -1 \end{pmatrix} \tag{15.16}$$

$$S_x \;\to\; \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix} \otimes \tfrac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \;=\; \frac{1}{2} \begin{pmatrix} 0 & 1 & & & & \\ 1 & 0 & & & & \\ & & 0 & 1 & & \\ & & 1 & 0 & & \\ & & & & 0 & 1 \\ & & & & 1 & 0 \end{pmatrix} \tag{15.17}$$

$$L_z \;\to\; \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} \;=\; \begin{pmatrix} 1 & & 0 & & 0 & \\ & 1 & & 0 & & 0 \\ 0 & & 0 & & 0 & \\ & 0 & & 0 & & 0 \\ 0 & & 0 & & -1 & \\ & 0 & & 0 & & -1 \end{pmatrix} \tag{15.18}$$

$$L_x \;\to\; \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} \;=\; \begin{pmatrix} 0 & & 1 & & 0 & \\ & 0 & & 1 & & 0 \\ 1 & & 0 & & 1 & \\ & 1 & & 0 & & 1 \\ 0 & & 1 & & 0 & \\ & 0 & & 1 & & 0 \end{pmatrix} \tag{15.19}$$

etc. Empty entries means a zero value that is implied by the fact that the operator act only on the "other" degree of freedom. This way of writing highlights the block structure of the matrices.

══════ [15.4] Rotations of a Composite system

We assume that we have a spin ℓ entity whose states are represented by the basis

$$|m_\ell = -\ell ... + \ell\rangle \tag{15.20}$$

and a spin s entity whose states are represented by the basis

$$|m_s = -s ... + s\rangle \tag{15.21}$$

The natural $(2\ell + 1) \times (2s + 1)$ basis for the representation of the composite system is defined as

$$|m_\ell, m_s\rangle \;=\; |m_\ell\rangle \otimes |m_s\rangle \tag{15.22}$$

A rotation of the ℓ entity is represented by the matrix

$$R \;=\; R^\ell \otimes \hat{1} \;=\; \mathrm{e}^{-i\Phi L_n} \otimes \hat{1} \;=\; \mathrm{e}^{-i\Phi L_n \otimes \hat{1}} \tag{15.23}$$

We have used the identity $f(A) \otimes \hat{1} = f(A \otimes \hat{1})$ which is easily established by considering the operation of both sides on a basis $|a, b\rangle$ that diagonalizes A. More generally we would like to rotate both the ℓ entity and the s entity. This two operations commute since they act on different degrees of freedom (unlike two successive rotation of the same entity). Thus we get

$$R \;=\; \mathrm{e}^{-i\Phi \hat{1} \otimes S_n}\, \mathrm{e}^{-i\Phi L_n \otimes \hat{1}} \;=\; \mathrm{e}^{-i\vec{\Phi}\cdot J} \tag{15.24}$$

where

$$J \;=\; L \otimes \hat{1} + \hat{1} \otimes S \;=\; L + S \tag{15.25}$$

From now on we use the conventional sloppy notations of physicists as in the last equality: the space over which the operator operates and the associated dimension of its matrix representation are implied by the context. Note that in full index notations the above can be summarized as follows:

$$\langle m_\ell m_s | R | m'_\ell m'_s \rangle \;=\; R^\ell_{m_\ell, m'_\ell} R^s_{m_s, m'_s} \tag{15.26}$$

$$\langle m_\ell m_s | J_i | m'_\ell m'_s \rangle \;=\; [L_i]_{m_\ell, m'_\ell} \delta_{m_s, m'_s} + \delta_{m_\ell, m'_\ell} [S_i]_{m_s, m'_s} \tag{15.27}$$

════ [15.5] Addition of angular momentum

It is important to realize that the basis states $|m_\ell, m_s\rangle$ are eigenstates of J_z, but not of J^2.

$$J_z |m_\ell, m_s\rangle \;=\; (m_\ell + m_s)|m_\ell, m_s\rangle \;\equiv\; m|m_\ell, m_s\rangle \tag{15.28}$$

$$J^2 |m_\ell, m_s\rangle \;=\; \text{superposition}\Big[\big|m_\ell[\pm 1], m_s[\mp 1]\big\rangle\Big] \tag{15.29}$$

The second expression is based on the observation that

$$J^2 = J_z^2 + \frac{1}{2}(J_+ J_- + J_- J_+) \tag{15.30}$$

$$J_\pm = L_\pm + S_\pm \tag{15.31}$$

This means that the representation is reducible, and can be written as a sum of irreducible representations. Using a conventional procedure we shall show later in this lecture that

$$(2\ell + 1) \otimes (2s + 1) \;=\; (2|\ell + s| + 1) \oplus \cdots \oplus (2|l - s| + 1) \tag{15.32}$$

It is called the "addition of angular momentum" theorem. The output of the "addition of angular momentum" procedure is a new basis $|j, m\rangle$ that satisfies

$$J^2 |j, m\rangle \;=\; j(j+1)|j, m\rangle \tag{15.33}$$

$$J_z |j, m\rangle \;=\; m|j, m\rangle \tag{15.34}$$

In the next sections we learn how to make the following decompositions:

$$2 \otimes 2 = 3 \oplus 1 \tag{15.35}$$
$$2 \otimes 3 = 4 \oplus 2$$

The first decomposition is useful in connection with the problem of two particles with spin $1/2$, where we can define a basis that includes three $j = 1$ states (the "triplet") and one $j = 0$ state (the "singlet"). The second example is useful in analyzing the Zeeman splitting of atomic levels.

===== [15.6] The Clebsch-Gordan-Racah coefficients

We shall see how to efficiently find the transformation matrix between the $|m_\ell, m_s\rangle$ and the $|j, m\rangle$ bases. The entries of the transformation matrix are called the Clebsch-Gordan-Racah Coefficients, and are commonly expressed using the Wigner 3j-symbol:

$$T_{m_\ell m_s, jm} \quad = \quad \langle m_\ell, m_s | j, m \rangle \quad = \quad (-1)^{\ell - s + m} \sqrt{2j + 1} \begin{pmatrix} \ell & s & j \\ m_\ell & m_s & -m \end{pmatrix} \tag{15.36}$$

Note that the Wigner 3j-symbol is non-zero only if its entries can be regarded as the sides of a triangle which is formed by 3 vectors of length ℓ and s and j whose projections m_ℓ and m_s and $-m$ sum to zero. This geometrical picture is implied by the addition of angular momentum theorem.

With the Clebsch-Gordan-Racah transformation matrix we can transform states and the operators between the two optional representations. In particular, note that J^2 is diagonal in the "new" basis, while in the "old basis" it can be calculated as follows:

$$[J^2]_{\text{old basis}} \quad \mapsto \quad \langle m_\ell', m_s' | J^2 | m_\ell, m_s \rangle \quad = \quad \sum \langle m_l', m_s' | j', m' \rangle \langle j', m' | J^2 | j, m \rangle \langle j, m | m_\ell, m_s \rangle \tag{15.37}$$

or in short

$$[J^2]_{\text{old basis}} \quad = \quad T[J^2]_{\text{diagonal}} T^\dagger \tag{15.38}$$

We shall see that in practical applications each representation has its own advantages.

===== [15.7] The inefficient decomposition method

Let us discuss as an example the case $\ell = 1$ and $s = 1/2$. In order to find J^2 we apparently have to do the following calculation:

$$J^2 \quad = \quad J_x^2 + J_y^2 + J_z^2 \quad = \quad \frac{1}{2} \left(J_+ J_- + J_- J_+ \right) + J_z^2 \tag{15.39}$$

The simplest term in this expression is the square of the diagonal matrix

$$J_z \quad = \quad L_z + S_z \quad \rightarrow \quad [6 \times 6 \ \ \text{matrix}] \tag{15.40}$$

We have additional terms in the J^2 expression that contain non-diagonal 6×6 matrices. To find them in a straightforward fashion can be time consuming. Doing the calculation of the matrix elements in the $|m_\ell, m_s\rangle$ basis, one realizes that most of the off-diagonal elements are zero: it is advised to use the (m_ℓ, m_s) diagram of the next section in order to identify which basis states are coupled. The result is

$$J^2 \rightarrow \begin{pmatrix} 15/4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 7/4 & \sqrt{2} & 0 & 0 & 0 \\ 0 & \sqrt{2} & 11/4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 11/4 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{2} & 7/4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 15/4 \end{pmatrix} \tag{15.41}$$

Next we have to diagonalize J^2 in order to get the "new" basis in which the representations decomposes into its irreducible components.

In the next section we shall introduce a more efficient procedure to find the matrix elements of J^2, and the "new" basis, using a "ladder operator picture". Furthermore, it is implied by the "addition of angular momentum" theorem that $3 \otimes 2 = 4 \oplus 2$, meaning that we have a $j = 3/2$ subspace and a $j = 1/2$ subspace. Therefore it is a-priori clear that after diagonalization we should get

$$J^2 \rightarrow \begin{pmatrix} (15/4) & 0 & 0 & 0 & 0 & 0 \\ 0 & (15/4) & 0 & 0 & 0 & 0 \\ 0 & 0 & (15/4) & 0 & 0 & 0 \\ 0 & 0 & 0 & (15/4) & 0 & 0 \\ 0 & 0 & 0 & 0 & (3/4) & 0 \\ 0 & 0 & 0 & 0 & 0 & (3/4) \end{pmatrix} \tag{15.42}$$

This by itself is valuable information. Furthermore, if we know the transformation matrix T we can switch back to the old basis by using a similarity transformation.

═══════ [15.8] The efficient decomposition method

In order to explain the procedure to build the new basis we consider, as an example, the addition of $\ell = 2$ and $s = \frac{3}{2}$. The figure below serves to clarify this example. Each point in the left panle represents a basis state in the $|m_\ell, m_s\rangle$ basis. The diagonal lines connect states that span the same J_z subspace, namely $m_\ell + m_s = \mathrm{const} \equiv m$. Let us call each such subspace a "floor". The upper floor $m = \ell + s$ contains only one state. The lower floor also contains only one state.
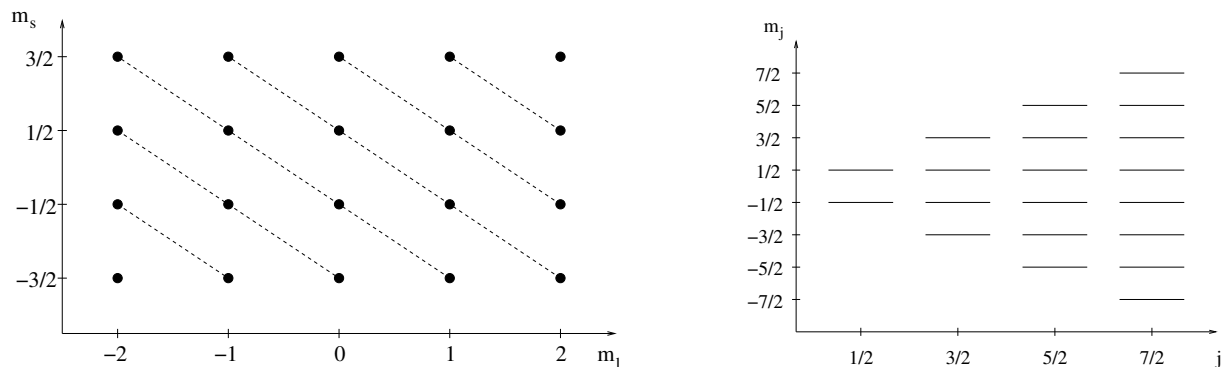
We recall that

$$J_z|m_\ell, m_s\rangle = (m_\ell + m_s)|m_\ell, m_s\rangle \tag{15.43}$$

$$S_-|m_\ell, m_s\rangle = \sqrt{s(s+1) - m_s(m_s - 1)}|m_\ell, m_s - 1\rangle \tag{15.44}$$

$$L_-|m_\ell, m_s\rangle = \sqrt{\ell(\ell+1) - m_\ell(m_\ell - 1)}|m_\ell - 1, m_s\rangle \tag{15.45}$$

$$J_- = S_- + L_- \tag{15.46}$$

$$J^2 = J_z^2 + \frac{1}{2}(J_+ J_- + J_- J_+) \tag{15.47}$$

Applying J_- or J_+ on a state takes us either one floor down or one floor up. By inspection we see that if J^2 operates on the state in the upper or in the lower floor, then we stay "there". This means that these states are eigenstates of J^2 corresponding to the eigenvalue $j = \ell + s$. Note that they could not belong to an eigenvalue $j > \ell + s$ because this would imply having larger (or smaller) m values.

Now we can use J_- in order to obtain the multiplet of $j = \ell + s$ states from the $m = \ell + s$ state. Next we look at the second floor from above and notice that we know the $|j = \ell + s, m = \ell + s - 1\rangle$ state, so by orthogonalization we can

find the $|j = \ell + s - 1, m = \ell + s - 1\rangle$ state. Once again we can get the whole multiplet by applying J_-. Going on with this procedure gives us a set of states as arranged in the right graph.

By suggesting the above procedure we have in fact proven the "addition of angular momentum" statement. In the displayed illustration we end up with 4 multiplets ($j = \frac{7}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2}$) so we have $5 \otimes 4 = 8 \oplus 6 \oplus 4 \oplus 2$. In the following sections we review some basic examples in detail.

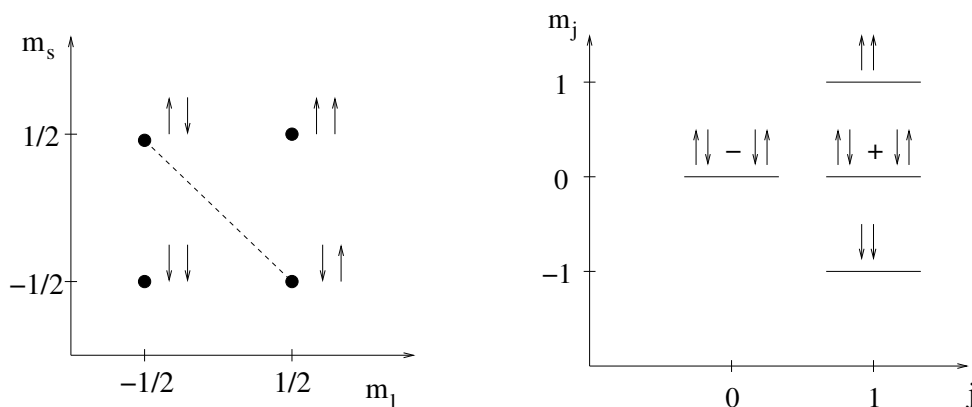## ═══════ [15.9] The case of $2 \otimes 2 = 3 \oplus 1$

Consider the addition of $\ell = \frac{1}{2}$ and $s = \frac{1}{2}$ (for example, two electrons). In this case the "old" basis is

$$|m_\ell, m_s\rangle = |\uparrow\uparrow\rangle, \ |\uparrow\downarrow\rangle, \ |\downarrow\uparrow\rangle, \ |\downarrow\downarrow\rangle \tag{15.48}$$

The "new" basis we want to find is

$$|j, m\rangle = \underbrace{|1, 1\rangle, |1, 0\rangle, |1, -1\rangle}, \underbrace{|0, 0\rangle} \tag{15.49}$$

These states are called triplet and singlet states.

The decomposition procedure gives:

$$
\begin{align}
|1, 1\rangle &= |\uparrow\uparrow\rangle \tag{15.50} \\
|1, 0\rangle &\propto J_-|\uparrow\uparrow\rangle = |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \tag{15.51} \\
|1, -1\rangle &\propto J_- J_-|\uparrow\uparrow\rangle = 2|\downarrow\downarrow\rangle \tag{15.52}
\end{align}
$$

By orthogonaliztion we get the singlet state, which after normalization is

$$|0, 0\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right) \tag{15.53}$$

Hence the transformation matrix from the old to the new basis is

$$T_{m_\ell, m_s | j, m} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{15.54}$$

The operator J^2 in the $|m_\ell, m_s\rangle$ basis is

$$\langle m'_\ell, m'_s|J^2|m_\ell, m_s\rangle = T \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} T^\dagger = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} \tag{15.55}$$
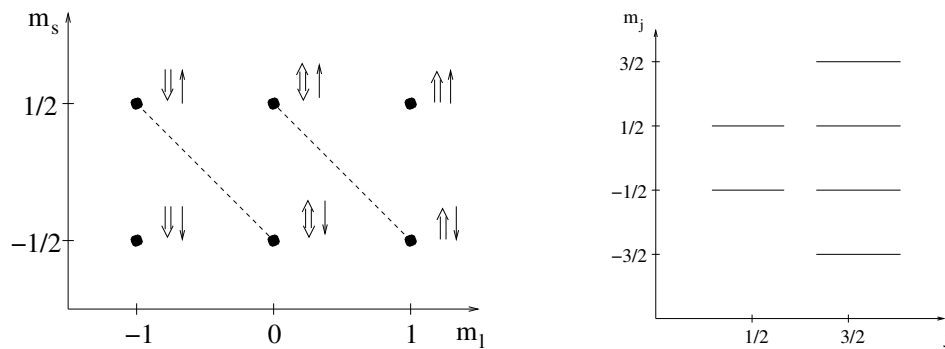
═══════ [15.10] The case of $3 \otimes 2 = 4 \oplus 2$

Consider the composite system of $\ell = 1$ and $s = \frac{1}{2}$.
In this case the "old" basis is

$$|m_\ell, m_s\rangle = |\Uparrow\uparrow\rangle, |\Uparrow\downarrow\rangle, |\Updownarrow\uparrow\rangle, |\Updownarrow\downarrow\rangle, |\Downarrow\uparrow\rangle, |\Downarrow\downarrow\rangle \tag{15.56}$$

The "new" basis we want to find is

$$|j, m\rangle = \underbrace{\left|\frac{3}{2}, \frac{3}{2}\right\rangle, \left|\frac{3}{2}, \frac{1}{2}\right\rangle, \left|\frac{3}{2}, -\frac{1}{2}\right\rangle, \left|\frac{3}{2}, -\frac{3}{2}\right\rangle}_{}, \underbrace{\left|\frac{1}{2}, \frac{1}{2}\right\rangle, \left|\frac{1}{2}, -\frac{1}{2}\right\rangle}_{} \tag{15.57}$$

The decomposition procedure is applied as in the previous section. Note that here the lowering operator L_- is associated with a $\sqrt{2}$ prefactor:

$$\left|\frac{3}{2}, \frac{3}{2}\right\rangle = |\Uparrow\uparrow\rangle \tag{15.58}$$

$$\left|\frac{3}{2}, \frac{1}{2}\right\rangle \propto J_-|\Uparrow\uparrow\rangle = |\Uparrow\downarrow\rangle + \sqrt{2}|\Updownarrow\uparrow\rangle \tag{15.59}$$

$$\left|\frac{3}{2}, -\frac{1}{2}\right\rangle \propto J_- J_-|\Uparrow\uparrow\rangle = 2\sqrt{2}|\Updownarrow\downarrow\rangle + 2|\Downarrow\uparrow\rangle \tag{15.60}$$

$$\left|\frac{3}{2}, -\frac{3}{2}\right\rangle \propto J_- J_- J_-|\Uparrow\uparrow\rangle = 6|\Downarrow\downarrow\rangle \tag{15.61}$$

By orthogonalization we get the starting point of the next multiplet, and then we use the lowering operator again:

$$\left|\frac{1}{2}, \frac{1}{2}\right\rangle \propto -\sqrt{2}|\Uparrow\downarrow\rangle + |\Updownarrow\uparrow\rangle \tag{15.62}$$

$$\left|\frac{1}{2}, -\frac{1}{2}\right\rangle \propto -|\Updownarrow\downarrow\rangle + \sqrt{2}|\Downarrow\uparrow\rangle \tag{15.63}$$

Hence the transformation matrix from the old to the new basis is

$$T_{m_\ell,m_s|j,m} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{1}{3}} & 0 & 0 & -\sqrt{\frac{2}{3}} & 0 \\ 0 & \sqrt{\frac{2}{3}} & 0 & 0 & \sqrt{\frac{1}{3}} & 0 \\ 0 & 0 & \sqrt{\frac{2}{3}} & 0 & 0 & -\sqrt{\frac{1}{3}} \\ 0 & 0 & \sqrt{\frac{1}{3}} & 0 & 0 & \sqrt{\frac{2}{3}} \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \tag{15.64}$$

and the operator J^2 in the $|m_\ell, m_s\rangle$ basis is

$$\langle m'_\ell, m'_s|J^2|m_\ell, m_s\rangle = T \begin{pmatrix} \frac{15}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{15}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{15}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{15}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{3}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{3}{4} \end{pmatrix} T^\dagger = \begin{pmatrix} \frac{15}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{7}{4} & \sqrt{2} & 0 & 0 & 0 \\ 0 & \sqrt{2} & \frac{11}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{11}{4} & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{2} & \frac{7}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{15}{4} \end{pmatrix} \tag{15.65}$$

This calculation is done in the Mathematica file *zeeman.nb*.

════ [15.11] The case of $(2\ell + 1) \otimes 2 = (2\ell + 2) \oplus (2\ell)$

The last example was a special case of a more general result which is extremely useful in studying the Zeeman Effect in atomic physics. We consider the addition of integer ℓ (angular momentum) and $s = \frac{1}{2}$ (spin). The procedure is exactly as in the previous example, leading to two multiplets: The $j = \ell + \frac{1}{2}$ multiplet and the $j = \ell - \frac{1}{2}$ multiplet. The final expression for the new basis states is:

$$\left| j = \ell + \frac{1}{2}, m \right\rangle = +\beta \left| m + \frac{1}{2}, \downarrow \right\rangle + \alpha \left| m - \frac{1}{2}, \uparrow \right\rangle \tag{15.66}$$

$$\left| j = \ell - \frac{1}{2}, m \right\rangle = -\alpha \left| m + \frac{1}{2}, \downarrow \right\rangle + \beta \left| m - \frac{1}{2}, \uparrow \right\rangle \tag{15.67}$$

where

$$\alpha = \sqrt{\frac{\ell + (1/2) + m}{2\ell + 1}}, \qquad\qquad \beta = \sqrt{\frac{\ell + (1/2) - m}{2\ell + 1}} \tag{15.68}$$

[16] Galilei group and the non-relativistic Hamiltonian

======== [16.1] The Representation of the Galilei Group

The defining realization of the Galilei group is over phase space. Accordingly, that natural representation is with functions that "live" in phase space. Thus the a-translated $\rho(x, v)$ is $\rho(x-a, v)$ while the u-boosted $\rho(x, v)$ is $\rho(x, v-u)$ etc.

The generators of the displacements are denoted $\mathbf{P}_x, \mathbf{P}_y, \mathbf{P}_z$, the generators of the boosts are denoted $\mathbf{Q}_x, \mathbf{Q}_y, \mathbf{Q}_z$, and the generators of the rotations are denoted $\mathbf{J}_x, \mathbf{J}_y, \mathbf{J}_z$. Thus we have 9 generators. It is clear that translations and boosts commute, so the only non-trivial structure constants of the Lie algebra have to do with the rotations:

$$[\mathbf{P}_i, \mathbf{P}_j] = \mathbf{0} \tag{16.1}$$

$$[\mathbf{Q}_i, \mathbf{Q}_j] = \mathbf{0} \tag{16.2}$$

$$[\mathbf{P}_i, \mathbf{Q}_j] = \mathbf{0} \qquad \text{(to be discussed)} \tag{16.3}$$

$$[\mathbf{J}_i, \mathbf{A}_j] = i\epsilon_{ijk}\mathbf{A}_k \qquad \text{for } \mathbf{A} = P, Q, J \tag{16.4}$$

Now we ask the following question: is it possible to find a faithful representation of the Galilei group that "lives" in configuration space. We already know that the answer is "almost" positive: We can represent pure quantum states using "wavefunctions" $\psi(x)$. These wavefunctions can be translated and rotated. On a physical basis it is also clear that we can talk about "boosted" states: this means to give the particle a different velocity. So we can also boost wavefunctions. On physical grounds it is clear that the boost should not change $|\psi(x)|^2$. In fact it is not difficult to figure out that the boost is realized by a multiplication of $\psi(x)$ by $e^{i(\mathsf{m}u)x}$. Hence we get the identifications $P_x \mapsto -i(d/dx)$ and $Q_x \mapsto -\mathsf{m}x$ for the generators. Still the wise reader should realize that in this "new" representation boosts and translations do not commute, while in case of the strict phase space realization they do commute!

On the mathematical side it would be nice to convince ourselves that the price of not having commutation between translations and boosts is inevitable, and that there is a unique representation (up to a gauge) of the Galilei group using "wavefunctions". This mathematical discussion should clarify that the "compromise" for having such a representation is: (1) The wavefunctions have to be complex; (2) The boosts commute with the translations only up to a phase factor. We shall see that the price that we have to pay is to add $\hat{1}$ as a tenth generator to the Lie algebra. This is similar to the discussion of the relation between SO(3) and SU(2). The elements of the latter can be regarded as "rotations" provided we ignore an extra "sign factor". Here rather than ignoring a "sign factor" we have to ignore a complex "phase factor".

Finally, we shall see that the most general form of the non-relativistic Hamiltonian of a spinless particle, and in particular its mass, are implied by the structure of the quantum Lie algebra.

======== [16.2] The Mathematical Concept of Mass

An element τ of the Galilei group is parametrized by 9 parameters. To find a strict (unitary) representation means to associate with each element a linear operator $U(\tau)$ such that $\tau^1 \otimes \tau^2 = \tau^3$ implies

$$U(\tau^1)U(\tau^2) = U(\tau^3) \tag{16.5}$$

Let us see why this strict requirement cannot be realized if we want a representation with "wavefunctions". Suppose that we have an eigenstate of $\hat{P}$ such that $\hat{P}|k\rangle = k|k\rangle$. since we would like to assume that boosts commute with translations it follows that also $U_{boost}|k\rangle$ is an eigenstate of $\hat{P}$ with the same eigenvalue. This is absurd, because it is like saying that a particle has the same momentum in all reference frames. So we have to replace the strict requirement by

$$U(\tau^1)U(\tau^2) = e^{i \times \text{phase}}U(\tau^3) \tag{16.6}$$

This means that now we have an extended group that "covers" the Galilei group, where we have an additional parameter (a phase), and correspondingly an additional generator ($\hat{\mathbf{1}}$). The Lie algebra of the ten generators is characterized by

$$[G_\mu, G_\nu] = i \sum_\lambda c^\lambda_{\mu\nu} G_\lambda \tag{16.7}$$

where $G_0 = \hat{\mathbf{1}}$ and the other nine generators are P_i, Q_i, J_i with $i = x, y, z$. It is not difficult to convince ourselves that without loss of generality this introduces one "free" parameter into the algebra (the other additional structure constants can be set to zero via appropriate re-definition of the generators). The "free" non-trivial structure constant m appears in the commutation

$$[\mathbf{P}_i, \mathbf{Q}_j] = i\mathsf{m}\delta_{ij} \tag{16.8}$$

which implies that boosts do not commute with translations.

════ [16.3] Finding the Most General Hamiltonian

Assume that we have a spinless particle for which the standard basis for representation is $|x\rangle$. With appropriate gauge of the x basis the generator of the translations is $P \mapsto -i(d/dx)$. From the commutation relation $[P, Q] = i\mathsf{m}$ we deduce that $Q = -\mathsf{m}\hat{x} + g(\hat{p})$, where $g()$ is an arbitrary function. With appropraite gauge of the momentum basis we can assume $Q = -\mathsf{m}\hat{x}$.

The next step is to observe that the effect of a boost on the velocity operator should be

$$U_{boost}(u)^{-1}\hat{v}U_{boost}(u) = \hat{v} + u \tag{16.9}$$

which implies that $[Q, \hat{v}] = -i$. The simplest possibility is $\hat{v} = \hat{p}/\mathsf{m}$. But the most general possibility is

$$\hat{v} = \frac{1}{\mathsf{m}}(\hat{p} - A(\hat{x})) \tag{16.10}$$

where A is an arbitrary function. This time we cannot gauge away A.

The final step is to recall the rate of change formula which implies the relation $\hat{v} = i[\mathcal{H}, \hat{x}]$. The simplest operator that will give the desired result for v is $\mathcal{H} = \frac{1}{2\mathsf{m}}(p - A(x))^2$. But the most general possibility involves a second undetermined function:

$$\mathcal{H} = \frac{1}{2\mathsf{m}}(\hat{p} - A(\hat{x}))^2 + V(x) \tag{16.11}$$

Thus we have determined the most general Hamiltonian that agrees with the Lie algebra of the Galilei group. In the next sections we shall see that this Hamiltonian is indeed invariant under Galilei transformations.

[17] Transformations and invariance

═══════ [17.1] Transformation of the Hamiltonian

First we would like to make an important distinction between passive ["Heisenberg"] and active ["Schrödinger"] points of view regarding transformations. The failure to appreciate this distinction is an endless source of confusion.

In classical mechanics we are used to the passive point of view. Namely, to go to another reference frame (say a displaced frame) is like a change of basis. Namely, we relate the new coordinates to the old ones (say $\tilde{x} = x - a$), and in complete analogy we relate the new basis $|\tilde{x}\rangle$ to the old basis $|x\rangle$ by a transformation matrix $T = e^{-ia\hat{p}}$ such that $|\tilde{x}\rangle = T|x\rangle = |x + a\rangle$.

However we can also use an active point of view. Rather than saying that we "change the basis" we can say that we "transform the wavefunction". It is like saying that "the tree is moving backwards" instead of saying that "the car is moving forward". In this active approach the transformation of the wavefunction is induced by $S = T^{-1}$, while the observables stay the same. So it is meaningless to make a distinction between old (x) and new $(\tilde{x})$ coordinates!

From now on we use the more convenient active point of view. It is more convenient because it is in the spirit of the Schrödinger (rather than Heisenberg) picture. In this active point of view observables do not transform. Only the wavefunction transforms ("backwards"). Below we discuss the associated transformation of the evolution operator and the Hamiltonian.

Assume that the transformation of the state as we go from the "old frame" to the "new frame" is $\tilde{\psi} = S\psi$. The evolution operator that propagates the state of the system from t_0 to t in the new frame is:

$$\tilde{U}(t, t_0) = S(t)U(t, t_0)S^{-1}(t_0) \tag{17.1}$$

The idea is that we have to transform the state to the old frame (laboratory) by S^{-1}, then calculate the evolution there, and finally go back to our new frame. We recall that the Hamiltonian is defined as the generator of the evolution. By definition

$$\tilde{U}(t + \delta t, t_0) = (1 - i\delta t\tilde{\mathcal{H}}(t))\tilde{U}(t, t_0) \tag{17.2}$$

Hence

$$\tilde{\mathcal{H}} \;=\; i\frac{\partial \tilde{U}}{\partial t}\tilde{U}^{-1} \;=\; i\left[\frac{\partial S(t)}{\partial t}US(t_0)^{-1} + S(t)\frac{\partial U}{\partial t}S(t_0)^{-1}\right]S(t_0)U^{-1}S(t)^{-1} \tag{17.3}$$

and we get the result

$$\tilde{\mathcal{H}} \;=\; S\mathcal{H}S^{-1} + i\frac{\partial S}{\partial t}S^{-1} \tag{17.4}$$

In practice we assume a Hamiltonian of the form $\mathcal{H} = h(x, p; V, A)$. Hence we get that the Hamiltonian in the new frame is

$$\tilde{\mathcal{H}} \;=\; h(SxS^{-1}, SpS^{-1}; V, A) + i\frac{\partial S}{\partial t}S^{-1} \tag{17.5}$$

Recall that "invariance" means that the Hamiltonian keeps its form, but the fields in the Hamiltonian may have changed. So the question is whether we can write the new Hamiltonian as

$$\tilde{\mathcal{H}} = h(x, p; \tilde{A}, \tilde{V}) \tag{17.6}$$

To have "symmetry" rather than merely "invariance" means that the Hamiltonian remains the same with $\tilde{A} = A$ and $\tilde{V} = V$. We are going to show that the following Hamiltonian is invariant under translations, rotations, boosts and gauge transformations:

$$\mathcal{H} = \frac{1}{2\mathsf{m}} \left(\hat{p} - \vec{A}(x) \right)^2 + V(x) \tag{17.7}$$

We shall argue that this is the most general non-relativistic Hamiltonian for a spinless particle. We shall also discuss the issue of time reversal (anti-unitary) transformations.

======= [17.2] Invariance Under Translations

$$
\begin{aligned}
T &= D(a) = \mathrm{e}^{-ia\hat{p}} \\
S &= T^{-1} = \mathrm{e}^{ia\hat{p}}
\end{aligned}
\tag{17.8}
$$

The coordinates (basis) transform with T, while the wavefunctions are transformed with S.

$$
\begin{aligned}
S\hat{x}S^{-1} &= x + a \\
S\hat{p}S^{-1} &= \hat{p} \\
Sf(\hat{x},\hat{p})S^{-1} &= f(S\hat{x}S^{-1}, S\hat{p}S^{-1}) = f(\hat{x} + a, \hat{p})
\end{aligned}
\tag{17.9}
$$

$$\tag{17.10}$$

Therefore the Hamiltonian is invariant with

$$
\begin{aligned}
\tilde{V}(x) &= V(x + a) \\
\tilde{A}(x) &= A(x + a)
\end{aligned}
\tag{17.11}
$$

======= [17.3] Invariance Under Gauge

$$
\begin{aligned}
T &= \mathrm{e}^{-i\Lambda(x)} \\
S &= \mathrm{e}^{i\Lambda(x)} \\
S\hat{x}S^{-1} &= \hat{x} \\
S\hat{p}S^{-1} &= \hat{p} - \nabla\Lambda(x) \\
Sf(\hat{x},\hat{p})S^{-1} &= f(S\hat{x}S^{-1}, S\hat{p}S^{-1}) = f(\hat{x}, \hat{p} - \nabla\Lambda(x))
\end{aligned}
\tag{17.12}
$$

Therefore the Hamiltonian is invariant with

$$
\begin{aligned}
\tilde{V}(x) &= V(x) \\
\tilde{A}(x) &= A(x) + \nabla\Lambda(x)
\end{aligned}
\tag{17.13}
$$

Note that the electric and the magnetic fields are not affected by this transformation.

More generally we can consider time dependent gauge transformations with $\Lambda(x, t)$. Then we get in the "new" Hamiltonian an additional term, leading to

$$
\begin{aligned}
\tilde{V}(x) &= V(x) - (d/dt)\Lambda(x, t) \\
\tilde{A}(x) &= A(x) + \nabla\Lambda(x, t)
\end{aligned}
\tag{17.14}
$$

In particular we can use the very simple gauge $\Lambda = ct$ in order to change the Hamiltonian by a constant ($\tilde{\mathcal{H}} = \mathcal{H} - c$).

═══════ [17.4] Boosts and Transformations to a Moving System

From an algebraic point of view a boost can be regarded as a special case of gauge:

$$
\begin{aligned}
T &= e^{i(\mathsf{m}u)x} \\
S &= e^{-i(\mathsf{m}u)x} \\
S\hat{x}S^{-1} &= \hat{x} \\
S\hat{p}S^{-1} &= \hat{p} + \mathsf{m}u
\end{aligned}
\tag{17.15}
$$

Hence $\tilde{V}(x) = V(x)$ and $\tilde{A}(x) = A(x) - \mathsf{m}u$. But a transformation to a moving frame is not quite the same thing. The latter combines a boost and a time dependent displacement. The order of these operations is not important because we get the same result up to a constant phase factor that can be gauged away:

$$
\begin{aligned}
S &= e^{i\text{phase}(u)}\, e^{-i(\mathsf{m}u)x}\, e^{i(ut)p} \\
S\hat{x}S^{-1} &= \hat{x} + ut \\
S\hat{p}S^{-1} &= \hat{p} + \mathsf{m}u
\end{aligned}
\tag{17.16}
$$

The new Hamiltonian is

$$
\tilde{\mathcal{H}} = S\mathcal{H}S^{-1} + i\frac{\partial S}{\partial t}S^{-1} = S\mathcal{H}S^{-1} - u\hat{p} = \frac{1}{2\mathsf{m}}(\hat{p} - \tilde{A}(x))^2 + \tilde{V}(x) + \text{const}(u)
\tag{17.17}
$$

where

$$
\begin{aligned}
\tilde{V}(x, t) &= V(x + ut, t) - u \cdot A(x + ut, t) \\
\tilde{A}(x, t) &= A(x + ut, t)
\end{aligned}
\tag{17.18}
$$

Thus in the new frame the magnetic field is the same (up to the displacement) while the electric field is:

$$
\tilde{\mathcal{E}} = -\frac{\partial \tilde{A}}{\partial t} - \nabla\tilde{V} = \mathcal{E} + u \times \mathcal{B}
\tag{17.19}
$$

In the derivation of the latter we used the identity

$$
\nabla(u \cdot A) - (u \cdot \nabla)A = u \times (\nabla \times A)
\tag{17.20}
$$

Finally we note that if we do not include the boost in S, then we get essentially the same results up to a gauge. By including the boost we keep the same dispersion relation: If in the lab frame $A = 0$ and we have $v = p/\mathsf{m}$, then in the new frame we also have $\tilde{A} = 0$ and therefore $v = p/\mathsf{m}$ still holds.

═══════ [17.5] Transformations to a rotating frame

Let us assume that we have a spinless particle held by a a potential $V(x)$. Assume that we transform to a rotating frame. We shall see that the transformed Hamiltonian will have in it a Coriolis force and a centrifugal force.

The transformation that we consider is

$$S = \mathrm{e}^{i(\vec{\Omega}t)\cdot \hat{L}} \tag{17.21}$$

The new Hamiltonian is

$$\tilde{\mathcal{H}} = S\mathcal{H}S^{-1} + i\frac{\partial S}{\partial t}S^{-1} = \frac{1}{2\mathsf{m}}p^2 + V(x) - \Omega\cdot\hat{L} \tag{17.22}$$

It is implicit that the new x coordinate is relative to the rotating frame of reference. Without loss of generality we assume $\vec{\Omega} = (0,0,\Omega)$. Thus we got Hamiltonian that looks very similar to that of a particle in a uniform magnetic field (see appropriate lecture):

$$\mathcal{H} = \frac{1}{2\mathsf{m}}(p - A(x))^2 + V(x) = \frac{p^2}{2\mathsf{m}} - \frac{\mathcal{B}}{2\mathsf{m}}L_z + \frac{\mathcal{B}^2}{8\mathsf{m}}(x^2 + y^2) + V(x) \tag{17.23}$$

The Coriolis force is the "magnetic field" $\mathcal{B} = 2\mathsf{m}\Omega$. By adding and subtracting a quadratic term we can write the Hamiltonian $\tilde{\mathcal{H}}$ in the standard way with

$$\tilde{V} = V - \frac{1}{2}\mathsf{m}\Omega^2(x^2 + y^2) \tag{17.24}$$
$$\tilde{A} = A + \mathsf{m}\vec{\Omega}\times r$$

The extra $-(1/2)\mathsf{m}\Omega^2(x^2 + y^2)$ term is called the centrifugal potential.

===== [17.6] Time Reversal transformations

Assume for simplicity that the Hamiltonian is time independent. The evolution operator is $U = \mathrm{e}^{-i\mathcal{H}t}$. If we make a *unitary* transformation T we get

$$\tilde{U} = T^{-1}\mathrm{e}^{-i\mathcal{H}t}T = \mathrm{e}^{-i(T^{-1}\mathcal{H}T)t} = \mathrm{e}^{-i\tilde{\mathcal{H}}t} \tag{17.25}$$

where $\tilde{\mathcal{H}} = T^{-1}\mathcal{H}T$. Suppose we want to reverse the evolution in our laboratory. Apparently we have to engineer T such that $T^{-1}\mathcal{H}T = -\mathcal{H}$. If this can be done the propagator $\tilde{U}$ will take the system backwards in time. We can name such T operation a "Maxwell demon" for historical reasons. Indeed for systems with spins such transformations have been realized using NMR techniques. But for the "standard" Hamiltonian $\mathcal{H} = \hat{p}^2/(2\mathsf{m})$ it is impossible to find a *unitary* transformation that do the trick for a reason that we explain below.

At first sight it seems that in classical mechanics there is a transformation that reverses the dynamics. All we have to do is to invert the sign of the velocity. Namely $p \mapsto -p$ while $x \mapsto x$. So why not to realize this transformation in the laboratory? This was Loschmidt's claim against Boltzman. Boltzman's answer was "go and do it". Why is it "difficult" to do? Most people will probably say that to reverse the sign of an Avogadro number of particles is tough. But in fact there is a better answer. In a sense it is impossible to reverse the sign even of one particle! If we believe that the dynamics of the system are realized by a Hamiltonian, then *the only physical transformations* are proper canonical transformations. Such transformations preserves the Poisson brackets, whereas $\{p \mapsto -p,\ x \mapsto x\}$ inverts sign. So it cannot be physically realized.

In quantum mechanical language we say that any physical realizable evolution process is described by a unitary operator. We claim that the transformation $p \mapsto -p$ while $x \mapsto x$ cannot be realized by any physical Hamiltonian. Assume that we have a unitary transformation T such that $T\hat{p}T^{-1} = -\hat{p}$ while $T\hat{x}T^{-1} = \hat{x}$. This would imply $T[\hat{x}, \hat{p}]T^{-1} = -[\hat{x}, \hat{p}]$. So we get $i = -i$. This means that such a transformation does not exist.

But there is a way out. Wigner has proved that there are two types of transformations that map states in Hilbert space such that the overlap between states remains the same. These are either unitary transformations or anti-unitary

transformations. The time reversal transformations that we are going to discuss are anti-unitary. They cannot be realized in an actual laboratory experiment. This leads to the distinction between "microreversibility" and actual "reversibility": It is one thing to say that a Hamiltonian has time reversal symmetry. It is a different story to actually reverse the evolution.

We shall explain in the next section that the "velocity reversal" transformation that has been mentioned above can be realized by an antiunitary transformation. We also explain that in the case of an antiunitary transformation we get

$$\tilde{U} \;=\; T^{-1}\mathrm{e}^{-i\mathcal{H}t}T \;=\; \mathrm{e}^{+i(T^{-1}\mathcal{H}T)t} \;=\; \mathrm{e}^{-i\tilde{\mathcal{H}}t} \tag{17.26}$$

where $\tilde{\mathcal{H}} = -T^{-1}\mathcal{H}T$. Thus in order to reverse the evolution we have to engineer T such that $T^{-1}\mathcal{H}T = \mathcal{H}$, or equivalently $[\mathcal{H}, T] = 0$. If such a T exists then we say that $\mathcal{H}$ has time reversal symmetry. In particular we shall explain that in the absence of a magnetic field the non-relativistic Hamiltonian has a time reversal symmetry.

There is a subtle distinction between the physical notion of time reversal invariance, as opposed to invariance under unitary operation. In the latter case, say "rotation", the given transformation T is well defined irrespective of the dynamics. Then we can check whether the "physical law" of the dynamics is "invariant"

$$\text{Given } T, \quad \forall A, \quad \exists \tilde{A}, \quad T^{-1}U[A]T = U[\tilde{A}] \tag{17.27}$$

In contrast to that time reversal invariance means:

$$\exists T, \quad \forall A, \quad \exists \tilde{A}, \quad U[A]^{-1} = TU[\tilde{A}]T^{-1} \tag{17.28}$$

For example, if A is the vector potential, time reversal invariance implies the transformation $\tilde{A} = -A$, which means that the time reversed dynamics can be realized by inverting the magnetic field. Thus, the definition of time reversal transformation is implied by the dynamics, and cannot be introduced out of context.

===== [17.7] Anti-unitary Operators

An anti-unitary operator has an anti-linear rather than linear property. Namely,

$$T\left(\alpha\left|\phi\right\rangle + \beta\left|\psi\right\rangle\right) = \alpha^{*}T\left|\phi\right\rangle + \beta^{*}T\left|\psi\right\rangle \tag{17.29}$$

An anti-unitary operator can be represented by a matrix T_{ij} whose columns are the images of the basis vectors. Accordingly $|\varphi\rangle = T|\psi\rangle$ implies $\varphi_i = T_{ij}\psi_j^*$. So its operation is complex conjugation followed by linear transformation. It is useful to note that $\tilde{H} = T^{-1}HT$ implies $\tilde{H}_{\mu\nu} = T_{i\mu}^{*}H_{ij}^{*}T_{j\nu}$. This is proved by pointing out that the effect of double complex conjugation when operating on a vector is canceled as far as its elements are concerned.

The simplest procedure to construct an anti-unitary operator is as follows: We pick an arbitrary basis $|r\rangle$ and define a diagonal anti-unitary operator K that is represented by the unity matrix. Such operator maps ψ_r to ψ_r^*, and has the property $K^2 = 1$. Note also that for such operator $\tilde{H}_{ij} = H_{ij}^*$. In a sense there is only one anti-unitary operator per choice of a basis. Namely, assume that T is represented by the diagonal matrix $\{\mathrm{e}^{i\phi_r}\}$. That means

$$T\left|r\right\rangle = \mathrm{e}^{i\phi_r}\left|r\right\rangle \tag{17.30}$$

Without loss of generality we can assume that $\phi_r = 0$. This is because we can gauge the basis. Namely, we can define a new basis $|\tilde{r}\rangle = \mathrm{e}^{i\lambda_r}|r\rangle$ for which

$$T\left|\tilde{r}\right\rangle = \mathrm{e}^{i(\phi_r - 2\lambda_r)}\left|\tilde{r}\right\rangle \tag{17.31}$$

By setting $\lambda_r = \phi_r/2$ we can make all the eigenvalues equal to one, and hence $T = K$. Any other antiunitary operator can be written trivially as $T = (TK)K$ where TK is unitary. So in practice any T is represented by complex

conjugation followed by a unitary transformation. Disregarding the option of having the "extra" unitary operation, time reversal symmetry $T^{-1} \mathcal{H} T = \mathcal{H}$ means that in the particular basis where T is diagonal the Hamiltonian matrix is real ($\mathcal{H}_{r,s}^* = \mathcal{H}_{r,s}$), rather than complex.

Coming back to the "velocity reversal" transformation it is clear that T should be diagonal in the position basis (x should remain the same). Indeed we can verify that such a T automatically reverses the sign of the momentum:

$$|k\rangle = \sum_x \mathrm{e}^{ikx} |x\rangle \tag{17.32}$$

$$T |k\rangle = \sum_x T \mathrm{e}^{ikx} |x\rangle = \sum_x \mathrm{e}^{-ikx} |x\rangle = |-k\rangle$$

In the absence of a magnetic field the kinetic term p^2 in the Hamiltonian has symmetry with respect to this T. Therefore we say that in the absence of a magnetic field we have time reversal symmetry. In which case the Hamiltonian is real in the position representation.

What happens if we have a magnetic field? Does it mean that there is no time reversal symmetry? Obviously in particular cases the Hamiltonian may have a different anti-unitary symmetry: if $V(-x) = V(x)$ then the Hamiltonian is symmetric with respect to the transformation $x \mapsto -x$ while $p \mapsto p$. The anti-unitary T in this case is diagonal in the p representation. It can be regarded as a product of "velocity reversal" and "inversion" ($x \mapsto -x$ and $p \mapsto -p$). The former is anti-unitary while the latter is a unitary operation.

If the particle has a spin we can define K with respect to the standard basis. The standard basis is determined by $\hat{x}$ and σ_3. However, $T = K$ is not the standard time reversal symmetry: It reverse the polarization if it is in the Y direction, but leave it unchanged if it is in the Z or in the X direction. We would like to have $T^{-1} \sigma T = -\sigma$. This implies that

$$T = \mathrm{e}^{-i\pi S_y} K = -i\sigma_y K \tag{17.33}$$

Note that $T^2 = (-1)^N$ where N is the number of spin $1/2$ particles in the system. This implies Kramers degeneracy for odd N. The argument goes as follows: If ψ is an eigenstate of the Hamiltonian, then symmetry with respect to T implies that also $T\psi$ is an eigenstate. Thus we must have a degeneracy unless $T\psi = \lambda\psi$, where λ is a phase factor. But this would imply that $T^2\psi = \lambda^2\psi$ while for odd N we have $T^2 = -1$. The issue of time reversal for particles with spin is further discussed in [**Messiah p.664**].

Dynamics and Driven Systems

[18] Transition probabilities

════════ [18.1] Time dependent Hamiltonians

To find the evolution which is generated by a time independent Hamiltonian is relatively easy. Such a Hamiltonian has eigenstates $|n\rangle$ which are the "stationary" states of the system. The evolution in time of an arbitrary state is:

$$|\psi(t)\rangle \;\; = \;\; \sum_n \mathrm{e}^{-iE_n t} \psi_n |n\rangle \tag{18.1}$$

But in general the Hamiltonian can be time-dependent $[\mathcal{H}(t_1), \mathcal{H}(t_2)] \neq 0$. In such case the strategy that was described above for finding the evolution in time loses its significance. In this case, there is no simple expression for the evolution operator:

$$\hat{U}(t, t_0) \;\; = \;\; \mathrm{e}^{-idt_N \mathcal{H}(t_N)} \cdots \mathrm{e}^{-idt_2 \mathcal{H}(t_2)} \mathrm{e}^{-idt_1 \mathcal{H}(t_1)} \;\; \equiv \;\; \mathrm{Texp}\left[-i \int_{t_0}^{t} \mathcal{H}(t') dt' \right] \tag{18.2}$$

where Texp denotes time-ordered exponential, that can be replaced by the ordinary *exp* if $\mathcal{H}$ is constant, but not in general.

Of special interest is the case where the Hamiltonian can be written as the sum of a time independent part $\mathcal{H}_0$ and a time dependent perturbation $V(t)$. In such case we can make the substitution

$$\mathrm{e}^{-idt_n \mathcal{H}(t_n)} \;\; = \;\; \mathrm{e}^{-idt_n \mathcal{H}_0} \left(1 - idt_n V(t_n)\right) \tag{18.3}$$

Next we can expand and rearrange the Texp sum as follows:

$$\hat{U}(t) \;\; = \;\; U_0(t, t_0) \;\; + \;\; (-i) \int_{t_0 < t_1 < t} dt_1 \; U_0(t, t_1) V(t_1) U_0(t_1, t_0) \tag{18.4}$$

$$+ \;\; (-i)^2 \iint_{t_0 < t_1 < t_2 < t} dt_2 dt_1 \; U_0(t, t_2) V(t_2) U_0(t_2, t_1) V(t_1) U_0(t_1, t_0) \;\; + \;\; \cdots \tag{18.5}$$

There are few cases where the calculation can be carried out analytically to infinite order (a nice example is the Landau-Zener problem). In many case, if the perturbation is weak enough, one is satisfied with the leading order approximation. Below we assume that the Hamiltonian can be written as a sum of a time independent part $\mathcal{H}_0$ and a time dependent perturbation. Namely,

$$\mathcal{H} \;\; = \;\; \mathcal{H}_0 + V \;\; = \;\; \mathcal{H}_0 + f(t) W \tag{18.6}$$

Using first order perturbation theory, we shall introduce a formula for calculating the probability of transition between unperturbed eigenstates. The formula can be obtained directly in "one line" derivation from the above expansion. But for pedagogical reason we shall repeat its derivation using a traditional iterative scheme.

════════ [18.2] The interaction picture

We would like to work in a basis such that $\mathcal{H}_0$ is diagonal:

$$\mathcal{H}_0 |n\rangle \;\; = \;\; E_n |n\rangle \tag{18.7}$$
$$|\Psi(t)\rangle \;\; = \;\; \sum_n \Psi_n(t) \, |n\rangle$$

The evolution is determined by the Schrödinger's equation:

$$i\frac{d\psi_n}{dt} = E_n\psi_n + \sum_{n'} V_{nn'}\Psi_{n'} \tag{18.8}$$

which can be written in a matrix style as follows:

$$i\frac{d}{dt}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} E_1\Psi_1 \\ E_2\Psi_2 \\ \vdots \end{pmatrix} + \begin{pmatrix} V_{11} & V_{12} & \cdots \\ V_{21} & V_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \end{pmatrix} \tag{18.9}$$

Without the perturbation we would get $\psi_n(t) = c_n\mathrm{e}^{-iE_nt}$, where c_n are constants. It is therefore natural to use the variation of parameters method, and to write

$$\Psi_n(t) = c_n(t)\,\mathrm{e}^{-iE_nt} \tag{18.10}$$

In other words, we represent the "wave function" by the amplitudes $c_n(t) = \psi_n(t)\mathrm{e}^{iE_nt}$ rather than by the amplitudes $\Psi_n(t)$. The Schrödinger's equation in the new representation takes the form

$$i\frac{dc_n}{dt} = \sum_{n'} \mathrm{e}^{i(E_n-E_{n'})t}\,V_{nn'}\,c_{n'}(t) \tag{18.11}$$

This is called the Schrödinger's equation in the "interaction picture". It is a convenient equation because the term on the right is assumed to be "small". Therefore, the amplitudes $c_n(t)$ change slowly. This equation can be solved using an iterative scheme which leads naturally to a perturbative expansion. The iteration are done with the integral version of the above equation:

$$c_n(t) = c_n(0) - i\sum_{n'}\int_0^t \mathrm{e}^{iE_{nn'}t'}\,V_{n,n'}\,c_{n'}(t')\,dt' \tag{18.12}$$

where $E_{nn'} = E_n - E_{n'}$. In each iteration we get the next order. Let us assume that the system has been prepared in level n_0. This means that the zero order solution is

$$c_n^{[0]}(t) = c_n(0) = \delta_{n,n_0} \tag{18.13}$$

We iterate once and get the first-order solution:

$$c_n(t) = \delta_{n,n_0} - i\int_0^t \mathrm{e}^{iE_{nn_0}t'}V_{n,n_0}dt' \tag{18.14}$$

It is instructive to consider constant perturbation (V does not depend on time). Doing the integral and going back to the standard representation we get the following result for the first-order transition amplitude:

$$\psi_n(t) = V_{n,n_0}\frac{\mathrm{e}^{-iE_nt} - \mathrm{e}^{-iE_{n_0}t}}{E_n - E_{n_0}}, \qquad [\text{constant perturbation, } n \neq n_0] \tag{18.15}$$

We notice that for very short times we get $\psi_n(t) \approx -iV_{n,n_0}t$, which reflects the definition of the matrix elements of the Hamiltonian as the "hopping" amplitude per unit of time. As long as the energy difference $(E_n - E_{n_0})$ is not resolved, this expression is merely modulated $\psi_n(t) \approx [-iV_{n,n_0}t]\mathrm{e}^{-iE_nt}$, reflecting the choice of the energy reference.

But for longer times the accumulation of the amplitude is suppressed due to the temporal oscillations of the integrand. If the perturbation is constant, the oscillation frequency of the integrand is $\omega = (E_n - E_{n'})$. If the perturbation is characterized by a frequency Ω, this oscillation frequency becomes $\nu = (E_n - E_{n'} - \Omega)$.

In order to illustrate the effect of the oscillating integrand, consider a problem in which the unperturbed Hamiltonian is "to be in some site". We can regard the possibility to move from site to site as a perturbation. The energy differences in the site problem are the gradients of the potential energy, which we call "electric field". The hopping amplitude is the same in each "hop" even if the hop into a potential wall. However, due to the potential difference the probability amplitude does not "accumulate" and therefore the particle is likely to be reflected. The reflection is not due to the lack of coupling between site, but due to the potential difference that induces "fields" that suppresses the transition probability.

======= [18.3] The transition probability formula

The expression we found for the wavefunction amplitudes using first-order perturbation theory can be written as:

$$c_n(t) \approx 1 \qquad\qquad \text{for } n = n_0 \tag{18.16}$$

$$c_n(t) = -iW_{n,n_0} \int_0^t f(t') e^{iE_{nn_0}t'} dt' \qquad \text{otherwise} \tag{18.17}$$

The latter expression for the transition amplitude can be written optionally as a Fourier transform (FT):

$$c_n(t) \approx -iW_{n,n_0} \, \text{FT}\,[f(t)] \tag{18.18}$$

We use here the convention that $f(t) = 0$ before and after the pulse. For example, if we turn on a constant perturbation for a finite duration, then $f(t)$ is a rectangle function. It is implicit that the FT is calculated at the frequency of the transition $\omega = E_n - E_{n_0}$, namely,

$$\text{FT}\,[f(t)] = \int_{-\infty}^{\infty} f(t') \, e^{iE_{n,n_0}t'} \, dt' \tag{18.19}$$

The associated expression for the transition probability is:

$$P_t(n|n_0) \approx |W_{n,n_0}|^2 \times \left| \text{FT}\,[f(t)] \right|^2 \tag{18.20}$$

======= [18.4] The effect of a constant or harmonic perturbation

We consider the following scenario: A particle is prepared in the state n_0, and then a constant perturbation is turned on for a time t. We want to know what is the probability of finding the particle at some later time in the state n. Using the transition probability formula we get

$$P_t(n|n_0) = |c_n(t)|^2 = |W_{nn_0}|^2 \left| \frac{1 - e^{i(E_n - E_{n_0})t}}{E_n - E_{n_0}} \right|^2 \tag{18.21}$$

We notice that the transition amplitude is larger to closer levels and smaller for distant levels.

The above expression can be regarded as a special case of a more general result that concerns harmonic perturbation:

$$f(t') = e^{-i\Omega t'} \qquad \text{for} \quad t' \in [0, t] \tag{18.22}$$

Recall that the Hamiltonian should be hermitian. Therefore this perturbation has a physical meaning only if it appears together with a conjugate term $e^{+i\Omega t'}$. In other words, the driving is done by a real field $2\cos(\Omega t')$ that changes periodically. Below we treat only "half" of the perturbation: the effect of the second half is obtained by making the replacement $\Omega \mapsto -\Omega$.

Using the transition probability formula with finite Ω we get the same integral as for constant perturbation with $E_n - E_{n_0}$ replaced by $E_n - E_{n_0} - \Omega$. Accordingly the result is

$$
P_t(n|n_0) \quad = \quad |W_{nn_0}|^2 \left| \frac{1 - e^{i(E_n - E_{n_0} - \Omega)t}}{E_n - E_{n_0} - \Omega} \right|^2 \quad = \quad |W_{n,n_0}|^2 \frac{2[1 - \cos(E_n - E_{n_0} - \Omega)t)]}{(E_n - E_{n_0} - \Omega)^2} \tag{18.23}
$$

$$
= \quad |W_{n,n_0}|^2 \frac{4\sin^2((E_n - E_{n_0}) - \Omega)t/2)}{(E_n - E_{n_0} - \Omega)^2} \quad = \quad |W_{n,n_0}|^2 \, t^2 \, \mathrm{sinc}^2((E_n - E_{n_0} - \Omega)t/2) \tag{18.24}
$$

Schematically we can write this result as follows:

$$
P_t(n|n_0) \quad = \quad 2\pi \, |W_{n,n_0}|^2 \, \delta_{2\pi/t}(E_n - E_{n_0} - \Omega) \, \times \, t \tag{18.25}
$$

The schematic way of writing emphasizes that if t is large enough the sinc^2 function becomes a narrow function of width $2\pi/t$ that resembles a delta function. Namely,

$$
\mathrm{sinc}(\nu) \quad \equiv \quad \frac{\sin(\nu)}{\nu} \tag{18.26}
$$

$$
\int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \mathrm{sinc}^2\left(\frac{\nu}{2}\right) \quad = \quad 1 \tag{18.27}
$$

======= [18.5] The Fermi golden rule (FGR)

The main transitions which are induced by a purely harmonic driving is to energy levels that obey the "resonance condition":

$$
(E_n - E_{n_0}) \quad \sim \quad \Omega \tag{18.28}
$$

From the expression we found, we see that the probability of transition to levels that obey $|E_n - (E_{n_0} + \Omega)| < 2\pi/t$ is proportional to t^2. That is what we would expect to get by the definition of the Hamiltonian as the probability amplitude for transitions per unit time. But the "width" of the area that includes these levels is proportional to $2\pi/t$. From this we conclude that the probability of transition to other levels grows linearly. We call the rate of transition to other levels Γ.

$$
\Gamma \quad = \quad \frac{2\pi}{\Delta} |W_{n,n_0}|^2 \quad = \quad 2\pi \varrho(E) \, |W_{n,n_0}|^2 \tag{18.29}
$$

The formula can be proved by calculating the probability to stay in level n_0:

$$
P(t) \quad = \quad 1 - \sum_{n(\neq n_0)} P_t(n|n_0) \quad = \quad 1 - \int \frac{dE}{\Delta} P_t(E|E_0) \quad = \quad 1 - \frac{2\pi t}{\Delta} |W_{n,n_0}|^2 \quad = \quad 1 - \Gamma t \tag{18.30}
$$

It is implicit in the above derivation that we assume a dense spectrum with well defined density of states. We also assume that the relevant matrix elements are all of the same order of magnitude.

Let us discuss the conditions for the validity of the Fermi golden rule picture. First-order perturbation theory is valid as long as $P(t) \approx 1$, or equivalently $\Gamma t \ll 1$. Hence a relevant time scale is the Wigner time

$$
t_\Gamma \quad = \quad \frac{1}{\Gamma} \tag{18.31}
$$

Another important time scale that gets into the game is the Heisenberg time which is defined as:

$$t_H = \frac{2\pi}{\Delta} \tag{18.32}$$

We distinguish below between the case of weak perturbation ($|W| \ll \Delta$), for which $t_H \ll t_\Gamma$ from the case of strong perturbation ($|W| > \Delta$), for which $t_H \gg t_\Gamma$.

In the case $|W| \ll \Delta$ first-order perturbation theory is still valid when $t = t_H$. If perturbation theory is valid up to this time then it is valid at any time, since after the Heisenberg time the (small) probability that has moved from the initial state to other energy levels oscillates, and does not grow further. This argument is based on the assumption that the difference $\nu = E_n - (E_{n_0} + \Omega)$ is of the order Δ, even for levels in the middle of the resonance. If there is an "exact" resonance, it is possible to show that the probability will oscillate between the two energy levels, as in the "two-site" problem, and there is no "cumulative" leakage of the probability to other levels.

In the case $|W| > \Delta$ first-order perturbation theory breaks down before the Heisenberg time. Then we must go to higher orders of perturbation theory. With some limitation we find the result:

$$P(t) = e^{-\Gamma t} \tag{18.33}$$

This means that there is a decay. In another lecture we analyze a simple model where we can get this result exactly. In the general case, this is an approximation that has, at best, limited validity. For an isolated system it can be justified on the basis of rezolvent theory (see separate lecture) assuming that a single pole is dominating. For a non-isolated system it can be justified on the basis of a Markovian picture.

Finally it should be clear that the FGR is irrelevant if the time is very short. Let us assume that Δ_b is the width of the energy-band whose levels E_n are coupled by W_{n,n_0} to the initial level E_{n_0}. Or optionally let us assume that the density of states has variation on some energy scale Δ_b. We define an associate time scale

$$t_c = \frac{2\pi}{\Delta_b} \tag{18.34}$$

During the time $t < t_c$ the total transition probability is possibly growing like t^2. The FGR holds only after the bandwidth Δ_b is "resolved", which can be written as $t \gg t_c$. If the driving source is noisy (the "other" version of Fermi golden rule) one identifies $t_c = \tau_c$ as the correlation time of the noise. The bottom line is that the Fermi golden rule in any of its variations is likely to be applicable during a finite time interval

$$t_c \ll t \ll t_H \tag{18.35}$$

[19] Transition rates

In the previous subsection we have derived an expression for the transition probability if the driving is purely harmonic. In this section we assume a noisy driving. The "noise" is characterized by a correlation function

$$\langle f(t)f(t') \rangle = F(t - t') \tag{19.1}$$

where the average is taken over realizations of $f(t)$. The Fourier transform of of the correlation function is the power spectrum of the noise $\tilde{F}(\omega)$. From the transition probability formula we get

$$P_t(n|m) = |W_{nm}|^2 \int_0^t \int_0^t \langle f(t')f(t'') \rangle \, e^{iE_{nm}(t'-t'')} \, dt'dt'' \approx |W_{nm}|^2 \, \tilde{F}(\omega{=}E_{nm}) \times t \tag{19.2}$$

where the approximation assumes that the duration of the noise is much larger compared with its correlation time τ_c. In practice we can distinguish 3 cases of interest: **(a)** White noise; **(b)** Low frequency noise; **(c)** Noisy periodic driving.

In the first case $\tilde{F}(\omega)$ is flat and wide, so it is enough to characterize it by its spectral intensity $\nu = \tilde{F}(\omega)$, and to write the above result as $P_t(n|m) = w_{nm}t$, where the transition rates are $w_{nm} = \nu|W_{nm}|^2$. In the second case $\tilde{F}(\omega)$ is narrow, with some spectral width $2\pi/\tau_c$, that is determined by the correlation time τ_c. We write $F(0) = \langle f^2 \rangle \equiv \varepsilon^2$ where ε is the RMS intensity of the noise. Then it follows that its peak spectral intensity is $\nu = \tilde{F}(0) = \varepsilon^2 \tau_c$. The third case refers to noisy harmonic driving that has a correlation time $\tau_c \gg 2\pi/\Omega$. In the latter case $\tilde{F}(\omega)$ is concentrated around the frequency Ω, and it is suggestive to re-write the expression for the transition rate schematically as follows:

$$w_{nm} \;\; = \;\; \varepsilon^2 \, |W_{n,m}|^2 \;\; 2\pi \delta_{2\pi/\tau_c}((E_n - E_m) - \Omega) \tag{19.3}$$

Note that ε can be absorbed into the definition of W. The above result for constant rate transition between levels is commonly regarded as a special version of the Fermi golden rule that we discussed in the previous lecture.

======= [19.1] Master equations

The above version of the FGR is commonly used in order to determine the rates constants in Master equations that provide a reduced description for the dynamics of a system that is coupled to a bath or to a noise source. Here we demonstrates how a Master equation is derived for the simplest case: system that is subjected to the influence of a white noise source.

Consider the Hamiltonian $\mathcal{H} = \mathcal{H}_0 + f(t)W$, were $f(t)$ represents white noise: that means that upon ensemble average $\langle f(t) \rangle = 0$, while $\langle f(t)f(t') \rangle = \nu \delta(t - t')$. The Liouville von-Neumann equation for the time evolution of ρ can be solved iteratively in order to determine $\rho(t + dt)$ given $\rho(t) \equiv \rho$, where dt is small time interval:

$$\rho(t + dt) \;\; = \;\; \rho - i \int_t^{t+dt} dt' \, [\mathcal{H}, \rho] - \int_t^{t+dt} \int_t^{t'} dt' dt'' \, [\mathcal{H}, [\mathcal{H}, \rho]] + ... \tag{19.4}$$

Averaging over realizations of $f(t)$ all the odd orders in this expansion vanish, while the leading dt contribution comes only from the zero order term that involves $\mathcal{H}_0$ and from the second order term that involves W. Consequently we get the following Master equation:

$$\frac{d\rho}{dt} = -i[\mathcal{H}_0, \rho] - \frac{1}{2}\nu[W, [W, \rho]] \tag{19.5}$$

In the most standard example $W = \hat{x}$, and the second term corresponds to the diffusion term $(\nu/2)\partial^2 \rho/\partial p^2$ in the classical Fokker-Plank equation.

In the weak noise limit the rate of the noise induced transitions becomes much smaller compared with the Bloch frequency of the coherent transitions. Then we can ignore all the highly oscillating terms that involve the off-diagonal terms, because they average to zero. Consequently we get the so-called Pauli mater equation for the probabilities p_n

$$\frac{d\boldsymbol{p}}{dt} \;\; = \;\; \mathcal{W} \, \boldsymbol{p} \qquad \mathcal{W} = \begin{pmatrix} -\Gamma_1 & w_{12} & ... \\ w_{21} & -\Gamma_2 & ... \\ ... & ... & ... \end{pmatrix} \tag{19.6}$$

In this equation the $\mathcal{W}$ matrix is in agreement with the FGR picture. Namely, the rate constants are $w_{nm} = \nu|W_{nm}|^2$, and the decay constants are $\Gamma_n = \sum_m w_{nm}$. We note that if we had interaction with a bath, then the ratio w_{12}/w_{21} would not be unity, but would favor downwards transitions.

The noise induced "diffusion" term in the master equation that we have derived is $W\rho W - (1/2)(WW\rho + \rho WW)$. We can regard it as a special case of the so-called Lindblad equation. The evolution of a non-isolated system is further discussed under *Special topics* in the lecture regarding *Quantum states, operations and measurements*. The presentation of the Master Equation formalism for a system that is coupled to a bath has been differed to *Lecture Notes in Statistical Mechanics and Mesoscopic*, arXiv:1107.0568

[20] The cross section in the Born approximation

======== [20.1] Cross Section

In both classical mechanics and quantum mechanics there are two types of problems: closed systems and open systems. We will discuss an open system. The dynamical problem that we will analyze is called a "scattering problem". For example, a wave that is scattered on a sphere. In a problem of this type the energy is given. We assume that there is an "incident particle flux" and we ask what is the "scattered flux".
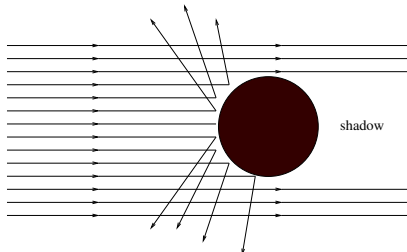
We notice that the sphere "hides" a certain area of the beam. The total hidden area is called the "total cross section" σ_{total}. Let us assume that we have a beam of particles with energy E and velocity v_E, so that the current density is:

$$J[\text{particles/time/area}] \quad = \quad \rho_0 v_E \tag{20.1}$$

where ρ_0 is the particle density. We write the scattered current as:

$$I_{\text{scattered}} \quad = \quad [\sigma_{\text{total}}] \times J \tag{20.2}$$

where the cross section σ_{total} is defined as the ratio of the scattered current $I_{\text{scattered}}$ to the incident particle flux density J. We notice that each area element of the sphere scatters to a different direction. Therefore, it is more interesting to talk about the differential cross section $\sigma(\Omega)$. In full analogy $\sigma(\Omega)d\Omega$ is defined by the formula:

$$I(k \in d\Omega | k_0) \quad = \quad [\sigma(\Omega)d\Omega] \times J \tag{20.3}$$

where k_0 denotes the initial momentum, while k is the final momentum. Here only the scattering into the angular element $d\Omega$ is detected.

======== [20.2] Cross section and rate of transition

For the theoretical discussion that will follow, it is convenient to think of the space as if it has a finite volume $L^3 = L_x L_y L_z$ with periodic boundary conditions. In addition we assume that the "incident" beam takes up the whole volume. If we normalize the particle density according to the volume then $\rho_0 = 1/L^3$. With this normalization, the flux J (particles per unit time) is actually the "probability current" (probability per unit time), and the current $I_{\text{scattered}}$ is in fact the scattering rate. Therefore an equivalent definition of the cross section is:

$$\Gamma(k \in d\Omega | k_0) \quad = \quad [\sigma(\Omega)d\Omega] \times \frac{1}{L^3} v_{\text{E}} \tag{20.4}$$

Given the scattering potential $U(r)$ we can calculate its Fourier transform $\tilde{U}(q)$

$$\tilde{U}(q) \quad = \quad \text{FT}[U(r)] \quad = \quad \int\int\int U(r)e^{-i\vec{q}\cdot\vec{r}}d^3r \tag{20.5}$$

Then we get from the Fermi golden rule (see derivation below) a formula for the differential cross section which is called the "Born approximation":

$$\sigma(\Omega) \quad = \quad \frac{1}{(2\pi)^2} \left(\frac{k_E}{v_E} \right)^2 |\tilde{U}(\vec{k}_\Omega - \vec{k}_0)|^2 \quad = \quad \left(\frac{\mathsf{m}}{2\pi} \right)^2 \left| \tilde{U}(\vec{k}_\Omega - \vec{k}_0) \right|^2 \tag{20.6}$$

The second expression assumes the non-relativistic dispersion relation $v_E = k_E/\mathsf{m}$. The Born approximation is a first-order perturbation theory approximation. It can be derived with higher order corrections within the framework of scattering theory.

═══════ [20.3] The DOS for a free particle

In order to use the Fermi golden rule we need an expression for the density of states of a free particle. In the past we defined $\varrho(E)dE$ as the number of states with energy $E < E_k < E + dE$. But in order to calculate the differential cross section we need a refined definition:

$$\varrho(\Omega, E)d\Omega dE \quad = \quad \text{Number of states } \vec{k} \in d\Omega \text{ with energy } E < E_k < E + dE \tag{20.7}$$

If we have a three-dimensional space with volume $L^3 = L_x L_y L_z$ and periodic boundary conditions, then the momentum states are:

$$k_{n_x, n_y, n_z} \quad = \quad \left(\frac{2\pi}{L_x} n_x, \frac{2\pi}{L_y} n_y, \frac{2\pi}{L_z} n_z \right) \tag{20.8}$$
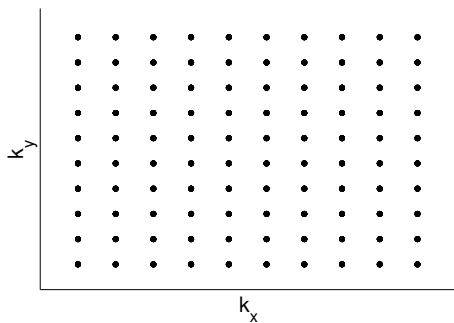
The number of states with a momentum that in a specified region of k space is:

$$\frac{dk_x \, dk_y \, dk_z}{\frac{2\pi}{L_x} \frac{2\pi}{L_y} \frac{2\pi}{L_z}} \quad = \quad \frac{L^3}{(2\pi)^3} \, d^3k \quad = \quad \frac{L^3}{(2\pi)^3} \, k^2 d\Omega \, dk \quad = \quad \frac{L^3}{(2\pi)^3} \, k_E^2 d\Omega \frac{dE}{v_E} \tag{20.9}$$

where we have moved to spherical coordinates and used the relation $dE = v_E dk$. Therefore, we find the result:

$$\varrho(\Omega, E)d\Omega dE \quad = \quad \frac{L^3}{(2\pi)^3} \frac{k_E^2}{v_E} d\Omega dE \tag{20.10}$$

════════ [20.4] Derivation of the Born formula

Let us assume that we have a flux of particles that are moving in a box with periodic boundary conditions in the z direction. As a result of the presence of the scatterer there are transitions to other momentum states (i.e. to other directions of motion). According to the Fermi golden rule the transition rate is:

$$\Gamma(k \in d\Omega | k_0) \quad = \quad 2\pi \left[\varrho(\Omega, E) d\Omega \right] |U_{k_\Omega, k_0}|^2 \tag{20.11}$$

By comparing with the definition of a cross section we get the formula:

$$\sigma(\Omega) \quad = \quad \frac{2\pi}{v_E} L^3 \, \varrho(\Omega, E) \, |U_{k_\Omega, k_0}|^2 \tag{20.12}$$

We notice that the matrix elements of the scattering potential are:

$$\langle \vec{k} | U(r) | \vec{k_0} \rangle \quad = \quad \int \frac{d^3x}{L^3} \, \mathrm{e}^{-ik \cdot r} U(r) \, \mathrm{e}^{ik_0 \cdot r} \quad = \quad \frac{1}{L^3} \int U(r) \, \mathrm{e}^{-i(k - k_0) \cdot r} d^3r = \frac{1}{L^3} \tilde{U}(k - k_0) \tag{20.13}$$

By substituting this expression and using the result for the density of states we get the Born formula.

════════ [20.5] Scattering by a spherically symmetric potential

In order to use the Born formula in practice we define our system of coordinates as follows: the incident wave propagates in the z direction, and the scattering direction is $\Omega = (\theta_\Omega, \varphi_\Omega)$. The difference between the k of the scattered wave and the k_0 of the incident wave is $\vec{q} = \vec{k} - \vec{k_0}$. Next we have to calculate $\tilde{U}(q)$ which is the Fourier transform of $U(r)$. If the potential is spherically symmetric we can use a rotated coordinate system for the calculation of the Fourier transform integral. Namely, we can use spherical coordinates such that $\theta = 0$ is the direction of $\vec{q}$. Consequently

$$\tilde{U}(q) \quad = \quad \int \int \int U(r) \mathrm{e}^{-iqr\cos(\theta)} d\varphi \, d\cos(\theta) r^2 dr \quad = \quad 4\pi \int_0^\infty U(r) \operatorname{sinc}(qr) \, r^2 dr \tag{20.14}$$

where the angular integration has been done using

$$\int_{-1}^1 \mathrm{e}^{-i\lambda s} ds = \left[\frac{\mathrm{e}^{-i\lambda s}}{-i\lambda} \right]_{-1}^1 = \frac{\mathrm{e}^{i\lambda} - \mathrm{e}^{-i\lambda}}{i\lambda} = \frac{2\sin(\lambda)}{\lambda} = 2\operatorname{sinc}(\lambda) \tag{20.15}$$

As an example consider $U(r) = 1/r$, for which we get $\tilde{U}(q) = 4\pi/q^2$ (Rutherford formula).
Next, we can go on calculating the total cross section:

$$\sigma_{\text{total}} \quad = \quad \int \int \sigma(\Omega) d\Omega \quad = \quad \frac{1}{(2\pi)^2} \left(\frac{k_E}{v_E} \right)^2 \int_0^\pi |\tilde{U}(q)|^2 \, 2\pi \sin \theta_\Omega d\theta_\Omega \tag{20.16}$$

We note that by simple trigonometry:

$$q = 2k_E \sin \left(\frac{\theta_\Omega}{2} \right) \qquad \leadsto \qquad dq = k_E \cos \left(\frac{\theta_\Omega}{2} \right) d\theta_\Omega \qquad \leadsto \qquad \sin \theta_\Omega d\theta_\Omega = \frac{q \, dq}{k_E^2} \tag{20.17}$$

Hence we can write the integral of the cross section as:

$$\sigma_{\text{total}} \quad = \quad \frac{1}{2\pi v_E^2} \int_0^{2k_E} |\tilde{U}(q)|^2 q \, dq \tag{20.18}$$

[21] Dynamics in the adiabatic picture

======= [21.1] The notion of adiabaticity

Consider a particle in a one dimensional box with infinite walls. We now move the wall. What happens to the particle? Let us assume that the particle has been prepared in a certain level. It turns out that if the wall is displaced slowly, the particle stays in the same level. This is called the "adiabatic approximation". We notice that staying in the same energy level means that the state of the particle changes! If the wall is moved very fast then the state of the particle does not have time to change. This is called the "sudden approximation". In the latter case the final state (after the displacement of the wall) is not an eigenstate of the (new) Hamiltonian. After a sudden displacement of the wall, the particle has to "ergodize" its state inside the box.

The fact that the energy of the particle decreases when we move the wall outwards, means that the particle is doing work. If the wall is displaced adiabatically, and then displaced back to its original location, then there is no net work done. In such case we say that the process is reversible. But if the displacement of the wall is not adiabatically slow, the particle makes transitions to other energy levels. This scattering to other energy levels is in general irreversible.

In the problem that we have considered above, the parameter X that we change is the length L of the box. Therefore $V = \dot{X}$ is the velocity at which the wall (or the "piston") is displaced. In other problems X could be any field. An important example is a particle in a ring where $X = \Phi$ is the magnetic flux through the ring, and EMF $= -\dot{X}$ is the electro motive force (by Faraday law). In problems of this type, the change in the parameter X can be very large, so we cannot use standard perturbation theory to analyze the evolution in time. Therefore, we would like to find another way to write Schrödinger's equation, so that $\dot{X}$ is the small parameter.

In the following section we transform the Schrödinger equation to the adiabatic basis. This can be regarded as a transformation to a moving frame. Namely, what we derive is a *special case* of the following general result:

$$\tilde{\mathcal{H}} \;\;=\;\; T^\dagger \mathcal{H} T \;-\; i T^\dagger \frac{\partial T}{\partial t} \tag{21.1}$$

See lecture "Transformations and invariance" for further discussion. The second term is the generator of the transformation to the moving frame, which is here the adiabatic basis.

======= [21.2] The Schrödinger equation in the adiabatic basis

We assume that we have Hamiltonian $\mathcal{H}(\hat{Q}, \hat{P}; X)$ that depends on a parameter X. The adiabatic states are the eigenstates of the instantaneous Hamiltonian:

$$\mathcal{H}(X) \; |n(X)\rangle \;\;=\;\; E_n(X) \; |n(X)\rangle \tag{21.2}$$

It is natural in such problems to work with the adiabatic basis and not with a fixed basis. We write the state of the system as:

$$|\Psi\rangle \;\;=\;\; \sum_n a_n(t) \, |n(X(t))\rangle \,, \qquad\qquad a_n(t) \equiv \langle n(X(t))|\Psi(t)\rangle \tag{21.3}$$

If we prepare the particle in the energy level n_0 and change X in adiabatically, then we shall see that $|a_n(t)|^2 \approx \delta_{n,n_0}$ at later times. We shall find a slowness condition for the validity of this approximation. Our starting point is the Schrödinger's equation

$$\frac{d\Psi}{dt} \;\;=\;\; -i\mathcal{H}(x, p; X(t)) \; \Psi \tag{21.4}$$

from which we get:

$$\frac{da_n}{dt} = \left\langle n \left| \frac{d}{dt} \Psi \right.\right\rangle + \left\langle \frac{d}{dt} n \left| \Psi \right.\right\rangle = -i \left\langle n \left| \mathcal{H} \psi \right.\right\rangle + \sum_m \left\langle \frac{d}{dt} n \left| m \right.\right\rangle \left\langle m \left| \Psi \right.\right\rangle \tag{21.5}$$

$$= -iE_n a_n + \dot{X} \sum_m \left\langle \frac{\partial}{\partial X} n \left| m \right.\right\rangle a_m \equiv -iE_n a_n + i\dot{X} \sum_m A_{nm} a_m \tag{21.6}$$

We conclude that in the adiabatic basis the effective Hamiltonian acquires an additional term, namely $\mathcal{H} \mapsto \mathcal{H} - \dot{X} A$. As an example consider the case where X is the position of a box that confine a particle, then we get in the moving frame $\tilde{H} = \mathcal{H} - \dot{X} \hat{p}$.

═══════ [21.3] The calculation of A_{nm}

Before we make further progress we would like to dwell on the calculation of the perturbation matrix A_{nm}. First of all we notice that for any X

$$\left\langle n \left| m \right.\right\rangle = \delta_{nm} \qquad \rightsquigarrow \qquad \frac{\partial}{\partial X} \left\langle n \left| m \right.\right\rangle = 0 \qquad \rightsquigarrow \qquad \left\langle \frac{\partial}{\partial X} n \left| m \right.\right\rangle + \left\langle n \left| \frac{\partial}{\partial X} m \right.\right\rangle = 0 \tag{21.7}$$

Which means that $\langle \partial n | m \rangle$ is anti-Hermitian, and therefore $-i \langle \partial n | m \rangle$ is Hermitian. If follows that

$$A_{nm} = -i \left\langle \frac{\partial}{\partial X} n \left| m \right.\right\rangle = i \left\langle n \left| \frac{\partial}{\partial X} m \right.\right\rangle = i \left\langle n \left| T^\dagger \frac{\partial T}{\partial X} \right| m \right\rangle \tag{21.8}$$

where $T(X)$ is the transformation to the moving frame, namely, $|n(X)\rangle = T(X) |n(0)\rangle$. For the diagonal elements we use the notation

$$A_n(X) = A_{nn} = i \left\langle n \left| \frac{\partial}{\partial X} n \right.\right\rangle \tag{21.9}$$

With regard to the off-diagonal elements one observes that

$$A_{nm} = \frac{-iV_{nm}}{E_n - E_m}, \qquad\qquad V_{nm} \equiv \left(\frac{\partial \mathcal{H}}{\partial X} \right)_{nm} \tag{21.10}$$

This is a very practical formula. Its proof is based on the following:

$$\left\langle n \left| \mathcal{H} \right| m \right\rangle = 0 \quad \text{for } n \neq m, \text{ for any } X \tag{21.11}$$

$$\rightsquigarrow \quad \frac{\partial}{\partial X} \left\langle n \left| \mathcal{H} \right| m \right\rangle = 0$$

$$\rightsquigarrow \quad \left\langle \frac{\partial}{\partial X} n \left| \mathcal{H} \right| m \right\rangle + \left\langle n \left| \frac{\partial}{\partial X} \mathcal{H} \right| m \right\rangle + \left\langle n \left| \mathcal{H} \right| \frac{\partial}{\partial X} m \right\rangle = 0$$

$$\rightsquigarrow \quad E_m \left\langle \frac{\partial}{\partial X} n \left| m \right.\right\rangle + V_{nm} + E_n \left\langle n \left| \frac{\partial}{\partial X} m \right.\right\rangle = 0$$

═══════ [21.4] The adiabatic condition

We found that in the adiabatic basis the Schrödinger's equation takes the form

$$\frac{da_n}{dt} = -iE_n a_n + i\dot{X} \sum_m A_{nm} a_m \equiv -i(E_n - \dot{X} A_n) a_n - i \sum_m W_{nm} a_m \tag{21.12}$$

For sake of analysis we separated above the diagonal part of the perturbation. We use the simplified notation $A_n = A_{nn}$, and packed the off-diagonal elements into the matrix $W_{nm} = -\dot{X}A_{nm}$, whose diagonal elements are zero. It should be noticed that the strength of the perturbation in this representation is determined by the rate $\dot{X}$ and not by the amplitude of the driving.

Let us write again the Schrodinger equation in the adiabatic basis, with the substitution of the explicit expression that we have derived for the perturbation W_{nm},

$$\frac{da_n}{dt} = -i(E_n - \dot{X}A_n)a_n + \dot{X}\sum_{m(\neq n)}\left(\frac{V_{nm}}{E_n - E_m}\right) a_m \tag{21.13}$$

If $\dot{X}$ is small enough, the perturbation matrix W is not able to induce transitions between levels, and we get the adiabatic approximation $|a_n(t)|^2 \approx \text{const}$. This means that the probability distribution does not change with time. In particular, if the particle is prepared in level n, then is stays in this level all the time.

From the discussion of first-order perturbation theory we know that we can neglect the coupling between two different energy levels if the absolute value of the matrix element is smaller compared with the energy difference between the levels. Assuming that all the matrix elements are comparable the main danger to the adiabaticity are transitions to neighboring levels. Therefore the adiabatic condition is $|W| \ll \Delta$ or

$$\dot{X} \ll \frac{\Delta^2}{\hbar\sigma} \tag{21.14}$$

where σ is the estimate for the matrix element V_{nm} that couples neighbouring levels.

An example is in order. Consider a particle in a box of length L. The wall is displaced at a velocity $\dot{X}$. Given that the energy of the particle is E we recall that the energy level spacing is $\Delta = (\pi/L)v_E$, while the coupling of neighbouring levels, based on a formula that we derive in the Hard Walls subsection (p.195), is

$$\sigma = \frac{1}{\mathsf{m}L}k_n^2 = \frac{1}{\mathsf{m}L}(\mathsf{m}v_E)^2 = \frac{1}{L}\mathsf{m}v_E^2 \tag{21.15}$$

It follows that the adiabatic condition is

$$\dot{X} \ll \frac{\hbar}{\mathsf{m}L} \tag{21.16}$$

Note that the result does not depend on E. This is not the typical case. In typical cases the density of states increases with energy, and consequently it becomes more difficult to satisfy the adiabatic condition.

It is worth pointing out that in the classical framework the adiabatic condition for a moving wall is $\dot{X} \ll v_E$. If the classical condition is violated the sudden approximation applies. If the classical condition is obeyed, but not the quantum adiabatic condition, the dynamics is semi-classical. Namely, in each collision with the moving wall the change of energy is $\Delta_{cl} = 2\mathsf{m}v_E\dot{X}$. In the semi-classical regime the energy changes in steps Δ_{cl} that are larger than Δ. This gives just the opposite condition to quantum adibaticity. For more details see [arXiv:cond-mat/0605591].

════ [21.5] The zero order adiabatic approximation

Assuming we can ignore the coupling between different levels, the adiabatic equation becomes

$$\frac{da_n}{dt} = -i(E_n - \dot{X}A_n)a_n \tag{21.17}$$

And its solution is:

$$a_n(t) = e^{i\Phi_n(t)} a_n(0) \tag{21.18}$$

where the accumulated phase is

$$\Phi_n(t) \;=\; \int_0^t \left(-E_n + \dot{X} A_n\right) dt' \;=\; -\int_0^t E_n dt' \;+\; \int_{X(0)}^{X(t)} A_n(X') dX' \tag{21.19}$$

As already observed the probability $|a_n(t)|^2$ to be in a specific energy level does not change in time. This is the adiabatic approximation. But it is interesting to look at the phase that the particle accumulates. Apart from the dynamical phase, the particle also accumulates a geometrical phase. An interesting case is when we several parameters in a cyclic manner. In this case, just as in the Aharonov-Bohm effect, the "geometrical phase" is regarded as "topological phase" or "Berry phase"

$$\Phi_{\text{Berry}} \;\equiv\; \oint A_n(X)\, dX \tag{21.20}$$

In fact, the Aharonov-Bohm effect can be viewed as a special case of the topological effect that has been explained above. In order to discuss further topological effects we have to generalize the derivation of the adiabatic equation. This will be done in the next lecture.

===== [21.6] Beyond the adiabatic approximation

Here we assume that we deal with one-parameter driving, accordingly the A_n can be gauged away, and the Φ_n is simply the integral over E_n. We can handle the adiabatic Hamiltonian within the framework of an "interaction picture", meaning that we substitute

$$a_n(t) \;=\; c_n(t)\, e^{i\Phi_n(t)} \tag{21.21}$$

hence getting the equation

$$\frac{dc_n}{dt} \;=\; \dot{X} \sum_{m(\neq n)} \frac{V_{nm}}{E_n - E_m} e^{-i(\Phi_n - \Phi_m)}\, c_m \tag{21.22}$$

Note the implicit time dependence of the energies and the matrix elements, due to their parametric dependence on $X = X(t)$. The leading order evaluation of the non-adiabatic transition probability is

$$P_t(n|m) \;=\; \left| \int_0^t \frac{V_{nm}}{E_n - E_m} e^{-i(\Phi_n - \Phi_m)}\, \dot{X} dt \right|^2 \tag{21.23}$$

It is illuminating to consider a constant rate process $\dot{X} = \text{const} \;(>0)$ and use dX rather than dt integration. Then the above expression takes the following schematic form:

$$P_t \;=\; \left| \int_{X_1}^{X_2} \frac{dX}{g(X)}\, \exp\left[-\frac{i}{\dot{X}} \phi(X) \right] \right|^2 \;\sim\; e^{-\text{const}/\dot{X}} \tag{21.24}$$

The approximation is based on the assumption that the integral is dominated by a single complex pole where $g(X) = 0$. For the simplest example of such calculation see the Landau-Zener dynamics subsection, where we present the analysis of the non-adiabatic two-level crossing.

[22] The Berry phase and adiabatic transport

In the following lectures we discuss the adiabatic formalism and the linear-response (Kubo) theory adopting the presentation and the notations as in [cond-mat/0307619]. Note that unlike most textbooks we write the Schrödinger equation in the adiabatic representation without switching to the "interaction picture".

━━━━━ [22.1] Geometric phase

Consider a parametric cycle in Hilbert space $C(t) = |\psi(t)\rangle\langle\psi(t)|$, where t is parameter, and it is assumed that the final "state" is the same as the initial "state". The question how the cycle is realized is irrelevant, hence an Hamiltonian is not specified. We can associate with the cycle so-called geometric phase as follows:

$$\gamma[C] \;\;=\;\; i \oint \langle\psi(t)|\partial_t\psi(t)\rangle\, dt \;\;\equiv\;\; \oint A_\psi dt \tag{22.1}$$

This is the "phase" that is accumulated by $\psi(t)$ during the cycle. The definition is non-ambiguous because it is invariant under gauge. Namely, if $\psi(t)$ is replaced by $\mathrm{e}^{-i\Lambda(t)}\psi(t)$ we get the same result. In is also independent of the t-parametrization. If $\psi(t)$ is an eigenstate of some parametric Hamiltonian $\mathcal{H}(t)$, then γ is called "Berry phase", and A_ψ is known as the "Berry connection".

━━━━━ [22.2] Parallel transport perspective

Let us assume that we want to perform "parallel transport" of an arrow (or of a spin) upon Earth. The coordinates of the manifold are $r = (\theta, \varphi)$, and the trajectory along which we go is $r(t)$. We can define a simple-minded parallel transport, such that the arrow keeps the same orientation with respect to a fixed reference frame. But we are interested in a different notion of "parallel transport" where an "up" arrow with respect to the surface of Earth remains "up", while a "down" arrow remains "down". We shall see that the two notions of "parallel transport" formally correspond to the "sudden limit" and to the "adiabatic limit" of quantum-mechanical processes. Most importantly, we shall see that the "Berry phase" naturally appears in the analysis of "parallel transport" irrespective of the quantum-mechanical context: it is merely a geometrical phase that is implied by the topology of the manifold.

There are several equivalent methods to visualize "parallel transport" on a sphere. Some methods (a,b) assume that the 2D manifold is embedded in a 3D Euclidean space, while the other methods (c,d,e) relay on the intrinsic topology of the surface. In options (a-c) we consider an SO(3) arrow. The transport of its perpendicular component is trivial, hence without loss of generality we consider arrows that are tangent to the surface. One find out that for a closed-cycle the rotation angle of a tangent vector equals the solid angle Ω of the surface-region that is encircled. In method (e) we consider an SU(2) spin, whose orientation is a superposition of "up" and "down" states. In the latter case the same rotation angle (Ω) is deduced from the "Berry phases" of the "up" and "down" polarizations. Below we provide details on methods (a-e).
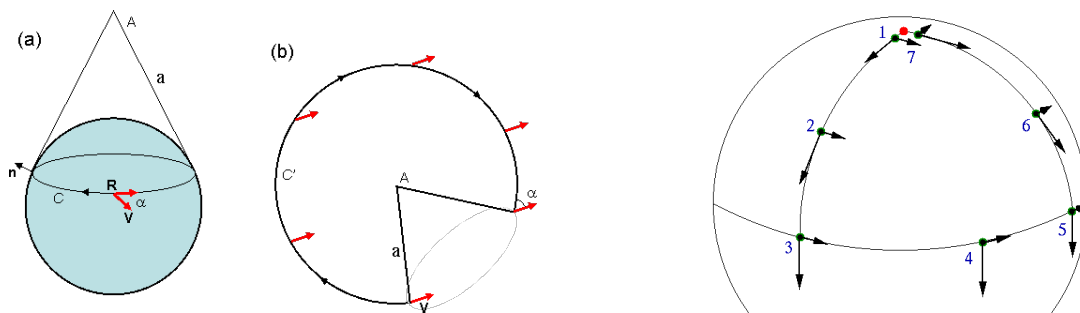
(a) **Projection method.**– We divide the trajectory $r(t)$ into small infinitesimal steps. In each step the arrow is parallel transported in the simple-minded Euclidean sense, but then it is projected back to the tangent direction. Note that the shortening of the length is second order in the step size, hence the arrows keeps its length in the limit of a continuous process.

(b) **Tangent plane method.**– At each point along the trajectory $r(t)$ we attach a flat piece of tangent plane. For

example, if we move along a line of constant latitude the union of all these pieces is a conical surface. This surface can be regarded as flat, and we can perform on it an Euclidean "parallel transport". See left panels of the figure [N.P.Ong website].

(c) Geodesic walk method.– We can always approximated $r(t)$ as a sum of infinitesimal geodesic steps. In the case of a sphere "geodesic" means to go along a big circle. The law of "parallel transport" is simple: the arrow should keep fixed angle with the geodesic. See right panel of the figure [N.Manini website].

(d) Metric connection method.– To each point $r = (x_1, x_2)$ on the surface we attach a set of "unit vectors" with which a metric is associated:

$$\overrightarrow{e}_n = \partial_n r = \frac{\partial r}{\partial x_n}, \qquad\qquad g_{nm} = \langle \overrightarrow{e}_n | \overrightarrow{e}_m \rangle = \langle \partial_n r | \partial_m r \rangle \qquad\qquad (22.2)$$

Then we can define so called *"connection"*, that can be derived from the metric:

$$\Gamma_{n,km} = \langle \overrightarrow{e}_n | \partial_k \overrightarrow{e}_m \rangle = \langle \partial_n r | \partial_k \partial_m r \rangle = \frac{1}{2} [\partial_k g_{nm} + \partial_m g_{kn} - \partial_n g_{km}] \qquad\qquad (22.3)$$

The metric connection allows us to calculate full derivatives:

$$|v\rangle = \sum_n v_n |\overrightarrow{e}_n\rangle, \qquad\qquad D_k |v\rangle = \sum_n \left[\partial_k v_n + \sum_m \Gamma_{n,km} v_m \right] |\overrightarrow{e}_n\rangle \qquad\qquad (22.4)$$

The construct $D = \partial + \Gamma$ is known as the "covariant derivative". It takes into account the explicit variation of the vector-components as well as the implicit parametric variation of the basis-vectors. We say that the vector v is parallel transported if $Dv = 0$. Accordingly Γ can be regarded as the generator of an orthogonal transformation that preservers the scalar product.

(e) Hermitian connection method.– We can repeat the formal derivation of the parallel transport law, considering transport of SU(2) spins instead of SO(3) arrows. To each point $r = (x_1, x_2)$ on the surface we attach a set basis vectors $|n(r)\rangle$. For example:

$$|\uparrow (\theta, \varphi)\rangle = \begin{pmatrix} \cos(\theta/2) \\ e^{i\varphi} \sin(\theta/2) \end{pmatrix}, \qquad\qquad |\downarrow (\theta, \varphi)\rangle = \begin{pmatrix} \sin(\theta/2) \\ -e^{i\varphi} \cos(\theta/2) \end{pmatrix} \qquad\qquad (22.5)$$

Then we can define an Hermitian connection, and an associate "covariant derivative" as follows:

$$D_k[\text{simple minded parallel transport}] = \partial_k + \langle n(r)|\partial_k m(r)\rangle \equiv \partial_k - iA_{nm}^k \qquad\qquad (22.6)$$

The requirement $D\psi = 0$ defines a simple-minded parallel transport, corresponding to the sudden-approximation in the quantum-dynamics context. We would like to define a different notion of "parallel transport" that respects "up" and "down" relative to the surface. Therefore the "connection" in the definition of the covariant derivative should be modified. In a fixed-basis frame we can write $D = \partial - i\Gamma$, while in the n-basis frame it should transforms into a diagonal matrix

$$D_k[\text{parametric parallel transport}] = \partial_k - i \left[\Gamma_{nm}^k + A_{nm}^k \right] \equiv \partial_k - i\tilde{A}_{nm}^k \qquad\qquad (22.7)$$

where $\tilde{A} = \text{diag}\{A_n\}$ is a diagonal matrix in the n-representation. In the concluding paragraph of this section we argue that A_n should be identified as the Berry connection, hence $\tilde{A}_{nm}^k = \delta_{n,m} A_{nm}^k$. Once this is established it follows automatically that for a cyclic parallel transport process $C_n(t) = |n(t)\rangle\langle n(t)|$, the transported $|n\rangle$ accumulates a phase that equals $\gamma_n = \gamma[C_n]$. Consequently, if we start at r_0 and go along a trajectory $r(t)$ back to r_0, then a tangent spin will rotate as follows:

$$|\uparrow (r_0)\rangle + |\downarrow (r_0)\rangle \quad \leadsto \quad e^{i\gamma_\uparrow [r]} |\uparrow (r_0)\rangle + e^{i\gamma_\downarrow [r]} |\downarrow (r_0)\rangle \qquad \text{RotationAngle} = -(\gamma_\uparrow - \gamma_\downarrow) \qquad\qquad (22.8)$$

Specifically if we go along the constant θ latitude line, the connection is $A_\uparrow^\varphi = -[\sin(\theta/2)]^2$, and one obtains $\gamma_\uparrow = -\Omega/2$, where $\Omega = 2\pi[1-\cos(\theta)]$. Similarly for a "down" spin one obtains $\gamma_\downarrow = +\Omega/2$. Hence the expected result for the rotation angle is recovered.

Natural hermitian connection.– To deduce the connection for an SO(3) arrow given the metric of the manifold is easy. To deduce the connection for an SU(2) spin requires further reasoning. What we want is to have a parallel transport law that preserves $|n\rangle\langle n|$. This means that "up" remains "up" and "down" remains "down". Namely $|\psi(t)\rangle = e^{i\gamma_n(t)}|n(t)\rangle$ should be qualified as a parallel-transport process, where $\gamma_n(t)$ still has to be determined. From such transport law it follows that $A_n = \partial_t\gamma_n$. We would like to argue that the proper determination of $\gamma_n(t)$ implies that A_n is the Berry connection.

At first sight it seems that the problem is ill-defined, and that $\gamma_n(t)$ can be chosen in an arbitrary way. The naive prescription would be $\gamma_n(t) = 0$. Clearly such prescription is gauge dependent: if we define a different basis $|\tilde{n}(r)\rangle = e^{-i\Lambda_n(r)}|n(r)\rangle$ we get a different rotation angle for a tangent vector. Even if we allow such gauge-dependent law of transport, still there is a problem. For a manifold with non-trivial topology (here it is a sphere) there is no way to have a well-defined gauge globally. With our choice of gauge the n states at the SouthPole remains ambiguous. Any gauge requires the exclusion of at least one point from the sphere, which is like saying that we are not dealing with a sphere...

The remedy for all this gauge-related complications is to define a parallel-transport law that does not depend on the gauge. Saying it differently, we claim that there is a natural way to define a gauge-invariant connection, such that "up" remains "up" and "down" remains "down". We first note that a change $|\delta\psi\rangle = |\psi(t+dt)\rangle - |\psi(t)\rangle$ can be decomposed into "parallel" and "transverse" components as follows:

$$|\delta\psi\rangle_\parallel \;=\; |\psi\rangle\langle\psi|\delta\psi\rangle \;=\; -iA_\psi|\psi\rangle \tag{22.9}$$

$$|\delta\psi\rangle_\perp \;=\; |\delta\psi\rangle - |\psi\rangle\langle\psi|\delta\psi\rangle \;=\; |\delta\psi\rangle + iA_\psi|\psi\rangle \tag{22.10}$$

Inspired by the "projection method" for constructing a parallel-transport process, the requirement for parallel transport becomes $|\delta\psi\rangle_\parallel = 0$. Note that in the SO(3) treatment the projection was onto the tangent direction, while here we are keeping the spin in the perpendicular ("parallel") direction. We realize that $|n(t)\rangle$ is not a proper parallel transport process. The remedy is to consider $|\psi(t)\rangle = e^{i\gamma_n(t)}|n(t)\rangle$ with $\partial_t\gamma_n = A_n(t)$, which is a gauge-invariant prescription. This implies that $\tilde{A} = \text{diag}\{A_n\}$ is the hermitian connection.

━━━━━ [22.3] The Berry curvature

We consider a set of basis states $\langle n(x)|$ that depend on a set of parameters $x = (x_1, x_2, x_3, ...)$. In the previous section we have motivated the definition of the hermitian connection matrix

$$A_{nm}^j(x) \;=\; i\hbar\left\langle n(x)\Big|\frac{\partial}{\partial x_j}m(x)\right\rangle \tag{22.11}$$

The hermiticity of the matrix can be deduced via differentiation by parts of $\partial_j\langle n(x)|m(x)\rangle = 0$. Furthermore, from differentiation by parts of $\partial_j\langle n(x)|\mathcal{H}|m(x)\rangle = 0$, we get for $n \neq m$ the following expressions:

$$A_{nm}^j(x) \;=\; \frac{i\hbar}{E_m - E_n}\left\langle n\left|\frac{\partial\mathcal{H}}{\partial x_j}\right|m\right\rangle \;\equiv\; -\frac{i\hbar\mathcal{F}_{nm}^j}{E_m - E_n} \tag{22.12}$$

It should be realized that A_{nm}^j is not gauge invariant. The effect of gauge transformation is

$$|n(x)\rangle \;\mapsto\; e^{-i\frac{\Lambda_n(x)}{\hbar}}|n(x)\rangle \tag{22.13}$$

$$A_{nm}^j \;\mapsto\; e^{i\frac{\Lambda_n - \Lambda_m}{\hbar}}A_{nm}^j + (\partial_j\Lambda_n)\delta_{nm}$$

We now focus on the the diagonal elements $A_n^j \equiv A_{nn}^j$. These are real, and transform as $A_n^j \mapsto A_n^j + \partial_j\Lambda_n$. Associated

with $A_n(x)$ is the gauge invariant 2-form which is called the "Berry curvature":

$$B_n^{kj} \;=\; \partial_k A_n^j - \partial_j A_n^k \;=\; -2\hbar \mathrm{Im}\langle \partial_k n | \partial_j n \rangle \;=\; -\frac{2}{\hbar}\mathrm{Im}\sum_m A_{nm}^k A_{mn}^j \tag{22.14}$$

This can be written in abstract notation as $B = \partial \wedge A$, and if not singular (see below) it has zero divergence $(\partial \wedge B = \partial \wedge \partial \wedge A = 0)$. The derivation of the following identity is straightforward:

$$B_n^{kj} \;=\; 2\hbar \sum_{m(\neq n)} \frac{\mathrm{Im}\left[\mathcal{F}_{nm}^k \mathcal{F}_{mn}^j \right]}{(E_m - E_n)^2} \tag{22.15}$$

From this expression it is evident that the sources of the divergenceless field B_n are located at point where it encounters a degeneracy with a neighbouring level. Also it is useful to notice that $\sum B_n = 0$, because the double summation results in a real expression inside the Im[]. The Berry phase can be regarded as the "flux" of B, namely,

$$\gamma_n \;=\; \oint A_n \cdot dr \;=\; \iint B_n \cdot ds \tag{22.16}$$

Using the same argumentation as in the discussion of Dirac monopoles (see [here]) we deduce that

$$\frac{1}{2\pi} \oiint B_n \cdot ds \;=\; \text{integer} \;\equiv\; \text{Chern number} \tag{22.17}$$

The mathematical digression below clarifies the analogy between B and the notion of magnetic field.

══════ [22.4] Digression - Geometrical Forms

Geometrical forms are the "vector analysis" generalization of the length, area and volume concepts to any dimension. In Euclidean geometry with three dimensions the basis for the usual vector space is $\hat{e}_1, \hat{e}_2, \hat{e}_3$. These are called 1-forms. We can also define a basis for surface elements (2-forms) and volume (3-form).

$$\hat{e}_{12} = \hat{e}_1 \wedge \hat{e}_2 \qquad\qquad \hat{e}_{23} = \hat{e}_2 \wedge \hat{e}_3 \qquad\qquad \hat{e}_{31} = \hat{e}_3 \wedge \hat{e}_1 \qquad\qquad \hat{e}_1 \wedge \hat{e}_2 \wedge \hat{e}_3 \tag{22.18}$$

By definition $\hat{e}_{21} = -\hat{e}_{12}$, and $\hat{e}_1 \wedge \hat{e}_2 \wedge \hat{e}_3 = -\hat{e}_2 \wedge \hat{e}_1 \wedge \hat{e}_3$ etc. There is a natural duality between 2-forms and 1-forms, namely $\hat{e}_{12} \mapsto \hat{e}_3$ and $\hat{e}_{23} \mapsto \hat{e}_1$ and $\hat{e}_{31} \mapsto \hat{e}_2$. This duality between surface elements and 1-forms does not hold in Euclidean geometry of higher dimension. For example in 4 dimensions the surface elements (2-forms) constitute $C_4^2 = 6$ dimensional space. In the latter case we have duality between the hyper-surface elements (3-forms) and the 1-forms, which are both 4 dimensional spaces. There is of course the simplest example of Euclidean geometry in 2 diemnsional space where 2-forms are regarded as either area or as volume and not as 1-form vectors. In general for N dimensional Euclidean geometry the k forms constitute a C_N^k dimensional vector space, and they are dual to the $(N-k)$ forms. We can multiply 1-forms as follows:

$$\left[\sum A_i \hat{e}_i\right] \wedge \left[\sum B_i \hat{e}_j\right] \;=\; \sum_{i,j} A_i A_j \hat{e}_i \wedge \hat{e}_j \;=\; \sum_{i<j}(A_i A_j - A_j A_i)\hat{e}_i \wedge \hat{e}_j \tag{22.19}$$

Note that $\hat{e}_i \wedge \hat{e}_i = \text{Null}$. This leads to the practical formula for a wedge product

$$(A \wedge B)_{ij} \;=\; A_i B_j - A_j B_i \tag{22.20}$$

Similarly we use the notation $(\partial \wedge A)_{ij} = \partial_i A_j - \partial_j A_i$. Note that in 3 dimensional Euclidean geometry we have the following association with conventional "vector analysis" notations:

$$\begin{aligned} \partial \wedge A &\;\mapsto\; \nabla \times A & \text{if } A \text{ is a 1-forms} \\ \partial \wedge B &\;\mapsto\; \nabla \cdot B & \text{if } B \text{ is a 2-forms} \end{aligned} \tag{22.21}$$

The above identifications are implied by the following:

$$
\begin{aligned}
\partial &= \partial_1 \hat{e}_1 + \partial_1 \hat{e}_2 + \partial_1 \hat{e}_3 \\
A &= A_1 \hat{e}_1 + A_2 \hat{e}_2 + A_3 \hat{e}_3 \\
B &= B_{12} \hat{e}_{12} + B_{23} \hat{e}_{23} + B_{31} \hat{e}_{31}
\end{aligned}
\tag{22.22}
$$

We now introduce a more flexible notations. We regard any scalar function $f(x)$ as a 0-form, and associate differential quantities with 1-forms and 2-forms as follows:

$$
w_f = f(x) \qquad w_A = \left[\sum_j A_j dx_j \right] \equiv A \cdot dr \qquad w_B = \left[\sum_{i<j} B_{ij} dx_i \wedge dx_j \right] \equiv B \cdot ds
\tag{22.23}
$$

we also use the notation $d = \sum_j \partial_j dx_j$ for full differential. With this notation a relation like $B = \partial \wedge A$ can be written as $w_B = d \wedge w_A$. The Stokes integral theorem is conventionally written as

$$
\oint A \cdot dr = \iint \partial \wedge A \cdot ds
\tag{22.24}
$$

This concerns 1-forms. The Divergence integral theorem concerns 2-forms. The generalized Stokes theorem relates the closed boundary integral over a k-form to an integral over a $(k+1)$-form within the interior. With the above notations it can be written as

$$
\oint w_A = \iint d \wedge w_A
\tag{22.25}
$$

where A is any k-form.

===== [22.5] Adiabatic evolution

The adiabatic equation is obtained from the Schrödinger equation by expanding the wavefunction in the x-dependent adiabatic basis:

$$
\begin{aligned}
\frac{d}{dt} |\psi\rangle &= -\frac{i}{\hbar} \mathcal{H}(x(t)) |\psi\rangle \\
|\psi\rangle &= \sum_n a_n(t) |n(x(t))\rangle \\
\frac{da_n}{dt} &= -\frac{i}{\hbar} E_n a_n + \frac{i}{\hbar} \sum_m \sum_j \dot{x}_j A_{nm}^j a_m
\end{aligned}
\tag{22.26}
$$

We define the perturbation matrix as

$$
W_{nm} = -\sum_j \dot{x}_j A_{nm}^j \qquad \text{for } n \neq m
\tag{22.27}
$$

and $W_{nm}^j = 0$ for $n = m$. Then the adiabatic equation can be re-written as follows:

$$
\frac{da_n}{dt} = -\frac{i}{\hbar}(E_n - \dot{x} A_n) a_n - \frac{i}{\hbar} \sum_m W_{nm} a_m
\tag{22.28}
$$

If we neglect the perturbation W, then we get the strict adiabatic solution:

$$|\psi(t)\rangle \;=\; \mathrm{e}^{-\frac{i}{\hbar}\left(\int_0^t E_n(x(t'))dt' - \int_{x(0)}^{x(t)} A_n(x)\cdot dx\right)} \, |n(x(t))\rangle \qquad (22.29)$$

The time dependence of this solution is exclusively via the x dependence of the basis states. On top, due to $A_n(x)$ we have the so called geometric phase. This can be gauged away unless we consider a closed cycle. For a closed cycle, the gauge invariant phase $\frac{1}{\hbar}\oint \vec{A}\cdot d\vec{x}$ is called the Berry phase.

With the above zero-order solution we can obtain the following result:

$$\langle \mathcal{F}^k\rangle \;=\; \left\langle \psi(t)\left|-\frac{\partial \mathcal{H}}{\partial x_k}\right|\psi(t)\right\rangle \;=\; -\frac{\partial}{\partial x_k}\,\langle n(x)|\,\mathcal{H}(x)\,|n(x)\rangle \qquad (22.30)$$

In the standard examples this corresponds to a conservative force or to a persistent current. From now on we ignore this trivial contribution to $\langle \mathcal{F}^k\rangle$, and look for the a first order contribution.

═════ [22.6] Adiabatic Transport

For linear driving (unlike the case of a cycle) the $A_n(x)$ field can be gauged away. Assuming further that the adiabatic equation can be treated as parameter independent (that means disregarding the dependence of E_n and W on x) one realizes that the Schrödinger equation in the adiabatic basis possesses stationary solutions. To first order these are:

$$|\psi(t)\rangle \;=\; |n\rangle + \sum_{m(\neq n)} \frac{W_{mn}}{E_n - E_m}|m\rangle \qquad (22.31)$$

Note that in a *fixed-basis representation* the above stationary solution is in fact time-dependent. Hence the explicit notations $|n(x(t))\rangle$ and $|m(x(t))\rangle$ are possibly more appropriate.

With the above solution we can write $\langle \mathcal{F}^k\rangle$ as a sum of zero order and first order contributions. From now on we ignore the zero order contribution, but keep the first order contribution:

$$\langle \mathcal{F}^k\rangle \;=\; -\sum_{m(\neq n)} \frac{W_{mn}}{E_n - E_m}\left\langle n\left|\frac{\partial \mathcal{H}}{\partial x_k}\right|m\right\rangle + \mathrm{CC} \;=\; \sum_j \left(i\sum_m A_{nm}^k A_{mn}^j + \mathrm{CC}\right)\dot{x}_j \;=\; -\sum_j B_n^{kj}\,\dot{x}_j \qquad (22.32)$$

For a general *stationary* preparation, either pure or mixed, one obtains

$$\langle \mathcal{F}^k\rangle = -\sum_j G^{kj}\,\dot{x}_j \qquad (22.33)$$

with

$$G^{kj} \;=\; \sum_n f(E_n)\,B_n^{kj} \qquad (22.34)$$

where $f(E_n)$ are weighting factors, with the normalization $\sum_n f(E_n) = 1$. For a pure state preparation $f(E_n)$ distinguishes only one state n, while for a canonical preparation $f(E_n) \propto \mathrm{e}^{-E_n/T}$, where T is the temperature. For a many-body system of non-interacting particles $f(E_n)$ is re-interpreted as the occupation function, so that $\sum_n f(E_n) = N$ is the total number of particles.

Thus we see that the assumption of a stationary first-order solution leads to a non-dissipative (antisymmetric) conductance matrix. This is known as either "adiabatic transport" or "geometric magnetism". In the next lecture we are going to see that "adiabatic transport" is in fact a special limit of the Kubo formula.

[23] Linear response theory and the Kubo formula

======== [23.1] Linear Response Theory

We assume that the Hamiltonian depends on several parameters, say three parameters:

$$\mathcal{H} = \mathcal{H}(\vec{r}, \vec{p}; \; x_1(t), x_2(t), x_3(t)) \tag{23.1}$$

and we define generalized forces

$$\mathcal{F}^k = -\frac{\partial \mathcal{H}}{\partial x_k} \tag{23.2}$$

Linear response means that

$$\langle \mathcal{F}^k \rangle_t = \sum_j \int_{-\infty}^{\infty} \alpha^{kj}(t - t') \; \delta x_j(t') dt' \tag{23.3}$$

where $\alpha^{kj}(\tau) = 0$ for $\tau < 0$. The expression for the response Kernel is known as the Kubo formula:

$$\alpha^{kj}(\tau) = \Theta(\tau) \frac{i}{\hbar} \langle [\mathcal{F}^k(\tau), \mathcal{F}^j(0)] \rangle_0 \tag{23.4}$$

where the average is taken with the assumed zero order stationary solution. Before we present the standard derivation of this result we would like to illuminate the *DC limit* of this formula, and to further explain the *adiabatic limit* that was discussed in the previous section.

======== [23.2] Susceptibility and DC Conductance

The Fourier transform of $\alpha^{kj}(\tau)$ is the generalized susceptibility $\chi^{kj}(\omega)$. Hence

$$[\langle \mathcal{F}^k \rangle]_\omega = \sum_j \chi_0^{kj}(\omega)[x_j]_\omega - \sum_j \mu^{kj}(\omega)[\dot{x}_j]_\omega \tag{23.5}$$

where the dissipation coefficient is defined as

$$\mu^{kj}(\omega) = \frac{\mathrm{Im}[\chi^{kj}(\omega)]}{\omega} = \int_0^\infty \alpha^{kj}(\tau) \frac{\sin(\omega\tau)}{\omega} d\tau \tag{23.6}$$

In the "DC limit" ($\omega \to 0$) it is natural to define the generalized conductance matrix:

$$G^{kj} = \mu^{kj}(\omega \sim 0) = \lim_{\omega \to 0} \frac{\mathrm{Im}[\chi^{kj}(\omega)]}{\omega} = \int_0^\infty \alpha^{kj}(\tau)\tau d\tau \tag{23.7}$$

Consequently the non-conservative part of the response can be written as a generalized Ohm law.

$$\langle \mathcal{F}^k \rangle = -\sum_j G^{kj} \; \dot{x}_j \tag{23.8}$$

It is convenient to write the conductance matrix as

$$G^{kj} \equiv \eta^{kj} + B^{kj} \tag{23.9}$$

where $\eta^{kj} = \eta^{jk}$ is the symmetric part of the conductance matrix, while $B^{kj} = -B^{jk}$ is the antisymmetric part. In our case there are three parameters so we can arrange the elements of the antisymmetric part as a vector $\vec{B} = (B^{23}, B^{31}, B^{12})$. Consequently the generalized Ohm law can be written in abstract notation as
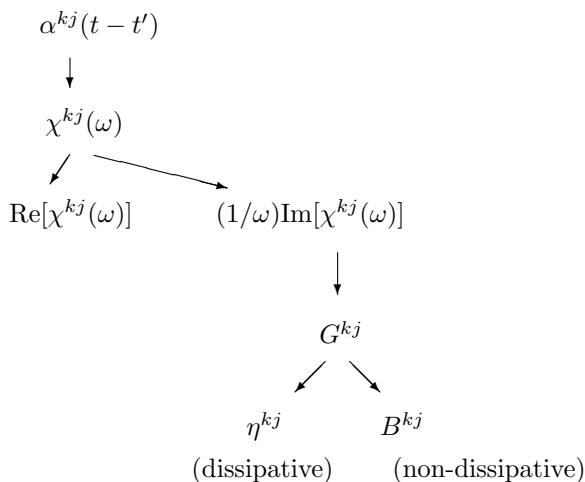
$$\langle \mathcal{F} \rangle = -\eta \cdot \dot{x} - B \wedge \dot{x} \tag{23.10}$$

where the dot product should be interpreted as matrix-vector multiplication, which involves summation over the index j. The wedge-product can also be regarded as a matrix-vector multiplication. It reduces to the more familiar cross-product in the case we have been considering - 3 parameters. The dissipation, which is defined as the rate at which energy is absorbed into the system, is given by

$$\dot{W} = -\langle \mathcal{F} \rangle \cdot \dot{x} = \sum_{kj} \eta^{kj} \, \dot{x}_k \dot{x}_j \tag{23.11}$$

which is a generalization of Joule's law. Only the symmetric part contributes to the dissipation. The contribution of the antisymmetric part is identically zero.

The conductance matrix is essentially a synonym for the term "dissipation coefficient". However, "conductance" is a better (less misleading) terminology: it does not have the (wrong) connotation of being specifically associated with dissipation, and consequently it is less confusing to say that it contains a non-dissipative component. We summarize the various definitions by the following diagram:

$$\alpha^{kj}(t - t')$$
$$\downarrow$$
$$\chi^{kj}(\omega)$$
$$\swarrow \qquad \searrow$$
$$\mathrm{Re}[\chi^{kj}(\omega)] \qquad (1/\omega)\mathrm{Im}[\chi^{kj}(\omega)]$$
$$\downarrow$$
$$G^{kj}$$
$$\swarrow \qquad \searrow$$
$$\eta^{kj} \qquad B^{kj}$$
$$\text{(dissipative)} \qquad \text{(non-dissipative)}$$

===== [23.3] Derivation of the Kubo formula

If the driving is not strictly adiabatic the validity of the stationary adiabatic solution that has been presented in the previous lecture becomes questionable. In general we have to take non-adiabatic transitions between levels into account. This leads to the Kubo formula for the response which we discuss below. The Kubo formula has many type of derivations. One possibility is to use the same procedure as in the previous lecture starting with

$$|\psi(t)\rangle = \mathrm{e}^{-iE_n t}|n\rangle + \sum_{m(\neq n)} \left[-i\boldsymbol{W}_{mn} \int_0^t \mathrm{e}^{i(E_n - E_m)t'} dt' \right] \mathrm{e}^{-iE_m t}|m\rangle \tag{23.12}$$

We shall not expand further on this way of derivation, which becomes quite subtle once we go beyond the stationary adiabatic approximation. A one line derivation of the Kubo formula is based on the interaction picture, and is presented in a dedicted section There are various different looking derivations of the Kubo formula that highlight the quantum-to-classical correspondence and/or the limitations of this formula. The advantage of the derivation below is that it also allows some extensions within the framework of a master equation approach that takes the environment into account.

For notational simplicity we write the Hamiltonian as

$$\mathcal{H} \ = \ \mathcal{H}_0 \ - \ f(t)V \tag{23.13}$$

We assume that the system, in the absence of driving, is prepared in a stationary state ρ_0. In the presence of driving we look for a first order solution $\rho(t) = \rho_0 + \tilde{\rho}(t)$. The equation for $\tilde{\rho}(t)$ is:

$$\frac{\partial \tilde{\rho}(t)}{\partial t} \ \approx \ -i[\mathcal{H}_0, \tilde{\rho}(t)] + if(t)[V, \rho_0] \tag{23.14}$$

Next we use the substitution $\tilde{\rho}(t) = U_0(t)\tilde{\tilde{\rho}}(t)U_0(t)^{-1}$, where $U_0(t)$ is the evolution operator which is generated by $\mathcal{H}_0$. Thus we eliminate from the equation the zero order term:

$$\frac{\partial \tilde{\tilde{\rho}}(t)}{\partial t} \ \approx \ if(t)[U_0(t)^{-1}VU_0(t), \rho_0] \tag{23.15}$$

The solution of the latter equation is straightforward and leads to

$$\rho(t) \ \approx \ \rho_0 + \int^t i \ [V(-(t-t')), \rho_0] \ f(t')dt' \tag{23.16}$$

where we use the common notation $V(\tau) = U_0(\tau)^{-1}VU_0(\tau)$.

Consider now the time dependence of the expectation value $\langle \mathcal{F} \rangle_t = \text{trace}(\mathcal{F}\rho(t))$ of an observable. Disregarding the zero order contribution, the first order expression is

$$\langle \mathcal{F} \rangle_t \ \approx \ \int^t i \ \text{trace}\left(\mathcal{F}[V(-(t-t')), \rho_0]\right) \ f(t')dt' \ = \ \int^t \alpha(t - t') \ f(t')dt'$$

where the response kernel $\alpha(\tau)$ is defined for $\tau > 0$ as

$$\alpha(\tau) = i \ \text{trace}\left(\mathcal{F}[V(-\tau), \rho_0]\right) \ = i \ \text{trace}\left([\mathcal{F}, V(-\tau)]\rho_0\right) \ = i\langle[\mathcal{F}, V(-\tau)]\rangle \ = i\langle[\mathcal{F}(\tau), V]\rangle \tag{23.17}$$

where we have used the cyclic property of the trace operation; the stationarity $U_0\rho_0U_0^{-1} = \rho_0$ of the unperturbed state; and the notation $\mathcal{F}(\tau) = U_0(\tau)^{-1}\mathcal{F}U_0(\tau)$.

[24] The Born-Oppenheimer picture

We now consider a more complicated problem, where x becomes a dynamical variable. The standard basis for the representation of the composite system is $|x, Q\rangle = |x\rangle \otimes |Q\rangle$. We assume a total Hamiltonian of the form

$$\mathcal{H}_{\text{total}} = \frac{1}{2\mathsf{m}} \sum_j p_j^2 + \mathcal{H}(Q, P; x) - f(t)V(Q) \tag{24.1}$$

Rather than using the standard basis, we can use the Born-Oppenheimer basis $|x, n(x)\rangle = |x\rangle \otimes |n(x)\rangle$. Accordingly the state of the combined system is represented by the wavefunction $\Psi_n(x)$, namely

$$|\Psi\rangle = \sum_{n,x} \Psi_n(x) \, |x, n(x)\rangle \tag{24.2}$$

The matrix elements of $\mathcal{H}$ are

$$\langle x, n(x)|\mathcal{H}|x_0, m(x_0)\rangle = \delta(x - x_0) \times \delta_{nm} E_n(x) \tag{24.3}$$

The matrix elements of $V(Q)$ are

$$\langle x, n(x)|V(Q)|x_0, m(x_0)\rangle = \delta(x - x_0) \times V_{nm}(x) \tag{24.4}$$

The matrix elements of p are

$$\langle x, n(x)|p_j|x_0, m(x_0)\rangle = (-i\partial_j \delta(x - x_0)) \times \langle n(x)|m(x_0)\rangle$$

The latter can be manipulated "by parts" leading to

$$\langle x, n(x)|p_j|x_0, m(x_0)\rangle = -i\partial_j \delta(x - x_0)\delta_{nm} - \delta(x - x_0)A_{nm}^j(x) \tag{24.5}$$

This can be summarized by saying that the operation of p_j on a wavefunction is like the differential operator $-i\partial_j - A_{nm}^j(x)$. Thus in the Born-Oppenheimer basis the total Hamiltonian takes the form

$$\mathcal{H}_{\text{total}} = \frac{1}{2\mathsf{m}} \sum_j (p_j - A_{nm}^j(x))^2 + \delta_{nm} E_n(x) - f(t)V_{nm}(x) \tag{24.6}$$

Assuming that the system is prepared in energy level n, and disregarding the effect of A and V, the adiabatic motion of x is determined by the effective potential $E_n(x)$. This is the standard approximation in studies of diatomic molecules, where x is the distance between the nuclei. If we treat the slow motion as classical, then the interaction with A can be written as

$$\mathcal{H}_{\text{interaction}}^{(1)} = -\sum_j \dot{x}_j A_{nm}^j(x) \tag{24.7}$$

This brings us back to the theory of driven systems as discussed in previous sections. The other interaction that can induce transitions between levels is

$$\mathcal{H}_{\text{interaction}}^{(2)} = -f(t)V_{nm}(x) \tag{24.8}$$

The analysis of molecular "wavepacket dynamics" is based on this picture.

The Green function approach

[25] The propagator and Feynman path integral

═══════ [25.1] The propagator

The evolution of a quantum mechanical system is described by a unitary operator

$$|\Psi(t)\rangle = U(t, t_0) |\Psi(t_0)\rangle \tag{25.1}$$

The Hamiltonian is defined by writing the infinitesimal evolution as

$$U(t + dt, t) = 1 - idt\mathcal{H}(t) \tag{25.2}$$

This expression has an imaginary i in order to make $\mathcal{H}$ a Hermitian matrix. If we want to describe continuous evolution we can "break" the time interval into N infinitesimal steps:

$$U(t, t_0) = (1 - idt_N\mathcal{H})\dots(1 - idt_2\mathcal{H})(1 - idt_1\mathcal{H}) \equiv \mathcal{T}e^{-i\int_{t_0}^{t}\mathcal{H}(t')dt'} \tag{25.3}$$

For a time independent Hamiltonian we get simply $U(t) = e^{-it\mathcal{H}}$ because of the identity $e^A e^B = e^{A+B}$ if $[A, B] = 0$.

If we consider a particle and use the standard position representation then the unitary operator is represented by a matrix $U(x|x_0)$. The time interval $[t_0, t]$ is implicit. We alway assume that $t > t_0$. Later it would be convenient to define the propagator as $U(x|x_0)$ for $t > t_0$ and as zero otherwise. The reason for this convention is related to the formalism that we are going to introduce later on.

═══════ [25.2] The Propagator for linear evolution

Consider a free particle in one dimension.

$$\mathcal{H} = \frac{p^2}{2\mathsf{m}} \tag{25.4}$$

The derivation of the next section leads to the result

$$U(x|x_0) = \left\langle x \left| e^{-i\frac{t}{2\mathsf{m}}p^2} \right| x_0 \right\rangle = \left(\frac{\mathsf{m}}{2\pi it}\right)^{\frac{1}{2}} e^{i\frac{\mathsf{m}}{2t}(x-x_0)^2} \tag{25.5}$$

Note that in the analogous study of stochastic diffusion, the generator is $-Dp^2$, and then we get the diffusion kernel $\propto \exp[-(x - x_0)^2/(4Dt)]$. If we take $t \to 0$ then $U \to \hat{1}$, and therefore $U(x|x_0) \to \delta(x - x_0)$.

For Hamiltonian that generates linear evolution in phase-space, the expression for the propagator comes out a Gaussian kernel. The calculation procedure will be explained later. For the harmonic oscillator

$$\mathcal{H} = \frac{p^2}{2\mathsf{m}} + \frac{1}{2}\mathsf{m}\Omega^2 x^2 \tag{25.6}$$

$$U(x|x_0) = \left(\frac{\mathsf{m}\Omega}{2\pi i \sin \Omega t}\right)^{\frac{1}{2}} e^{i\frac{\mathsf{m}\Omega}{2\sin \Omega t}[\cos \Omega t(x^2+x_0^2)-2xx_0]} \tag{25.7}$$

Note that in the analogous study of thermal equilibrium the non-normalized probability matrix of the canonical state is formally the same expression with $t \mapsto -i\beta$.

═════ [25.3] Propagator for free particle - derivation

We first clarify that the following kernels become delta functions in the $a \to \infty$ limit:

$$\sqrt{\frac{a}{2\pi}}\exp\left[-\frac{1}{2}ar^2\right]; \qquad \sqrt{\frac{a}{\pi}}\cos\left[-\frac{1}{2}ar^2\right]; \qquad \sqrt{\frac{a}{\pi}}\sin\left[-\frac{1}{2}ar^2\right]; \qquad \sqrt{\frac{a}{i2\pi}}\exp\left[\frac{i}{2}ar^2\right] \qquad (25.8)$$

The last expression is formally obtained from the first expression by the replacement $a \mapsto -ia$. But this procedure is misleading, and also vague with respect to the meaning of $\sqrt{i}$. It is better to regard the last expression as the sum of "cos" and "sin" kernels. The proper normalization is implied by the integral

$$\int_{-\infty}^{\infty}\cos\left(\frac{1}{2}r^2\right)dr \;=\; \sqrt{2}\int_0^{\infty}\frac{\cos u}{\sqrt{u}}du \;=\; \sqrt{\pi} \qquad (25.9)$$

Therefore the "area" of $\exp[i\cdots]$ is $(1+i)\sqrt{\pi} = \sqrt{i2\pi}$, with the convention $\sqrt{i} = \exp(+i\pi/4)$. Note that for negative a we get the opposite phase.

The derivation of the expression for the propagator in the case of a free particle goes as follows. For clarity we use units such that $\mathsf{m} = 1$:

$$\left\langle x\left|e^{-i\frac{1}{2}tp^2}\right|x_0\right\rangle \;=\; \sum_k \langle x|k\rangle\, e^{-i\frac{1}{2}tk^2}\langle k|x_0\rangle \;=\; \int\frac{dk}{2\pi}e^{-i\frac{1}{2}tk^2+ik(x-x_0)} \qquad (25.10)$$

This is formally an inverse FT of a Gaussian, and one obtains the desired result, which is formally a Gaussian that has an imaginary variance it. The more careful procedure is to complete the squares, and to split the remaining integral into "cos" and "sin" as in the calculation of the previous paragraph. This leads to

$$\langle x|e^{-i\frac{1}{2}tp^2}|x_0\rangle \;=\; \frac{1}{\sqrt{2\pi it}}\left[\cos\frac{1}{2t}(x-x_0)^2 + i\sin\frac{1}{2t}(x-x_0)^2\right] \;\equiv\; \frac{1}{\sqrt{2\pi it}}e^{\frac{i(x-x_0)^2}{2t}} \qquad (25.11)$$

For oscillator one may be tempted to use a similar procedure, namely, to transform the kernel from the basis that diagonalize the Hamiltonian. But the simpler procedure is to use the Feynman path-integral procedure as described below.

═════ [25.4] Gaussian integrals

Consider a quadradic form over $x = (x_1, x_2, \cdots, x_N)$. It can be written as

$$\mathcal{A}[x] \;=\; \frac{1}{2}\sum_{i,j}A_{i,j}x_ix_j \qquad (25.12)$$

where $A_{i,j}$ is a real symmetric matrix. Such matrix can be diagonalized in a "k" basis with eigenvalues a_k. The Gaussian integral is

$$\int d[x]e^{-\mathcal{A}[x]} \;=\; \prod_k\int d\tilde{x}_k\, e^{-\frac{1}{2}a_k\tilde{x}_k^2} \;=\; \sqrt{\mathrm{Det}\left(\frac{2\pi}{A}\right)} \qquad (25.13)$$

Below we are going to use the Stationary Phase Approximation for the estimate of an integral over $\exp(i\mathcal{A}[x])$, where $\mathcal{A}[x]$ is called *the action*. The main contribution to the integral comes from the point $x = \bar{x}$, which is in fact a trajectory. For this stationary point, the first variation of the action is zero. For simplicity of notation let us assume that $N = 1$. The stationary point is determined by the equation $\mathcal{A}'(x) = 0$. We expand near this point:

$$\mathcal{A}(x) \;=\; \mathcal{A}(\bar{x}) + \frac{1}{2}\mathcal{A}''(\bar{x})(x-\bar{x})^2 + \ldots \qquad (25.14)$$

and then the Gaussian integral becomes

$$\int e^{\imath \mathcal{A}(x)}dx \approx e^{\imath \mathcal{A}(\bar{x})} \int e^{\imath \frac{1}{2}\mathcal{A}''(\bar{x})(x-\bar{x})^2}dx = \sqrt{\frac{i2\pi}{\mathcal{A}''(\bar{x})}} e^{\imath \mathcal{A}(\bar{x})} \tag{25.15}$$

The generalization of this expression for any N is straightforward. Namely, inside the square-root we will have a determinant of $A_{i,j} = \partial_i \partial_j \mathcal{A}[\bar{x}]$. The further $N \to \infty$ generalization to handle integration over trajectories $x(t)$ is further discussed below.

====== [25.5] The Feynman Path Integrals

How can we find the propagator $U(x|x_0)$ for the general Hamiltonian $\mathcal{H} = \frac{p^2}{2\mathsf{m}} + V(x)$? The idea is to write $\langle x|e^{-\imath t \mathcal{H}}|x_0\rangle$ as a convolution of small time steps:

$$\langle x|e^{-\imath t \mathcal{H}}|x_0\rangle = \sum_{x_1, x_2, \ldots x_{N-1}} \langle x|e^{-\imath \delta t_N \mathcal{H}}|x_{N-1}\rangle \cdots \langle x_2|e^{-\imath \delta t_2 \mathcal{H}}|x_1\rangle \langle x_1|e^{-\imath \delta t_1 \mathcal{H}}|x_0\rangle \tag{25.16}$$

Now we have to find the propagator for each infinitesimal step. At first sight it looks as if we just complicated the calculation. But then we recall that for infinitesimal operations we have:

$$e^{\varepsilon A + \varepsilon B} \approx e^{\varepsilon A}e^{\varepsilon B} \approx e^{\varepsilon B}e^{\varepsilon A} \qquad \text{for any } A \text{ and } B \tag{25.17}$$

This is because the higher order correction can be made as small as we want. So we write

$$\left\langle x_j \left| e^{-\imath \delta t (\frac{p^2}{2\mathsf{m}} + V(x))} \right| x_{j-1} \right\rangle \approx \left\langle x_j \left| e^{-\imath \delta t V(x)} e^{-\imath \delta t \frac{p^2}{2\mathsf{m}}} \right| x_{j-1} \right\rangle \approx \left(\frac{\mathsf{m}}{2\pi \imath dt_j} \right)^{\frac{1}{2}} e^{\imath \frac{\mathsf{m}}{2dt_j}(x_j - x_{j-1})^2 - dt_j V(x_j)} \tag{25.18}$$

and get:

$$U(x|x_0) = \int dx_1 dx_2 \ldots dx_{N-1} \left(\frac{\mathsf{m}}{2\pi \imath dt} \right)^{\frac{N}{2}} e^{i\mathcal{A}[x]} \equiv \int d[x] \, e^{i\mathcal{A}[x]} \tag{25.19}$$

where $\mathcal{A}[x]$ is called the *action*.

$$\mathcal{A}[x] = \sum_{j=1}^{N-1} \left[\frac{\mathsf{m}}{2dt}(x_j - x_{j-1})^2 - dt V(x) \right] = \int \left(\frac{1}{2}\mathsf{m}\dot{x}^2 - V(x) \right) dt = \int \mathcal{L}(x, \dot{x})dt \tag{25.20}$$

More generally, if we include the vector potential in the Hamiltonian, then we get the Lagrangian

$$\mathcal{L}(x, \dot{x}) = \frac{1}{2}\mathsf{m}\dot{x}^2 - V(x) + A(x)\dot{x} \tag{25.21}$$

and the action becomes

$$\mathcal{A}[x] = \int \left(\frac{1}{2}\mathsf{m}\dot{x}^2 - V(x) \right) dt + \int A(x) \cdot dx \tag{25.22}$$

The calculation of the propagator for e.g. Harmonic Oscillator requires the calculation of the determinant of the matrix $A_{i,j}$ that is defined by inspection of of the time-discretized action, and then taking the $N \to \infty$ limit. However, a

shortcut is available if we use the Van-Vleck formula of the next section, that provides an exact result for Hamiltonians that generate linear evolution.

════ [25.6] The semiclassical approximation

The generalization of the Stationary Phase Approximation that we have discussed previously, for the purpose of evaluating the multi-dimensional integral over $d[x]$, is immediate. The stationary point is the trajectory for which the first order variation is zero ($\delta\mathcal{A} = 0$). This leads to Lagrange equation, hence the "stationary point" is identified as the classical trajectory. Consequently we get the semiclassical (Van-Vleck) approximation:

$$U(x|x_0) = \int d[x]\, e^{i\mathcal{A}[x]} \approx \sum_{cl} \left(\frac{1}{i2\pi}\right)^{d/2} \left|\det\left(-\frac{\partial^2\mathcal{A}_{cl}}{\partial x \partial x_0}\right)\right|^{1/2} e^{i\mathcal{A}_{cl}(x,x_0)-i(\pi/2)\nu_{cl}} \tag{25.23}$$

This formula is written above for a system that has d degrees of freedom. The determinant is $d \times d$. Without loss of generality, we discuss below the derivation for $d = 1$, such that the "det" notation can be omitted. This formula requires to find the classical trajectories that connect x to x_0 given the time t. There might be more than a single classical path. So in general we might have *interference* of several contributions. For each trajectory we have to calculate the classical action $\mathcal{A}_{cl}$ and determine its Morse-Maslov index ν_{cl}, as explained below.

The derivation of the semiclassical Van-Vleck formula is based on a stationary phase approximation, which requires expansion of the action functional to second order around the classical trajectory, and performing the Gaussian integral. The formula becomes exact for quadratic Hamiltonians, for which the expansion does not include higher order terms. Let us illustrate the procedure for a particle in one dimension assuming potential $V(x)$ and time interval $t \in [t_0, t_f]$. The action is expanded as follows:

$$\mathcal{A}[x(t) + \delta x(t)] = \int_{t_0}^{t_f} dt \left[\frac{1}{2}\mathsf{m}\dot{x}^2 - V(x)\right] + \int_0^t dt\,\delta x\,[-\mathsf{m}\ddot{x} - V'(x)] + \int_0^t dt\,\delta x\left[-\mathsf{m}\frac{d^2}{dt^2} - V''(x)\right]\delta x \tag{25.24}$$

Note that we have use integration-by-parts to convert integral over $\dot{f}(t)\dot{g}(t)$ into integral over $-f(t)\ddot{g}(t)$. By definition, the first-order variation is zero for a classical trajectory $x_{cl}(t)$. Thus the above expansion takes the following form:

$$\mathcal{A}[x_{cl}(t) + \psi(t)] = \mathcal{A}_{cl}(x, x_0) + 0 + \int_0^t dt\,\psi(t)\boldsymbol{Q}\psi(t) \tag{25.25}$$

The quadratic term involves a differential operator $\boldsymbol{Q}$ that is mathematically equivalent to a Schrodinger Hamiltonian (if the time variable is regarded as a position variable):

$$\boldsymbol{Q}\psi(t) = -\mathsf{m}\frac{d^2}{dt^2}\psi(t) - V''(x_{cl}(t))\psi(t), \qquad t \in [t_0, t_f] \tag{25.26}$$

In order to perform the Gaussian integration we have to evaluate the determinant of $\boldsymbol{Q}$. This can be done via diagonalization. Namely, we have to solve the eigenvalue equation $\boldsymbol{Q}\psi = \lambda\psi$ with Dirichlet boundary conditions $\psi(t_0) = \psi(t_f) = 0$. For very short $t_f - t_0$ this is formally the same as the equation for the eigenstates of a particle in a narrow rectangular well, hence all the $N-1$ eigenvalues are positive. Consequently, after the Gaussian integration, the pre-exponential $(i2\pi)^{-N/2}$ factor is get multiplied by $(i2\pi)^{(N-1)/2}$. The net prefactor is $(i2\pi)^{-1/2}$. However, for larger t_f, some of the eigenvalues can become negative, which implies that x_{cl} is a saddle point and no longer a minimum for the action. The Morse-Maslov index ν_{cl} counts the number of negative eigenvalues. For example, for harmonic oscillator $V''(x_{cl}) = \mathsf{m}\omega^2$, the eigenvalues are $a_n = -\mathsf{m}\omega^2 + \mathsf{m}[(\pi/t)n]^2$ with $n = 1, 2, \cdots$, and therefore the number of negative eigenvalues is determined by $\omega t/\pi$.

From the above reasoning it follows that the Morse-Maslov index ν_{cl} counts the number of conjugate points along the classical trajectory. A conjugate point (in time) is defined as the time t_f when the above linearized equation has a $\lambda=0$ solution. This implies that $x(t_f)$ is on a caustic or a focal point of trajectories. If the time is short the Morse-Maslov index equals zero, and then both this index and the absolute value that encloses the determinant can

be omitted from the Van-Vleck expression. In the case of a reflection from a wall, the Morse index is $+\mathbf{1}$ for each collision. This is correct for "soft" wall, as we proved above for harmonic osccilator. In the case of "hard" wall the standard semiclassical result for ν_{cl} breaks down, and the correct result turns out to be $+\mathbf{2}$ for each collision. The latter rule is implied by the **Dirichlet** boundary conditions. Note, that it would be $+\mathbf{0}$ in the case of **Neumann** boundary conditions.

We have clarified the determination of the Morse-Maslov index, which provides a phase-factor for each classical trajectory. Now we turn to clarify the *weight* of the trajectory. Let us first look how $U(x|x_0)$ of a free particle is obtained from the Van-Vleck expression. The action $\mathcal{A}[x]$ for the free particle is

$$\mathcal{A}[x] \quad = \quad \int_0^t \frac{1}{2}\mathsf{m}\dot{x}^2 dt'. \tag{25.27}$$

Given the end points we find the classical path

$$x_{cl} \quad = \quad x_0 + \frac{x - x_0}{t}t' \tag{25.28}$$

and hence

$$\mathcal{A}_{cl}(x, x_0) \quad = \quad \int_0^t \frac{1}{2}\mathsf{m}\left(\frac{x - x_0}{t}\right)^2 dt' \quad = \quad \frac{\mathsf{m}}{2t}(x - x_0)^2 \tag{25.29}$$

We also observe that

$$\text{weight} \quad = \quad -\frac{\partial^2 \mathcal{A}_{cl}}{\partial x \partial x_0} \quad = \quad \frac{\mathsf{m}}{t} \quad \equiv \quad \text{spreading slope} \tag{25.30}$$

This agree with the exact result. The latter expression has a simple phase-space interpretation within the Wigner function formalism: it is simply the decreasing overlap due to spatial spreading of an initial squeezed state. Namely, define $|\psi\rangle = U|x_0\rangle$ and $|\chi\rangle = |x\rangle$, then $|U(x|x_0)|^2 = \text{Prob}(\chi|\psi) = \text{trace}(\rho^\chi \rho^\psi)$.
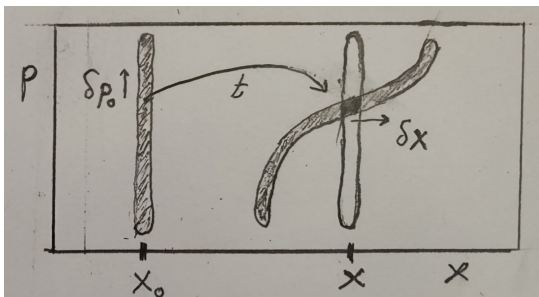
Inspired by phase-space interpretation of the *weight* factor, we can use it as the starting point for a general derivation that bypasses the burden of a lengthy procedure for direct evaluation of the determinant. The key observation is that this weight is simply the overlap that is illustrated in the schematic figure above. This overlap is determined by the *slope* of the spreading distribution at the target position x. For a free particle the spreading is $\delta x = (\delta p/\mathsf{m})t$, and therefore the spreading slope is m/t. In order to get a more general result we recall that the derivatives of the classical action relative to the end-points are $\partial \mathcal{A}_{cl}/\partial x_f = p_f$ and $\partial \mathcal{A}_{cl}/\partial x_0 = -p_0$. Accordingly the mixed derivative of the action provides $-dp_0/dx$, from which one can deduce the spreading δx in position as a result of dispersion δp_0 in the initial momentum. This generalization implies immediately the validity of the general formula.

The expression for the propagator of an harmonic oscillator can be easily obtained from the Van-Vleck formula. Optionally one can use a direct technique in order to calculate the determinant of the Gaussian integral, and the result comes out the same. In the Wigner function formalism the quantum propagator for any such Hamiltonian, that generates linear evolution in (x, p), comes out identical with the classical Liouville propagator, namely, describing motion along classical trajectories.

[26] The resolvent and the Green function

═══════ [26.1] The resolvent

The resolvent is defined in the complex plane as

$$G(z) = \frac{1}{z - \mathcal{H}} \tag{26.1}$$

In case of a bounded system it has poles at the eigenvalues. We postpone for later the discussion of unbounded systems. It is possibly more illuminating to look on the matrix elements of the resolvent

$$G(x|x_0) = \langle x|G(z)|x_0\rangle = \sum_n \frac{\psi^n(x)\psi^n(x_0)^*}{z - E_n} \equiv \sum_n \frac{q_n}{z - E_n} \tag{26.2}$$

where $\psi^n(x) = \langle x|n\rangle$ are the eigenstates of the Hamiltonian. If we fix x and x_0 and regard this expression as a function of z this is formally the complex representation of an electric field in a two dimensional electrostatic problem.

We can look on $G(x|x_0)$, with fixed $z = E$ and x_0, as a wavefunction in the variable x. We see that $G(x|x_0)$ is a superposition of eigenstates. If we operate on it with $(E - \mathcal{H})$ the coefficients of this superposition are multiplied by $(E - E_k)$, and because of the completeness of the basis we get $\delta(x - x_0)$. This means that $G(x|x_0)$ satisfies the Schrodinger equation with the complex energy E and with an added source at $x = x_0$. Namely,

$$(E - \mathcal{H})G(x|x_0) = \delta(x - x_0) \tag{26.3}$$

This is simply the standard representation of the equation $(z - \mathcal{H})G = \hat{1}$ which defines the matrix inversion $G = 1/(z - \mathcal{H})$. The wavefunction $G(x|x_0)$ should satisfy that appropriate boundary conditions. If we deal with a particle in a box this means Dirichlet boundary conditions. In the case of an unbounded system the issue of boundary conditions deserves further discussion (see later).

The importance of the Green functions comes from its Fourier transform relation to the propagator. Namely,

$$FT\left[\Theta(t)\mathrm{e}^{-\gamma t}\, U(t) \right] = iG(\omega + i\gamma) \tag{26.4}$$

where $\Theta(t)$ is the step function, $\Theta(t)U(t)$ is the "propagator", and $\mathrm{e}^{-\gamma t}$ is an envelope function that guarantees convergence of the FT integral. Later we discuss the limit $\gamma \to 0$.

We note that we can extract from the resolvent useful information. For example, we can get the energy eigenfunction by calculation the residues of $G(z)$. The Green functions, which we discuss in the next section are obtained (defined) as follows:

$$G^\pm(\omega) = G(z = \omega \pm i0) = \frac{1}{\omega - \mathcal{H} \pm i0} \tag{26.5}$$

From this definition follows that

$$\mathrm{Im}[G^+] \equiv -\frac{i}{2}(G^+ - G^-) = -\pi\delta(E - \mathcal{H}) \tag{26.6}$$

From here we get expression for the density of states $\varrho(E)$ and for the local density of states $\rho(E)$, where the latter is with respect to an arbitrary reference state Ψ

$$\varrho(E) = -\frac{1}{\pi}\mathsf{trace}\Big(\mathrm{Im}[G^+(E)] \Big) \tag{26.7}$$

$$\rho(E) = -\frac{1}{\pi}\Big\langle \Psi\Big| \mathrm{Im}[G^+(E)] \Big|\Psi\Big\rangle$$

Further applications of the Green functions will be discussed later on.

Concluding this section we note that from the above it should become clear that there are three methods of calculating the matrix elements of the resolvent:

- Summing as expansion in the energy basis
- Solving an equation (Helmholtz for a free particle)
- Finding the Fourier transform of the propagator

Possibly the second method is the simplest, while the third one is useful in semiclassical schemes.

===== [26.2] Mathematical digression

Let us summarize some useful mathematical facts that are related to the theory of the resolvent. First of all we have the following identity for a decomposition into "principal" and "singular" parts:

$$\frac{1}{\omega + i0} \quad = \quad \frac{\omega}{\omega^2 + 0^2} - i\frac{0}{\omega^2 + 0^2} \quad = \quad \frac{1}{\omega} - i\pi\delta(\omega) \tag{26.8}$$

where 0 is an infinitesimal. An optional proof of this identity in the context of contour integration is based on deforming the contour into a semicircle in the upper complex half plane, and then displacing the pole to be on the real axis. Then the first term is contributed by the principal part, while the second term is contributed by the semicircle.

The following Fourier transform relation is extremely useful, and we would like to establish it both in the forward and in the backward directions:

$$\mathrm{FT}\left[\Theta(t)\right] \quad = \quad \frac{i}{\omega + i0} \tag{26.9}$$

An equivalent relation is

$$\mathrm{FT}\left[\Theta(t) - \frac{1}{2}\right] \quad = \quad \frac{i}{\omega} \qquad \text{[the FT that gives the principal part]} \tag{26.10}$$

In the forward direction the proof is based on taking the $\gamma \to 0$ limit of

$$\mathrm{FT}\left[\Theta(t)\mathrm{e}^{-\gamma t}\right] = \int_0^\infty \mathrm{e}^{-(\gamma - i\omega)t}dt = \frac{1}{\gamma - i\omega} \tag{26.11}$$

Note that this is not the same as

$$\mathrm{FT}\left[\mathrm{e}^{-\gamma|t|}\right] = \frac{2\gamma}{\omega^2 + \gamma^2} \qquad \text{[the FT that gives the singular part]} \tag{26.12}$$

In the backward direction the simplest is to use contour integration:

$$\int_{-\infty}^\infty \frac{d\omega}{2\pi}\left[\frac{i\mathrm{e}^{-i\omega t}}{\omega + i0}\right] \quad = \quad 2\pi i \times \text{Residue} \qquad \text{[for } t > 0 \text{ the contour is closed in the lower half plane]} \tag{26.13}$$

The other possibility is to stay with the original contour along the real axis, but to split the integrand into principal part and singular part. The integral over the principal part is in-fact the inverse Fourier transform of i/ω. Its calculation is based on the elementary integral

$$\int_{-\infty}^{+\infty} \frac{\sin(ax)}{x}dx \quad = \quad \text{Sign}(a)\,\pi \quad = \quad \pm\pi \tag{26.14}$$

═══════ [26.3] The Green function of a bounded particle

In order to get insight into the mathematics of $G^+(z)$ we first consider how $G(z)$ looks like for a particle in a very large box. To be more specific we can consider a particle in a potential well or on a ring. In the latter case it means periodic boundary conditions rather than Dirichlet boundary conditions. Later we would like to take the length L of the box to be infinite so as to have a "free particle". Expanding $\psi(x) = \langle x|G(z)|x_0\rangle$ in the energy basis we get the following expressions:

$$
\langle x|G_{\text{well}}(z)|x_0\rangle \;=\; \frac{2}{L}\sum_n \frac{\sin(k_n x)\sin(k_n x_0)}{z - E_n} \tag{26.15}
$$

$$
\langle x|G_{\text{ring}}(z)|x_0\rangle \;=\; \frac{1}{L}\sum_n \frac{e^{ik_n(x-x_0)}}{z - E_n}
$$

where the real k_n correspond to a box of length L. As discussed in the previous lecture, this sum can be visualized as the field which is created by a string of charges along the real axis. If we are far enough from the real axis we get a field which is the same as that of a smooth distribution of "charge". Let us call it the "far field" region. As we take the volume of the box to infinity the "near field" region, whose width is determined by the level spacing, shrinks and disappears. Then we are left with the "far field" which is the resolvent of a free particle. The result should not depend on whether we consider Dirichlet of periodic boundary conditions.

The summation of the above sums is technically too difficult. In order to get an explicit expression for the resolvent we recall that $\psi(x) = \langle x|G(z)|x_0\rangle$ is the solution of a Schrodinger equation with complex energy z and a source at $x = x_0$. The solution of this equation is

$$
\langle x|G(z)|x_0\rangle = -i\frac{\mathsf{m}}{k}e^{ik|x-x_0|} + Ae^{ikx} + Be^{-ikx} \tag{26.16}
$$

where $k = (2\mathsf{m}z)^{1/2}$ corresponds to the complex energy z. The first term satisfies the matching condition at the source, while the other two terms are "free waves" that solve the associated homogeneous equation. The coefficients A and B should be adjusted such that the boundary conditions are satisfied. For the "well" we should ensure the Dirichlet boundary conditions $\psi(x) = 0$ for $x = 0, L$, while for the "ring" we should ensure the periodic boundary conditions $\psi(0) = \psi(L)$ and $\psi'(0) = \psi'(L)$.

Let us try to gain some insight for the solution. If z is in the upper half plane then we can write $k = k_E + i\alpha$ where both k_E and α are positive(!) real numbers. This means that a propagating wave (either right going or left going) exponentially decays to zero in the propagation direction, and exponentially explodes in the opposite direction. It is not difficult to conclude that in the limit of a very large L the coefficients A and B become exponentially small. In the strict $L \to \infty$ limit we may say that $\psi(x)$ should satisfy "outgoing boundary conditions". If we want to make analytical continuation of $G(z)$ to the lower half plane, we should stick to these "outgoing boundary conditions". The implication is that $\psi(x)$ in the lower half plane exponentially explodes at infinity.

An optional argument that establishes the application of the outgoing boundary conditions is based on the observation that the FT of the retarded $G^+(\omega)$ gives the propagator. The propagator is identically zero for negative times. If we use the propagator to propagate a wavepacket, we should get a non-zero result for positive times and a zero result for negative times. In the case of an unbounded particle only outgoing waves are consistent with this description.

═══════ [26.4] Analytic continuation

The resolvent is well defined for any z away from the real axis. We define $G^+(z) = G(z)$ in the upper half of the complex plane. As long as we discuss bounded systems this "definition" looks like a duplication. The mathematics becomes more interesting once we consider unbounded systems with a continuous energy spectrum. In the latter case there are circumstances that allow analytic continuation of $G^+(z)$ into the lower half of the complex plane. This analytical continuation, if exists, would not coincide with $G^-(z)$.

In order to make the discussion of analytical continuation transparent let us assume, without loss of generality, that

we are interested in the following object:

$$f(z) = \langle\Psi|G(z)|\Psi\rangle = \sum_n \frac{q_n}{z - E_n} \tag{26.17}$$

The function $f(z)$ with $z = x + iy$ can be regarded as describing the electric field in a two dimensional electrostatic problem. The field is created by charges that are placed along the real axis. As the system grows larger and larger the charges become more and more dense, and therefore in the "far field" the discrete sum $\sum_n$ can be replaced by an integral $\int \varrho(E)dE$ where $\varrho(E)$ is the smoothed density of states. By "far field" we mean that $\mathrm{Im}[z]$ is much larger compared with the mean level spacing and therefore we cannot resolve the finite distance between the charges. In the limit of an infinite system this becomes exact for any finite (non-zero) distance from the real axis.

In order to motivate the discussion of analytical continuation let us consider a typical problem. Consider a system built of two weakly coupled 1D regions. One is a small "box" and the other is a very large "surrounding". The barrier between the two regions is a large delta function. According to perturbation theory the zero order states of the "surrounding" are mixed with the zero order bound states of the "box". The mixing is strong if the energy difference of the zero order states is small. Thus we have mixing mainly in the vicinity of the energies E_r where we formerly had bound states of the isolated "box". Let us assume that Ψ describes the initial preparation of the particle inside the "box". Consequently we have large q_n only for states with $E_n \approx E_r$. This means that we have an increased "charge density" in the vicinity of energies E_r. It is the LDOS rather than the DOS which is responsible for this increased charge density. Now we want to calculate $f(z)$. What would be the implication of the increased charge density on the calculation?

In order to understand the implication of the increased charge density on the calculation we recall a familiar problem from electrostatics. Assume that we have a conducting metal plate and a positive electric charge. Obviously there will be an induced negative charge distribution on the metal plate. We can follow the electric field lines through the plate, from above the plate to the other side. We realize that we can replace all the charge distribution on the plate by a single negative electric charge (this is the so called "image charge").

bounded system   continuum   ● image
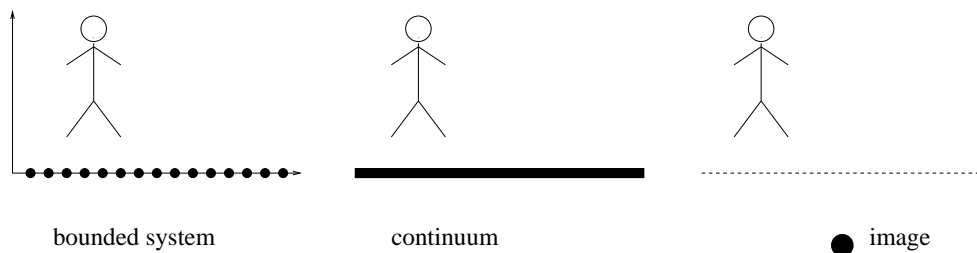
Returning to the resolvent, we realize that we can represent the effect of the increased "charge density" using an "image charge" which we call a "resonance pole". The location of the "resonance pole" is written as $E_r - i(\Gamma_r/2)$. Formally we say that the resonance poles are obtained by the analytic continuation of $G(z)$ from the upper half plane into the lower half plane. In practice we can find these poles by looking for complex energies for which the Schrodinger equation has solutions with "outgoing" boundary conditions. In another section we give an explicit solution for the above problem. Assume that this way or another we find an approximation for $f(z)$ using such "image charges":

$$f(E) = \langle\Psi|G^+(E)|\Psi\rangle = \sum_n \frac{q_n}{E - (E_n - i0)} = \sum_r \frac{Q_r}{E - (E_r - i(\Gamma_r/2))} + \text{smooth background} \tag{26.18}$$

We observe that the sum over n is in fact an integral, while the sum over r is a discrete sum. So the analytic continuation provides a simple expression for $G(z)$. Now we can use this expression in order to deduce physical information. We immediately find the LDOS can be written as as sum over Lorentzians. The Fourier transform of the LDOS is the survival amplitude, which comes out a sum over exponentials. In fact we can get the result for the survival amplitude directly by recalling that $\Theta(t)U(t)$ is the FT of $iG^+(\omega)$. Hence

$$\langle\Psi|U(t)|\Psi\rangle = \sum_r Q_r \mathrm{e}^{-iE_r t - (\Gamma_r/2)t} + \text{short time corrections} \tag{26.19}$$

If Ψ involves contribution from only one resonance, then the probability to stay inside the "box" decreases exponentially with time. This is the type of result that we would expect form either Wigner theory or from the Fermi Golden rule. Indeed we are going later to develop a perturbation theory for the resolvent, and to show that the expression for Γ in leading order is as expected.

========= [26.5] The Green function via direct diagonalization

For a free particle the eigenstates are known and we can calculate the expression by inserting a complete set and integrating. From now on we set $\mathsf{m} = 1$ in calculations, but we restore it in the final result.

$$
\begin{aligned}
G^+(x|x_0) &= \sum_{\boldsymbol{k}} \langle x|\boldsymbol{k}\rangle \frac{1}{E - \frac{1}{2}k^2 + i0}\langle \boldsymbol{k}|x_0\rangle \\
&= \int \frac{d\boldsymbol{k}}{(2\pi)^d} \mathrm{e}^{i\boldsymbol{k}\cdot\mathbf{r}} \frac{1}{E - \frac{1}{2}k^2 + i0}
\end{aligned}
\tag{26.20}
$$

where d is the dimension of the space. In order to compute this expression we define $\vec{r} = \vec{x} - \vec{x_0}$ and choose our coordinate system in such a way that the $\hat{z}$ direction will coincide with the direction of $\mathbf{r}$.

$$
G^+(x|x_0) = \int \frac{2\mathrm{e}^{ikr\cos\theta}}{k_E{}^2 - k^2 + i0}\frac{d\Omega k^{d-1}dk}{(2\pi)^d}
\tag{26.21}
$$

where $k_E = \sqrt{2\mathsf{m}E}$ is the wavenumber for a particle with energy E. The integral is a d-dimensional spherical integral. The solutions of $|\mathbf{k}| = k$ in 1D give two k's, while in 2D and 3D the k's lie on a circle and on a sphere respectively. We recall that Ω_d is $2, 2\pi, 4\pi$ in 1D, 2D and 3D respectively, and define averaging over all directions for a function $f(\theta)$ as follows:

$$
\langle f(\theta)\rangle_d = \frac{1}{\Omega_d}\int f(\theta)d\Omega
\tag{26.22}
$$

With this definition we get

$$
\langle \mathrm{e}^{ikr\cos\theta}\rangle_d = \begin{cases} \cos(kr), & \text{d=1;} \\ \mathrm{J}_0(kr), & \text{d=2;} \\ \mathrm{sinc}(kr), & \text{d=3.} \end{cases}
\tag{26.23}
$$

where $\mathrm{J}_0(x)$ is the zero order *Bessel function of the first kind*. Substituting these results and using the notation $z = kr$ we get in the 3D case:

$$
\begin{aligned}
G^+(\mathbf{r}) &= \frac{1}{\pi^2 r}\frac{1}{2}\int_{-\infty}^{\infty}\frac{z\sin z}{z_E{}^2 - z^2 + i0}dz = \frac{1}{\pi^2 r}\frac{1}{4i}\int_{-\infty}^{\infty}\frac{z(\mathrm{e}^{iz} - \mathrm{e}^{-iz})}{z_E{}^2 - z^2 + i0}dz \\
&= \frac{1}{\pi^2 r}\frac{1}{4i}\left[-\int \frac{z\mathrm{e}^{iz}}{(z - (z_E + i0))(z + (z_E + i0))}dz + \int \frac{z\mathrm{e}^{-iz}}{(z - (z_E + i0))(z + (z_E + i0))}dz\right] \\
&= \frac{1}{2\pi r}\sum_{\text{poles}}\mathrm{Res}[f(z)] = \frac{1}{2\pi r}\left[-\frac{1}{2}\mathrm{e}^{iz_E} - \frac{1}{2}\mathrm{e}^{-i(-z_E)}\right] = -\frac{\mathsf{m}}{2\pi}\frac{\mathrm{e}^{ik_E r}}{r}
\end{aligned}
\tag{26.24}
$$
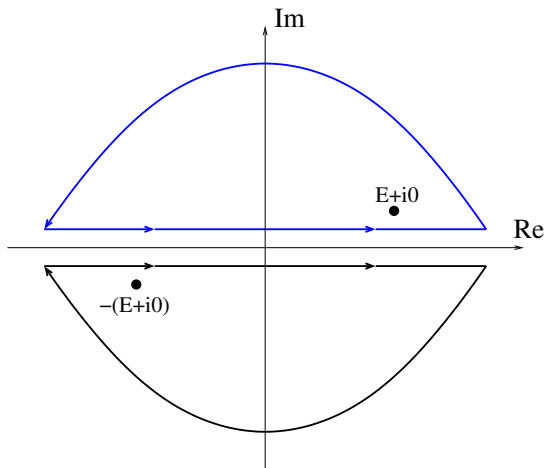
The contour of integration (see figure) has been closed in the upper half of the plane for the term containing e^{iz}, and in the lower half for the term with e^{-iz}, so the arc at infinity add zero contribution. Then the contour has been deformed, so the contribution for each term comes from one of the poles at $\pm(z_E + i0)$. We see that the solution is a variation on the familiar Coulomb law.

══════ [26.6] Solving the Helmholtz equation in 1D/2D/3D

The simplest method to find the Green function is by solving the Schrodinger equation with a source and appropriate boundary conditions. In the case of a free particle we get the Helmholtz equation which is a generalization of the Poisson equation of electrostatic problems:

$$(\nabla^2 + k_E{}^2)G(\mathbf{r}|\mathbf{r}_0) = -q\delta(\mathbf{r} - \mathbf{r}_0) \tag{26.25}$$

where the "charge" in our case is $q = -2\mathsf{m}/\hbar^2$. For $k_E = 0$ this is the Poisson equation and the solution is the Coulomb law. For $k_E \neq 0$ the solution is a variation on Coulomb law. We shall explore below the results in case of a particle in 3D, and then also for 1D and 2D.

The 3D case:

In the 3D case the "Coulomb law" is:

$$G(\mathbf{r}|\mathbf{r}_0) = \frac{q}{4\pi|\mathbf{r} - \mathbf{r}_0|} \cos(k_E|\mathbf{r} - \mathbf{r}_0|) \tag{26.26}$$

This solution still has a gauge freedom, just as in electrostatics where we have a "free constant". We can add to this solution any "constant", which in our case means an arbitrary (so called "free wave") solution of the homogeneous equation. Note that any "free wave" can be constructed from a superpostion of planar waves. In particular the "spherical" free wave is obtained by averaging $e^{i\mathbf{k}\cdot\mathbf{r}}$ over all directions. If we want to satisfy the "outgoing wave" boundary conditions we get:

$$G(r) = \frac{q}{4\pi r} \cos(k_E r) + i\frac{q}{4\pi r} \sin(k_E r) = \frac{q}{4\pi r}e^{ik_E r} = -\frac{\mathsf{m}}{2\pi r}e^{ik_E r} \tag{26.27}$$

The solutions for 1D and 2D can be derived in the same way.

The 1D case:

In the one dimensional case the equation that determines the Green function is

$$\left(\frac{\partial^2}{\partial x^2} + k_E^2\right)G(x) = -q\delta(x) \tag{26.28}$$

where for simplicity we set $x_0 = 0$. The delta function source requires a jump of the derivative $G'(+0) - G'(-0) = -q$. Using different phrasing: in order for the second derivative to be a delta function the first derivative must have a step function. Thus, when $k_E = 0$ we get the 1D Coulomb law $G(x) = -(q/2)|x|$, but for $k_E \neq 0$ we have a variation on Coulomb law

$$G(x) = -\frac{q}{2k_E}\sin(k_E|x|) \tag{26.29}$$

(see figure). To this we can add any 1D free wave. In order to satisfy the "outgoing waves" boundary conditions we add $\cos(kx) = \cos(k|x|)$ to this expression, hence we get the retarded Green's function in 1D

$$G(x) = i\frac{q}{2k_E}e^{ik_E|x|} = -i\frac{m}{k_E}e^{ik_E|x|} \tag{26.30}$$
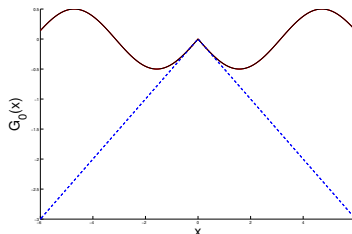
The 2D case:

In two dimensions for $k_E = 0$ we use Gauss' law to calculate the electrostatic field that goes like $1/r$, and hence the electrostatic potential is $G(r) = -(1/(2\pi))\ln r$. for $k_E \neq 0$ we get the modulated result

$$G(r) = -\frac{q}{4}Y_0(k_E r) \tag{26.31}$$

where $Y_0(x)$ is the Bessel function of the second kind

$$Y_0'(x) = -Y_1(x) \tag{26.32}$$
$$Y_0(x) \sim \sqrt{\frac{2}{\pi x}}\sin(x - \frac{\pi}{4}) \quad , \quad \text{for large } x$$

The second independent solution of the associated homogeneous equation is the Bessel function of the first kind $J_0(x)$. Adding this "free wave" solution leads to a solution that satisfies the "outgoing wave" boundary conditions. Hence we get the retarded Green's function in 2D

$$G(r) = i\frac{q}{4}H_0(k_E r) = -i\frac{m}{2}H_0(k_E r) \tag{26.33}$$

where $H_0(x) = J_0(x) + iY_0(x)$ is the Hankel function.

═══════ [26.7] Green function for a quasi 1D network

There is a very simple expression for the Green function of a particle that has energy E in a quasi 1D network (see "QM is practice" section):

$$G(x|x_0) = -i\frac{1}{v_E} \sum_p A_p(E)\, e^{ik_E L_p} \tag{26.34}$$

where p labels trajectories that start at x_0 and end at x. The length of a given trajectory is L_p, while $A_p(E)$ is the product of transmission and reflection amplitudes due to scattering at the nodes of the network. The proof of this formula is a straightforward generalization of the standard 1D case: The function $\Psi(x) = G(x|x_0)$ satisfies the Schrodinger equation for any $x \neq x_0$, and in particular the matching conditions at the nodes are satisfied by construction. At x_0 the function $\Psi(x)$ has the same discontinuity as in the standard 1D case, because for the direct trajectory $L_p = |x - x_0|$ has a jump in its derivative. This discontinuity reflects having a source at $x = x_0$ as required.

Delta scatterer.– Possibly the simplest quasi 1D networks, is a line with one node. Assuming that this node is a delta barrier, it is characterized by a reflection coefficient r and by a transmission coefficient $t = 1 + r$, where

$$r = -\frac{i(u/v_E)}{1 + i(u/v_E)} \tag{26.35}$$

Accordingly the Green function is

$$G(x|x_0) = -i\frac{1}{v_E}\left[e^{ik_E|x-x_0|} + r e^{ik_E(|x|+|x_0|)} \right] \tag{26.36}$$

This expression becomes appealing if we adopt a 3D-scattering perspective. Namely, it is the sum over a direct trajectory and a scattered trajectory. This is not an "accident". This becomes clear if we use a different procedure to derive this expression. For this purpose we write the expression for the delta function potential in Dirac notations as follows:

$$V(x) = u\delta(x) = |0\rangle u \langle 0| \tag{26.37}$$

For this type of potential we derive in the next lecture an *inversion formula*. It allows a direct calculation of the rezolvant. Namely,

$$G = \frac{1}{(E-H_0)-V} = G_0 + \frac{1}{1-u\mathcal{G}}G_0 V G_0 \equiv G_0 + G_0 T G_0 \tag{26.38}$$

where $\mathcal{G} = \langle 0|G_0|0\rangle = -i(1/v_E)$. Thus we get

$$T = \left(\frac{1}{1-u\mathcal{G}}\right)V = \frac{u}{1+i(u/v_E)}\delta(x) \tag{26.39}$$

The operator T is like effective V that incorporates all higher-orders of the scattering process. The formula for $G(x|x_0)$ is directly obtained from $G = G_0 + G_0 T G_0$, hence including a direct term, and a look-alike first-order scattering term with reflection coefficient r that incorporates all higher orders in u. Note that the reflected wave has amplitude r, while the transmited wave has amplitde $t = 1 + r$, which is the sum of incident and scattered wave. The scattering is isotropic (same r for both directions).

====== [26.8] Semiclassical evaluation of the Green function

The semiclassical procedure, based on the Van-Vleck formula, provides a common approximation for all the special cases that have been discussed above, and also allows further generalization. The Green function is the FT of the propagator:

$$G(x|x_0) \ \sim \ \int_0^\infty e^{i\mathcal{A}_{cl}(x,x_0)+iEt} dt \ \sim \ e^{i\mathcal{S}_{cl}(x,x_0)} \tag{26.40}$$

In order to derive the last expression one applies the stationary phase approximation for the evaluation of the dt integral. The stationary point is determined by the equation $E_{cl} = E$ where $E_{cl} \equiv -d\mathcal{A}_{cl}/dt$. The reduced action is defined as

$$\mathcal{S}_{cl}(x,x_0) \ = \ \mathcal{A}_{cl} + Et \ = \ \int_0^t [\mathcal{L}_{cl} + E] dt \ = \ \int_{x(0)}^{x(t)} p_{cl} \cdot dx \tag{26.41}$$

It is implicit in this definition that the reduced action is evaluated for a classical trajectory that has energy E and connects the points $x(0)$ and $x(t)$, and likewise the classical momentum p_{cl} is evaluated along this trajectory. In 1D $p_{cl} = \sqrt{2\mathsf{m}(E - V(x))} + A(x)$, and accordingly the particle acquires Adx phase and approximately $-Vdt$ phase in addition to the unperturbed $k_E dx$ phase along dx segment of its path.

====== [26.9] The boundary integral method

The Schrödinger equation $\mathcal{H}\psi = E\psi_0$ can be written as $\mathcal{H}_E\psi = 0$ where

$$\mathcal{H}_E = -\nabla^2 + U_E(r) \tag{26.42}$$

with $U_E(r) = U(r) - E$. Green's function solves the equation $\mathcal{H}_E G(r|r_0) = -q\delta(r - r_0)$ with $q = -2\mathsf{m}/\hbar^2$. In this section we follow the convention of electrostatics and set $q = 1$. From this point on we use the following (generalized) terminology:

Laplace equation [no source]:	$\mathcal{H}_E\psi(r) = 0$	(26.43)
Poisson equation:	$\mathcal{H}_E\psi(r) = \rho(r)$	(26.44)
Definition of the Coulomb kernel:	$\mathcal{H}_E G(r|r_0) = \delta(r - r_0)$	(26.45)

The solution of the Poisson equation is unique up to an arbitrary solution of the associated Laplace equation. If the charge density $\rho(r)$ is real, then the imaginary part of $\psi(r)$ is a solution of the Laplace equation. Therefore without loss of generality we can assume that $\psi(r)$ and $G(r|r_0)$ are real. From the definition of the Coulomb kernel it follows that the solution of the Poisson equation is

$$\text{Coulomb law:} \qquad \psi(r) \ = \ \int G(r|r')\rho(r')dr' \tag{26.46}$$

In particular we write the solution which is obtained if we have a charged closed boundary $r = r(s)$. Assuming that the charge density on the boundary is $\sigma(s)$ and that the dipole density (see discussion below) is $d(s)$ we get:

$$\psi(r) \ = \ \oint \Big([G(r|s)]\sigma(s) + [\partial_s G(r|s)]d(s) \Big) ds \tag{26.47}$$

We use here the obvious notation $G(r|s) = G(r|r(s))$. The normal derivative $\partial = \vec{n} \cdot \nabla$ is taken with respect to the source coordinate, where $\vec{n}$ is a unit vector that points outwards.

It should be obvious that the obtained $\psi(r)$ solves the Laplace equation in the *interior* region, as well as in the *exterior* region, while across the boundary it satisfies the matching conditions

Gauss law:
$$\partial\psi(s^+) - \partial\psi(s^-) = -\sigma(s) \qquad (26.48)$$
$$\psi(s^+) - \psi(s^-) = d(s) \qquad (26.49)$$

These matching conditions can be regarded as variations of Gauss law. They are obtained by integrating the Poisson equation over an infinitesimal range across the boundary. The charge density $\sigma(s)$ implies a jump in the electric field $-\partial\psi(s)$. The dipole density $d(s)$ is formally like a very thin parallel plates capacitor, and it implies a jump in the potential $\psi(s)$.

Let us ask the inverse question: Given a solution of Laplace equation in the interior region, can we find $\sigma(s)$ and $d(s)$ that generate it? The answer is *yes*. In fact, as implied from the discussion below, there are infinitely many possible choices. But in particular there is one unique choice that gives $\psi(r)$ inside and *zero* outside. Namely, $\sigma(s) = \partial\psi(s)$ and $d(s) = -\psi(s)$, where $\psi(s) = \psi(r(s))$. Thus we get:

The bounday integral formula:
$$\psi(r) = \oint \Big([G(r|s)]\partial\psi(s) - [\partial_s G(r|s)]\psi(s) \Big) ds \qquad (26.50)$$

The bounday integral formula allows to express the $\psi(r)$ at an arbitrary point inside the domain using a boundary integral over $\psi(s)$ and its normal derivative $\partial\psi(s)$.

The standard derivation of the boundary integral formula is based on formal algebraic manipulations with Green's theorem. We prefer below a simpler physics-oriented argumentation. If $\psi(r)$ satisfies Laplace equation in the *interior*, and it is defined to be *zero* in the exterior, then it satisfies (trivially) the Laplace equation also in the *exterior*. On top it satisfies the Gauss matching conditions with $\sigma(s) = \partial\psi(s^-)$ and $d(s) = -\psi(s^-)$. Accordingly it is a solution of the Poisson equation with $\sigma(s)$ and $d(s)$ as sources. But for the same $\sigma(s)$ and $d(s)$ we can optionally obtain another solutions of the Poisson equation from the bounday integral formula. The two solutions can differ by a solution of the associated Laplace equation. If we supplement the problem with zero boundary conditions at infinity, the two solutions have to coincide.

For the case where the wave function vanishes on the boundary $\psi(s) = 0$ the expression becomes very simple

$$\psi(r) = \oint G(r|s')\varphi(s')ds' \qquad (26.51)$$

where $\varphi(s) = \partial\psi(s)$, and in particular as we approach the boundary we should get:

$$\int G(s|s')\varphi(s')ds' = 0 \qquad (26.52)$$

An obvious application of this formula leads to a powerful numerical method for finding eigenfunctions. This is the so called *boundary integral method*. Let us consider the problem of a particle in a billiard potential. Our Green's function is (up to a constant)

$$G(s|s') = Y_0(k_E|r(s) - r(s')|) \qquad (26.53)$$

If we divide the boundary line into N segments then for any point on the boundary the equality $\int G(s|s')\varphi(s')ds' = 0$ should hold, so:

$$\sum_j A_{ij}\varphi_j = 0 \qquad \text{with} \quad A_{ij} = Y_0(k_E|r(s_i) - r(s_j)|) \qquad (26.54)$$

Every time the determinant $\det(A)$ vanishes we get a non trivial solution to the equation, and hence we can construct an eigenfunction. So all we have to do is plot the determinant $\det(A)$ as a function of k_E. The points where $\det(A)$ equals zero are the values of k_E for which the energy E is an eigenvalue of the Hamiltonian $\mathcal{H}$.

[27] Perturbation theory

════════ [27.1] Perturbation theory for the resolvent

Let us assume that we know how to invert analytically a matrix A. Next we are asked to invert $A - B$ where B is "small". If $A = 1$ the formal expansion is a geometric sum, and this can be generalized. Namely,

$$\frac{1}{(1-B)} \quad = \quad (1-B)^{-1} \quad = \quad \sum_{n=0}^{\infty} B^n \tag{27.1}$$

$$\frac{1}{A-B} \quad = \quad (A(1-A^{-1}B))^{-1} \quad = \quad (1-A^{-1}B)^{-1}A^{-1} \quad = \quad \sum_n (A^{-1}B)^n A^{-1}$$

$$= \quad \frac{1}{A} + \frac{1}{A}B\frac{1}{A} + \frac{1}{A}B\frac{1}{A}B\frac{1}{A} + \dots \tag{27.2}$$

In general exact summation is not possible, and we have to truncate the sum one way or another. But there is a special case of interest if $B = |\psi\rangle \lambda \langle\psi|$. Then we can sum the expansion to get a closed expression:

$$\frac{1}{A-B} \quad = \quad \frac{1}{A} + \left(\frac{1}{1-\lambda g}\right)\frac{1}{A}B\frac{1}{A} \tag{27.3}$$

where $g = \langle\psi|A^{-1}|\psi\rangle$. Note that for $A = 1$ this identity can be easily confirmed by selecting an basis that contains ψ as its first state, such that the matrix in the denominator is $\text{diag}\{1-\lambda, 1, 1, 1, ...\}$.

The formal expansion of $(A - B)^{-1}$ can be used for the calculation of the resolvent. One obtains:

$$G(z) \quad = \quad \frac{1}{z-\mathcal{H}} \quad = \quad \frac{1}{z-(\mathcal{H}_0+V)} \quad = \quad \frac{1}{(z-\mathcal{H}_0)-V} \tag{27.4}$$

$$= \quad G_0(z) + G_0(z)VG_0(z) + G_0(z)VG_0(z)VG_0(z) + \dots \tag{27.5}$$

Or, in matrix representation

$$G(x|x_0) = G_0(x|x_0) + \int G_0(x|x_2)dx_2\langle x_2|V|x_1\rangle dx_1 G_0(x_1|x_0) + \dots \tag{27.6}$$

Note that for the scalar potential $\hat{V} = u(\hat{x})$ we get

$$G(x|x_0) = G_0(x|x_0) + \int dx' G_0(x|x')u(x')G_0(x'|x_0) + \dots \tag{27.7}$$

════════ [27.2] Perturbation Theory for the Propagator

For the Green function we get

$$G^+(\omega) = G_0^+(\omega) + G_0^+(\omega)VG_0^+(\omega) + G_0^+(\omega)VG_0^+(\omega)VG_0^+(\omega) + \dots \tag{27.8}$$

Recall that

$$G^+(\omega) \to FT \to -i\Theta(\tau)U(\tau) \tag{27.9}$$

Then from the convolution theorem it follows that

$$(-i)[\Theta(t)U(t)] = (-i)[\Theta U_0(t)] + (-i)^2 \int dt' [\Theta(t-t')U(t-t')] [V] [\Theta(t')U_0(t')] + \dots \tag{27.10}$$

which leads to

$$U(t) = U_0(t) + \sum_{n=1}^{\infty} (-i)^n \int_{0<t_1<t_2<\dots<t_n<t} dt_n \dots dt_2 dt_1 \, U_0(t-t_n)V \dots U_0(t_2-t_1)VU_0(t_1) \tag{27.11}$$

for $t > 0$ and zero otherwise. This can be illustrated diagrammatically using Feynman diagrams.

Let us see how we use this expression in order to get the transition probability formula. The first order expression for the evolution operator is

$$U(t) = U_0 - i \int dt' \, U_0(t-t')VU_0(t') \tag{27.12}$$

Assume that the system is prepared in an eigenstate m of the unperturbed Hamiltonian, we get the amplitude to find it after time t in another eigenstate n is

$$\langle n|U(t)|m\rangle = e^{-iE_n t}\delta_{nm} - i \int dt' \, e^{-iE_n(t-t')}\langle n|V|m\rangle e^{-iE_m t'} \tag{27.13}$$

If $n \neq m$ it follows that:

$$P_t(n|m) = |\langle n|U(t)|m\rangle|^2 = \left| \int_0^t dt' V_{nm} e^{i(E_n - E_m)t'} \right|^2 \tag{27.14}$$

═════ [27.3] Perturbation theory for the evolution

In this section we review the elementary approach to solve the evolution problem via an iterative scheme with the Schrodinger equation. Then we make the bridge to a more powerful procedure. Consider

$$|\Psi\rangle = \sum_n \Psi_n(t)|n\rangle \tag{27.15}$$

It follows that:

$$i\frac{\partial \Psi_n}{\partial t} = E_n \Psi_n + \sum_{n'} V_{nn'} \Psi_{n'} \tag{27.16}$$

We want to solve in the method which is called "variation of parameters", so we set:

$$\Psi_n(t) = c_n(t)e^{-iE_n t} \tag{27.17}$$

Hence:

$$\frac{dc_n}{dt} = -i \sum_{n'} e^{i(E_n - E_{n'})t} V_{nn'} c_{n'}(t) \tag{27.18}$$

From the zero order solution $c_n(t) = \delta_{n,m}$ we get after one iteration:

$$c_n(t) = \delta_{nm} - i \int_0^t dt' e^{i(E_n - E_m)t'} V_{nm} \tag{27.19}$$

In order to make the connection with the formal approach of the previous and of the next section we write

$$c_n = e^{iE_n t} \Psi_n = \langle n | U_0^{-1} U(t) | m \rangle \equiv \langle n | U_I(t) | m \rangle \tag{27.20}$$

and note that

$$e^{i(E_n - E_m)t} V_{nm} = \langle n | U_0(t)^{-1} V U_0(t) | m \rangle \equiv \langle n | V_I(t) | m \rangle \tag{27.21}$$

Hence the above first order result can be written as

$$\langle n | U_I(t) | m \rangle = \delta_{nm} - i \int_0^t \langle n | V_I(t') | m \rangle \, dt' \tag{27.22}$$

In the next sections we generalize this result to all orders.

═══════ [27.4] The Interaction Picture

First we would like to recall the definition of time ordered exponentiation

$$U(t, t_0) = (1 - i dt_N \mathcal{H}(t_N)) \ldots (1 - i dt_2 \mathcal{H}(t_2))(1 - i dt_1 \mathcal{H}(t_1)) \equiv \mathcal{T} e^{-i \int_{t_0}^t \mathcal{H}(t') dt'} \tag{27.23}$$

Previously we have assumed that the Hamiltonian is not time dependent. But in general this is not the case, so we have to keep the time order. The parenthesis in the above definition can be "opened" and then we can assemble the terms of order of dt. Then we get the expansion

$$
\begin{aligned}
U(t, t_0) &= 1 - i(dt_N \mathcal{H}(t_N)) \cdots - i(dt_1 \mathcal{H}(t_1)) + (-i)^2 (dt_N \mathcal{H}(t_N))(dt_{N-1} \mathcal{H}(t_{N-1})) + \ldots \\
&= 1 - i \int_{t_0 < t' < t} \mathcal{H}(t') dt' + (-i)^2 \int_{t_0 < t' < t'' < t} \mathcal{H}(t'') \mathcal{H}(t') dt'' dt' + \ldots \\
&= \sum_{n=0}^{\infty} (-i)^n \int_{t_0 < t_1 < t_2 \cdots < t_n < t} dt_n \ldots dt_1 \mathcal{H}(t_n) \ldots \mathcal{H}(t_1)
\end{aligned} \tag{27.24}
$$

Note that if $\mathcal{H}(t') = \mathcal{H}$ is not time dependent then we simply get the usual Taylor expansion of the exponential function where the $1/n!$ prefactors would come from the time ordering limitation.

The above expansion is not very useful because the sum is likely to be divergent. What we would like to consider is the case

$$\mathcal{H} = \mathcal{H}_0 + V \tag{27.25}$$

where V is a small perturbation. The perturbation V can be either time dependent or time independent. It is convenient to regard the evolution as a sequence of "free" evolution during $[t_0, 0]$, an interaction at $t = 0$, and a later "free" evolution during $[0, t]$. Consequently we define a unitary operator U_I such that $U(t, t_0) = U_0(t, t_0) U_I U_0(0, t_0)$. Accordingly $U_I = \mathbf{1}$ if $V = 0$. Otherwise U_I gives the effect of the interaction as if it happened at the reference time $t = 0$. For simplicity we adopt from now on the convention $t_0 = 0$, and use the notation $U(t)$ instead of $U(t, t_0)$. Thus

$$U_I \equiv U_0(t)^{-1} U(t) \tag{27.26}$$

We also define the following notation

$$V_I(t) = U_0(t)^{-1} V U_0(t) \tag{27.27}$$

By definition of $\mathcal{H}$ as the generator of the evolution:

$$\frac{d}{dt}U(t) = -i(\mathcal{H}_0 + V) U(t) \tag{27.28}$$

Consequently:

$$\frac{d}{dt}U_I = -iV_I(t) U_I \tag{27.29}$$

The solution is by time ordered exponentiation

$$U_I = \mathcal{T} \exp\left(-i\int_0^t V_I(t')dt'\right) = \sum_{n=0}^{\infty}(-i)^n \int_{0<t_1<t_2\cdots<t_n<t} dt_n \ldots dt_1 \, V_I(t_n)\ldots V_I(t_1) \tag{27.30}$$

Which can be written formally as

$$U_I = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_0^t dt_n \ldots dt_1 \, \mathcal{T}V_I(t_n)\ldots V_I(t_1) \tag{27.31}$$

Optionally we can switch back to the Schrodinger picture:

$$U(t) = \sum_{n=0}^{\infty}(-i)^n \int_{0<t_1<t_2<\cdots<t_n<t} dt_n \ldots dt_2 dt_1 \, U_0(t - t_n)V \ldots U_0(t_2 - t_1)VU_0(t_1) \tag{27.32}$$

The latter expression is more general than the one which we had obtained via FT of the resolvent expansion, because here V is allowed to be time dependent.

════ [27.5] The Kubo formula

Consider the special case of having a time dependent perturbation $V = -f(t)\hat{B}$. The first order expression for the evolution operator in the interaction picture is

$$U_I(t) = 1 + i\int_0^t A_I(t')f(t')dt' \tag{27.33}$$

where $A_I(t)$ is A in the interaction picture. If our interest is in the evolution of an expectation value of another observable $\hat{A}$, then we have the identity

$$\langle A \rangle_t = \langle \psi(t)|A|\psi(t)\rangle = \langle \psi|A_H(t)|\psi\rangle = \langle \psi|U_I(t)^{-1}A_I(t)U_I(t)|\psi\rangle \tag{27.34}$$

To leading order we find

$$\langle A \rangle_t = \langle A_I(t)\rangle + \int_0^t \alpha(t,t')f(t')dt' \tag{27.35}$$

where the linear response kernel is given by the Kubo formula:

$$\alpha(t, t') = i\langle [A_I(t), B_I(t')] \rangle \tag{27.36}$$

In the above formulas expectation values without subscript are taken with the state ψ. It should be clear that the Kubo formula is merely the interaction picture version of the "rate of change" formula: The rate of change of the expectation value of A is determined by the expectation value of the commutator $[\mathcal{H}, A]$, hence in the interaction picture it is determined by the expectation value of $[V_I, A_I]$.

════ [27.6] The S operator

The formula that we have found for the evolution operator in the interaction picture can be re-written for an evolution that starts at $t = -\infty$ (instead of $t = 0$) and ends at $t = \infty$. For such scenario we use the notation $\hat{S}$ instead of U_I and write:

$$\hat{S} = \sum_{n=0}^{\infty} \frac{(-i)^n}{N!} \int_{-\infty}^{+\infty} dt_n \ldots dt_1 \, \mathcal{T} V_I(t_n) \ldots V_I(t_1) \tag{27.37}$$

It is convenient to regard $t = -\infty$ and $t = \infty$ as two well defined points in the far past and in the far future respectively. The limit $t \to -\infty$ and $t \to \infty$ is ill defined unless $\hat{S}$ is sandwiched between states in the same energy shell, as in the context of time independent scattering.

The S operator formulation is useful for the purpose of obtaining an expression for the temporal cross-correlation of (say) two observables A and B. The type of system that we have in mind is (say) a Fermi sea of electrons. The interest is in the the ground state ψ of the system which we can regard as the "vacuum state". The object that we want to calculate, written in the Heisenberg / Schrodinger / Interaction pictures is

$$
\begin{align}
C_{BA}(t_2, t_1) &= \langle \psi | B_H(t_2) A_H(t_1) | \psi \rangle \tag{27.38} \\
&= \langle \psi | U(t_2)^{-1} B \, U(t_2, t_1) \, A \, U(t_1) | \psi \rangle \tag{27.39} \\
&= \langle \psi | U_I(t_2)^{-1} B_I(t_2) \, U_I(t_2, t_1) \, A_I(t_1) \, U_I(t_1) | \psi \rangle \tag{27.40}
\end{align}
$$

where it is implicitly assumed that $t_2 > t_1 > 0$, and we use the notation $U_I(t_2, t_1) = U_I(t_2) U_I(t_1)^{-1}$, which is the evolution operator in the interaction picture referenced to the time t_1 rather than to $t=0$. Note that $\hat{S} = U_I(\infty, -\infty)$. Assuming that ψ is obtained from the non-interacting ground state ϕ via an adiabatic switching of the perturbation during the time $-\infty < t < 0$ we can rewrite this expression as follows:

$$
\begin{align}
C_{BA}(t_2, t_1) &= \langle \phi | U_I(\infty, -\infty)^{-1} U_I(\infty, t_2) B_I(t_2) U_I(t_2, t_1) A_I(t_1) U_I(t_1, -\infty) | \phi \rangle \tag{27.41} \\
&= \langle \phi | \hat{S}^\dagger \, \mathcal{T} \, \hat{S} \, B_I(t_2) \, A_I(t_1) | \phi \rangle \tag{27.42}
\end{align}
$$

In the last line it is implicit that one should first substitute the expansion for $\hat{S}$, and then (prior to integration) perform the time ordering of each term. The Gell-Mann-Low theorem rewrites the above expression as follows:

$$\langle \psi | \mathcal{T} B_H(t_2) A_H(t_1) | \psi \rangle = \frac{\langle \phi | \mathcal{T} \hat{S} B_I(t_2) A_I(t_1) | \phi \rangle}{\langle \phi | \hat{S} | \phi \rangle} = \langle \phi | \mathcal{T} \hat{S} B_I(t_2) A_I(t_1) | \phi \rangle_{\text{connected}} \tag{27.43}$$

The first equality follows from the observation that due to the assumed adiabaticity the operation of $\hat{S}$ on ϕ is merely a multiplication by a phase factor. The second equality is explained using a diagrammatic language. Each term in the perturbative expansion is illustrated by a Feynman diagram. It is argued that the implicit unrestricted summation of the diagrams in the numerator equals to the restricted sum over all the connected diagrams, multiplied by the unrestricted summation of vacuum-to-vacuum diagrams (as in the numerator). The actual diagrammatic calculation is carried out by applying Wick's theorem. The details of the diagrammatic formalism are beyond the scope of our presentation.

[28] Complex poles from perturbation theory

══════ [28.1] Models of interest

In this section we solve the particle decay problem using perturbation theory for the resolvent. We are going to show that for this Hamiltonian the analytical continuation of the resolvent has a pole in the lower part of the complex z-plane. The imaginary part ("decay rate") of the pole that we find is the same as we found by either the Fermi golden rule or by the exact solution of the Schrödinger equation.

We imagine that we have an "unperturbed problem" with one energy level $|0\rangle$ of energy E_0 and a continuum of levels $|k\rangle$ with energies E_k. A model of this kind may be used for describing tunneling from a metastable state. Another application is the decay of an excited atomic state due to emission of photons. In the latter case the initial state would be the excited atomic state without photons, while the continuum are states such that the atom is in its ground state and there is a photon. Schematically we have

$$\mathcal{H} = \mathcal{H}_0 + V \tag{28.1}$$

where we assume

$$\langle k|V|0\rangle = \sigma_k \qquad \text{(coupling to the continuum)} \tag{28.2}$$
$$\langle k'|V|k\rangle = 0 \qquad \text{(no transitions within the continuum)}$$

Due to gauge freedom we can assume that the coupling coefficients are real numbers without loss of generality. The Hamiltonian matrix can be illustrated as follows:

$$\mathcal{H} = \begin{pmatrix}
E_0 & \sigma_1 & \sigma_2 & \sigma_3 & . & . & . & \sigma_k & . \\
\sigma_1 & E_1 & 0 & 0 & . & . & . & 0 & . \\
\sigma_2 & 0 & E_2 & 0 & . & . & . & 0 & . \\
\sigma_3 & 0 & 0 & E_3 & . & . & . & 0 & . \\
. & . & . & . & . & . & . & 0 & . \\
. & . & . & . & . & . & . & 0 & . \\
. & . & . & . & . & . & . & 0 & . \\
\sigma_k & 0 & 0 & 0 & 0 & 0 & 0 & E_k & . \\
. & . & . & . & . & . & . & . & .
\end{pmatrix} \tag{28.3}$$

We later assume that the system under study is prepared in state $|0\rangle$ at an initial time ($t=0$), and we want to obtain the probability amplitude to stay in the initial state at a later times.

It is important to notice the following (a) we take one state and neglect other states in the well. (b) we assume that V allows transitions from this particular state in the well (zero state $|0\rangle$) into the $|k\rangle$ states in the continuum, while we do not have transitions in the continuum itself. These assumptions allow us to make exact calculation using perturbation theory to infinite order. The advantage of the perturbation theory formalism is that it allows the treatment of more complicated problems for which exact solutions cannot be found.

══════ [28.2] Heuristic approach

The Hamiltonian of the previous section is of the form

$$\mathcal{H} = \mathcal{H}_0 + V = \begin{pmatrix} H_0^P & 0 \\ 0 & H_0^Q \end{pmatrix} + \begin{pmatrix} 0 & V^{PQ} \\ V^{QP} & 0 \end{pmatrix} \tag{28.4}$$

and the wavefunction can be written as

$$\Psi = \begin{pmatrix} \psi \\ \chi \end{pmatrix} \tag{28.5}$$

In the decay problem of the previous section H_0^P is a 1×1 matrix, and H_0^Q is an $\infty \times \infty$ matrix. The perturbation allows transitions between P and Q states. In the literature it is customary to define projectors $\mathcal{P}$ and $\mathcal{Q}$ on the respective sub-spaces.

$$\mathcal{P} + \mathcal{Q} \;=\; \hat{1} \tag{28.6}$$

Our interest is focused only in the ψ piece of the wavefunction, which describes the state of the particle in the P space. On the other hand we assume that $\mathcal{H}$ has a continuous spectrum, and therefore any E above the ground state defines a stationary state via the equation

$$\begin{pmatrix} H_0^P & V^{PQ} \\ V^{QP} & H_0^Q \end{pmatrix} \begin{pmatrix} \psi \\ \chi \end{pmatrix} = E \begin{pmatrix} \psi \\ \chi \end{pmatrix} \tag{28.7}$$

From the second raw of the above equation it follows that $\chi = G^Q V^{QP} \psi$, where $G_0^Q = 1/(E - H_0^Q)$. Consequently the reduced equation for ψ is obtained from the first raw of the matrix equation

$$\left[H_0^P + V^{PQ} G^Q V^{QP} \right] \psi = E\psi \tag{28.8}$$

The second term in the square brackets $\Sigma(E) = V^{PQ} G_0^Q V^{QP}$ is the so called "self energy". Using the vague prescription $E \mapsto E + i0$ we can split it into an effective potential due to so called "polarization cloud" (also known as Lamb shift) and an imaginary part due to FGR decay:

$$H^P \;=\; H_0^P + \Delta - i\Gamma/2 \tag{28.9}$$

$$\Delta_{ij} \;=\; \sum_{k \in Q} \frac{V_{ik} V_{kj}}{E - E_k} \tag{28.10}$$

$$\Gamma_{ij} \;=\; 2\pi \sum_{k \in Q} V_{ik} V_{kj} \delta(E - E_k) \tag{28.11}$$

We argue that H^P generates the time evolution of ψ within P space. This effective Hamiltonian is non-hermitian because probability can escape to the Q space. It can be diagonalized so as to get the decay modes of the system. Each mode is characterized by its complex energy $E_r - i(\Gamma_r/2)$. Note that the effective Hamiltonian is non-hermitian and therefore the eigen-modes are in general non-orthogonal [see discussion of generalized spectral decomposition in the Fundementals I section].

The advantage of the above treatment is its technical simplicity. However, the mathematical significance of the $E \mapsto E + i0$ prescription is vague. We therefore turn to a more formal derivation of the same result, which illuminates how the non-hermiticity emerges once the Q continuum is eliminated.

▬▬▬▬ [28.3] The $P + Q$ formalism

We want to calculate the resolvent. But we are interested only in the single matrix element $(0,0)$ because we want to know the probability to stay in the $|0\rangle$ state:

$$\text{survival probability} \;=\; \left| \text{FT}\Big[\langle 0|G(\omega)|0 \rangle \Big] \right|^2 \tag{28.12}$$

Here $G(\omega)$ is the retarded Green function. More generally we may have several states in the well. In such a case instead of $P = |0\rangle\langle 0|$ we have

$$P = \sum_{n \in \text{well}} |n\rangle\langle n| \tag{28.13}$$

If we prepare the particle in an arbitrary state Ψ inside the well, then the probability to survive in the same state is

$$\text{survival probability} \;=\; \left| \text{FT}\Big[\, \langle \Psi | G(\omega) | \Psi \rangle \,\Big] \right|^2 \;=\; \left| \text{FT}\Big[\, \langle \Psi | G^P(\omega) | \Psi \rangle \,\Big] \right|^2 \tag{28.14}$$

Namely, we are interested only in one block of the resolvent which we call

$$G^P(z) = \mathcal{P} G(z) \mathcal{P} \tag{28.15}$$

Using the usual expansion we can write

$$
\begin{aligned}
G^P \;=\;& PGP = P\frac{1}{z-(H_0+V)}P = P(G_0 + G_0 V G_0 + \dots)P \\
=\;& PG_0P + PG_0(P+Q)V(P+Q)G_0P + PG_0(P+Q)V(P+Q)G_0(P+Q)V(P+Q)G_0P + \dots \\
=\;& G_0^P + G_0^P \Sigma^P G_0^P + G_0^P \Sigma^P G_0^P \Sigma^P G_0^P + \dots \\
=\;& \frac{1}{z-(H_0^P + \Sigma^P)}
\end{aligned}
\tag{28.16}
$$

where the "self energy" term

$$\Sigma^P = V^{PQ} G_0^Q V^{QP} \tag{28.17}$$

represents the possibility of making a round trip out of the well. Note that only even order terms contribute to this perturbative expansion because we made the simplifying assumption that the perturbation does not have "diagonal blocks". In our problem Σ^P is a 1×1 matrix that we can calculate as follows:

$$
\begin{aligned}
\Sigma^P \;=\;& \sum_k \langle 0|V|k\rangle \langle k|G_0|k\rangle \langle k|V|0\rangle = \sum_k \frac{|V_k|^2}{E - E_k + i0} \\
=\;& \sum_k \frac{|V_k|^2}{E - E_k} - i\pi \sum_k |V_k|^2 \delta(E-E_k) \;\equiv\; \Delta_0 - i(\Gamma_0/2)
\end{aligned}
\tag{28.18}
$$

In the last step we have implicitly assumed that our interest is in the retarded Green function. We have identified as before the Fermi golden rule rate

$$\Gamma_0 = 2\pi \sum_k |V_k|^2 \delta(E-E_k) \;\equiv\; 2\pi \varrho(E)\,|V|^2 \tag{28.19}$$

Thus, the resolvent is the 1×1 matrix.

$$G^P(z) = \frac{1}{z-(H_0^P+\Sigma^P)} = \frac{1}{z-(\varepsilon_0+\Delta_0)+i(\Gamma_0/2)} \tag{28.20}$$

We see that due to the truncation of the Q states we get a complex Hamiltonian, and hence the resolvent has a pole in the lower plane. The Fourier transform of this expression is the survival amplitude. After squaring it gives a simple exponential decay $e^{-\Gamma t}$.

Scattering Theory

[29] The plane wave basis

There are several different conventions for the normalization of plane waves:
- Box normalized plane waves $|n\rangle$
- Density normalized plane waves $|k\rangle$
- Energy shell normalized plane waves $|E, \Omega\rangle$

We are going to be very strict in our notations, else errors are likely. We clarify the three conventions first in the 1D case, and later in the 3D case, and then to remark on energy shell bases in general.

═══════ [29.1] Plane waves in 1D

The most intuitive basis set originates from quantization in a box with periodic boundary conditions (a torus):

$$|n\rangle \longrightarrow \frac{1}{\sqrt{L}} e^{ik_n x} \tag{29.1}$$

where

$$k_n = \frac{2\pi}{L} n \tag{29.2}$$

Orthonormality:

$$\langle n|n'\rangle = \delta_{n,n'} \tag{29.3}$$

Completeness:

$$\sum_n |n\rangle\langle n| = \hat{1} \tag{29.4}$$

The second convention is to have the density normalized to unity:

$$|k\rangle \longrightarrow e^{ikx} \tag{29.5}$$

Orthonormality:

$$\langle k|k'\rangle = 2\pi\delta(k - k') \tag{29.6}$$

Completeness:

$$\int |k\rangle \frac{dk}{2\pi} \langle k| = \hat{1} \tag{29.7}$$

Yet there is a third convention which assumes that the states are labeled by their energy, and by another index that indicate the direction.

$$|E, \Omega\rangle = \frac{1}{\sqrt{v_E}} |k_\Omega\rangle \longrightarrow \frac{1}{\sqrt{v_E}} e^{ik_\Omega x} \tag{29.8}$$

where $0 < E < \infty$ and Ω is the direction of propagation with $n_\Omega = \pm 1$, hence

$$k_\Omega = n_\Omega k_E = \pm\sqrt{2mE} \tag{29.9}$$

Orthonormality:

$$\langle E, \Omega | E', \Omega' \rangle = 2\pi \delta(E - E') \delta_{\Omega \Omega'} \tag{29.10}$$

Completeness:

$$\int \frac{dE}{2\pi} \sum_\Omega |E, \Omega\rangle \langle E, \Omega| \;=\; \hat{1} \tag{29.11}$$

In order to prove the orthonormality we note that $dE = v_E dk$ and therefore

$$\delta(E - E') = \frac{1}{v_E} \delta(k - k') \tag{29.12}$$

The energy shell normalization of plane waves in 1D is very convenient also for another reason. We see that the probability flux of the plane waves is normalized to unity. We note that this does not hold in more than 1D. Still also in more than 1D, the S matrix formalism reduces the scattering problem to 1D channels, and therefore this property is very important in general.

════════ [29.2] Plane waves in 3D

The generalization of the box normalization convention to the 3D case is immediate. The same applied to the density normalized plane waves:

$$|\vec{k}\rangle \longrightarrow e^{i\vec{k}\vec{x}} \tag{29.13}$$

Orthonormality:

$$\langle \vec{k} | \vec{k}' \rangle = (2\pi)^3 \delta^3(\vec{k} - \vec{k}') \tag{29.14}$$

Completeness:

$$\int |\vec{k}\rangle \frac{d^3k}{(2\pi)^3} \langle \vec{k}| = \hat{1} \tag{29.15}$$

The generalization of the energy shell normalization convention is less trivial:

$$|E, \Omega\rangle = \frac{1}{2\pi} \frac{k_E}{\sqrt{v_E}} |\vec{k}_\Omega\rangle \longrightarrow \frac{1}{2\pi} \frac{k_E}{\sqrt{v_E}} e^{i\vec{k}_\Omega \cdot \vec{x}} \tag{29.16}$$

where we define the direction by $\Omega = (\theta, \varphi)$, with an associated unit vector $\vec{n}_\Omega$ and a wavenumber

$$\vec{k}_\Omega = k_E \vec{n}_\Omega \tag{29.17}$$

Orthonormality:

$$\langle E, \Omega | E', \Omega' \rangle = 2\pi \delta(E - E') \delta^2(\Omega - \Omega') \tag{29.18}$$

Completeness:

$$\int \frac{dE}{2\pi} \int |E,\Omega\rangle d\Omega \langle E,\Omega| = \hat{1} \tag{29.19}$$

To prove the identities above we note that

$$d^3k = k^2 dk d\Omega \ = \ k_E^2 \frac{dE}{v_E} d\Omega \ = \ k_E^2 \frac{dE}{v_E} d\varphi d\cos\theta \tag{29.20}$$

and

$$\delta^3(\vec{k} - \vec{k}') \ = \ \frac{v_E}{k_E^2} \delta(E - E') \delta^2(\Omega - \Omega') \ = \ \frac{v_E}{k_E^2} \delta(E - E') \delta(\varphi - \varphi') \delta(\cos\theta - \cos\theta') \tag{29.21}$$

In general we have to remember that any change of the "measure" is associated with a compensating change in the normalization of the delta functions.

══════ [29.3] Optional energy shell bases

Instead of the standard energy shell basis $|E,\Omega\rangle$ one can use some other basis $|E,a\rangle$, where a is a quantum number that labels the different basis states. In particular in 3D problem it is convenient to use the $|E,\ell m\rangle$ basis, such that

$$\langle E,\ell m | E',\ell'm'\rangle \ = \ 2\pi\delta(E' - E) \ \delta_{\ell,\ell'} \ \delta_{m,m'} \tag{29.22}$$

In position representation

$$\langle r,\Omega | E,\ell m\rangle \ = \ 2\frac{k_E}{\sqrt{v_E}} \ j_\ell(k_E r) \ Y^{\ell m}(\Omega) \tag{29.23}$$

This wavefunction is properly normalized as an energy-shell basis state. In order to establish this normalization, note that the asymptotic behaviour of the spherical Bessel function is $j_\ell(kr) \sim \sin(kr - \text{phase})/(kr)$, which implies the orthogonality relation

$$\int_0^\infty r^2 dr \, j_\ell(kr) \, j_\ell(k'r) \ = \ \frac{\pi}{2kk'}\delta(k - k') \tag{29.24}$$

From here, using the same procedure as in previous sections, the energy-shell normalization is implied. As in the 1D case, the $|E,\ell m\rangle$ wavefunctions are also "flux normalized": the flux of both the ingoing and the outgoing wave components equals unity.

[30] Scattering in the T-matrix formalism

======= [30.1] The Scattering States

Our purpose is to solve the Schrödinger's equation for a given energy E.

$$(\mathcal{H}_0 + V)\Psi = E\Psi \tag{30.1}$$

If we rearrange the terms, we get:

$$(E - \mathcal{H}_0 - V)\Psi = 0 \tag{30.2}$$

In fact we want to find scattering solutions. These are determined uniquely if we define what is the "incident wave" and require outgoing boundary conditions for the scattered component. Thus we write Ψ as a superposition of a free wave and a scattered wave,

$$\Psi = \phi + \Psi^{scatt} \tag{30.3}$$

The scattered wave Ψ^{scatt} is required to satisfy outgoing boundary conditions. The free wave ϕ is any solution of:

$$\mathcal{H}_0\phi = E\phi \tag{30.4}$$

Substituting, we obtain:

$$(E - \mathcal{H}_0 - V)\Psi^{scatt} = V\phi \tag{30.5}$$

with the solution $\Psi^{scatt} = G^+V\phi$, leading to:

$$\Psi \;\; = \;\; (1 + G^+V)\phi \tag{30.6}$$

======= [30.2] The Lippman Schwinger equation

The explicit solution for Ψ that was found in the previous section is in typically useless, because it is difficult to get G. A more powerful approach is to write an integral equation for Ψ. For this purpose we re-arrange the differential equation as

$$(E - \mathcal{H}_0)\Psi = V\Psi \tag{30.7}$$

Using exactly the same procedure as in the previous section we get

$$\Psi = \phi + G_0^+V\Psi \tag{30.8}$$

This Lippman Schwinger equation can be solved for Ψ using standard techniques (see example in the next section). More generally closed analytical solutions cannot be obtained. Still if V is small we can try to find a solution iteratively, starting with the free wave as a zero order solution. This leads to a perturbative expansion for Ψ which we are going to derive in a later section using a simpler approach.

====== [30.3] Example: scattering by a regularized delta function

Let us demonstrate the procedure of solving Lippman Schwinger equation for scattering on a delta potential $u\delta(x)$ in one dimension. The relation $\Psi = \phi + G_0^+ V \Psi$ is written as

$$\Psi(x) \quad = \quad \mathrm{e}^{ikx} - i\frac{u}{v_E}\Psi(0)\mathrm{e}^{ik|x|} \tag{30.9}$$

Setting $x = 0$ we obtain a closed equation for the unknown wave amplitude $\Psi(0)$, whose solution leads to

$$\Psi(x) \quad = \quad \mathrm{e}^{ikx} + r\mathrm{e}^{ik|x|}, \qquad\qquad r = \frac{-i(u/v_E)}{1 + i(u/v_E)} \tag{30.10}$$

where r is identified as the reflection coefficient, while the transmission coefficient is $t = 1 + r$.

It is instructive to consider the more general case of scattering by a regularized delta function in any dimension, and with any dispersion relation. This generalization is also known as s-scattering. In particular it illuminates how a divergent series for the T matrix (see next section) can give a finite result, and why in the absence of regularization a delta function does not scatter in more than one dimension. By a regularized delta function we mean a potential $V(x) = u\delta(x)$ in $d = 1, 2, 3$ dimensions, whose non-zero matrix elements are

$$V_{k,k'} \quad = \quad \frac{u}{L^d}, \qquad\qquad \text{for } |k|, |k'| < \Lambda \tag{30.11}$$

with large momentum cutoff Λ. For clarity of physical units we assume box L^d normalization of the k basis. The Lippman Schwinger equation reads

$$\Psi(x) \quad = \quad \phi(x) + \sum_{k,k'}\langle x|G_0^+|k\rangle V_{k,k'}\langle k'|\Psi\rangle \tag{30.12}$$

The sum over k and k' factorizes, hence the second term in the right hand side can be approximated as $uG_0^+(x|0)\Psi(0)$. Setting $x = 0$ we obtain a closed equation for the unknown wave amplitude $\Psi(0)$, whose solution leads to

$$\Psi(x) \quad = \quad \phi(x) + G_0^+(x|0)\ u_{\text{eff}}\phi(0), \qquad\qquad u_{\text{eff}} \quad = \quad \frac{u}{1 - u\mathcal{G}(E)} \tag{30.13}$$

where $\mathcal{G}(E) = G_0^+(0|0)$. The above expression for $\Psi(x)$ can be written as $\Psi = (1 + G_0^+ T)\phi$ where

$$T \quad = \quad u_{\text{eff}}\ \delta(x) \tag{30.14}$$

In the next section we further discuss the significance of T, which can be regarded as a renormalized version of the potential $V = u\delta(x)$.

We now turn to discuss the practical calculation of $\mathcal{G}(E)$. From the definition it follows that in $d = 1, 2, 3$ dimensions

$$\mathcal{G}(E) \quad = \quad G_0^+(0|0) \quad = \quad \frac{1}{L^d}\sum_k \frac{1}{E - E_k + i0} \quad = \quad \int_0^\Lambda \frac{d\vec{k}}{(2\pi)^d}\left(\frac{1}{E - E_k + i0}\right) \tag{30.15}$$

The k summation should be treated with the appropriate integration measure. It equals $-i/v_E$ for a non-regularized Dirac delta function in one dimension. In higher dimensions $\mathcal{G}(E)$ has a real part that diverges, which implies that the scattering goes to zero. The regularization makes $\mathcal{G}(E)$ finite. In three dimensions we get $\mathcal{G}(E) = -(\mathsf{m}/\pi^2)\Lambda_E$ where

$$\Lambda_E = -2\pi^2 \int_0^\Lambda \frac{d^3k}{(2\pi)^3}\frac{1}{k_E^2 - k^2 + i0} = \Lambda - \frac{1}{2}k_E \log\left(\frac{\Lambda + k_E}{\Lambda - k_E}\right) + i\frac{\pi}{2}k_E \tag{30.16}$$

Another interesting case to consider is having (say) a constant density of states with a threshold energy. The divergence of $\mathcal{G}(E)$ near a threshold is logarithmic. It is quite amusing that the second order as well as all the higher terms in perturbation theory are divergent, while their sum goes to zero...

======= [30.4] Perturbation Theory for the Scattering State

Going back to the formal solution for Ψ we can substitute there the perturbative expansion of G

$$G = G_0 + G_0 V G_0 + G_0 V G_0 V G_0 + \ldots \tag{30.17}$$

leading to

$$\Psi = (1 + G^+ V)\phi = \phi + G_0 V \phi + G_0 V G_0 V \phi + \ldots \tag{30.18}$$

As an example consider the typical case of scattering by a potential $V(x)$. In this case the above expansion to leading order in space representation is:

$$\Psi(x) = \phi(x) + \int G_0(x, x') V(x') \phi(x') \, dx' \tag{30.19}$$

======= [30.5] The T matrix

It is customary to define the T matrix as follows

$$T \;\; = \;\; V + V G_0 V + V G_0 V G_0 V + \ldots \;\; = \;\; V + V G V \tag{30.20}$$

The T matrix can be regarded as a "corrected" version of the potential V, so as to make the following first order look-alike expression exact:

$$G \;\; = \;\; G_0 + G_0 T G_0 \tag{30.21}$$

Or the equivalent expression for the wavefunction:

$$\Psi = \phi + G_0^+ T \phi \tag{30.22}$$

Later it is convenient to take matrix elements in the unperturbed basis of free waves:

$$\begin{aligned} V_{\alpha\beta} \;\; &= \;\; \langle \phi^\alpha | V | \phi^\beta \rangle \\ T_{\alpha\beta}(E) \;\; &= \;\; \langle \phi^\alpha | T(E) | \phi^\beta \rangle \end{aligned} \tag{30.23}$$

In principle we can take the matrix elements between any states. But in practice our interest is in states that have the same energy, namely $E_\alpha = E_\beta = E$. Therefore it is convenient to use two indexes (E, a), where the index a distinguishes different free waves that have the same energy. In particular a may stand for the "direction" (Ω) of the plane wave. Thus in practice we are interested only in matrix elements "on the energy shell":

$$T_{ab}(E) = \langle \phi^{E,a} | T(E) | \phi^{E,b} \rangle \tag{30.24}$$

One should be very careful to handle correctly the different measures that are associated with different type of indexes. In particular note that in 3D:

$$T_{\Omega,\Omega_0} = \frac{1}{v_E} \left(\frac{k_E}{2\pi} \right)^2 T_{k_\Omega, k_{\Omega_0}} \tag{30.25}$$

===== [30.6] Scattering states in 1D problems

In this section we look for a scattering solution that originates from the free wave $|k_0\rangle$. Using the result of a previous section we write $\Psi = \phi^{k_0} + G_0^+ T \phi^{k_0}$ with

$$\phi^{k_0}(r) \quad = \quad e^{ik_0 x} \qquad \text{[density normalized]} \tag{30.26}$$

In Dirac notations:

$$|\Psi\rangle \quad = \quad |\phi^{k_0}\rangle + G_0^+ T |\phi^{k_0}\rangle \tag{30.27}$$

In space representation:

$$\langle x|\Psi\rangle \quad = \quad \langle x|\phi^{k_0}\rangle + \langle x|G_0^+ T|\phi^{k_0}\rangle \tag{30.28}$$

or in "old style" notation:

$$\Psi(x) \quad = \quad \phi^{k_0}(x) + \int G_0^+(x|x_0)dx_0 \langle x_0|T|k_0\rangle \tag{30.29}$$

In 1D problems the Green function is

$$G_0^+(x|x_0) \quad = \quad \langle x|G_0^+|x_0\rangle \quad = \quad -\frac{i}{v_E} e^{ik_E|x-x_0|} \tag{30.30}$$

Thus we get:

$$\psi(x) \quad = \quad e^{i\vec{k_0}x} - \frac{i}{v_E} \int e^{ik_E|x-x_0|} dx_0 \langle x_0|T|k_0\rangle \tag{30.31}$$

By observation of the left asymptotic region we deduce that the reflection coefficient is

$$r \quad = \quad -\frac{i}{v_E} \langle -k_0|T|k_0\rangle \quad = \quad -i\langle E,-|T|E,+\rangle \tag{30.32}$$

By observation of the right asymptotic region we deduce that the transmission coefficient is

$$t \quad = \quad 1 - \frac{i}{v_E} \langle k_0|T|k_0\rangle \quad = \quad 1 - i\langle E,+|T|E,+\rangle \quad \equiv \quad 1 + r_0 \tag{30.33}$$

We note that conservation of probability implies $|r|^2 + |t|^2 = 1$. With the substitution of the above relations it follows that

$$|r|^2 + |r_0|^2 \quad = \quad -2\text{Re}[r_0] \tag{30.34}$$

This is a special example for an "optical theorem" that we shall discuss later on: it relates the total cross section (here the left hand side) to the "forward" scattering amplitude (r_0). Note that t is the sum of the forward scattering with the incident wave. In the special case of delta scattering we have $r_0 = r$ and consequently we deduce that the scattering phase shift satisfies

$$\cos(\theta) \quad = \quad -|r| \tag{30.35}$$

═══════ [30.7] Scattering states in 3D problems

The derivation is the 3D case follows the same procedure as in the 1D case. The incident wave is

$$\phi^{k_0}(r) \;=\; e^{i\vec{k_0}\cdot\vec{r}} \qquad \text{[density normalized]} \tag{30.36}$$

and the implied scattering state is

$$\Psi(r) \;=\; \phi^{k_0}(r) + \int G_0^+(r|r_0)dr_0\langle r_0|T|k_0\rangle \tag{30.37}$$

where

$$G_0^+(r|r_0) = \langle r|G_0^+|r_0\rangle = -\frac{\mathsf{m}}{2\pi}\frac{e^{ik_E|r-r_0|}}{|r-r_0|} \tag{30.38}$$

Thus we get

$$\Psi(r) = \phi^{k_0}(r) - \frac{\mathsf{m}}{2\pi}\int \frac{e^{ik_E|r-r_0|}}{|r-r_0|}\langle r_0|T|k_0\rangle\,dr_0 \tag{30.39}$$

So far everything is exact. Now we want to get a simpler expression for the asymptotic form of the wavefunction. Note that from the experimental point of view only the "far field" region (far away from the target) is of interest. The major observation is that the dr_0 integration is effectively bounded to the scattering region $|r| < r_0$ where the matrix elements of V and hence of T are non-zero. Therefore for $|r| \gg |r_0|$ we can use the approximation

$$|\vec{r}-\vec{r_0}| = \sqrt{(\vec{r}-\vec{r_0})^2} = \sqrt{|r|^2 - 2\vec{r}\cdot\vec{r_0} + \mathcal{O}(|r_0|^2)} \approx |r|\left[1 - \vec{n}_\Omega\cdot\frac{\vec{r_0}}{|r|}\right] = |r| - \vec{n}_\Omega\cdot\vec{r_0} \tag{30.40}$$

Here and below we use the following notations:

$$\begin{aligned}
\vec{r} &\equiv |r|\vec{n}_\Omega \\
\Omega &= (\theta,\varphi) = \text{spherical coordinates} \\
\vec{n}_\Omega &= (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \\
\vec{k}_\Omega &= k_E\vec{n}_\Omega
\end{aligned} \tag{30.41}$$
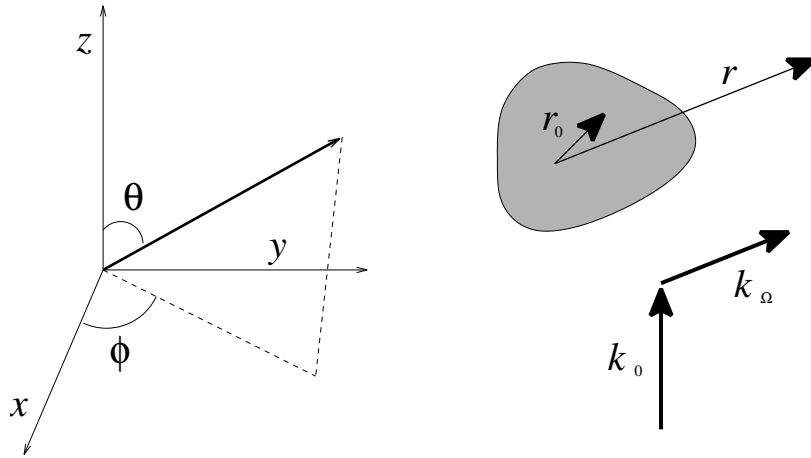
With the approximation above we get:

$$\Psi(r) \approx e^{i\vec{k}_0 \cdot \vec{r}} - \frac{\mathsf{m}}{2\pi} \frac{e^{ik_E|r|}}{r} \int e^{-i\vec{k}_\Omega \cdot \vec{r}_0} \langle r_0|T|k_0 \rangle \, dr_0 \equiv e^{i\vec{k}_0 \cdot \vec{r}} + f(\Omega) \frac{e^{ik_E|r|}}{|r|} \tag{30.42}$$

where

$$f(\Omega) = -\frac{\mathsf{m}}{2\pi} \langle \vec{k}_\Omega|T(E)|\vec{k}_0 \rangle \tag{30.43}$$

It follows that the differential cross section is

$$\frac{d\sigma}{d\Omega} = |f(\Omega)|^2 = \left(\frac{\mathsf{m}}{2\pi\hbar}\right)^2 \left|\frac{1}{\hbar}T_{k_\Omega, k_0}\right|^2 \tag{30.44}$$

This formula assumes density normalized plane waves. It relates the scattering which is described by $f(\Omega)$ to the T matrix. It can be regarded as a special case of a more general relation between the S matrix and the T matrix, as discussed in later sections (and see in particular the discussion of the "optical theorem" below).

====== [30.8] Born approximation and beyond

For potential scattering the first order approximation $T \approx V$ leads to the Born approximation:

$$f(\Omega) = -\frac{\mathsf{m}}{2\pi} \langle \vec{k}_\Omega|T(E)|\vec{k}_0 \rangle \approx -\frac{\mathsf{m}}{2\pi} \tilde{V}(q) \tag{30.45}$$

where $\vec{q} = \vec{k}_\Omega - \vec{k}_0$ and $\tilde{V}(\vec{q})$ is the Fourier transform of $V(\vec{r})$. The corresponding formula for the cross section is consistent with the Fermi golden rule.

It is customary in high energy physics to take into account higher orders. The various terms in the expansion are illustrated using Feynman diagrams. However, there are circumstance where we can gain better insight by considering the analytical properties of the Green function. In particular we can ask what happens if G has a pole at some complex energy $z = E_r - i(\Gamma_r/2)$. Assuming that the scattering is dominated by that resonance we get that the cross section has a Lorentzian line shape. More generally, If there is an interference between the resonance and the non-resonant terms then we get a Fano line shape. We shall discuss further resonances later on within the framework of the S matrix formalism.

====== [30.9] The Optical Theorem

From the energy-shell matrix elements of the T operator we can form an object that later we identify as the S matrix:

$$S_{ab} = \delta_{ab} - i\langle E, a|T|E, b \rangle \tag{30.46}$$

Using a more sloppy notation the equation above can be written as $S = 1 - iT$. We should remember that S is not an operator, and that S_{ab} are not the matrix elements of an operator. In contrast to that T_{ab} are the on-shell matrix elements of an operator. This relation assumes that the energy shell basis states are *properly* normalized.

The S matrix, as we define it later, is unitary. So we have $S^\dagger S = 1$, and therefore we conclude that the T matrix should satisfy the following equality:

$$(T^\dagger - T) = iT^\dagger T \tag{30.47}$$

In particular we can write:

$$\langle a_0|T - T^\dagger|a_0 \rangle = -i \sum_a \langle a_0|T|a \rangle \langle a|T^\dagger|a_0 \rangle \tag{30.48}$$

and we get:

$$\sum_a |T_{aa_0}|^2 = -2\mathrm{Im}[T_{a_0a_0}] \tag{30.49}$$

This so called "optical theorem" establishes a connection between the "cross section" and the forward scattering amplitude $T_{a_0a_0}$. It should be clear that if this relation holds in one particular energy-shell basis, then it holds also in any other (properly normalized) energy shell basis. In 3D scattering problems we can write one of the following expressions:

$$\sum_{\ell,m} |\langle \phi^{E,\ell,m}|T|\phi^{E,l_0,m_0}\rangle|^2 = -2\mathrm{Im}[\langle \phi^{E,l_0,m_0}|T|\phi^{E,l_0,m_0}\rangle] \tag{30.50}$$

$$\sum_{\Omega} |\langle \phi^{E,\Omega}|T|\phi^{E,\Omega_0}\rangle|^2 = -2\mathrm{Im}[\langle \phi^{E,\Omega_0}|T|\phi^{E,\Omega_0}\rangle]$$

Using the relations

$$|E,\Omega\rangle = \frac{1}{\sqrt{v_E}}\frac{k_E}{2\pi}|k_\Omega\rangle \tag{30.51}$$

$$f(\Omega) = -\frac{\mathsf{m}}{2\pi}\langle \vec{k}_\Omega|T(E)|\vec{k}_0\rangle$$

we get

$$\int |\langle \vec{k}_\Omega|T|\vec{k}_0\rangle|^2 d\Omega = -2v_E\left(\frac{2\pi}{k_E}\right)^2 \mathrm{Im}[\langle \vec{k}_0|T|\vec{k}_0\rangle] \tag{30.52}$$

Or the more familiar version:

$$\sigma_{\text{total}} = \int |f(\Omega)|^2 d\Omega = \frac{4\pi}{k_E}\mathrm{Im}[f(0)] \tag{30.53}$$

═══════ [30.10] Subtleties in the notion of cross section

Assume that we have a scattering state Ψ. We can write it as a sum of "ingoing" and "outgoing" waves or as a sum of "incident" and "scattered" waves. This is not the same thing!

$$\Psi = \Psi_{ingoing} + \Psi_{outgoing} \tag{30.54}$$

$$\Psi = \Psi_{incident} + \Psi_{scattered}$$

The "incident wave" is a "free wave" that contains the "ingoing" wave with its associated "outgoing" component. It corresponds to the $\mathcal{H}_0$ Hamiltonian. The "scattered wave" is what we have to add in order to get a solution to the scattering problem with the Hamiltonian $\mathcal{H}$. In the case of the usual boundary conditions it contains only an "outgoing" component.
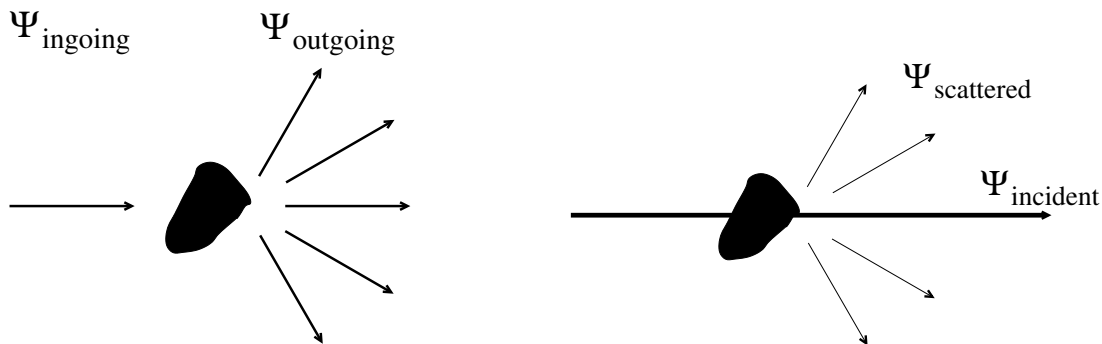
Below is an illustration of the 1D case where we have just two directions of propagation (forwards and backwards):
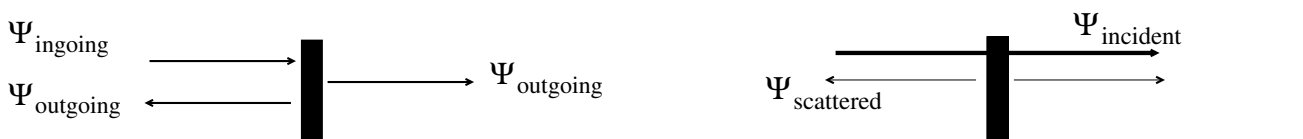
The S matrix gives the amplitudes of the outgoing wave, while the $T = i(\hat{1} - S)$ matrix gives the amplitudes of the scattered component (up to a phase factor). Let us consider extreme case in order to clarify this terminology. If we have in the above 1D geometry a very high barrier, then the outgoing wave on the right will have zero amplitude. This means that the scattered wave must have the same amplitude as the incident wave but with the opposite sign.

In order to define the "cross section" we assume that the incident wave is a density normalized ($\rho = 1$) plane wave. This is like having a current density $J = \rho v_E$. If we regard the target as having some "area" σ then the scattered current is

$$I_{scattered} = (\rho v_E) \times \sigma \tag{30.55}$$

It is clear from this definition that the units of the cross section are $[\sigma] = L^{d-1}$. In particular in 1D geometry the "differential cross section" into channel a, assuming an incident wave in channel a_0 is simply

$$\sigma_a = |T_{a,a_0}|^2 \tag{30.56}$$

and by the "optical theorem" the total cross section is

$$\sigma_{\text{total}} = -2\text{Im}[T_{a_0,a_0}] \tag{30.57}$$

The notion of "cross section" is problematic conceptually because it implies that it is possible for the scattered flux to be larger than the incident flux. This is most evident in the 1D example that we have discussed above. We see that the scattered wave is twice the incident wave, whereas in fact the forward scattering cancels the outgoing component of the incident wave. Later we calculate the cross section of a sphere in 3D and get twice the classical cross section ($2\pi a^2$). The explanation is the same - there must be forward scattering that is equal in magnitude (but opposite in sign) to the outgoing component of the incident wave in order to create a "shadow region" behind the sphere.

[31] Scattering in the S-matrix formalism

════════ [31.1] Channel Representation

Before we define the S matrix, Let us review some of the underlying assumptions of the S matrix formalism. Define

$$\rho(x) = |\Psi(x)|^2 \tag{31.1}$$

The continuity equation is

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot J \tag{31.2}$$

We are working with a time-independent Hamiltonian and looking for stationary solutions, hence:

$$\nabla \cdot J = 0 \tag{31.3}$$

The standard basis for representation is $|x\rangle$. We assume that the wave function is separable outside of the scattering region. Accordingly we arrange the basis as follows:

$$|x \in \text{inside}\rangle = \text{the particle is located inside the scattering region} \tag{31.4}$$
$$|a, r\rangle = \text{the particle is located along one of the outside channels}$$

and write the quantum state in this representation as

$$|\Psi\rangle \;=\; \sum_{x \in \text{inside}} \varphi(x)\,|x\rangle \;+\; \sum_{a,r} R_a(r)\,|a, r\rangle \tag{31.5}$$

The simplest example for a system that has (naturally) this type of structure is a set of 1D wires connected together to some "dot". In such geometry the index a distinguishes the different wires. Another, less trivial example, is a lead connected to a "dot". Assuming for simplicity 2D geometry, the wavefunction in the lead can be expanded as

$$\Psi(x) \;=\; \Psi(r, s) \;=\; \sum_a R_a(r)\chi^a(s) \tag{31.6}$$

where the channel functions (waveguide modes) are:

$$\chi^a(s) \;=\; \sqrt{\frac{2}{\ell}} \sin\left(\left(\frac{\pi}{\ell}a\right) s\right) \qquad \text{with } a = 1, 2, 3 \ldots \text{ and } 0 < s < \ell \tag{31.7}$$

In short, we can say that the wavefunction outside of the scattering region is represented by a set of radial functions:

$$\Psi(x) \;\mapsto\; R_a(r) \qquad \text{where } a = 1, 2, 3 \ldots \text{ and } 0 < r < \infty \tag{31.8}$$

The following figures illustrate several examples for scattering problems (from left to right): three connected wires, dot-waveguide system, scattering in spherical geometry, and inelastic scattering. The last two systems will be discussed below and in the exercises.
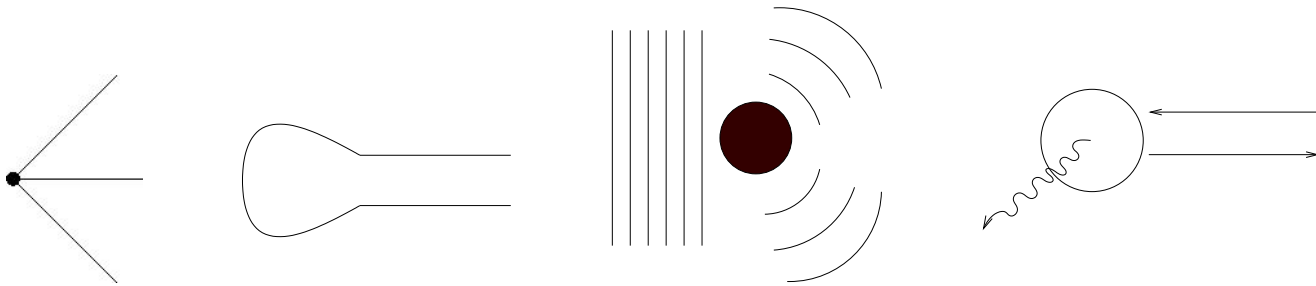
════ [31.2] The Definition of the S Matrix

Our Hamiltonian is time-independent, so the energy E is a good quantum number, and therefore the Hamiltonian $\mathcal{H}$ is block diagonal if we take E as one index of the representation. For a given energy E the Hamiltonian has an infinite number of eigenstates which form the so called "energy shell". For example in 3D for a given energy E we have all the plane waves with momentum $|\vec{k}| = k_E$, and all the possible superpositions of these waves. Once we are on the energy shell, it is clear that the radial functions should be of the form

$$R_a(r) \quad = \quad A_a R^{E,a,-}(r) - B_a R^{E,a,+}(r) \tag{31.9}$$

For example, in case of a waveguide

$$R^{E,a,\pm}(r) \quad = \quad \frac{1}{\sqrt{v_a}}\, e^{\pm i k_a r} \qquad \text{[flux normalized]} \tag{31.10}$$

where the radial momentum in channel a corresponds to the assumed energy E,

$$k_a \quad = \quad \sqrt{2\mathsf{m}\left(E - \frac{1}{2\mathsf{m}}\left(\frac{\pi}{\ell}a\right)^2\right)} \tag{31.11}$$

and the velocity $v_a = k_a/\mathsf{m}$ in channel a is determined by the dispersion relation. Thus on the energy shell the wavefunctions can be represented by a set of ingoing and outgoing amplitudes:

$$\Psi(x) \quad \longmapsto \quad (A_a, B_a) \qquad \text{with } a = 1, 2, 3 \ldots \tag{31.12}$$

But we should remember that not all sets of amplitudes define a stationary energy state. In order to have a valid energy eigenstate we have to match the ingoing and outgoing amplitudes on the boundary of the scattering region. The matching condition is summarized by the S matrix.

$$B_b \quad = \quad \sum_a S_{ba} A_a \tag{31.13}$$

By convention the basis radial functions are "flux normalized". Consequently the current in channel a is $I_a = |B_a|^2 - |A_a|^2$ and from the continuity equation it follows that

$$\sum_a |B_a|^2 \quad = \quad \sum_a |A_a|^2 \tag{31.14}$$

From here follows that the S matrix is unitary. The unitarity of the S matrix sometimes implies surprising consequences. For example: in 1D the transmission from-left-to-right must be equal to the transmission from-right-to-left. More generally: if we have a system with two different leads $\mathbf{1}$ and $\mathbf{2}$ then $\sum_{a \in \mathbf{1}, b \in \mathbf{2}} |S_{ba}|^2 = \sum_{a \in \mathbf{2}, b \in \mathbf{1}} |S_{ba}|^2$. The latter observation is essential for the theory of the two-terminal Landauer conductance.

In order to practice the definition of the S matrix consider a system with a single 2D lead. Let us assume that the lead has 3 open channels. That means that k_a is a real number for $a = 1, 2, 3$, and becomes imaginary for $a > 3$. The $a > 3$ channels are called "closed channels" or "evanescent modes". They should not be included in the S matrix because if we go far enough they contribute nothing to the wavefunction (their contribution decays exponentially). Thus we have a system with 3 open channels, and we can write

$$
R_1(r) = \frac{1}{\sqrt{v_1}}(A_1 e^{-ik_1 r} - B_1 e^{+k_1 r}) \tag{31.15}
$$

$$
R_2(r) = \frac{1}{\sqrt{v_2}}(A_2 e^{-ik_2 r} - B_2 e^{+k_2 r})
$$

$$
R_3(r) = \frac{1}{\sqrt{v_3}}(A_3 e^{-ik_3 r} - B_3 e^{+k_3 r})
$$

and

$$
\begin{pmatrix} B_1 \\ B_2 \\ B_3 \end{pmatrix} = \mathbf{S} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix} \tag{31.16}
$$

Simple examples for S matrices are provided in the "delta junction" sections of the "Boxes and Networks" lecture.

===== [31.3] Scattering states

Let us define the unperturbed Hamiltonian $\mathcal{H}_0$ as that for which the particle cannot make transitions between channels. Furthermore without loss of generality the phases of $R^{a\pm}(r)$ is chosen such that $S_{ab} = \delta_{ab}$, or equivalently $B_a = A_a$, should give the "free wave" solutions. We label the "free" energy states that correspond to the Hamiltonian $\mathcal{H}_0$ as $|\phi\rangle$. In particular we define a complete set $|\phi^\alpha\rangle$, that are indexed by $\alpha = (E, a)$, Namely, we define

$$
|\phi^\alpha\rangle = |\phi^{E_\alpha a_\alpha}\rangle \longmapsto \delta_{a, a_\alpha}(R^{a-}(r) - R^{a+}(r)) \tag{31.17}
$$

The following figure illustrates how the "free wave" $|\phi^{E,2}\rangle$ of a three wire system looks like.
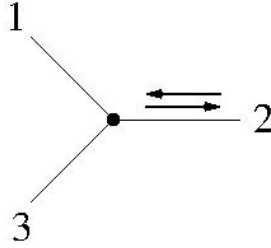
It is clear that the states $|\phi^{E,a}\rangle$ form a complete basis. Now we take the actual Hamiltonian $\mathcal{H}$ that permits transitions between channels. The general solution is written as

$$
|\Psi^\alpha\rangle \longmapsto A_a R^{a-}(r) - B_a R^{a+}(r) \tag{31.18}
$$

where $B_a = S_{ab} A_b$ or the equivalent relation $A_a = (S^{-1})_{ab} B_b$. In particular we can define the following sets of solutions:

$$
|\Psi^{\alpha+}\rangle = |\Psi^{E_\alpha a_\alpha +}\rangle \longmapsto \delta_{a, a_\alpha} R^{a-}(r) - S_{a, a_\alpha} R^{a+}(r) \tag{31.19}
$$

$$
|\Psi^{\alpha-}\rangle = |\Psi^{E_\alpha a_\alpha -}\rangle \longmapsto (S^{-1})_{a, a_\alpha} R^{a-}(r) - \delta_{a, a_\alpha} R^{a+}(r)
$$

The set of (+) states describes an incident wave in the a_α channel ($A_a = \delta_{a,a_\alpha}$) and a scattered wave that satisfies "outgoing" boundary conditions. The sign convention is such that $|\phi^\alpha\rangle$ is obtained for $\boldsymbol{S} = 1$. The set of (−) states is similarly defined. We illustrate some of these states in the case of a three wire system.
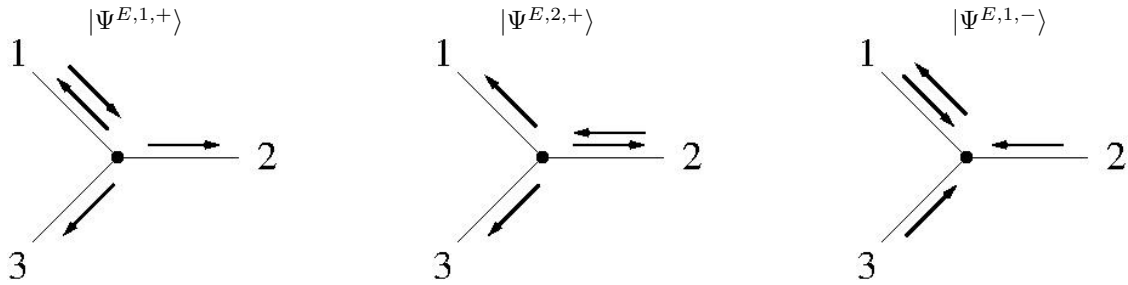
[31.4] Time reversal in scattering theory

It is tempting to identify the (−) scattering states as the time reversed version of the (+) scattering states. This is indeed correct in the absence of a magnetic field, when we have time reversal symmetry. Otherwise it is wrong. We shall clarify this point below.

Assuming that we have the solution

$$|\Psi^{E,a_0,+}\rangle \longmapsto \delta_{a,a_0}\mathrm{e}^{-ikx} - S_{a,a_0}\mathrm{e}^{+ikx} \tag{31.20}$$

The time reversed state is obtained via complex conjugation:

$$\mathcal{T}|\Psi^{E,a_0,+}\rangle \longmapsto \delta_{a,a_0}\mathrm{e}^{ikx} - (S^*)_{a,a_0}\mathrm{e}^{-ikx} \tag{31.21}$$

This should be contrasted with

$$|\Psi^{E,a_0,-}\rangle \longmapsto (S^{-1})_{a,a_0}\mathrm{e}^{-ikx} - \delta_{a,a_0}\mathrm{e}^{ikx} \tag{31.22}$$

We see that the two coincide (disregarding a global minus) only if

$$S^* = S^{-1} \tag{31.23}$$

which means that the S matrix should be symmetric ($S^{\mathrm{T}} = S$). This is the condition for having time reversal symmetry in the language of scattering theory.

[31.5] Orthonormality of the scattering states

The (+) states form a complete orthonormal basis. Also the (−) states form a complete orthonormal basis. The orthonormality relation and the transformation that relates the two basis sets are

$$\langle E_1, a_1, +|E_2, a_2, +\rangle = 2\pi\delta(E_1 - E_2)\delta_{a_1,a_2} \tag{31.24}$$
$$\langle E_1, a_1, -|E_2, a_2, -\rangle = 2\pi\delta(E_1 - E_2)\delta_{a_1,a_2} \tag{31.25}$$
$$\langle E_1, a_1, -|E_2, a_2, +\rangle = 2\pi\delta(E_1 - E_2)S_{a_1,a_2} \tag{31.26}$$

The last equality follows directly from the definition of the S matrix. Without loss of generality we prove this lemma for the 3 wire system. For example let us explain why it is true for $a_1 = 1$ and $a_2 = 2$. By inspection of the figure in

a previous section we see that the singular overlaps comes only from the first and the second channels. Disregarding the "flux" normalization factor the singular part of the overlap is

$$\langle E_1, 1, -|E_2, 2, +\rangle\Big|_{\text{singular}} \quad = \quad \int_0^\infty \left[-\mathrm{e}^{ikr}\right]^* \left[-S_{12}\mathrm{e}^{+ik_0r}\right] dr + \int_0^\infty \left[(S^{-1})_{21}\mathrm{e}^{-ikr}\right]^* \left[\mathrm{e}^{-ik_0r}\right] dr \qquad (31.27)$$

$$= \quad \int_0^\infty S_{12}\mathrm{e}^{-i(k-k_0)r} dr + \int_{-\infty}^0 S_{12}\mathrm{e}^{-i(k-k_0)r} dr \quad = \quad 2\pi\delta(k-k_0)S_{12}$$

where is the second line we have changed the dummy integration variables of the second integral from r to $-r$, and used $(S^{-1})_{21}^* = S_{12}$. If we restore the "flux normalization" factor we get the desired result. One can wonder what about the non-singular contributions to the overlaps. These may give, and indeed give, an overlap that goes like $1/(E \pm E_0)$. But on the other hand we know that for $E \neq E_0$ the overlap should be exactly zero due to the orthogonality of states with different energy (the Hamiltonian is Hermitian). If we check whether all the non-singular overlaps cancel, we find that this is not the case. What is wrong? The answer is simple. In the above calculation we disregarded a non-singular overlap which is contributed by the scattering region. This must cancel the non-singular overlap in the outside region because as we said, the Hamiltonian is Hermitian.

===== **[31.6] Getting the S matrix from the T matrix**

In this section we present a relation between the S matrix and the T matrix. The derivation of this relations goes as follows: On the one hand we express the overlap of the ingoing and outgoing scattering states using the S matrix. On the other hand we express it using the T matrix. Namely,

$$\langle \Psi^{E_1,a_1,-}|\Psi^{E_2,a_2,+}\rangle \quad = \quad 2\pi\delta(E_1 - E_2)\, S_{a_1a_2}$$
$$\langle \Psi^{E_1,a_1,-}|\Psi^{E_2,a_2,+}\rangle \quad = \quad 2\pi\delta(E_1 - E_2)\,(\delta_{a_1a_2} - iT_{a_1a_2}) \qquad (31.28)$$

By comparing the two expressions we deduce the relation between the S matrix and the T matrix:

$$S_{a_1a_2} \quad = \quad \delta_{a_1a_2} - iT_{a_1a_2} \qquad (31.29)$$

or in abstract notation $S = 1 - iT$. Another way to re-phrase this relation is to say that the S matrix can be obtained from the matrix elements of an $\hat{S}$ operator:

$$\langle \phi^{E_1,a_1}|\hat{S}|\phi^{E_2,a_2}\rangle \quad = \quad 2\pi\delta(E_1 - E_2)\, S_{a_1a_2} \qquad (31.30)$$

where the $\hat{S}$ operator is the evolution operator in the interaction picture. Within the framework of the time dependent approach to scattering theory the latter relation is taken as the definition for the S matrix. The two identities that we prove in the previous and in this section establish that the time-independent definition of the S matrix and the time dependent approach are equivalent. The rest of this section is dedicated to the derivation of the T matrix relation.

First order derivation.– We recall that the scattering states are defined as the solution of $\mathcal{H}\Psi = E\Psi$ and they can be expressed as

$$\Psi^{E_2,a_2,+} \quad = \quad \left(1 + G_0^+(E_2)V + ...\right) \phi^{E_2,a_2} \qquad (31.31)$$
$$\Psi^{E_1,a_1,-} \quad = \quad \left(1 + G_0^-(E_1)V + ...\right) \phi^{E_1,a_1} \qquad (31.32)$$

Hence

$$\langle \Psi^{E_1,a_1,-}|\Psi^{E_2,a_2,+}\rangle \quad = \quad \langle \phi^{E_1,a_1}|\phi^{E_2,a_2}\rangle + \langle \phi^{E_1,a_1}|VG_0^+(E_1) + G_0^+(E_2)V|\phi^{E_2,a_2}\rangle + ... \qquad (31.33)$$

$$= \quad \langle \phi^{E_1,a_1}|\phi^{E_2,a_2}\rangle + \left[\frac{1}{E_1 - E_2 + i0} + \frac{1}{E_2 - E_1 + i0}\right] \langle \phi^{E_1,a_1}|V|\phi^{E_2,a_2}\rangle + ... \qquad (31.34)$$

$$= \quad 2\pi\delta(E_1 - E_2)\delta_{a_1a_2} - i2\pi\delta(E_1 - E_2)\langle \phi^{E_1,a_1}|V|\phi^{E_2,a_2}\rangle + ... \qquad (31.35)$$

Full derivation.– We recall that the scattering states can be expressed as

$$\Psi^{E_2,a_2,+} = (1 + G^+(E_2)V)\phi^{E_2,a_2} = \left(1 + \frac{1}{E_2 - \mathcal{H} + i0}V\right)\phi^{E_2,a_2} \tag{31.36}$$

$$\Psi^{E_1,a_1,-} = (1 + G^-(E_1)V)\phi^{E_1,a_1} = \left(1 + \frac{1}{E_1 - \mathcal{H}_0 - i0}T(E_1)^\dagger\right)\phi^{E_1,a_1} \tag{31.37}$$

where the last equality relays on $GV = G_0T$. In the following calculation we use the first identity for the "ket", and after that the second identity for the "bra":

$$\begin{aligned}
\langle\Psi^{E_1,a_1,-}|\Psi^{E_2,a_2,+}\rangle &= \left\langle\Psi^{E_1,a_1,-}\left|1 + \frac{1}{E_2 - \mathcal{H} + i0}V\right|\phi^{E_2,a_2}\right\rangle \\
&= \left\langle\Psi^{E_1,a_1^-}\left|1 + \frac{1}{E_2 - E_1 + i0}V\right|\phi^{E_2,a_2}\right\rangle \\
&= \left\langle\phi^{E_1,a_1}\left|\left[1 + T(E_1)\frac{1}{E_1 - \mathcal{H}_0 + i0}\right]\left[1 + \frac{V}{E_2 - E_1 + i0}\right]\right|\phi^{E_2,a_2}\right\rangle \\
&= \left\langle\phi^{E_1,a_1}\left|\left[1 + \frac{T(E_1)}{E_1 - E_2 + i0}\right]\right|\phi^{E_2,a_2}\right\rangle + \left\langle\phi^{E_1,a_1}\left|\frac{V + T(E_1)G_0^+(E_1)V}{E_2 - E_1 + i0}\right|\phi^{E_2,a_2}\right\rangle \\
&= \left\langle\phi^{E_1,a_1}\left|1 + \frac{T(E_1)}{E_1 - E_2 + i0}\right|\phi^{E_2,a_2}\right\rangle + \left\langle\phi^{E_1,a_1}\left|\frac{T(E_1)}{E_2 - E_1 + i0}\right|\phi^{E_2,a_2}\right\rangle \\
&= 2\pi\delta(E_1 - E_2)\delta_{a_1 a_2} - i2\pi\delta(E_1 - E_2)\left\langle\phi^{E_1,a_1}|T(E_1)|\phi^{E_2,a_2}\right\rangle
\end{aligned} \tag{31.38}$$

where before the last step we have used the relation $V + TG_0V = T$.

▬▬▬ [31.7] The Wigner time delay

A given element of the S matrix can be written as

$$S_{ab} = \sqrt{g}e^{i\theta} \tag{31.39}$$

where $0 < g < 1$ is interpreted as either transmission or reflection coefficient, while θ is called phase shift. The cross section is related to g while the Wigner time delay that we discuss below is related to θ. The Wigner time delay is defined as follows:

$$\tau_{\text{delay}}(E) = \hbar\frac{d\theta}{dE} \tag{31.40}$$

Consider for example the time delay in the case of a scattering on a "hard" sphere of radius R. We shall see that in such case we have a smooth energy dependence $\theta \approx -2kR$ and consequently we get the expected result $\tau \approx -2R/v_E$. On the other hand we shall consider the case of a scattering on a shielded well. If the energy is off resonance we get the same result $\tau \approx -2R/v_E$. But if E is in the vicinity of a resonance, then we can get a very large (positive) time delay $\tau \sim \hbar/\Gamma_r$, where Γ_r is the so called "width" of the resonance. This (positive) time delay reflects "trapping" and it is associated with an abrupt variation of the cross section as discussed in a later section.

Let us explain the reasoning that leads to the definition of the Wigner time delay. For this purpose we consider the propagation of a Gaussian wavepacket in a given channel:

$$\Psi(x) = \int dk \, e^{-\sigma^2(k-k_0)^2}\sqrt{g}\exp\left[i\left(k(x - x_0) + \theta - Et\right)\right] \tag{31.41}$$

where both g and θ and E are functions of k. In order to determine the position $\bar{x}$ of the wavepaket we use the stationary phase approximation. Disregarding the Gaussian envelope, and regarding g as constant at the energy

range of interest, most of contribution to the dk integral comes from the k region where the phase is stationary. This leads to

$$x - x_0 + \frac{d\theta}{dk} - \frac{dE}{dk}t = 0 \tag{31.42}$$

The position $\bar{x}$ of the wavepacket is determined by the requirement that the above equation should have a solution for $k \sim k_0$. Thus we get

$$\bar{x} = x_0 + v_{\text{group}} \times (t - \tau_{\text{delay}}) \tag{31.43}$$

where $v_{\text{group}} = (dE/dk)$ is the group velocity for $k = k_0$ and τ_{delay} is the Wigner time delay as defined above. How this is related to a scattering problem? Consider for example scattering on one dimensions where we have "left" and "right" channels. Assume that the wavepacket at $t = 0$ is an undistorted Gaussian with $\theta = 0$. The initial wavepacket is centered on the "left" around $\bar{x} = x_0$ with momentum $\bar{k} = k_0$. We would like to know how $\bar{x}$ evolves with time before and after the scattering. Say that we observe the transmitted part of the wavepacket that emerges in the "right" channel. Following the above analysis we conclude that the effect of introducing $\theta \neq 0$ is the Wigner time delay.

===== [31.8] The Friedel phase and the DOS

The issue that we discuss in this section is how to determine the number $\mathcal{N}(E)$ of energy levels in the scattering region if we know how the S matrix depends on the energy E. This would be the number of no interacting Fermions that can be accommodated there at zero temperature. More precisely what we can extract from $S(E)$ is the density of states $\varrho(E)$ in the scattering region. To have a clear idea of the physical picture it is best to imagine a single lead system, where the lead is a waveguide with $\mathcal{M}$ modes, and the "depth" of the scattering region is L. In such system

$$\varrho(E) \quad \sim \quad \mathcal{M} \times v_{\text{E}} \frac{\pi}{L} \quad \sim \quad \mathcal{M} \times \tau_{\text{delay}} \tag{31.44}$$

where $\tau_{\text{delay}} \sim L/v_{\text{E}}$ is the semiclassical estimate for the time delay. We shall see that the so called Friedel-sum-rule is merely a refinement of the latter formula. In complete analogy with the Wigner formula, that express τ_{delay} as the E derivative of the scattering phase shift, we are going to express $\varrho(E)$ as the E derivative of the "Friedel phase".

The most illuminating way to define the energy levels of the scattering region is to impose Dirichlet boundary condition at the $r = 0$ section. This leads to the equation (say for 3 modes):

$$\mathbf{S} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix} = \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix} \tag{31.45}$$

This equation has a non-trivial solution if and on if

$$\det\left(\mathbf{S}(E) - \mathbf{1}\right) = 0 \tag{31.46}$$

Form this condition we can extract the eigen-energies. Recall that the S matrix is unitary. Therefore its $\mathcal{M}$ complex eigenvalues $e^{i\theta_r}$ are located on a circle. We get zero determinant in the above equation each time that one of the eigen-phases cross through $\theta = 0$. Thus the mean level spacing is simply $2\pi/\mathcal{M}$ divided by the average "velocity" $d\theta/dE$. This leads to

$$\varrho(E) = \frac{1}{2\pi}\left(\frac{d\theta_{\text{E}}}{dE}\right) = \frac{1}{2\pi i}\text{trace}\left(\frac{dS}{dE}S^\dagger\right) \tag{31.47}$$

where the Friedel phase is $\theta_{\text{E}} = \sum_r \theta_r$. The last equality is easily derived by calculating the trace in the basis in which S is diagonal.

A straightforward generalization of the above considerations allow to calculate the number of fermions that are emitted from the scattering region if a parameter X is being varied very very slowly such that at any moment we have zero temperature occupation. The result can be written as $dN = -GdX$ where

$$ G = \frac{1}{2\pi i}\mathsf{trace}\left(\frac{dS}{dX}S^\dagger\right) \tag{31.48} $$

The further generalization of this relation to multi-lead geometry has been discussed by Brouwer following the work of Buttiker Pretre and Thomas, and is known as the scattering approach to quantum pumping.

===== [31.9] Phase shifts and resonances

If we have only one wire (hence one channel) the S matrix is 1×1, and accordingly we can write

$$ S_{00} = \exp[i2\delta_0(E)] \tag{31.49} $$
$$ T_{00} = -\mathrm{e}^{i\delta_0}2\sin(\delta_0) \tag{31.50} $$

where $\delta_0(E)$ is known as the phase shift. If the scattering potential is short range one can use a matching procedure in order to determine the phase shift. This will be discussed in the next lecture. Another possibility is to use perturbation theory via the T matrix formalism:

$$ T_{00} = V_{00} + (VGV)_{00} = \text{Born expansion} \tag{31.51} $$

It is essential to calculate the matrix elements using properly flux-normalized free waves:

$$ |\phi^E\rangle = \frac{1}{\sqrt{v_E}}\mathrm{e}^{-ik_E r} - \frac{1}{\sqrt{v_E}}\mathrm{e}^{+ik_E r} = -i\frac{1}{\sqrt{v_E}}2\sin(k_E r) \tag{31.52} $$

There are two limiting cases of particular interest.

- First order non-resonant scattering by a weak potential V
- Resonant scattering which is dominated by a single pole of G

In the case of scattering by a weak potential we can use the first order Born approximation for the T matrix:

$$ T_{00} \approx V_{00} = \langle\phi^E|V|\phi^E\rangle = \frac{4}{v_E}\int_0^\infty V(r)\left(\sin(k_E r)\right)^2 dr \tag{31.53} $$

The assumption of weak scattering implies $\delta_0 \ll 1$, leading to the first order Born approximation for the phase shift:

$$ \delta_0^{\mathrm{Born}} \approx -\frac{2}{v_E}\int_0^\infty V(r)\left(\sin(k_E r)\right)^2 dr \tag{31.54} $$

This formula is similar to the WKB phase shift formula. It has a straightforward generalization to any ℓ which we discuss in the context of spherical geometry. We note that we have manged above to avoid the standard lengthy derivation of this formula, which is based on the Wronskian theorem (Messiah p.404).

The other interesting case is resonant scattering where

$$ T_{00} \approx (VGV)_{00} = \frac{\langle\phi^E|V|r\rangle\langle\tilde{r}|V|\phi^E\rangle}{E - E_r + i(\Gamma_r/2)} \tag{31.55} $$

From the optical theorem $2\text{Im}[T_{00}] = -|T_{00}|^2$ we can deduce that the numerator, if it is real, must equal Γ_r. Thus we can write this approximation in one of the following equivalent ways:

$$T_{00} = \frac{\Gamma_r}{E - E_r + i(\Gamma_r/2)} \tag{31.56}$$

$$S_{00} = \frac{E - E_r - i(\Gamma_r/2)}{E - E_r + i(\Gamma_r/2)} \tag{31.57}$$

$$\tan(\delta_\ell) = -\frac{\Gamma_r/2}{E - E_r} \tag{31.58}$$

Note that if the optical theorem were not satisfied by the approximation we would not be able to get a meaningful expression for the phase shift. In order to prove the equivalence of the above expressions note that δ_0 can be regarded as the polar phase of the complex number $z = (E-E_r) - i(\Gamma_r/2)$.

The Wigner time delay is easily obtained by taking the derivative of $\delta_0(E)$ with respect to the energy. This gives a Lorentzian variation of τ_{delay} as a function of $(E-E_r)$. Namely,

$$\tau_{\text{delay}} = \frac{\Gamma_r}{(E - E_r)^2 + (\Gamma_r/2)^2} \tag{31.59}$$

The width of the Lorentzian is Γ_r, and the time delay at the center of the resonance is of order $\hbar/\Gamma_r$.

[32] Scattering in quasi 1D geometry

In this lecture we consider various scattering problems is which the radial functions are $\exp(\pm ik_a r)$, where a is the channel index. In order to find a scattering solution we have to use a *matching* procedure. Namely the ingoing and outgoing free wave solutions should match an interior solution within the scattering region. This requirement imposes a boundary condition that relates the wavefunction amplitude and its derivative on the boundary. The simplest example for this class of systems is a network that consists of $\mathcal{M}$ semi 1D wires that are connected at one junction. The problem of s-scattering ($\ell = 0$) in spherical geometry is formally the same as $\mathcal{M}=1$ "semi 1D wire" problem. We shall discuss the general case (any ℓ) in a later lecture. The 1D scattering problem on a line, where we have "left" and "right" leads, is formally an $\mathcal{M}=2$ "semi 1D wire" system. Then it is natural to consider less trivial $\mathcal{M}$ channel systems that can be regarded as generalizations of the 1D problem, including scattering in waveguides and multi-lead geometries. Also *inelastic* scattering in 1D can be formally re-interpreted as an $\mathcal{M}$ channel "semi 1D wire" problem.

════ [32.1] The matching procedure

In this section we would like to outline a procedure for finding an exact result for the phase shift is quasi 1D one channel geometry. This procedure will allow us to analyze s-scattering by "hard" spheres as well as by "deep" wells. The key assumption is that we have a finite range potential which is contained within the region $r < R$. The boundary of the scattering region at $r = R$ is fully characterized by the logarithmic derivative $\tilde{k}_0(E)$. The definition of the latter is as follows: given the energy E, one finds the regular solution $\psi(r)$ of the Schrodinger equation in the interior ($r \leq R$) region; Typically this solution is required to satisfy Dirichlet boundary conditions at the origin $r = 0$; Once the regular solution is known, the logarithmic derivative at the boundary is calculated as follows:

$$\tilde{k}_0 \;=\; \left[\frac{1}{\psi(r)} \frac{d\psi(r)}{dr} \right]_{r=R} \tag{32.1}$$

The derivative should be evaluated at the *outer* side of the boundary. For each problem $\tilde{k}_0(E)$ should be evaluated from scratch. But once it is known we can find both the $E < 0$ bound states and the $E > 0$ scattering states of the system. It is useful the consider the simplest example: square well of radius a that has potential floor V_0. It is convenient to set the boundary at $R = a$. The regular solution in the interior region is $\Psi(r) \propto \mathrm{SIN}(\alpha_{\mathrm{in}} r)$, where SIN is either sin or sinh function. Accordingly the logarithmic derivative at the boundary is

$$\tilde{k}_0(E) \;=\; \alpha_{\mathrm{in}} \mathrm{COT}(\alpha_{\mathrm{in}} a), \qquad \text{where} \;\; \alpha_{\mathrm{in}} = \sqrt{2\mathsf{m}|E - V_0|} \tag{32.2}$$

Finding the bound states: In the case of a bound state the wavefunction at the outside region is $\psi(r) \propto \exp(-\alpha_E r)$. The matching with the interior solution gives the equation

$$\tilde{k}_0(E) \;=\; -\alpha_E \qquad \text{where } \alpha_E = \sqrt{2\mathsf{m}|E|} \tag{32.3}$$

This equation determines the eigen-energies of the system. In order to have bound states $\tilde{k}_0$ should become negative. This is indeed the case with square well ($V_0 < 0$) if its depth $|V_0|$ is large enough.

Finding the scattering states: For positive energies we look for scattering states. We define $k = k_E = \sqrt{2\mathsf{m}E}$. The scattering solution in the outside region is

$$\Psi(r) \;=\; A\mathrm{e}^{-ikr} - B\mathrm{e}^{ikr} \;=\; A(\mathrm{e}^{-ikr} - \mathrm{e}^{i2\delta_0}\mathrm{e}^{ikr}) \;=\; C\sin(kr + \delta_0) \tag{32.4}$$

where δ_0 is the phase shift. The matching with the interior solution gives the equation

$$k\cot(ka + \delta_0) \;=\; \tilde{k}_0 \tag{32.5}$$

This equation can be written as $\tan(\delta_0 - \delta_0^\infty) = k/\tilde{k}_0$, where $\delta_0^\infty = -ka$ is the solution for "hard sphere scattering".

Thus the explicit solution for the phase shift is

$$\delta_0 \;=\; \delta_0^\infty + \arctan(\frac{k}{\tilde{k}_0}) \tag{32.6}$$

It is clear that in practical problems the boundary $r = R$ is an arbitrary radius in the "outside" region. It is most natural to extrapolate the outside solution into the the region $r < R$ as if the potential there is zero. Then it is possible to define the logarithmic derivative $\bar{k}_0$ of the extrapolated wavefunction at $r = 0$. This function contains the same information as $\tilde{k}_0$, while the subtlety of fixing an arbitrary R is being avoided. From the above analysis we get

$$\bar{k}_0(E) \;=\; \left[\frac{1}{\psi(r)}\frac{d\psi(r)}{dr}\right]_{r=0} \;=\; k\cot(\delta_0(E)) \;=\; \frac{\tilde{k}_0 + k\tan(ka)}{k - \tilde{k}_0\tan(ka)} \tag{32.7}$$

At low energies, in the limit $k \to 0$, this expression takes the simpler form $\bar{k}_0 = ((1/\tilde{k}_0) - a)^{-1}$.

[32.2] Low energy scattering

Of particular interest is the long-wavelength limit, which means $kR \ll 1$ where R is the radius of the scattering region. Then the regular solution for $r \sim R$, where the potential is zero, has the form $\psi(r) \propto r - a_{\mathrm{s}}$. This implies by definition that for low energy $\delta_0 = -ka_{\mathrm{s}}$. The parameter a_{s} is called the scattering length. Given a_s, it follows from the above definition that the log derivative, referenced to the origin, is $\bar{k}_0 = -1/a_{\mathrm{s}}$. More generally it is customary to expand the log-derivative at the origin as follows:

$$\bar{k}_0(E) \;\equiv\; k\cot(\delta_0(E)) \;=\; -\frac{1}{a_{\mathrm{s}}} + \frac{1}{2}r_{\mathrm{s}}k^2 + ... \tag{32.8}$$

Thus a_s is merely a parameter in the expression for phase shift in the limit of low energies. If this phase shift is small it can be expressed as $\delta_0 = -ka_{\mathrm{s}}$. For a sphere of radius R and potential V_0 one obtains $a_s = R$ in the hard sphere limit ($V_0 = \infty$). As V_0 is decreased one obtains $a_s \approx (2/3)\mathsf{m}R^3V_0$. For negative V_0 ("spherical well") one obtains $a_s = R - (1/\alpha)\tan(\alpha R)$, where $\alpha = \sqrt{2\mathsf{m}|V_0|}$.

At this stage we mention a common terminology that might look strange at first sight. Referring to a square well it is clear that is $|V_0|$ is very small the potential has no bound state. We can regard such potential as a broadened delta function $V(r) = u\delta(r)$ that has $u < 0$. In such situation we have $\delta_0 > 0$ and $a_s < 0$, which should be contrasted with hard sphere. Such $u < 0$ scattering potential is called "attractive". As $|V_0|$ becomes larger it can accommodate a bound state, and it behaves like a $u > 0$ delta potential with $\delta_0 < 0$ and $a_s > 0$. Such scattering potential is called "repulsive". The bound state energy of the such "repulsive" potential is determined from the matching condition that has been discussed in the previous section, leading to

$$E_{\mathrm{bound}} \;=\; -\frac{1}{2\mathsf{m}a_{\mathrm{s}}^2} \tag{32.9}$$

It should be clear that this solution is meaningful provided the assumptions $a_{\mathrm{s}} \gg R$ and $|E_{\mathrm{bound}}| < \Delta$ are satisfied. Here Δ is the range within which a_s can be regarded as a constant.

From the definition of the scattering length it follows that for weak scattering it can be expressed as $\delta_0 = -ka_{\mathrm{s}}$. In a later section we shall see that in 3D this means that the total s-scattering cross section is

$$\sigma_{\mathrm{total}} \;=\; \frac{4\pi}{k^2}\sin^2(\delta_0) \;\approx\; 4\pi a_{\mathrm{s}}^2 \tag{32.10}$$

A delta function $V(x) = u\,\delta^3(x)$ in 3D has a zero total cross section. Still from the first order Born approximation for the T matrix we get as an artifact

$$\sigma_{\mathrm{total}} \;=\; 4\pi\left(\frac{\mathsf{m}}{2\pi}u\right)^2 \tag{32.11}$$

It is therefore common to describe an s-scatterer that is characterize by a scattering length a_s, as a delta scatterer with $u = 2\pi a_s/\mathsf{m}$. One should be very careful with the latter point of view.

====== [32.3] Inelastic scattering by a delta scatterer

We consider inelastic scattering on a delta scatterer in one dimension [arXiv:0801.1202]

$$\mathcal{H} \;=\; \frac{p^2}{2\mathsf{m}} + Q\delta(x) + \mathcal{H}_{\text{scatterer}} \tag{32.12}$$

The scatterer is assumed to have energy levels n with eigenvalues E_n. It should be clear that inelastic scattering of a spinless particle by a multi level atom is mathematically equivalent to inelastic scattering of a multi level atom by some static potential. Outside of the scattering region the total energy of the system (particle plus scatterer) is

$$\mathcal{E} \;=\; \epsilon_k + E_n \tag{32.13}$$

We look for scattering states that satisfy the equation

$$\mathcal{H}|\Psi\rangle = \mathcal{E}|\Psi\rangle \tag{32.14}$$

The scattering channels are labeled as

$$\boldsymbol{n} = (n_0, n) \tag{32.15}$$

where $n_0 = \text{left,right}$. We define

$$k_{\boldsymbol{n}} = \sqrt{2m(\mathcal{E} - E_n)} \qquad \text{for } n \in \text{open} \tag{32.16}$$
$$\alpha_{\boldsymbol{n}} = \sqrt{-2m(\mathcal{E} - E_n)} \qquad \text{for } n \in \text{closed} \tag{32.17}$$

later we use the notations

$$v_{\boldsymbol{n}} = k_{\boldsymbol{n}}/\mathsf{m} \tag{32.18}$$
$$u_{\boldsymbol{n}} = \alpha_{\boldsymbol{n}}/\mathsf{m} \tag{32.19}$$

and define diagonal matrices $\boldsymbol{v} = \text{diag}\{v_n\}$ and $\boldsymbol{u} = \text{diag}\{u_n\}$. The channel radial functions are written as

$$R(r) = A_n e^{-ik_n r} + B_n e^{+ik_n r} \qquad \text{for } n \in \text{open} \tag{32.20}$$
$$R(r) = C_n e^{-\alpha_n r} \qquad \text{for } n \in \text{closed} \tag{32.21}$$

where $r = |x|$. Next we derive expression for the $2N \times 2N$ transfer matrix $\boldsymbol{T}$ and for the $2N \times 2N$ scattering matrix $\boldsymbol{S}$, where N is the number of open modes. The wavefunction can be written as

$$\Psi(r, n_0, Q) = \sum_n R_{n_0, n}(r)\chi^n(Q) \tag{32.22}$$

The matching equations are

$$\Psi(0, \text{right}, Q) = \Psi(0, \text{left}, Q) \tag{32.23}$$
$$\frac{1}{2\mathsf{m}}\left[\Psi'(0, \text{right}, Q) + \Psi'(0, \text{left}, Q)\right] = \hat{Q}\Psi(0, Q) \tag{32.24}$$

The operator $\hat{Q}$ is represented by the matrix Q_{nm} that has the block structure

$$Q_{nm} = \begin{pmatrix} Q_{vv} & Q_{vu} \\ Q_{uv} & Q_{uu} \end{pmatrix} \tag{32.25}$$

For sake of later use we define

$$M_{nm} = \begin{pmatrix} \frac{1}{\sqrt{v}} Q_{vv} \frac{1}{\sqrt{v}} & \frac{1}{\sqrt{v}} Q_{vu} \frac{1}{\sqrt{u}} \\ \frac{1}{\sqrt{u}} Q_{uv} \frac{1}{\sqrt{v}} & \frac{1}{\sqrt{u}} Q_{uu} \frac{1}{\sqrt{u}} \end{pmatrix} \tag{32.26}$$

The matching conditions lead to the following set of matrix equations

$$\begin{align}
A_R + B_R &= A_L + B_L \tag{32.27} \\
C_R &= C_L \tag{32.28} \\
-i\boldsymbol{v}(A_R - B_R + A_L - B_L) &= 2Q_{vv}(A_L + B_L) + 2Q_{vu}C_L \tag{32.29} \\
-\boldsymbol{u}(C_R + C_L) &= 2Q_{uv}(A_L + B_L) + 2Q_{uu}C_L \tag{32.30}
\end{align}$$

from here we get

$$\begin{align}
A_R + B_R &= A_L + B_L \tag{32.31} \\
A_R - B_R + A_L - B_L &= i2(\boldsymbol{v})^{-1}\mathcal{Q}(A_L + B_L) \tag{32.32}
\end{align}$$

where

$$\mathcal{Q} = Q_{vv} - Q_{vu}\frac{1}{(\boldsymbol{u} + Q_{uu})}Q_{uv} \tag{32.33}$$

The set of matching conditions can be expressed using a transfer matrix formalism that we discuss in the next subsection, where

$$\mathcal{M} = \frac{1}{\sqrt{\boldsymbol{v}}}\mathcal{Q}\frac{1}{\sqrt{\boldsymbol{v}}} = M_{vv} - M_{vu}\frac{1}{1 + M_{uu}}M_{uv} \tag{32.34}$$

═══ [32.4] Finding the S matrix from the transfer matrix

The set of matching conditions in the delta scattering problem can be written as

$$\begin{pmatrix} \tilde{B}_R \\ \tilde{A}_R \end{pmatrix} = \boldsymbol{T}\begin{pmatrix} \tilde{A}_L \\ \tilde{B}_L \end{pmatrix} \tag{32.35}$$

where $\tilde{A}_n = \sqrt{v_n}A_n$ and $\tilde{B}_n = \sqrt{v_n}B_n$. The transfer $2N \times 2N$ matrix can be written in block form as follows:

$$\boldsymbol{T} = \begin{pmatrix} \boldsymbol{T}_{++} & \boldsymbol{T}_{+-} \\ \boldsymbol{T}_{-+} & \boldsymbol{T}_{--} \end{pmatrix} = \begin{pmatrix} 1 - i\mathcal{M} & -i\mathcal{M} \\ i\mathcal{M} & 1 + i\mathcal{M} \end{pmatrix} \tag{32.36}$$

The $\boldsymbol{S}$ matrix is defined via

$$\begin{pmatrix} \tilde{B}_L \\ \tilde{B}_R \end{pmatrix} = \boldsymbol{S}\begin{pmatrix} \tilde{A}_L \\ \tilde{A}_R \end{pmatrix} \tag{32.37}$$

and can be written in block form as

$$\boldsymbol{S_{n,m}} \;\;=\;\; \begin{pmatrix} \boldsymbol{S_R} & \boldsymbol{S_T} \\ \boldsymbol{S_T} & \boldsymbol{S_R} \end{pmatrix} \tag{32.38}$$

A straightforward elimination gives

$$\boldsymbol{S} \;\;=\;\; \begin{pmatrix} -\boldsymbol{T}_{--}^{-1}\boldsymbol{T}_{-+} & \boldsymbol{T}_{--}^{-1} \\ \boldsymbol{T}_{++}-\boldsymbol{T}_{-+}\boldsymbol{T}_{--}^{-1}\boldsymbol{T}_{+-} & \boldsymbol{T}_{+-}\boldsymbol{T}_{--}^{-1} \end{pmatrix} \;\;=\;\; \begin{pmatrix} (1+i\mathcal{M})^{-1}-1 & (1+i\mathcal{M})^{-1} \\ (1+i\mathcal{M})^{-1} & (1+i\mathcal{M})^{-1}-1 \end{pmatrix} \tag{32.39}$$

Now we can write expressions for $\boldsymbol{S_R}$ and for $\boldsymbol{S_T}$ using the $\mathcal{M}$ matrix.

$$\boldsymbol{S_T} \;\;=\;\; \frac{1}{1+i\mathcal{M}} = 1 - i\mathcal{M} - \mathcal{M}^2 + i\mathcal{M}^3 + ... \tag{32.40}$$
$$\boldsymbol{S_R} \;\;=\;\; \boldsymbol{S_T} - \boldsymbol{1} \tag{32.41}$$

====== **[32.5] Elastic scattering by a delta in a waveguide**

The *elastic* scattering of a spinless particle by a regularized delta scatterer in a waveguide is mathematically the same problem as that of the previous section. We have

$$Q = c\delta(y - y_0) \tag{32.42}$$

for which

$$Q_{\mathrm{nm}} \;\;=\;\; c \int \chi_n \delta(y - y_0) \chi_m \mathrm{dy} \;\;=\;\; c\, \chi^n(y_0)\chi^m(y_0) \tag{32.43}$$

Given the total energy we define

$$M_{nm} \;\;=\;\; \frac{1}{\sqrt{|v_n|}} Q_{nm} \frac{1}{\sqrt{|v_m|}} \;\;\equiv\;\; \begin{pmatrix} M_{vv} & M_{vu} \\ M_{uv} & M_{uu} \end{pmatrix} \tag{32.44}$$

Regularization means that one impose a cutoff on the total number of coupled channels, hence M is a finite (truncated) matrix. Using the formula for inverting a matrix of the type $1 - aa^\dagger$, we first obtain $\mathcal{M}$ and then obtain

$$S_R = \frac{iM_{vv}}{1 + i\,\mathsf{trace}[M_{vv}] + \mathsf{trace}[M_{uu}]} \tag{32.45}$$

Let us consider what happens as we change the total energy: Each time that a new channels is opened the scattering cross section becomes zero. Similarly, if we remove the regularization we get zero scattering for any energy because of the divergent contribution of the closed channels.

====== **[32.6] Transmission through a tight-binding network**

Consider a network that consists of N sites and described by Hamiltonian $\mathcal{H}_I$. We can attach a lead to a site of the network, or in general we attach several leads to different points. We would like to calculate the S matrix in this configuration. For this purpose we apply the T matrix formalism, combined with the "P+Q" formalism where "P" is the network and "Q" are the leads.

The lead is regarded as a chain of sites ($x = 1, 2, 3, ...$) with hopping amplitude $-c_0$. Accordingly a free "wave" with wavenumber k has energy and velocity as follows:

$$\epsilon = -2c_0 \cos(k) \tag{32.46}$$
$$v = 2c_0 \sin(k), \qquad \text{mass} \equiv 1/(2c_0) \tag{32.47}$$

The flux-normalized free wave in a disconnected lead is

$$\varphi(x) = \frac{2}{\sqrt{v}} \sin(kx), \qquad \text{Note: } \varphi(1) = \frac{\sqrt{v}}{c_0} \tag{32.48}$$

The Green function due a source at the first site is

$$G^{\text{lead}}(x|1) = -\frac{1}{c_0} e^{ikx} \qquad \text{Note: } G(1|1) = \frac{\epsilon - iv}{2c_0^2} \tag{32.49}$$

The hopping amplitude between the $x = 1$ site of the lead that is labeled as a, and a contact point the network that is labeled as n_a, will be denoted $-c_\gamma$. Later we shall define the dimensionless coupling parameter $\gamma = (c_\gamma/c_0)^2$. If we have M leads it is convenient to pack the couplings in a rectangular $M \times N$ contact matrix Q that is composed of zeros and ones, such that $V_{a,n} = -c_\gamma Q_{a,n}$. The Green function of the network can be calculated using the "P+Q" expression

$$G(n|m) = \left[\frac{1}{\epsilon - \mathcal{H}_0 - V^\dagger G^{\text{lead}} V} \right]_{n,m} = \left[\frac{1}{\epsilon - \mathcal{H}_0 - \frac{\gamma}{2}(\epsilon - iv)Q^\dagger Q} \right]_{n,m} \tag{32.50}$$

The scattering matrix is expressed as $\boldsymbol{S} = \boldsymbol{1} - i\boldsymbol{T}$, where the T matrix elements are

$$\boldsymbol{T}_{a,b} = = \langle \varphi^a | VGV^\dagger | \varphi^b \rangle = \left[\frac{\gamma v}{\epsilon - \mathcal{H}_{\text{eff}} + i\frac{\gamma v}{2}Q^\dagger Q} \right]_{n_a, n_b} \tag{32.51}$$

where n_a and n_b are the contact sites of lead a and lead b, and the definition of $\mathcal{H}_{\text{eff}}$ is implied from the expression for $G(n|m)$. Note that the $Q^\dagger Q$ term implies that the on-site potential at the contact sites becomes complex.

Assume that the network represents a 1D wire segment to which leads are attached at the endpoint. Ideal contacts corresponds to $\gamma = 1$. It is instructive to consider the continuum limit of the T matrix expression for such a setup. This limit corresponds to small k at the bottom of the band where $\epsilon \approx -2c_0$. One observes that the effective Hamiltonian becomes

$$\mathcal{H}_{\text{eff}} = \mathcal{H}_0 - c_0 Q^\dagger Q \tag{32.52}$$

This Hamiltonian corresponds to Neumann boundary conditions. The reasoning is as follows: If we place a negative delta $-[1/(2\mathsf{m}a)]\delta(x-a)$ at an infinitesimal distance a from the endpoint $x = 0$ of the segment, it forces the derivative to be zero. In a tight-binding model this is like having a potential $-c_0$ at the first site.

════ [32.7] Transmission through a cavity

Consider a cavity to which a lead is attached. We would like to calculate the S matrix in this configuration. One possibility is to take the continuum limit of the network model that we have solved in the previous section. This leads to the so-called Weidenmuller formula:

$$\boldsymbol{S} = \boldsymbol{1} - iWGW = \boldsymbol{1} - iW \frac{1}{E - \mathcal{H}_{\text{eff}} + i(W^\dagger W/2)} W^\dagger \tag{32.53}$$

where $\mathcal{H}_{\text{eff}}$ is the Hamiltonian of the cavity with Neumann boundary conditions on the surface of the scattering region. It is convenient to find a complete set $\varphi^{(n)}(x)$ of cavity eigenfunctions. Then the expression for the contact matrix takes the form

$$W_{a,n} \quad = \quad \sqrt{v_a} \int \chi^a(s) \varphi^{(n)}(x(s)) \ ds \tag{32.54}$$

where $\chi^a(s)$ are the channel functions and s is the transverse coordinate. Conventionally the Weidenmuller formula is derived from the so called $\boldsymbol{R}$ matrix formalism, which we outline below.

The Fisher-Lee relation.– Before we go on it is appropriate to point out the duality between the Weidenmuller formula and the Fisher-Lee relation. The latter expresses the Green function $G(s|s_0)$ using the S matrix as given. The surface coordinates s and s_0 indicate points $x(s)$ and $x(s')$ on the boundary of the scattering region. The standard derivation goes as follows [Datta]: We place a source at the lead and use the S matrix to define the boundary conditions on the surface $x(s)$ of the scattering region. We solve for the outgoing amplitudes and find that

$$G(s|s_0) \quad = \quad i \sum_{ab} \frac{1}{\sqrt{v_a}} \chi^a(s) \ (\boldsymbol{S} - \boldsymbol{1})_{ab} \ \frac{1}{\sqrt{v_b}} \chi^b(s_0) \tag{32.55}$$

This relation can be inverted:

$$\boldsymbol{S}_{ab} \quad = \quad \delta_{ab} \ - \ i\sqrt{v_a v_b} \int \chi^a(s) \ G(s|s_0) \ \chi^b(s_0) \ ds ds_0 \quad \equiv \quad \left[1 - iWGW^\dagger \right]_{a,b} \tag{32.56}$$

The latter expression has the same expected structure that is anticipated from T matrix theory, and therefore should be equivalent to the Weidenmuller formula. Inserting a complete basis of cavity eigenstates for the representation of the Green function, the integral over s becomes a sum over n, and the definition of W is implied. Still this perspective does not provide a practical procedure for the choice of the n basis, and for the evaluation of $G_{n,n'}$.

The R matrix formalism.– We would like to describe a formulation that opens the way for a powerful numerical procedure for finding the $\boldsymbol{S}$ matrix of a cavity-lead system. The idea is to reduce the scattering problem to a bound state problem by chopping the leads. It can be regarded as a generalization of the one-dimensional phase shift method where the outer solution is matched to an interior solution. The latter is characterized by its log derivative on the boundary. In the same spirit the $\boldsymbol{R}$ matrix is defined through the relation

$$\Psi(s) \quad = \quad \int \boldsymbol{R}(s, s') \partial \Psi(s') \ ds' \tag{32.57}$$

If we decompose this relation into channels we can rewrite it as

$$\Psi_a \quad = \quad \sum_b \boldsymbol{R}_{ab} \partial \Psi_b \tag{32.58}$$

Expressing Ψ_a and $\partial \Psi_a$ as the sum and the difference of the ingoing and the outgoing amplitudes A_a and B_a, one finds a simple relation between the $\boldsymbol{R}$ matrix and the $\boldsymbol{S}$ matrix:

$$\boldsymbol{R}_{ab} \quad = \quad i \frac{1}{\sqrt{k_a k_b}} \left(\frac{1 - \boldsymbol{S}}{1 + \boldsymbol{S}} \right)_{ab} \tag{32.59}$$

The inverse relation is

$$\boldsymbol{S} \quad = \quad \frac{1 + i\sqrt{\boldsymbol{k}}\boldsymbol{R}\sqrt{\boldsymbol{k}}}{1 - i\sqrt{\boldsymbol{k}}\boldsymbol{R}\sqrt{\boldsymbol{k}}} \tag{32.60}$$

From the Green theorem it follows that

$$\boldsymbol{R}(s, s') \quad = \quad -\frac{\hbar^2}{2\mathsf{m}} G^N(s'|s) \tag{32.61}$$

where G^N is the Green function of the interior with Neumann boundary conditions on the surface of the scattering region. If we find a complete set of interior eigenfunctions then

$$G^N(s'|s) \quad = \quad \sum_n \frac{\varphi^{(n)}(s')\varphi^{(n)}(s)}{E - E_n} \tag{32.62}$$

and consequently

$$\boldsymbol{R}_{ab} \quad = \quad -\frac{1}{2} \sum_n \left(\frac{W_{an}}{\sqrt{k_a}}\right) \frac{1}{E - E_n} \left(\frac{W_{bn}}{\sqrt{k_b}}\right) \tag{32.63}$$

The corresponding result for the $\boldsymbol{S}$ matrix is obtained by expanding $(1 + x)/(1 - x) = 1 + 2(...)$ with the identification of $(...)$ as the diagrammatic expression of the resolvent. This leads to the Weidenmuller formula.

[33] Scattering in a spherical geometry

Of special interest is the scattering problem in 3D geometry. We shall consider in this lecture the definitions of the channels and of the S matrix for this geometry. Later analyze in detail the scattering by a spherically symmetric target. In the latter case the potential $V(r)$ depends only on the distance from the origin. In order to find the scattering states we can perform separation of variables, where ℓ and m are good quantum numbers. In the (ℓ, m) subspace the equation for the radial function $u(r) = rR(r)$ reduces to a one dimensional Schrödinger equation on the $0 < r < \infty$ axis, with effective potential

$$V_{\text{eff}}(r) \quad = \quad V(r) + \frac{(\ell+1)\ell}{2\mathrm{m}r^2} \tag{33.1}$$

To avoid divergence in $R(r)$ we have to use the boundary condition $u(0) = 0$, as if there is an infinite wall at $r = 0$.

Most textbooks focus on the Coulomb interaction $V(r, \theta, \varphi) = -\alpha/r$ for which the effective radial potential is $V_{\text{eff}}(r) = -\alpha/r + \beta/r^2$. This is an extremely exceptional potential as discussed with regard to the spectrum of the Hydrogen atom. In the present context the following observations are important:

- It does not feature a centrifugal barrier.
- Consequently there are no resonances with the continuum.
- It has an infinite rather than a finite number of bound states.

As opposed to that, we are going to consider below, as a generic example, scattering on a spherical target which we call either "sphere" or "well". The parameters that characterize the sphere are its radius a, the height of the potential floor V, and optionally the the shielding barrier u. Namely,

$$V(r, \theta, \varphi) \quad = \quad V\Theta(a - r) + u\delta(r - a) \tag{33.2}$$

Disregarding the shielding the effective radial potential is $V_{\text{eff}}(r) = V\Theta(a - r) + \beta/r^2$. We consider first hard sphere ($V_0 = \infty$) and later on the scattering on a spherical well ($V_0 < 0$). The effective potential for 3 representative values of V is illustrated in panels (a)-(b)-(c) of the following figure. In panels (d) we illustrate, for sake of comparison, the effective potential in the case of a Coulomb interaction.
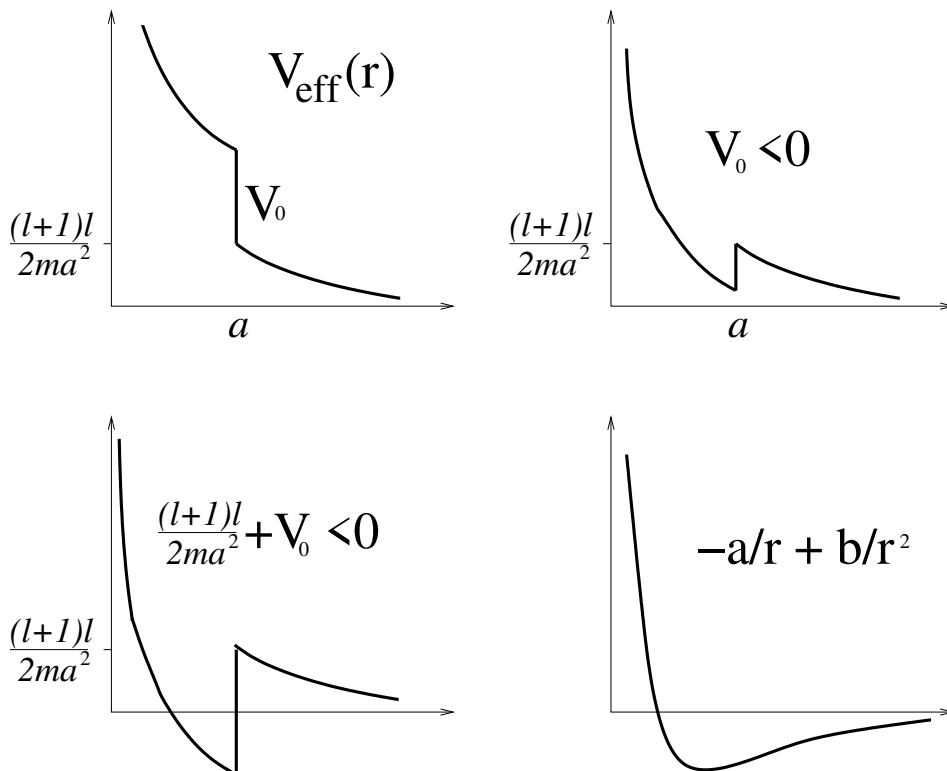
Classically it is clear that if the impact parameter b of a particle is larger than the radius a of the scattering region then there is no scattering at all. The impact parameter is the distance of the particle trajectory (extrapolated as a straight line) from form the scattering center. Hence its angular momentum is $\ell = \mathsf{m}vb$. Thus the semiclassical condition for non-negligible scattering can be written as

$$b < a \qquad \Leftrightarrow \qquad \ell < ka \qquad \Leftrightarrow \qquad \frac{\ell^2}{2\mathsf{m}a^2} < E \tag{33.3}$$

The last version is interpreted as the condition for reflection from the centrifugal barrier (see Fig). In the channels where the semiclassical condition is not satisfied we expect negligible scattering. (no phase shift). This semiclassical expectation assumes that the "forbidden" region is unaccessible to the particle, hence it ignores the possibility of tunneling and resonances that we shall discuss later on. Whenever we neglect the latter possibilities, the scattering state is simply a free wave which is described by the spherical Bessel function $j_\ell(kr)$, where $k = k_E = \sqrt{2\mathsf{m}E}$. For $kr \ll \ell$ this spherical Bessel function is exponentially small due to the centrifugal barrier, and therefore it is hardly affected by the presence of the sphere.

===== [33.1] The spherical Bessel functions

Irrespective of whether the scattering potential is spherically symmetric or not the Schrodinger equation is separable outside of the scattering region. This means that we can expand any wavefunction that satisfies $\mathcal{H}\Psi = E\Psi$ in the outside region as follows:

$$\Psi(x) = \sum_{\ell,m} R_{\ell,m}(r) Y^{\ell m}(\theta, \varphi) \tag{33.4}$$

The channel index is $a = (\ell, m)$ while $\Omega = (\theta, \varphi)$ is analogous to the s of the 2D lead system. The $Y^{\ell m}$ are the channel functions. In complete analogy with the case of 1D geometry we can define the following set of functions:

$$
\begin{aligned}
h_\ell^+(kr) &\leftrightarrow e^{ikr} \\
h_\ell^-(kr) &\leftrightarrow e^{-ikr} \\
j_\ell(kr) &\leftrightarrow \sin(kr) \\
n_\ell(kr) &\leftrightarrow \cos(kr)
\end{aligned}
\tag{33.5}
$$

Note that the right side equals the left side in the special case $\ell = 0$, provided we divide by r. This is because the semi-1D radial equation becomes literally the 1D Schrödinger equation only after the substitution $R(r) = u(r)/r$.

In what follows we use Messiah convention p.489. Note that other textbooks may use different sign convention. The relation between the functions above is defined as follows:

$$h_\ell^\pm \;=\; n_\ell(kr) \pm i j_\ell(kr) \tag{33.6}$$

We note that the $j_\ell(r)$ are regular at the origin, while the $n_\ell(r)$ are singular at the origin. Therefore only the former qualify as global "free waves". The $\ell = 0$ functions are:

$$
\begin{aligned}
j_0(kr) &= \frac{\sin(kr)}{kr} \\
n_0(kr) &= \frac{\cos(kr)}{kr}
\end{aligned}
\tag{33.7}
$$

More generally

$$
\begin{aligned}
j_\ell(x) &= \sqrt{\frac{\pi}{2x}} J_{\ell+\frac{1}{2}}(x) = (-x)^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\sin x}{x} \\
n_\ell(x) &= \sqrt{\frac{\pi}{2x}} Y_{\ell+\frac{1}{2}}(x) = (-x)^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\cos x}{x}
\end{aligned}
$$

The asymptotic behavior for $kr \gg \ell+1$ is:

$$
\begin{aligned}
h_\ell^\pm(kr) &\sim (\mp i)^\ell \; \frac{\mathrm{e}^{\pm ikr}}{kr} \\
n_\ell(kr) &\sim \frac{\cos(kr - \frac{\pi}{2}\ell)}{kr} \\
j_\ell(kr) &\sim \frac{\sin(kr - \frac{\pi}{2}\ell)}{kr}
\end{aligned}
\tag{33.8}
$$

The short range $kr \ll \ell+1$ behavior is:

$$
\begin{aligned}
n_\ell(kr) &\approx (2l-1)!! \left(\frac{1}{kr}\right)^{\ell+1} \left[1 + \frac{1}{2(2l-1)}(kr)^2 + \ldots\right] \\
j_\ell(kr) &\approx \frac{(kr)^\ell}{(2l+1)!!} \left[1 - \frac{1}{2(2l+3)}(kr)^2 + \ldots\right]
\end{aligned}
\tag{33.9}
$$

===== [33.2] Free spherical waves

On the energy shell we write the radial wavefunctions as

$$
R_{\ell m}(r) = A_{\ell m} R^{E,\ell m,-}(r) - B_{\ell m} R^{E,\ell,m,+}(r)
\tag{33.10}
$$

where in complete analogy with the 1D case we define

$$
R^{E,\ell m,\pm}(r) = \frac{k}{\sqrt{v}} h_\ell^\pm(kr)
\tag{33.11}
$$

where $v = k/\mathsf{m}$. The asymptotic behavior of the spherical Hankel functions is $(\mp i)^\ell \mathrm{e}^{\pm ikr}/(kr)$. From this follows that the flux of the above radial functions is indeed normalized to unity as required. Also the sign convention that we use for $R^{E,\ell m,\pm}(r)$ is appropriate because the free waves are indeed given by

$$
\phi^{E,\ell m}(r,\theta,\varphi) = \left[R^{lm-}(r) - R^{lm+}(r)\right] Y^{\ell m}(\theta,\varphi) = -i\frac{k}{\sqrt{v}} 2j_\ell(kr)\, Y^{\ell m}(\theta,\varphi)
\tag{33.12}
$$

This spherical free wave solution is analogous to the planar free wave $|\phi^{E,\Omega}\rangle \mapsto \mathrm{e}^{ik\vec{n}_\Omega \cdot \vec{x}}$. If we decide (without loss of generality) that the planar wave is propagating in the z direction, then we can use the following expansion in order to express a planar wave as a superposition of spherical waves:

$$
\mathrm{e}^{ikz} = \sum_\ell (2\ell+1)\, (i)^\ell\, P_\ell(\cos(\theta))\, j_\ell(kr)
\tag{33.13}
$$

We note that we have only $m = 0$ basis functions because there is no dependence on the angle φ. In different phrasing one may say that a plane wave that propagates in the z direction has $L_z = 0$ angular momentum. Using the identity

$$
Y^{\ell 0} = \sqrt{\frac{2\ell+1}{4\pi}} P_\ell(\cos(\theta))
\tag{33.14}
$$

we can write

$$
\mathrm{e}^{ikz} = \sum_{\ell,m=0} \sqrt{(2l+1)\pi}\, (i)^{\ell+1} \frac{\sqrt{v}}{k}\, \phi^{E,\ell,m}(r,\theta,\varphi)
\tag{33.15}
$$

which makes it easy to identify the ingoing and the outgoing components:

$$(e^{ikz})_{\text{ingoing}} = \sum_{\ell m} A_{\ell m} Y^{\ell m}(\theta, \varphi) R^{\ell m -}(r) \tag{33.16}$$

$$(e^{ikz})_{\text{outgoing}} = -\sum_{\ell m} B_{\ell m} Y^{\ell m}(\theta, \varphi) R^{\ell m +}(r)$$

where

$$B_{\ell m} = A_{\ell m} = \delta_{m,0} \sqrt{(2l+1)\pi} \ (i)^{\ell+1} \ \frac{\sqrt{v}}{k} \tag{33.17}$$

This means that the incident flux in channel $(\ell, 0)$ is simply

$$i_{\text{incident}} = \left[\frac{\pi}{k^2}(2\ell+1)\right] v \tag{33.18}$$

The expression in the square brackets has units of area, and has the meaning of cross section. The actual cross section (see next section) contains an additional factor that express how much of the incident wave is being scattered. The maximum fraction that can be scattered is 400% as explained in the next section.

====== [33.3] The scattered wave, phase shifts, cross section

In the past we were looking for a solution which consists of incident plane wave plus scattered component. Namely,

$$\Psi(r) = e^{ik_0 z} + f(\Omega)\frac{e^{ikr}}{r} \tag{33.19}$$

From the decomposition of the incident plane wave it is implied that the requested solution is

$$\Psi_{\text{incident}} = \sum_{\ell m} A_{\ell m}[R^{\ell m -}(r) - R^{\ell m +}(r)]Y^{\ell m}(\theta, \varphi) \tag{33.20}$$

$$\Psi_{\text{scattered}} = \sum_{\ell m}(A_{\ell m} - B_{\ell m})R^{\ell m +}(r)Y^{\ell m}(\theta, \varphi)$$

where

$$A_{\ell m} = \delta_{m,0} \sqrt{(2l+1)\pi} \ (i)^{\ell+1} \ \frac{\sqrt{v}}{k} \tag{33.21}$$

$$B_{\ell m} = S_{\ell m, \ell' m'} \ A_{\ell' m'}$$

$$(A_{\ell m} - B_{\ell m}) = iT_{\ell m, \ell' m'} \ A_{\ell' m'}$$

Of major interest is the case where the target has spherical symmetry. In such case the S matrix is diagonal:

$$S_{\ell m, \ell' m'}(E) = \delta_{\ell \ell'} \delta_{mm'} \ e^{2i\delta_\ell} \tag{33.22}$$

$$T_{\ell m, \ell' m'}(E) = -\delta_{\ell \ell'} \delta_{mm'} \ e^{i\delta_\ell} \ 2\sin(\delta_\ell)$$

Consequently we get

$$\Psi_{\text{scattered}} = -\sum_{\ell} T_{\ell\ell} \sqrt{(2\ell+1)\pi} \ (i)^{\ell} \ Y^{\ell 0}(\theta, \varphi)h_\ell^+(kr) \quad \sim \quad f(\Omega)\frac{e^{ikr}}{r} \tag{33.23}$$

with

$$f(\Omega) \;=\; -\frac{1}{k}\sum_{\ell}\sqrt{(2\ell+1)\pi}\; T_{\ell\ell}\; Y^{\ell 0}(\theta,\varphi) \tag{33.24}$$

It follows that

$$\sigma_{\text{total}} \;=\; \int |f(\Omega)|^2 d\Omega \;=\; \frac{\pi}{k^2}\sum_{\ell}(2\ell+1)|T_{\ell\ell}|^2 \;=\; \frac{4\pi}{k^2}\sum_{\ell}(2\ell+1)|\sin(\delta_{\ell})|^2 \tag{33.25}$$

By inspection of the scattered wave expression we see that the scattered flux in each of the $(\ell, m{=}0)$ channels can be written as $i_\ell = \sigma_\ell v$, where the partial cross section is

$$\sigma_\ell \;=\; |T_{\ell\ell}|^2 \times \left[(2\ell+1)\frac{\pi}{k^2}\right] \;=\; (2\ell+1)|\sin(\delta_\ell)|^2\,\frac{4\pi}{k^2} \tag{33.26}$$

It is important to realize that the scattered flux can be as large as 4 times the corresponding incident flux. The maximum is attained if the scattering induces a $\pi/2$ phase shift which inverts the sign of the incident wave. In such case the scattered wave amplitude should be twice the incident wave with an opposite sign.

===== [33.4] Finding the phase shift from T matrix theory

We can get expressions for $T_{\ell\ell} = V_{\ell\ell} + (VGV)_{\ell\ell}$ using the Born expansion, and hence to get approximations for the phase shift δ_ℓ and for the partial cross section σ_ℓ. The derivation is the same as in the quasi 1D $\ell{=}0$ case. The flux-normalized free waves are

$$\phi^{E\ell m}(r,\theta,\varphi) \;=\; -i\frac{k}{\sqrt{v}}2j_\ell(kr)Y^{\ell m}(\theta,\varphi) \tag{33.27}$$

The first order result for the phase shift is

$$\delta_\ell^{\text{Born}} \;\approx\; \langle \phi^{E\ell m}|V|\phi^{E\ell m}\rangle \;=\; -\frac{2}{\hbar v}\int_0^\infty V(r)\,(krj_l(kr))^2\,dr \tag{33.28}$$

while in the vicinity of resonances we have

$$\delta_\ell \;=\; \delta_\ell^{bkg} - \arctan\left(\frac{\Gamma_r/2}{E-E_r}\right) \tag{33.29}$$

where δ_ℓ^{bkg} is a slowly varying "background" phase that represent the non-resonant contribution.

There are two physical quantities which are of special interest and can be deduced from the phase shift. One is the time delay that we already have discussed in the quasi one dimensional context. The other is the cross section:

$$\sigma_\ell(E) \;=\; (2\ell+1)\frac{4\pi}{k^2}|\sin(\delta_\ell)|^2 \tag{33.30}$$

For resonant scattering the "line shape" of the cross section versus energy is typically Breit-Wigner and more generally of Fano type. The former is obtained if we neglect δ_ℓ^∞, leading to

$$\sigma_\ell \;=\; (2\ell+1)\frac{4\pi}{k^2}\frac{(\Gamma_r/2)^2}{(E-E_r)^2+(\Gamma_r/2)^2} \tag{33.31}$$

We see that due to a resonance the partial cross section σ_ℓ can attain its maximum value (the so called "unitary limit"). If we take δ_ℓ^∞ into account we get a more general result which is known as Fano line shape:

$$\sigma_\ell \;=\; (2\ell+1)\frac{4\pi}{k^2}\left(\frac{1}{1+q^2}\right)\frac{[\varepsilon+q]^2}{\varepsilon^2+1} \tag{33.32}$$

where $\varepsilon = (E - E_r)/(\Gamma/2)$ is the scaled energy, and $q = -\cot(\delta_\ell^\infty)$ is the so called Fano asymmetry parameter. The Breit-Wigner peak is obtained in the limit $q \to \infty$, while a Breit-Wigner dip (also known as anti-resonance) is obtained for $q = 0$.

======= [33.5] Scattering by a soft sphere

Assuming that we have a soft sphere ($|V|$ is small), we would like to evaluate the phase shift using the Born approximation. Evidently the result makes sense only if the phase shift comes out small ($\delta_\ell \ll 1$). There are two limiting cases. If $ka \ll \ell+1$ we can use the short range approximation of the spherical Bessel function to obtain

$$\delta_\ell^{\text{Born}} \;\approx\; -\frac{2}{(2\ell+3)\left[(2l+1)!!\right]^2}\frac{\mathsf{m}V}{\hbar^2}a^2(ka)^{2\ell+1} \tag{33.33}$$

On the other hand, if $ka \gg \ell+1$ we can use the "far field" asymptotic approximation of the spherical Bessel function which implies $[krj_\ell(kr)]^2 \approx [\sin(kr)]^2 \approx 1/2$. Then we obtain

$$\delta_\ell^{\text{Born}} \;\approx\; -\frac{1}{\hbar v}Va \;\;=\;\; -\frac{\mathsf{m}V}{\hbar^2}a^2(ka)^{-1} \tag{33.34}$$

======= [33.6] Finding the phase shift by matching

We would like to generalize the quasi one-dimensional matching scheme to any ℓ. First we have to find the radial function for $0 < r < a$ and define the logarithmic derivative

$$k_\ell = \left(\frac{1}{R(r)}\frac{dR(r)}{dr}\right)_{r=a} \tag{33.35}$$

Note that we use here $R(r)$ and not $u(r)$ and therefore in the $\ell = 0$ case we get $k_0 = \tilde{k}_0 - (1/a)$. The solution in the outside region is

$$
\begin{aligned}
R(r) \;&=\; Ah_\ell^-(kr) - Bh_\ell^+(kr) \\
&=\; A(h_\ell^-(kr) - \mathrm{e}^{i2\delta_\ell}h_\ell^+(kr)) \\
&=\; C(\cos(\delta_\ell)j_\ell(kr) + \sin(\delta_\ell)n_\ell(kr))
\end{aligned}
\tag{33.36}
$$

We do not care about the normalization because the matching equation involves only logarithmic derivatives:

$$k\frac{\cos(\delta)j' + \sin(\delta)n'}{\cos(\delta)j + \sin(\delta)n} = k_\ell \tag{33.37}$$

solving this equation for $\tan(\delta_\ell)$ we get

$$\tan(\delta_\ell) = -\frac{k_\ell j_\ell(ka) - kj_\ell'(ka)}{k_\ell n_\ell(ka) - kn_\ell'(ka)} \tag{33.38}$$

which can also be written as:

$$\mathrm{e}^{i2\delta_\ell} = \left(\frac{h_\ell^-}{h_\ell^+}\right) \frac{k_\ell - (h_\ell'^-/h_\ell^-)k}{k_\ell - (h_\ell'^+/h_\ell^+)k} \tag{33.39}$$

In order to go from the first expression to the second note that if $\tan(\delta) = a/b$ determines the phase of a complex number $z = a + ib$ then $(a + ib)/(a - ib) = \mathrm{e}^{i2\delta}$. Thus we have expressions for the phase shift given the log derivative of the regular solution on the boundary of the scattering region.

======= [33.7] Scattering by a hard sphere

The phase shifts for a hard sphere ($V \to \infty$) can be found from the phase shift formula of the previous section using $k_\ell \to \infty$, leading to

$$\tan(\delta_\ell^\infty) = -\frac{j_\ell(ka)}{n_\ell(ka)} \tag{33.40}$$

or equivalently

$$\mathrm{e}^{i2\delta_\ell^\infty} = \frac{h_\ell^-(ka)}{h_\ell^+(ka)} \tag{33.41}$$

From the first version it is convenient to derive the result

$$\delta_\ell^\infty \approx -\frac{1}{(2\ell+1)!!(2\ell-1)!!}(ka)^{2\ell+1} \qquad \text{for } \ell \gg ka \tag{33.42}$$

where we have used the short range expansions $j_\ell \propto r^\ell$ and $n_\ell \propto 1/r^{\ell+1}$. From the second version it is convenient to derive the result

$$\delta_\ell^\infty = -\arg(h_\ell^+(ka)) \approx -(ka - \frac{\pi}{2}\ell) \qquad \text{for } \ell \ll ka \tag{33.43}$$

where we have used the asymptotic expression $h_\ell^+ \sim (-\imath)^\ell \, \mathrm{e}^{ikr}/r$.

Small hard sphere: In the case of a small sphere ($ka \ll 1$) we have $1 \gg \delta_0 \gg \delta_1 \gg \delta_2 \dots$ and the $\ell = 0$ cross section is dominant

$$\delta_0 = -(ka) \tag{33.44}$$

Hence

$$\sigma_{\text{total}} = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1)\sin^2(\delta_\ell) \approx \frac{4\pi}{k^2}\sin^2(\delta_0) \approx 4\pi a^2 \tag{33.45}$$

We got a σ that is 4 times bigger than the classical one. The scattering is isotropic because only the $\ell = 0$ component contributes to the scattered wave.

Large hard sphere: Now we turn to the case of a large sphere ($ka \gg 1$). We neglect all δ_ℓ for which $\ell > ka$. For the non-vanishing phase shifts we get

$$\begin{aligned} \delta_\ell &= -(ka) & \text{for } \ell = 0, 2, 4, \dots \\ \delta_\ell &= -(ka) + \tfrac{\pi}{2} & \text{for } \ell = 1, 3, 5, \dots \end{aligned} \tag{33.46}$$

hence

$$
\begin{aligned}
\sigma_{total} &= \frac{4\pi}{k^2}\left(\sum_{\ell=0,2\ldots ka}(2l+1)\sin^2(ka) + \sum_{\ell=1,3\ldots ka}(2l+1)\cos^2(ka)\right) \quad (33.47) \\
&\approx \frac{4\pi}{k^2}\sum_{\ell=0,1\ldots ka}^{\ell=ka}(2l+1)\frac{1}{2} \approx \frac{2\pi}{k^2}\int_0^{ka}2x\,dx = \frac{2\pi}{k^2}(ka)^2 = 2\pi a^2
\end{aligned}
$$

This time the result is 2 times the classical result. The factor of 2 is due to forward scattering which partially cancels the incident wave so as to create a shadow region behind the sphere.

======= [33.8] Summary of results for scattering on a sphere

We have discussed scattering on a "hard sphere", on a "deep well", and on a "soft sphere". Now we would like to put everything together, and to draw an (a, V) diagram for the results in the different regimes. It is useful to notice that there are 3 length-scales that determine the cross-section. These are the radius a of the sphere, the de-Brolie wavelength which is related to $k = (2\mathsf{m}E)^{1/2}$, and a potential-related scale $k_V = (2\mathsf{m}V)^{1/2}$.
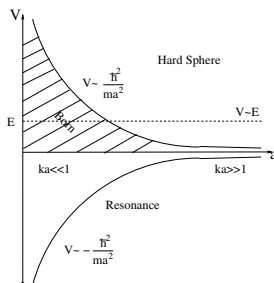
Let us discuss the various regimes in this diagram. It is natural to begin with a small sphere. A small sphere means that the radius is small compared with the De-Broglie wavelength ($ka < 1$). The cross section is dominated by s-scattering ($\ell = 0$), namely, $\sigma_0 = 4\pi\sin^2(\delta_0)/k^2$. We have 3 possible results:

$$
\begin{aligned}
\delta_0^{\text{Hard}} &\approx -(ka) \\
\delta_0^{\text{Born}} &\approx -\frac{2}{3}\left[\frac{\mathsf{m}V}{\hbar^2}a^2\right](ka) \\
\delta_0^{\text{Resonance}} &= \frac{\pi}{2} \quad [\text{unitary limit, diffraction}]
\end{aligned}
$$

We see that the crossover from "soft" to "hard" happens at $V \sim \Delta$ where $\Delta \equiv \hbar^2/(\mathsf{m}a^2)$ is the energy scale that is associated with energy level-spacing in a region of width a. The resonances appear when $V \le E$. If we had equally-spaced resonances, we would get enhanced diffractive scattering for $V = E - n\Delta$.

We now consider the case of a large sphere ($ka \gg 1$). For small impact parameter ($\ell \ll ka$) we have either the Born or the hard sphere approximations:

$$
\begin{aligned}
\delta_\ell^{\text{Hard}} &= \mathcal{O}(1) \\
\delta_\ell^{\text{Born}} &\approx -\frac{V}{\hbar v}a
\end{aligned}
$$

Comparing these expressions, we see that the crossover from "hard" to "soft" happens at $|V| \sim v/a$. For $V \le E$ we expect to see fluctuations due to the merging of resonances. On the average a large sphere with very negative V is not much different from a large sphere with very positive V. In both cases the wavefunction is expelled from the scattering region.

QM in Practice (part I)

[34] Overview of prototype model systems

Below we consider some simple one-particle closed systems in 0D/1D/2D/3D. Later we further illuminate and analyze some prototype problems.

Discrete site systems: Consider an N site systems. Each site is regarded as a zero dimensional (0D) object, sometimes called "dot". In the condense matter context these are known as "tight binding models". The simplest is the two site ($N = 2$) system. If we want to have non-trivial topology we must consider at least a 3-site ($N = 3$) system. Next we can construct N-site chains, or rings or networks or so called tight-binding arrays. If we regard these models as a coarse grained description of motion in free space, then the hopping amplitude per unit time between two nearby sites i and j is determined by the mass of the particle (m) and by the hopping distance (a):

$$K_{ij} \quad = \quad -\frac{1}{2\mathsf{m}a^2} \tag{34.1}$$

Network systems: A one dimensional (1D) segment can be regarded as the continuum limit of a 1D chain. If the particle in confined between two ends, the model is know as "infinite well" or as 1D box with hard walls. If there are periodic boundary conditions, the model is know as "1D ring". Several "1D boxes" can be connected into a network: each 1D segment is called "bond", and the junctions are called "vortices". The simplest is a "delta junction" that connects two wires: If we regard the junction as a barrier $u\delta(x)$ the coupling between wire wavefunctions is

$$U_{nm} \quad = \quad -\frac{1}{4\mathsf{m}^2 u} \left[\frac{d\psi^{(n)}}{dr}\right]_0 \left[\frac{d\psi^{(m)}}{dr}\right]_0 \tag{34.2}$$

An unconnected endpoint of a 1D segment can be regarded as "hard wall". If this hard wall can be displaced, it can be regarded as a "piston". The perturbation due to a small displacement dL is

$$W_{nm} \quad = \quad -\frac{dL}{2\mathsf{m}} \left[\frac{d\psi^{(n)}}{dr}\right]_0 \left[\frac{d\psi^{(m)}}{dr}\right]_0 \tag{34.3}$$

1D systems: In the more general class of 1D systems the confining potential is not stepwise, but changes smoothly. The simplest example is "a well with soft walls", such as the harmonic oscillator, where the potential is $V(x) = x^2$. The prototype example for anharmonic potential, with a dividing separatrix in phase space, is the pendulum where $V(x) = \cos(x)$.

2D systems: Genuine 2D systems are chaotic. If the potential floor is flat, and the walls are "hard", they are called "billiards". These serve as prototype models for "quantum chaos" studies. But if the system has (say) rectangular or cylindrical symmetry then the problem reduces back to 1D.

3D systems: Genuine 3D systems are rarely considered. Typically people consider models with spherical symmetry (e.g. the Hydrogen atom) where the problem is reduced to 1D, while the perturbations that do not respect the high symmetry are treated using a few-level approximation.

Interacting particles: The treatment of non-interacting system with Bosons or with Fermions reduces to one-particle analysis. In order to have new physics we have to take into account interactions. The prototype models (Kondo / Hubburd) assume that the interaction is of the type $U \propto (\hat{n} - 1)\hat{n}$ where $\hat{n} = a_1^\dagger a_1$ is the simplest non-trivial possibility in the case of Bosons, while $\hat{n} = a_1^\dagger a_1 + a_2^\dagger a_2$ is the simplest non-trivial possibility in the case of Fermions.

System-bath models: If we have few distinguished degrees of freedom that we call "system", and all the other degrees of freedoms form a weakly coupled background that we call "environment", then there is a sense in using a system-bath model in order to describe the (reduced) dynamics of the system. Typically the environment is characterized by its fluctuations, and then modeled as a large collection of harmonic oscillators.

[35] Discrete site systems

Two site model.– The simplest non-trivial network that we can imagine is of course a two site system. Without loss of generality we can write the Hamiltonian with a real hopping amplitude c, namely,

$$\mathcal{H} = \begin{pmatrix} \epsilon/2 & c \\ c & -\epsilon/2 \end{pmatrix} \quad = \quad \frac{\epsilon}{2}\sigma_z + c\sigma_x \quad = \quad \vec{\Omega} \cdot \vec{S} \tag{35.1}$$

where $\vec{\Omega} = (2c, 0, \epsilon)$. We can define the occupation operator of (say) the first site as

$$\hat{\mathcal{N}}_1 \quad \equiv \quad |1\rangle\langle 1| \quad \equiv \quad \frac{1}{2}(1 + \sigma_z) \tag{35.2}$$

The definition of the current that comes out from this site is implied by the "rate of change formula", namely

$$\hat{\mathcal{I}}_{1 \to 2} \quad \equiv \quad -i[\mathcal{H}, \mathcal{N}_1] \quad = \quad -c\sigma_y \tag{35.3}$$

So we have the continuity equation

$$\frac{d}{dt}\langle\hat{\mathcal{N}}_1\rangle \quad = \quad -\langle\hat{\mathcal{I}}_{1 \to 2}\rangle, \qquad\qquad \langle\hat{\mathcal{N}}_1\rangle = |\psi_1|^2, \qquad\qquad \langle\hat{\mathcal{I}}_{1 \to 2}\rangle = 2c\,\mathrm{Im}[\psi_2^*\psi_1] \tag{35.4}$$

General site model.– The generalization from a two site system to an N site system is straightforward. Assuming that the one-particle Hamiltonian in the standard (position) basis is represented by a matrix H_{ij}, we define occupation operators and current operators as follow:

$$\hat{\mathcal{N}}_i \quad \equiv \quad |i\rangle\langle i| \tag{35.5}$$

$$\hat{\mathcal{I}}_{i \to j} \quad \equiv \quad -i\Big[|j\rangle H_{ji}\langle i| - |i\rangle H_{ij}\langle j|\Big] \tag{35.6}$$

so as to have the continuity equation

$$\frac{d}{dt}\langle\hat{\mathcal{N}}_i\rangle \quad = \quad -\sum_j \langle\hat{\mathcal{I}}_{i \to j}\rangle \tag{35.7}$$

Chain model.– Of particular important is the the standard tight binding model where we have a chain of N sites with near neighbor hopping. For simplicity we assume periodic boundary conditions, which is like saying that we have a closed ring. We also use length units such that the sites are positioned at $x = 1, 2, 3....$ The Hamiltonian, with real hopping amplitudes $-c$, can be written as

$$\mathcal{H} \quad = \quad -c(\hat{D} + \hat{D}^{-1}) + V(\hat{x}) \quad = \quad -2c\cos(\hat{p}) + V(\hat{x}) \tag{35.8}$$

where D is the one site displacement operator. The definition of the velocity operator is implied by the "rate of change formula", namely

$$\hat{v} \quad = \quad i[\mathcal{H}, \hat{x}] \quad = \quad ic(\hat{D} - \hat{D}^{-1}) \quad = \quad 2c\sin(p) \tag{35.9}$$

Note that for small velocities we have linear dispersion relation $v = (1/\mathsf{m})p$, where the mass is $\mathsf{m} = 1/(2c)$. If distance between the sites were a rather then unity one would conclude the identification $c = 1/(2\mathsf{m}a^2)$.

Lattices.– It is interesting to consider a generalizations of the simple chain model, where the motion is on a lattice. For example: the case of 1D chain with alternating lattice constant $(a, b, a, b, ...)$. In the latter case we get two energy bands rather than one. For further information consult textbooks on Solid State Physics.

[36] Two level dynamics

═══════ [36.1] Bloch sphere picture of the dynamics

The most general Hamiltonian for a particle with spin $\frac{1}{2}$ is:

$$\mathcal{H} \;=\; \vec{\Omega} \cdot \vec{S} = \Omega_x S_x + \Omega_y S_y + \Omega_z S_z \tag{36.1}$$

where $\vec{S} = \frac{1}{2}\vec{\sigma}$. The evolution operator is:

$$U(t) \;=\; \mathrm{e}^{-it\hat{\mathcal{H}}} \;=\; \mathrm{e}^{-i(\vec{\Omega}t)\cdot\vec{S}} \;=\; R(\vec{\Phi}(t)) \tag{36.2}$$

where $\vec{\Phi}(t) = \vec{\Omega}t$. This means that the spin makes precession. It is best to represent the state of the spin using the polarization vector $\vec{M}$. Then we can describe the precession using a classical-like, so called "Bloch sphere picture". The formal derivation of this claim is based on the relation between $M(t)$ and $\rho(t)$. We can write it either as $M(t) = \mathsf{trace}(\sigma\rho(t))$ or as an inverse relation $\rho(t) = (1 + \vec{M}(t)\cdot\sigma)/2$. In the former case the derivation goes as follows:

$$\begin{aligned} M_i(t) &\;=\; \mathsf{trace}(\sigma_i \rho(t)) = \mathsf{trace}(\sigma_i(t)\rho) \\ &\;=\; \mathsf{trace}((R^{-1}\sigma_i R)\rho) = \mathsf{trace}((R^E_{ij}\sigma_j)\rho) = R^E_{ij}(\Phi(t))\ M_j(0) \end{aligned} \tag{36.3}$$

where we have used the evolution law $\rho(t) = U(t)\rho(0)U(t)^{-1}$ and the fact that $\vec{\sigma}$ is a vector operator.

We notice that the evolution of any system whose states form a dim=2 Hilbert space can always be described using a precession picture. The purpose of the subsequent exposition is (i) to show the power of the precession picture as opposed to diagonalization; (ii) To explain the notion of small versus large perturbations. With appropriate gauge of the standard basis the Hamiltonian can be written as:

$$\mathcal{H} \;=\; \begin{pmatrix} \epsilon/2 & c \\ c & -\epsilon/2 \end{pmatrix} \;=\; \frac{\epsilon}{2}\sigma_z + c\sigma_x \;=\; \vec{\Omega}\cdot\vec{S}, \qquad\qquad \vec{\Omega} = (2c, 0, \epsilon) \tag{36.4}$$

In the case of a symmetric system ($\epsilon = 0$) we can find the eigenstates and then find the evolution by expanding the initial state at that basis. The frequency of the oscillations equals to the energy splitting of the eigen-energies. But once ($\epsilon \neq 0$) this scheme becomes very lengthy and intimidating. It turns out that it is much much easier to use the analogy with spin 1/2. Then it is clear, just by looking at the Hamiltonian that the oscillation frequency is

$$\Omega \;=\; \sqrt{(2c)^2 + \epsilon^2} \tag{36.5}$$

and hence the eigenenergies are $E_\pm = \pm\Omega/2$. Furthermore, it is clear that the precession axis is tilted relative to the z axis with an angle

$$\theta \;=\; \arctan(2c/\epsilon) \tag{36.6}$$

Accordingly the eigenstates can be obtained from the $\uparrow$ and from the $\downarrow$ states by rotating them an angle θ around the y axis:

$$|+\rangle = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2) \end{pmatrix}, \qquad\qquad |-\rangle = \begin{pmatrix} -\sin(\theta/2) \\ \cos(\theta/2) \end{pmatrix} \tag{36.7}$$

If we are interested in studying the dynamics there is no need to expand the initial state at this basis. It is much easier to use write the explicit expression for the evolution operator:

$$U(t) \;=\; R(\vec{\Phi}(t)) \;=\; \cos(\Omega t/2) - i\sin(\Omega t/2)\Big[\cos\theta\ \boldsymbol{\sigma}_z + \sin\theta\ \boldsymbol{\sigma}_x\Big] \tag{36.8}$$

Let us assume that initially the system is in the "up" state. We get that the state after time t is

$$|\psi(t)\rangle \;=\; U(t)|\uparrow\rangle \;=\; \left[\cos(\Omega t/2) - i\cos\theta\sin(\Omega t/2)\right]|\uparrow\rangle - i\left[\sin\theta\sin(\Omega t/2)\right]|\downarrow\rangle \tag{36.9}$$

Let us define $P(t)$ as the probability to be found after time t in the same state. Initially we have $P(0) = 1$. We can easily find the explicit expression for $P(t)$ without having to do any diagonalization of the Hamiltonian. Rather we exploit the explicit expression above and get

$$P(t) \;=\; \left|\langle\uparrow|\psi(t)\rangle\right|^2 \;=\; 1 - \sin^2(\theta)\sin^2\left(\frac{\Omega t}{2}\right) \tag{36.10}$$

This result is called the Rabi Formula. We see that in order to have nearly complete transitions to the other site after half a period, we need a very strong coupling ($c \gg \epsilon$). In the opposite limit ($c \ll \epsilon$) the particle tends to stay in the same site, indicating that the eigenstates are barely affected.

We note that the Rabi Formula can be optionally derived by considering the precession of the polarization vector $M(t)$. This procedure is on the one hand more illuminating, but on the other requires better geometrical insight: One should realize that the inclination angle of $M(t)$ oscillates between the values 0 and 2θ. Therefore $M_z(t)$ oscillates between the maximal value $M_z = 1$ and the minimal value $M_z = \cos(2\theta)$. Using the relation $P(t) = (1 + M_z(t))/2$ one concludes that $P(t)$ oscillates with the frequency Ω between the maximal value 1 and the minimal value $(\cos(\theta))^2$ leading to the Rabi Formula.

══════ [36.2] Landau-Zener dynamics

A prototype adiabatic process is the Landau-Zener crossing of two levels. The Hamiltonian is

$$\mathcal{H} \;=\; \frac{1}{2}\begin{pmatrix} \alpha t & \kappa \\ \kappa & -\alpha t \end{pmatrix} \;=\; \frac{1}{2}\alpha t \sigma_3 + \frac{1}{2}\kappa\sigma_1 \tag{36.11}$$

Let us assume that the system is prepared at $t = -\infty$ in the lower ("-") level (which is the "up" state). We want to find what is the probability to find the system at $t = \infty$ in the upper ("+") level (which is again the "up" state!). The exact result is know as the Landau-Zener formula:

$$P_{\text{LZ}} \;=\; P_\infty(+|-) \;=\; P_\infty(\uparrow\,|\,\uparrow) \;=\; \exp\left[-\frac{\pi}{2}\frac{\kappa^2}{\alpha}\right] \tag{36.12}$$

Exact solution.– The straightforward way to derive this formula is to sum the Texp terms up to infinite order:

$$\langle\uparrow|U(t,t_0)|\uparrow\rangle = \; e^{-i\frac{\alpha}{4}(t^2 - t_0^2)} \;+\; \iint_{t_0 < t_1 < t_2 < t} dt_2 dt_1 \; \left(-i\frac{\kappa}{2}\right)^2 e^{-i\frac{\alpha}{4}\left((t^2 - t_2^2) - (t_2^2 - t_1^2) + (t_1^2 - t_0^2)\right)}$$

$$+ \iint\iint dt_4 dt_3 dt_2 dt_1 \; \left(-i\frac{\kappa}{2}\right)^4 e^{-i\frac{\alpha}{4}\left((t^2 - t_4^2) - (t_4^2 - t_3^2) + (t_3^2 - t_2^2) - (t_2^2 - t_1^2) + (t_1^2 - t_0^2)\right)} \;+\; \cdots \tag{36.13}$$

where time ordering of the integration variables is required. Each term represent a sequence of spin flips that are induced by the perturbation. Obviously only even orders appear in the calculation of $P(\uparrow\,|\,\uparrow)$. Dropping phase factor, rescaling the time variables, and taking the integration limits to infinity we get

$$\langle\uparrow|U(t,t_0)|\uparrow\rangle \;=\; \sum_{n=0}^{\infty}\left(-i\frac{\kappa}{2}\frac{1}{\sqrt{\alpha}}\right)^{2n} \iint\cdots\iint dt_{2n}\cdots dt_1 \; \exp\left[-\frac{i}{2}\left(t_1^2 - t_2^2 + t_3^2\cdots - t_{2n}^2\right)\right] \tag{36.14}$$

Following Kayanuma [Appendix] we note that the time-ordered integral can be calculated using the following trick: the nth term can be regarded as describing a train of n pulses; New integration variables $\tau_j = t_{2j} - t_{2j-1}$ and $\tilde{t}_j$ are

defined; The τ_j is the length of the pulse and the $\tilde{t}_j$ is its reduced time; The latter is the value of t_j if the pulses were of zero length. Consequently one obtains integrals that are symmetric under time permutation, and can be factorized into elementary Gaussian integrals, leading to $\pi^n/n!$. Thus we get

$$\langle \uparrow |U(t,t_0)| \uparrow \rangle \;\; = \;\; \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{\pi}{4} \frac{\kappa^2}{\alpha} \right)^n \;\; = \;\; \exp\left[-\frac{\pi}{4} \frac{\kappa^2}{\alpha} \right] \tag{36.15}$$

For pedagogical purpose we consider below the standard procedures for obtaining *approximations* for the Landau-Zener formula.

Diabatic approximation.– For a "fast" sweep, aka diabatic process, the problem can be treated using conventional (fixed basis) perturbation theory. The first order result requires the calculation of $p = |\langle \downarrow |U(t,t_0)| \uparrow \rangle|^2$. Performing the time integration one obtains $p \approx (\pi/2)[\kappa^2/\alpha]$, in consistency with the leading order term in the expansion of P_{LZ}. Optionally the same result is obtained from the Schrodinger equation for the amplitude $c_\downarrow(t)$ in the interaction picture:

$$\frac{dc_\downarrow(t)}{dt} \;\; = \;\; -i\frac{\kappa}{2} \exp\left[-i\frac{1}{2}\alpha t^2 \right] c_\uparrow(t) \tag{36.16}$$

Setting $c_\uparrow(t) \mapsto 1$ and performing the time integration, one obtains the same first order estimate for p.

Adiabatic approximation.– In order to analyze the Landau-Zener transition in the adiabatic regime we write the Schrodinger equation in the adiabatic basis, and write the analogous equation for the amplitude $c_+(t)$. The instantaneous eigenenergies are $E_\pm = \pm(1/2)\Omega$, with

$$\Omega(t) = \sqrt{(\alpha t)^2 + \kappa^2} \tag{36.17}$$

and the associated eigenstates are $|+\rangle$ and $|-\rangle$, as defined in the previous section, with

$$\theta(t) \;\; = \;\; \arctan\left(\kappa/(\alpha t) \right). \tag{36.18}$$

Note that $\theta = \pi$ at $t = -\infty$ evolves to $\theta = 0$ at $t = \infty$. In our choice of gauge the adiabatic eigenstates have real amplitudes, and therefore the Berry "vector potential" comes out zero. At the same time the non-zero element of the perturbation matrix W_{nm} is

$$W_{+-} \;\; = \;\; i\frac{\alpha}{E_+ - E_-} \left[\frac{1}{2}\sigma_3 \right]_{+-} \;\; = \;\; -i\frac{\alpha \sin(\theta)}{2\Omega} \;\; = \;\; -i\frac{\alpha\kappa}{2\Omega^2} \;\; = \;\; -\frac{i}{2}\frac{\alpha}{\kappa}\left[\frac{1}{(\alpha t/\kappa)^2 + 1} \right] \tag{36.19}$$

Following the standard procedure as in time-dependent perturbation theory we substitute

$$a_\pm(t) \;\; = \;\; c_\pm(t) \, \exp\left[-i \int^t E_\pm dt' \right] \tag{36.20}$$

Using the rescaled variable $\tau = \alpha t/\kappa$, and changing to $\tau = \sinh(z)$, the expression for the dynamical phase is

$$\Phi(t) \;\; = \;\; \frac{\kappa^2}{\alpha} \int^\tau d\tau \sqrt{\tau^2 + 1} \;\; = \;\; \frac{\kappa^2}{\alpha} \times \frac{1}{2}\left(z + \frac{1}{2}\sinh(2z) \right) \tag{36.21}$$

Thus for the amplitude $c_+(t)$ we get the equation

$$\frac{dc_+(t)}{dt} \;\; = \;\; -\frac{1}{2}\frac{\alpha}{\kappa}\left[\frac{1}{(\alpha t/\kappa)^2 + 1} \right] e^{i\Phi(t)} c_-(t) \tag{36.22}$$

Starting with the zero order solution ($c_-(t) \mapsto -1$), and performing the time integration, one obtains the first order adiabatic estimate for the amplitude $c_+(t)$, leading to

$$P_{\text{LZ}} \approx \left| \frac{1}{2} \int_{-\infty}^{\infty} \frac{1}{\tau^2 + 1}\, e^{i\Phi(\tau)} d\tau \right|^2 = \left| \frac{1}{2} \int_{-\infty}^{\infty} \frac{1}{\cosh(z)}\, e^{i\Phi(z)} dz \right|^2 \tag{36.23}$$

In order to evaluate this integral one can use contour integration. The explicit expression for the phase Φ as a function of $z = x + iy$ is

$$\Phi(z) = \frac{\kappa^2}{\alpha} \times \frac{1}{2} \left[\left(x + \frac{1}{2}\sinh(2x)\cos(2y) \right) + i \left(y + \frac{1}{2}\cosh(2x)\sin(2y) \right) \right] \tag{36.24}$$

The original contour of integration is $y = 0$, but we would like to deform it into the complex plane so as to get rid of the rapid oscillations of the phase factor, and have instead a smooth monotonic variation. The details can be found in section VI of [arXiv]. The deformed contour is displayed in Fig4 there. The phase is pure imaginary along the curves C_- and C_+. At $z_0 = 0 + i(\pi/2)$ we have $\Phi = i(\pi/4)\kappa^2/\alpha$, while $\cosh z \approx i(z - z_0)$. Consequently we have a pole leading to the same exponent as in the Landau-Zener result. The prefactor come out $(\pi/3)^2$. The derivation of the correct prefactor, which is unity, requires either exact solution of the differential equation using parabolic cylinder functions, or otherwise iterations of the above procedure to infinite order.

===== [36.3] Adiabatic transfer from level to level

A practical problem which is encountered in Chemical Physical applications is how to manipulate coherently the preparation of a system. Let us as assume that an atom is prepared in level $|E_a\rangle$ and we want to have it eventually at level $|E_b\rangle$. We have in our disposal a laser source. This laser induce AC driving that can couple the two levels. The frequency of the laser is ω and the induced coupling is Ω. The detuning is defined as $\delta = \omega - (E_b - E_a)$. Once the laser is turned "on" the system starts to execute Bloch oscillation. The frequency of these oscillation is $\tilde{\Omega} = (\Omega^2 + \delta^2)^{1/2}$. This is formally like the coherent oscillations of a particle in a double well system. Accordingly, in order to simplify the following discussion we are going to use the terminology of a site-system. Using this terminology we say that with a laser we control both the energy difference δ and the coupling Ω between the two sites.

By having exact resonance ($\delta = 0$) we can create "complete" Bloch oscillations with frequency Ω. This is formally like the coherent oscillations of a particle in a symmetric double well system. In order to have 100% transfer from state $|E_a\rangle$ to state $|E_b\rangle$ we have to keep $\delta = 0$ for a duration of exactly half period ($t = \pi/\Omega$). In practice this is impossible to achieve. So now we have a motivation to find a practical method to induce the desired transfer.

There are two popular methods that allow a robust 100% transfer from state $|E_a\rangle$ to state $|E_b\rangle$. Both are based on an adiabatic scheme. The simplest method is to change δ gradually from being negative to being positive. This is called "chirp". Formally this process is like making the two levels "cross" each other. This means that a chirp induced transfer is just a variation of the Landau-Zener transition that we have discussed in the previous section.

There is another so called "counter intuitive scheme" that allows a robust 100% transfer from state $|E_a\rangle$ to state $|E_b\rangle$, which does not involve a chirp. Rather it involves a gradual turn-on and then turn-off of two laser sources. The first laser source should couple the (empty) state $|E_b\rangle$ to a third level $|E_c\rangle$. The second laser source should couple the (full) state $|E_a\rangle$ to the same third level $|E_c\rangle$. The second laser is tuned on while the first laser it turned off. It is argued in the next paragraph that this scheme achieves the desired transfer. Thus within the framework of this scheme it looks as if a transfer sequence $a \mapsto c \mapsto b$ is realized using a counter intuitive sequence $c \mapsto b$ followed by $a \mapsto c$.

The explanation of the "counter intuitive scheme" is in fact very simple. All we have to do is to draw the adiabatic energy levels $E_-(t)$ and $E_0(t)$ and $E_+(t)$ as a function of time, and then to figure out what is the "identity" of (say) the middle level at each stage. Initially only the first laser in "on" and therefore $|E_b\rangle$ and $|E_c\rangle$ split into "even" and "odd" superpositions. This means that initially $E_0(t)$ corresponds to the full state $|E_a\rangle$. During the very slow switching process an adiabatic evolution takes place. This means that the system remains in the middle level. At the end of the process only the second laser is "on" and therefore, using a similar argumentation, we conclude that $E_0(t)$ corresponds to the state $|E_b\rangle$. The conclusion is that a robust 100% transfer from state $|E_a\rangle$ to state $|E_b\rangle$ has been achieved.

[37] A few site system with Bosons

Formally, we can regard a Bosonic site as an Harmonic mode. With each site ($j = 1, ..., L$) we can associate a creation operator $\boldsymbol{a}_j^\dagger$, and an occupation operator $\boldsymbol{n}_j = \boldsymbol{a}_j^\dagger \boldsymbol{a}_j$. A double well system with Bosons has formally the same Hilbert space as that of spin $N/2$ particle. This will be discussed in details below. The generalization of this statement for an L site system is straightforward, as discussed in the following paragraph.

The one particle states form an L dimensional Hilbert space. The set of unitary transformations within this space is the $SU(L)$ group. Let us call these transformation generalized "rotations". If we have N particles in L sites then the dimensionality of Hilbert space is

$$\mathcal{N} \;\; = \;\; \frac{(N{+}L{-}1)!}{(L{-}1)!(N{+}L{-}1)!} \tag{37.1}$$

For the $L = 2$ system we have $\mathcal{N} = N{+}1$ basis states $|n_1, n_2\rangle$ with $n_1 + n_2 = N$. We can "rotate" the whole system using $\dim(N)$ matrices. Thus we obtain a $\dim(N)$ representation of the $SU(L)$ group. By definition these "rotations" can be expressed as a linear combination of the $SU(L)$ generators J_μ, and they all commute with $\hat{N}$. The manybody Hamiltonian $\mathcal{H}$ may contain "non linear" terms such as J_μ^2 that correspond to interactions between the particles. Accordingly $\mathcal{H}$ of an interacting system is not merely a "rotation".

═══════ [37.1] A two site system with N Bosons

We discuss in what follows the Bose-Hubbard Hamiltonian for N Bose particles in a two site system. Defining $s = N/2$ we shall see that the Hamiltonian can be regarded as describing a spin entity. The dimension of the Hilbert space is $\mathcal{N} = N + 1 = 2s + 1$. Later we assume $N \gg 1$. The Hamiltonian is

$$\mathcal{H} \;\; = \;\; \sum_{j=1,2} \left[\mathcal{E}_j \boldsymbol{n}_j + \frac{U}{2}(\boldsymbol{n}_j - 1)\boldsymbol{n}_j \right] - \frac{K}{2}(\boldsymbol{a}_2^\dagger \boldsymbol{a}_1 + \boldsymbol{a}_1^\dagger \boldsymbol{a}_2) \tag{37.2}$$

where K represents the hopping, and U is the interaction, and $\mathcal{E} = \mathcal{E}_2 - \mathcal{E}_1$ is the potential bias. The total number of particles $n_1 + n_2 = N$ is constant of the motion. the dimensionless parameters of the model are

$$u \equiv \frac{NU}{K}, \qquad\qquad \varepsilon \equiv \frac{\mathcal{E}}{K} \tag{37.3}$$

These are the parameters that appear in the *classical* equations of motion after proper re-scaling of the units. In the full quantum treatment $1/N$ plays the role of dimensionless Plank constant. This becomes transparent if we adopt action-angle variables $(\boldsymbol{n}_j, \boldsymbol{\varphi}_j)$, that are defined via $\boldsymbol{a}_j = \sqrt{n_j}e^{i\varphi_j}$, and write the equation of motion with the re-scaled variables $\tilde{n}_j := n_j/N$. In the quantum context $e^{i\varphi_j}$ can be regarded as a defected translation operator, namely,

$$\boldsymbol{a}_j \;\; = \;\; \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix} \;\; = \;\; \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \sqrt{1} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{3} \end{pmatrix} \;\; = \;\; e^{i\varphi_j}\sqrt{\boldsymbol{n}_j} \tag{37.4}$$

The occupation space is truncated at $n = 0$, therefore $e^{i\varphi_j}$ annihilates the ground state, and accordingly it is not a unitary operator. However, if our interest is focused on dynamics in large n regions, this issue becomes insignificant.

The Hamiltonian for a given N is formally equivalent to the Hamiltonian of a spin $s = N/2$ entity. Defining

$$S_z \;\; \equiv \;\; \frac{1}{2}(\hat{n}_1 - \hat{n}_2) \;\; \equiv \;\; \boldsymbol{n} \tag{37.5}$$

$$S_+ \;\; \equiv \;\; \hat{a}_1^\dagger \hat{a}_2 \tag{37.6}$$

we can re-write the Hamiltonian as

$$\mathcal{H} \;=\; U\hat{S}_z^2 - \mathcal{E}\hat{S}_z - K\hat{S}_x + \text{const} \tag{37.7}$$

In the absence of interaction this is like having a spin in magnetic field with precession frequency $\Omega = (K, 0, \mathcal{E})$. More generally, in order to analyze the dynamics it is useful to to treat the Hamiltonian as classical. From the Poisson brackets of $\mathcal{H}$ with S_j one derives equations of motion for the Bloch vector. Both N and the energy E are constant of motion, and therefore the generated trajectories are along $\mathcal{H}(S_x, S_y, S_z) = E$ contours of the Bloch sphere $S_x^2 + S_y^2 + S_z^2 \equiv (N/2)^2$. Assuming for simplicity that $\mathcal{E} = 0$, one realizes that for $NU > K$ the $S_x = -N/2$ fixed-point becomes unstable, and a separatrix appears as in the following illustration. Consequently, the upper-energy states exhibit self-trapping, as opposed to the low-energy region, around $S_x = N/2$, where Rabi-like oscillations are observed.
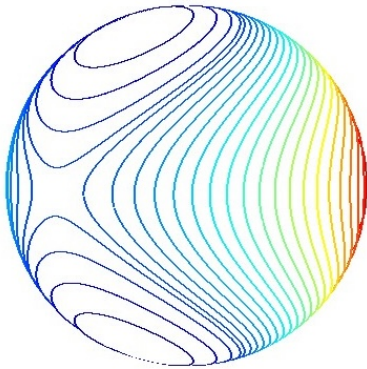
In order to further analyze the dynamics for finite U, it is more convenient to re-write the Hamiltonian with canonically conjugate variables $\hat{n}$ and $\varphi \equiv \varphi_1 - \varphi_2$. Using a classical perspective, or ignoring negligible commutation error, the Hamiltonian takes the following from

$$\mathcal{H} \;=\; U\boldsymbol{n}^2 \;-\; \mathcal{E}\boldsymbol{n} \;-\; K\sqrt{(N/2)^2 - \boldsymbol{n}^2}\,\cos(\boldsymbol{\varphi}) \tag{37.8}$$

In the $n \sim 0$ region of phase space $\mathcal{H}$ resembles the so-called Josephson Hamiltonian, which is formally the Hamiltonian of a mathematical pendulum

$$\mathcal{H}_{\text{Josephson}} \;=\; E_C(\boldsymbol{n} - n_0)^2 \;-\; E_J\cos(\boldsymbol{\varphi}) \tag{37.9}$$

with $E_c = U$ and $E_J = KN/2$, while $n_0 = \mathcal{E}/(2U)$. The Josephson Hamiltonian is an over-simplification because it does not capture correctly the global topology of phase space, which is *sphere* and not a *cylinder*. However it correctly captures that Rabi-like oscillation around $\varphi = 0$, and the self trapping outside of the separatrix region.

======= [37.2] An L site chain with N Bosons

Consider bosons in a 1D chain of length L with periodic boundary conditions. The Hamiltonian is

$$\mathcal{H} \;=\; \sum_{j=1}^{L}\left[\frac{U}{2}\boldsymbol{a}_j^\dagger\boldsymbol{a}_j^\dagger\boldsymbol{a}_j\boldsymbol{a}_j - \frac{K}{2}\left(\boldsymbol{a}_{j+1}^\dagger\boldsymbol{a}_j + \text{h.c.}\right)\right] \tag{37.10}$$

Here K is the hopping frequency, U is the on-site interaction, and $j \bmod(L)$ labels the sites $x_j = j$, where the lattice constant is chosen as the unit length. If we treat this Hamiltonian as classical, we can derive from it equations of motions that are known as the discrete non-linear Schrodinger (DNLS) equation, or as the discrete Gross-Pitaevskii equation. Namely,

$$i\frac{da_j}{dt} \;=\; \left(\mathcal{E}_j + U|a_j|^2\right)a_j - \frac{K}{2}\left(a_{j+1} + a_{j-1}\right) \tag{37.11}$$

Optionally we can define creation operators in the momentum representation

$$\boldsymbol{b}_k^\dagger \quad = \quad \frac{1}{\sqrt{L}} \sum_j e^{ikx_j}\, \boldsymbol{a}_j^\dagger \tag{37.12}$$

Then the Hamiltonian takes the form

$$\mathcal{H} \quad = \quad \sum_k \epsilon_k \boldsymbol{b}_k^\dagger \boldsymbol{b}_k \ + \ \frac{U}{2L} \sum_{\langle k_1..k_4 \rangle} \boldsymbol{b}_{k_4}^\dagger \boldsymbol{b}_{k_3}^\dagger \boldsymbol{b}_{k_2} \boldsymbol{b}_{k_1} \tag{37.13}$$

Here $\epsilon_k = -K\cos(k)$, and the summation is over all the k values that satisfy $k_1 + k_2 = k_3 + k_4 \mod(L)$.

Consider condensation of N particles in the $k{=}0$ momentum orbital:

$$|\Psi^{(0)}\rangle \quad = \quad \frac{1}{\sqrt{N!}} \left(\boldsymbol{b}_0^\dagger\right)^N |0\rangle \tag{37.14}$$

The number of particle is constant of motion and therefore we can substitute in the kinetic part of the Hamiltonian $\boldsymbol{b}_0^\dagger \boldsymbol{b}_0 = N - \sum \boldsymbol{b}_k^\dagger \boldsymbol{b}_k$. In the vicinity of $\Psi^{(0)}$ we can further simplify the interaction part of the Hamiltonian. The "largest" term $\boldsymbol{b}_0^\dagger \boldsymbol{b}_0^\dagger \boldsymbol{b}_0 \boldsymbol{b}_0$ is merely a constant and can be dropped. Terms of the type $\boldsymbol{b}_k^\dagger \boldsymbol{b}_0^\dagger \boldsymbol{b}_0 \boldsymbol{b}_k \approx N \boldsymbol{b}_k^\dagger \boldsymbol{b}_k$ can be absorbed into the kinetic part. The justification for $\boldsymbol{b}_0^\dagger \boldsymbol{b}_0 \approx N$ in the vicinity of the ground state is as follows: we inspect the matrix representation of $\mathcal{H}$ in the orbital-Fock basis; and we realized that the replacement $\sqrt{n_0} \mapsto \sqrt{N}$ implies $\mathcal{O}(1/N)$ error that can be neglected. Additionally, we have to keep the leading non-trivial terms in the interaction which involve creation or destruction of pairs. Consequently, we approximate the Hamiltonian by a quadratic form

$$\mathcal{H}_0 \quad = \quad \sum_{k \neq 0} \varepsilon_k \boldsymbol{b}_k^\dagger \boldsymbol{b}_k \ + \ \Delta \sum_{q>0} \left(\boldsymbol{b}_{-q}^\dagger \boldsymbol{b}_{+q}^\dagger + \boldsymbol{b}_{-q} \boldsymbol{b}_{+q} \right) \tag{37.15}$$

where

$$\varepsilon_k = (\epsilon_k - \epsilon_0) + \Delta, \qquad\qquad \Delta = \frac{NU}{L} \tag{37.16}$$

This Hamiltonian is trivially separable with respect to q, and each term can be diagonalized by the Bogolyubov transformation

$$\boldsymbol{c}_{+q}^\dagger \quad = \quad u\boldsymbol{b}_{+q}^\dagger + v\boldsymbol{b}_{-q} \tag{37.17}$$
$$\boldsymbol{c}_{-q}^\dagger \quad = \quad u\boldsymbol{b}_{-q}^\dagger + v\boldsymbol{b}_{+q} \tag{37.18}$$

The above transformation can be written compactly as $\boldsymbol{c}_q^\dagger = u_q \boldsymbol{b}_q^\dagger + v_q \boldsymbol{b}_{-q}$, with q that can be either positive or negative, where

$$u_q = \cosh(\theta/2), \qquad v_q = \sinh(\theta/2), \qquad \tanh(\theta) = \frac{\Delta}{\varepsilon_q} = \frac{\Delta}{\Delta + (\epsilon_q - \epsilon_0)} \tag{37.19}$$

The Hamiltonian takes the form

$$\mathcal{H}_0 \quad = \quad \sum_{q \neq 0} \omega_q \boldsymbol{c}_q^\dagger \boldsymbol{c}_q \ \equiv \ \sum_{q \neq 0} \omega_q \tilde{\boldsymbol{n}}_q \tag{37.20}$$

where $\tilde{\boldsymbol{n}}_q$ are the occupation operators of the Bogoliubov quasi-particles. The excitation frequencies are

$$
\omega_q \;\; = \;\; \sqrt{\varepsilon_q^2 - \Delta^2} \;\; = \;\; \sqrt{[(\epsilon_q - \epsilon_0) + 2\Delta](\epsilon_q - \epsilon_0)} \tag{37.21}
$$

Note that the $\pm q$ degeneracy is removed if time reversal is broken (rotating ring). The excitation frequencies for small quasi-momentum q are associated with phase-modes that have approximately a linear dispersion relation $\omega_q \approx cq$, and therefore regarded as sound waves (phonons) with velocity $c = \sqrt{NUK/L}$. The ground-state of the Hamiltonian is the product state of having all the excitation modes "empty", meaning $c_q|\text{GS}\rangle = 0$. This equation is easily solved for each mode, and consequently one obtains

$$
|\text{GS}\rangle \;\; \propto \;\; \prod_{q \neq 0} e^{-(v/u)\boldsymbol{b}^\dagger_{-q}\boldsymbol{b}^\dagger_q}|\text{vacuum}\rangle \tag{37.22}
$$

We note that in the analogous treatment for interacting fermions, one obtains the same equations for the BCS ground sate. For Fermionic creation operator A it is customary to expand the exponent as $e^A = 1 + A$ because $A^2 = 0$, and write the product as $\prod[u - v\boldsymbol{b}^\dagger_{-q}\boldsymbol{b}^\dagger_q]$.

════ [37.3] The mean field approximation

Within the framework of the *proper* semiclassical treatment the quantum state is described as a distribution of points in phase space. The *proper* semiclassical treatment propagate those points using the classical equations of motion for the action-variables $\dot{n}_j$ and $\dot{\varphi}_j$. The mean-field approximation further assumes that in any time the state of the system looks like a coherent state. Such a state corresponds to a Gaussian-like distribution is phase space ("minimal wavepacket"). The mean field is defines as follows:

$$
\psi_j \;\; = \;\; \langle \boldsymbol{a}_j \rangle \;\; = \;\; \left\langle \sqrt{n_j} e^{\boldsymbol{\varphi}_j} \right\rangle \;\; \approx \;\; \sqrt{\langle n_j \rangle}\, e^{\langle \boldsymbol{\varphi}_j \rangle} \tag{37.23}
$$

The last approximation is valid as long as the spreading of the "cloud" can be ignored. As U/K is increased beyond a critical value there is a quantum phase transition of the ground-state form Superfluid to Mott insulator. The latter features equal population of the sites (definite values $n_j = N/L$, and associated uncertainty in φ_j), hence $\psi_j = 0$.

In the continuum limit we use the notation $\psi(x)$, and in leading order obtain the Gross-Pitaevskii (GP) equation:

$$
i\frac{d\psi(x)}{dt} \;\; = \;\; \left[V(x) + g_s|\psi(x)|^2 - \frac{1}{2\mathsf{m}}\nabla^2 \right]\psi(x) \tag{37.24}
$$

The potential $V(x)$ corresponds to the $\mathcal{E}_i$ of the DNLS equation, and the inverse mass $1/\mathsf{m}$ reflects the hopping amplitude K. In addition to that we have the interaction parameter g_s that corresponds to U multiplied by the volume of a site. It also can be related to the scattering length using the relation $g_s = 4\pi a_s/\mathsf{m}$.

The ground state of the GP equation is a uniform state that features $|\psi^{(0)}|^2 = \text{const}$. Without loss of generality we set $\psi^{(0)}$ as a real positive number. The GP equation of motion can be linearized around this solution, using the substitution

$$
\psi(x;t) \;\; \equiv \;\; \psi^{(0)} + u(x)e^{-i\omega t} - v(x)^* e^{+i\omega t} \tag{37.25}
$$

The eigen-modes are found. They correspond to the Bogoliubov quasi-particles. We use here the same "sign convention" for v as in the quantum second-quantized treatment. With this convention $v = u$ signifies phase-modes as opposed to $v = -u$ that signifies amplitude modes. Note that Bogoliubov excitations feature $0 < v < u$, and become phase-mode for $q \to 0$, aka Goldstone excitations. The prediction of gapped Higgs amplitude modes requires to go beyond the Bogoliubov approximation. The terms phase/amplitude refer here to the order parameter $\psi(x)$ and not to the density $n(x)$ of the particles. Oscillations of $\psi(x)$ reflect transitions of particles between the condensate and the excited orbitals.

There are various ways to justify the GP equation in a proper quantum perspective. Possibly the most common approach is based on regarding the semiclassical "cloud" as a *coherent state*. This perspective requires further mathematical discussion. We first recall how it is defined for harmonic-oscillator, and then discuss how the concept is generalized in the many-body context.

The harmonic oscillator is described by canonical coordinates (q, p), and one defines destruction operator $\boldsymbol{a}_0 = 2^{-1/2}(\boldsymbol{q} + i\boldsymbol{p})$. The coherent state $\alpha = 2^{-1/2}(\bar{q} + i\bar{p})$ is defined as the phasespace translation $\boldsymbol{D}(\alpha)$ of the ground state $|0\rangle$, namely

$$
\begin{aligned}
\boldsymbol{D}(\alpha) &= e^{-i\bar{q}\boldsymbol{p} + i\bar{p}\boldsymbol{q}} = e^{\alpha \boldsymbol{a}^\dagger - \alpha * \boldsymbol{a}} & (37.26) \\
|\alpha\rangle &= \boldsymbol{D}(\alpha) |0\rangle & (37.27)
\end{aligned}
$$

One can define a destruction operator $\boldsymbol{a}_\alpha = \boldsymbol{a}_0 - \alpha$ around the α phasespace location. In the Heisenberg picture $\boldsymbol{D}^\dagger \boldsymbol{a}_0 \boldsymbol{D} = \boldsymbol{a}_0 + \alpha$, which can equivalently written as $\boldsymbol{D}\boldsymbol{a}_0\boldsymbol{D}^\dagger = \boldsymbol{a}_\alpha$. Considering general time evolution that is generated by some Hamiltonian, the leading semiclassical approximation is analogously written as

$$
\boldsymbol{U}(t) \, \boldsymbol{a}^\dagger_{\alpha(0)} \, \boldsymbol{U}(t)^\dagger \approx \boldsymbol{a}^\dagger_{\alpha(t)} \tag{37.28}
$$

where $\alpha(t)$ satisfies Hamilton's equations of motion. In view of the manybody generalization below we referred here to the creation operator $a^\dagger$.

Perelomov and Gilmore have generalized the concept of coherent states in a way that allows application in the manybody context. Considering a system of bosons in an M site system, we define creation operators $\hat{a}^\dagger_j$, with $j = 1, ..., M$. Then we define an operator that creates particle in orbital α as follows:

$$
\boldsymbol{a}^\dagger_\alpha = \sum_{j=1}^{M} \alpha_j \boldsymbol{a}^\dagger_j, \qquad \text{where } \sum_{j=1}^{M} |\alpha_j|^2 = 1 \tag{37.29}
$$

Consequently, we can generate a set of coherent states as follows:

$$
|\alpha\rangle = \frac{1}{\sqrt{N}} \left[\boldsymbol{a}^\dagger_\alpha \right]^N |\text{vacuum}\rangle \tag{37.30}
$$

All those α states can be regarded as SU(M) "rotations" of an arbitrarily selected coherent state α_0. This is completely analogous to the harmonic oscillator, where all the α states are "translations" of each other. For the evolution of a coherent state we deduce from the above discussion the semiclassical approximation

$$
\boldsymbol{U}(t) |\alpha(0)\rangle \approx |\alpha(t)\rangle \tag{37.31}
$$

where $\alpha(t)$ satisfies Hamilton's equations of motion. This is what we called *mean field theory*: the manybody evolution is derived from a single classical trajectory that is generated by the classical Hamiltonian.

We use the following terminolgy: α indicates phase space location; and $|\alpha\rangle$ is a coherent state that is supported by α. Such state describes condensation of particles in a single *orbital* (single particle state) that is parametrized by α. For a two site system (dimer) the common paramterization is

$$
\alpha_{\text{dimer}} = \left(\cos(\theta) e^{-i\varphi/2}, \sin(\theta) e^{i\varphi/2} \right) \tag{37.32}
$$

hence phasespace is the Bloch sphere, with spherical coordinates (θ, φ) that describe the population imbalance and the relative phase. Note that the eigenstates of the dimer are associated with strips that are stretched along contour lines $H(\varphi, \theta) = E$ of the Hamiltonian. The $|n\rangle$ states are the eigenstates of the $K = 0$ Hamiltonian. In particular the $|n{=}N\rangle$ state (all the particles are in the first site) is a Gaussian-like wavepacket which is concentrated in the NorthPole. By rotation we get from it all the other coherent states. coherent states.

[38] A few site system with Fermions

════════ [38.1] A two-site system with one particle

The problem of "positioning a particle of spin $1/2$ in a specific location" is formally identical to the problem of "putting a particle in a two-site system". In both cases the system is described by a two-dimensional Hilbert space $\dim = 2$. Instead of discussing an electron that can be either "up" or "down", we shall discuss a particle that can be either in site 1 or in site 2. In other words, we identify the states as: $|1\rangle = |\uparrow\rangle$ and $|2\rangle = |\downarrow\rangle$.
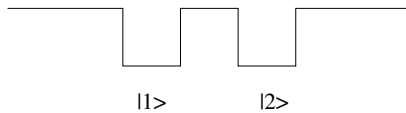
The standard basis is the position basis $|x = 1\rangle$, $|x = 2\rangle$. The representation of the operator $\hat{x}$ is:

$$\hat{x} \to \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} = 1 + \frac{1}{2}\left(1 - \sigma_3\right), \qquad\qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{38.1}$$

The translation operator can be optionally regarded as a reflection operator:

$$\hat{R} = \hat{D} \to \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_1 \tag{38.2}$$

where σ_1 is the first Pauli matrix. The k states are defined as the eigenstates of the latter operator, hence they are the even and the odd superpositions:

$$|k = 0\rangle = |+\rangle = \frac{1}{\sqrt{2}}\left(|1\rangle + |2\rangle\right) \tag{38.3}$$
$$|k = \pi\rangle = |-\rangle = \frac{1}{\sqrt{2}}\left(|1\rangle - |2\rangle\right)$$

Note the formal analogy with spin $1/2$ system: $|+\rangle = |\to\rangle$ represents spin polarized right, while $|-\rangle = |\leftarrow\rangle$ represents spin polarized left.

════════ [38.2] A two site system with two different particles

In this case the Hilbert space is four dimensional: $\dim = (2 \times 2) = 4$. If the two particles are different (for example, a proton and a neutron) then each state in the Hilbert space is "physical". The standard basis is:

$|1,1\rangle = |1\rangle \otimes |1\rangle$ - particle A in site 1, particle B in site 1
$|1,2\rangle = |1\rangle \otimes |2\rangle$ - particle A in site 1, particle B in site 2
$|2,1\rangle = |2\rangle \otimes |1\rangle$ - particle A in site 2, particle B in site 1
$|2,2\rangle = |2\rangle \otimes |2\rangle$ - particle A in site 2, particle B in site 2

The transposition operator $\hat{T}$ swaps the location of the particles:

$$\hat{T}|i,j\rangle = |j,i\rangle \tag{38.4}$$

We must not make confusion between the transposition operator and the reflection operators:

$$\hat{T} \mapsto \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \qquad\qquad \hat{R} \mapsto \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \tag{38.5}$$

Instead of the basis $|1,1\rangle$, $|1,2\rangle$, $|2,1\rangle$, $|2,2\rangle$, we may use the basis $|A\rangle$, $|1,1\rangle$, $|S\rangle$, $|2,2\rangle$, where we have defined:

$$|A\rangle = \frac{1}{\sqrt{2}}\left(|1,2\rangle - |2,1\rangle\right), \qquad\qquad |S\rangle = \frac{1}{\sqrt{2}}\left(|1,2\rangle + |2,1\rangle\right) \tag{38.6}$$

The state $|A\rangle$ is anti-symmetric under transposition, and all the others are symmetric under transposition.

====== [38.3] Placing together two identical particles

The motivation for discussing this system stems from the question: is it possible to place two electrons in the same location so that one of the spins is up and the other is down, or maybe they can be oriented differently. For example, one spin left and one right, or one right and the other up. We shall continue using the terminology of the previous section. We may deduce, from general symmetry considerations that the quantum state of identical particles must be an eigenstate of the transposition operator (otherwise we could conclude that the particles are not identical). It turns out that we must distinguish between two types of identical particles. According to the "spin and statistics theorem", particles with half-odd-integer spins (fermions) must be in an antisymmetric state. Particles with integer spins (bosons) must be in a symmetric state.

Assume that we have two spin zero particles. Such particles are Bosons. There is no problem to place two (or more) Bosons at the same site. If we want to place two such particles in two sites, then the collection of possible states is of dimension 3 (the symmetric states), as discussed in the previous section.

Electrons have spin 1/2, and therefore they are Fermions. Note that the problem of placing "two electron in one site" is formally analogous to the hypothetical system of placing "two spinless electrons in two sites". Thus the physical problem is formally related to the discussion in the previous section, and we can use the same notations. From the requirement of having an antisymmetric state it follows that if we want to place two electrons at the same location then there is only one possible state which is $|A\rangle$. This state is called the "singlet state". We discuss this statement further below.

Let us try to be "wise guys". Maybe there is another way to squeeze to electrons into one site? Rather than placing one electron with spin "up" and the other with spin "down" let us try a superposition of the type $|\rightarrow\leftarrow\rangle - |\leftarrow\rightarrow\rangle$. This state is also antisymmetric under transposition, therefore it is as "good" as $|A\rangle$. Let us see what it looks like in the standard basis. Using the notations of the previous section:

$$
\begin{aligned}
\frac{1}{\sqrt{2}}\left(|+-\rangle - |-+\rangle\right) &= \frac{1}{\sqrt{2}}\left(|+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle\right) \\
&= \frac{1}{2\sqrt{2}}\left((|1\rangle + |2\rangle) \otimes (|1\rangle - |2\rangle)\right) - \frac{1}{2\sqrt{2}}\left((|1\rangle - |2\rangle) \otimes (|1\rangle + |2\rangle)\right) \\
&= -\frac{1}{\sqrt{2}}\left(|1\rangle \otimes |2\rangle - |2\rangle \otimes |1\rangle\right) = -|A\rangle
\end{aligned}
\tag{38.7}
$$

So, we see that mathematically it is in fact the same state. In other words: the antisymmetric state is a single state and it does not matter if we put one electron "up" and the other "down", or one electron "right" and the other "left". Still let us try another possibility. Let us try to put one electron "up" and the other "right". Writing $|\uparrow\rightarrow\rangle$ in the standard basis using the notation of the previous section we get

$$|1\rangle \otimes |+\rangle = \frac{1}{\sqrt{2}}|1\rangle \otimes (|1\rangle + |2\rangle) = \frac{1}{\sqrt{2}}(|1,1\rangle + |1,2\rangle) \tag{38.8}$$

This state is not an eigenstate of the transposition operator, it is neither symmetric nor anti-symmetric state. Therefore it is not physical.

Anti-bunching.– If we place two (spinless) fermions in a two site system, the probability to find them both in the same site is zero. This is the opposite of the bosonic case where we have *bunching*. Say that we place one boson in oribial $|+\rangle$ and one in $|-\rangle$. The 2-body state is $|+-\rangle + |-+\rangle$. Going back to the site basis we get $|11\rangle - |22\rangle$, with zero probability to find them one in site 1 and one in site 2.

[39] Boxes and Networks

A 1D segment can be regarded as the continuum limit of a discrete tight-binding chain. If the particle in confined between two ends, the model is know as "infinite well" or as "1D box". If there are periodic boundary conditions, the model is know as "1D ring". Several "1D boxes" can be connected into a network: each 1D segment is called "bond", and the junctions are called "vortices".

The ends of an isolated bond can be regarded as *hard walls*. It is easily argued that the wavefunction should satisfy Dirichlet boundary conditions at the boundary of a hard wall. The perturbation which is created by an infinitesimal displacement of the wall is finite (see section below).

The coupling between two wavefunctions in a network due to the introduction of a connecting *junction* can be deduced by considering a wire which is divided by a high $u\delta(x)$ barrier (see section below).

We characterize a network by specifying the lengths $\{L_a\}$ of the bonds, and the the potentials u at each vertex. Given this information we would like to find the eigenfunctions and the eigenenergies. We describe below two procedures for that purpose: one is based on a straightforward generalization of the standard matching conditions, while the other is based on the scattering matrix formalism.

===== [39.1] Hard walls

Let us assume that we have a particle in a one dimensional box of length L, such that $V(x) = 0$ within the interval $0 < x < L$. We assume Dirichlet boundary conditions at $x = 0$, while at $x = L_0$ we assume a potential step, such that $V(x) = V_0$ for $x > L_0$. We are going to see that if we take the limit $V_0 \to \infty$, then this implies Dirichlet boundary conditions at $x = L_0$ too.

The wavefunction of nth eigenstate has to satisfy the Dirichlet boundary conditions at $x = 0$, and therefore has to be of the form

$$
\psi(x) = \begin{cases} A\sin(kx) & \text{for } 0 < x < L \\ Be^{-\alpha x} & \text{for } x > L \end{cases}
\tag{39.1}
$$

where

$$
\begin{aligned}
k &= \sqrt{2\mathsf{m}E} \\
\alpha &= \sqrt{2\mathsf{m}(V_0 - E)} \approx \sqrt{2\mathsf{m}V_0}
\end{aligned}
\tag{39.2}
$$

The normalization factor at the limit $V_0 \to \infty$ is $A = (2/L)^{1/2}$. It would be convenient later to make the replacement $A \mapsto (-1)^n A$, in order to have the same sign for $\psi(x)$ at $x \sim L$. The matching condition at $x = L$ is:

$$
\left.\frac{\psi`(x)}{\psi(x)}\right|_{x=L-0} = \left.\frac{\psi`(x)}{\psi(x)}\right|_{x=L+0} = -\alpha
\tag{39.3}
$$

Consequently the eigenvalue equation is

$$
k\cot(kL) = -\alpha
\tag{39.4}
$$

In the limit $V_0 \to \infty$ the equation becomes $\sin(kL) = 0$ which implies that the unperturbed eigen-energies are $E_n = k_n^2/2\mathsf{m}$ with $k_n = (\pi/L)n$. In this limit we see that the matching condition at $x = L$ simply forces the wave-function to be zero there. Thus we have established that Hard walls implies Dirichlet boundary conditions.

Perturbation due to wall displacement.– We would like to find the perturbation due to a small shift dL in the position of the wall. We keep V_0 finite, but assume that it is very very large. We shall take the strict limit $V_0 \to \infty$ only at the end of the calculation. For $L = L_0$ the unperturbed Hamiltonian after digonalization is

$$
[\mathcal{H}_0]_{nm} = \frac{1}{2\mathsf{m}}\left(\frac{\pi}{L_0}n\right)^2 \delta_{nm}
\tag{39.5}
$$

If we displace the wall a distance dL the new Hamiltonian becomes $\mathcal{H} = \mathcal{H}_0 + dLW$. We ask what are the matrix elements W_{nm} of this perturbation. At first sight it looks as if to displace an "infinite wall" constitutes "infinite perturbation" and hence $W_{nm} = \infty$. But in fact it is not like that. We shall see that

$$W_{nm} = -\frac{\pi^2}{\mathsf{m}L_0^3}nm, \qquad \text{[note sign convention]} \tag{39.6}$$

It is easily verified that the diagonal terms $W_{nn}dL$ of the perturbation matrix give correctly the first order shift dE_n of the energy levels due to the dL displacement.

Derivation.– The Hamiltonian of the unperturbed system, and the Hamiltonian after we have displaced the wall a distance dL are respectively

$$\mathcal{H}_0 = \frac{p^2}{2\mathsf{m}} + V(x), \qquad \mathcal{H} = \frac{p^2}{2\mathsf{m}} + \tilde{V}(x) \tag{39.7}$$

The perturbation is:

$$\delta V(x) = \tilde{V}(x) - V(x) \equiv dL \times W \tag{39.8}$$

which is a rectangle of width dL and height $-V_0$. It follows that the matrix elements of the perturbation are

$$W_{nm} = \frac{1}{dL}\int_L^{L+dL} \psi^{(n)}(x)[-V_0]\psi^{(m)}(x)dx = -V_0\psi^{(n)}(L)\psi^{(m)}(L) \tag{39.9}$$

The "matching conditions" allow to express $\psi(0)$ using its derivative as $-(1/\alpha)\psi'(0)$, leading to

$$W_{nm} = -\frac{1}{2\mathsf{m}}\left(\frac{d}{dx}\psi^{(n)}(L)\right)\left(\frac{d}{dx}\psi^{(m)}(L)\right) \tag{39.10}$$

The last expression has only an implicit dependence on V_0, through the derivatives of the wavefunctions at $x = L$. Obviously the limit $V_0 \to \infty$ gives a well defined finite result:

$$\frac{d}{dx}\psi^{(n)}(x)\bigg|_{x=L} = \sqrt{\frac{2}{L}}k_n = \left[\frac{2\pi^2}{L^3}\right]^{1/2}n \tag{39.11}$$

leading to the result for W_{nm} that has been cited in the introduction to this derivation.

═══ [39.2] The two-terminal delta junction

The simplest non-trivial example for an S matrix, is for a system which is composed of two 1D wires labeled as $i = 1, 2$, attached by a junction that is modeled as a delta barrier $u\delta(x)$. Using the standard "s-scattering" convention the channel wavefunctions are written as $\Psi(r) \propto A_i\exp(-ikr) - B_i\exp(ikr)$ where $r = |x|$. The linear relation between the As and the Bs is determined by the matching conditions. The matching conditions for the channel wavefunction at the origin $r = 0$ in the case of a delta barrier are further discussed in the next subsection, where it is also generalized to the case of having a junction with $\mathcal{M}$ wires. The S matrix which is implied by these matching conditions is

$$\boldsymbol{S} = -\begin{pmatrix} r & t \\ t & r \end{pmatrix}, \qquad \text{[such that } \boldsymbol{S}=\boldsymbol{1} \text{ for } u=\infty] \tag{39.12}$$

with

$$v \equiv (2E/\mathsf{m})^{1/2} \tag{39.13}$$

$$t = \frac{1}{1 + i(u/v)} \tag{39.14}$$

$$r = -1 + t \tag{39.15}$$

There is a more elegant way to re-write this expression. Define the phase

$$\gamma_0 \equiv -\text{phase}(v + iu) \tag{39.16}$$

Then it follows that

$$|t|^2 = (\cos(\gamma_0))^2 \qquad \text{phase}(t) = \gamma_0 \tag{39.17}$$

$$|r|^2 = (\sin(\gamma_0))^2 \qquad \text{phase}(r) = \gamma_0 - (\pi/2) \tag{39.18}$$

In practice it is more convenient to use in the present context an ad-hoc convention of writing a raw-swapped $\tilde{\boldsymbol{S}}$ matrix, corresponding to the re-definition of the outgoing amplitudes as $\tilde{B}_1 = -B_2$ and $\tilde{B}_2 = -B_1$, namely,

$$\tilde{\boldsymbol{S}} = \begin{pmatrix} t & r \\ r & t \end{pmatrix} = e^{i\gamma} \begin{pmatrix} \sqrt{g}e^{i\phi} & -i\sqrt{1-g}e^{-i\alpha} \\ -i\sqrt{1-g}e^{i\alpha} & \sqrt{g}e^{-i\phi} \end{pmatrix} \qquad \text{[such that } \tilde{\boldsymbol{S}}=\mathbf{1} \text{ for } u=0] \tag{39.19}$$

with $\alpha = \phi = 0$, and $\gamma = \gamma_0$, and

$$g = |t|^2 = \frac{1}{1 + (u/v_E)^2} = (\cos(\gamma_0(E)))^2 \tag{39.20}$$

The advantage of the ad-hoc convention is the possibility to regard $u = 0$ as the unperturbed Hamiltonian, and to use the $\boldsymbol{T}$ matrix formalism to find the $\tilde{\boldsymbol{S}}$ matrix. All the elements of the $\boldsymbol{T}$ matrix equal to the same number T, and the equality $\tilde{\boldsymbol{S}} = \mathbf{1} - i\boldsymbol{T}$ implies that $r = -iT$ and $t = 1 - iT$.

════ [39.3] The multi-terminal delta junction

The simplest junction is composed of $\mathcal{M} = 2$ wires that are connected at one point. We can model such a junction as a delta barrier $V(x) = u\delta(x)$. The matching condition at $x = 0$ is implied by the Schrodinger equation, and relates the jump in the derivative to the value of the wavefuntion at that point.

$$\frac{1}{2\mathsf{m}} \left[\partial\psi(+0) - \partial\psi(-0)\right] = u \, \psi(0) \tag{39.21}$$

A more elegant way of writing this relation is

$$\sum_{a=1}^{M} \frac{d\psi_a}{dr}\bigg|_{r=0} = \mathcal{M} \, \mathsf{m} u \, \psi(0) \tag{39.22}$$

with $\mathcal{M} = 2$. The derivative of the radial functions $\psi_1(r) = \psi(-r)$ and $\psi_2(r) = \psi(+r)$ is with respect to the radial coordinate $r = |x|$. It is implicit that these wavefuntions should have the same value at the meeting point $r = 0$. If we have $\mathcal{M}$ wires connected at one point we can define a generalized "delta junction" using the same matching condition. Say that we have $a = 1, 2, 3$ leads. The matching conditions at the junction are $\psi_1(0) = \psi_2(0) = \psi_3(0) \equiv \psi(0)$ while

the sum over the radial derivatives should equal $\mathcal{M}\mathsf{m}u\psi(0)$. This means that the sum over the outgoing currents is zero.

More generally a junction can be fully characterized by its S matrix. So we can ask what is the S matrix of a delta junction. It is straightforward to find out that the S matrix which is implied by the above matching conditions is

$$\boldsymbol{S}_{ab} = \delta_{ab} - \frac{2}{\mathcal{M}}\left(\frac{1}{1+i(u/v_E)}\right) \qquad \text{[such that } \boldsymbol{S}{=}\boldsymbol{1} \text{ for } u{=}\infty\text{]} \qquad (39.23)$$

For $u = 0$ we get zero reflection if $\mathcal{M} = 2$, while if $\mathcal{M} = 3$ we get

$$\boldsymbol{S} = \begin{pmatrix} +1/3 & -2/3 & -2/3 \\ -2/3 & +1/3 & -2/3 \\ -2/3 & -2/3 & +1/3 \end{pmatrix} \qquad (39.24)$$

In the limit $\mathcal{M} \to \infty$ we get total reflection.

Sometimes we want to treat the connecting junction as a perturbation. Consider for example the simplest possibility of having two 1D boxes connected at $x = 0$ hence forming a double well structure which is described by a Hamiltonian $\mathcal{H}(x, p; u)$ in which the barrier is represented by $V(x) = u\delta(x)$. The eigenstates n of the unperturbed Hamiltonian $\mathcal{H}(x, p; \infty)$ are those of the left box together with those of the right box. We want to have an explicit expression for the perturbation W_{nm} due to the coupling at $x = 0$. Note that W is defined as the difference $\mathcal{H}(u) - \mathcal{H}(\infty)$ so it is not the same as $V = \mathcal{H}(u) - \mathcal{H}(0)$. We can obtain the total perturbation W from a sequence of infinitesimal variations of the barrier height starting from $u = \infty$. Namely,

$$\mathcal{H}(u) \;=\; \mathcal{H}(\infty) - \int_u^\infty \left(\frac{\partial \mathcal{H}}{\partial u}\right)\, \mathrm{d}u' \;\equiv\; \mathcal{H}(\infty) + W \qquad (39.25)$$

For any value of u the Hilbert space of the system is spanned by a set of (real) eigenfunction labeled by n. The matrix elements for an infinitesimal variation of the barrier height is

$$\left(\frac{\partial \mathcal{H}}{\partial u}\right)_{nm} \;=\; \psi^{(n)}(0)\,\psi^{(m)}(0) \;=\; \frac{1}{(2\mathsf{m}u)^2}\left[\frac{d\psi^{(n)}}{dr}\right]_0 \left[\frac{d\psi^{(m)}}{dr}\right]_0 \qquad (39.26)$$

where is the last step we have used the matching conditions in order to express the wave function by the total radial derivative. As long as the barrier has small transmission ($g \ll 1$), the nth and the mth states remain similar to the unperturbed states and accordingly, upon integration, we get the result [arXiv:0807.2572]

$$W_{nm} \;=\; -\frac{1}{4\mathsf{m}^2 u}\left[\frac{d\psi^{(n)}}{dr}\right]_0 \left[\frac{d\psi^{(m)}}{dr}\right]_0 \qquad (39.27)$$

The d/dr in this expression is the total radial derivative, but in fact the contribution comes from one term only, because the unperturbed wavefunction of a given eigenstate $\psi^{(n)}$ is non-zero only in one box.

══════ [39.4] Finding the eigenstates of a network

Consider a network which is composed of b bonds and v vertexes. The wavefunction on bond $a \equiv (i, j)$ that connects vertex i to vertex j is written as

$$\psi_a(x) \;=\; B_a \mathrm{e}^{ik_a x} + A_a \mathrm{e}^{-ik_{\tilde{a}} x} \qquad (39.28)$$

where $0 < x < L_a$ is the position of the particle along the bond with the origin at vertex i. Note that the wavefunction on $\tilde{a} = (j, i)$ is with $A_{\tilde{a}} = B_a \mathrm{e}^{ik_a L_a}$ and $B_{\tilde{a}} = A_a \mathrm{e}^{-ik_{\tilde{a}} L_a}$. The wavenumber is $k_a = \sqrt{2\mathsf{m}E} + (\phi_a/L_a)$, where ϕ_a is

determined by the vector potential. Note that $\phi_{\tilde{a}} = -\phi_a$. For simplicity we assume below that there is no magnetic field, and accordingly $k_{\tilde{a}} = k_a$.

The most economical way to represent the wavefunction is by a vector $\psi \mapsto \{\psi_1, \psi_2, ..., \psi_v\}$ that contains the wave amplitudes at the vertexes. If we know this vector then we can construct the whole wavefunction on bond $a = (i, j)$ using the formula

$$\psi_a(x) = \frac{1}{\sin(k_a L_a)} \Big[\psi_i \sin(k_a(L_a - x)) + \psi_j \sin(k_a x) \Big] \tag{39.29}$$

The in order to find the eigenstates we simply have to write the v matching conditions of the vertexes, and look for the energies E for which there is non-trivial solution for this homogeneous set of equations.

Optionally the wavefunction can be represented by the vector $A = \{A_a\}$ of length $2b$, or equivalently by the vector $B = \{B_a\}$. The wavefunction and its gradient in a particular vertex are related to the latter as follows:

$$\psi = B + A \tag{39.30}$$
$$\partial\psi = ik \times (B - A) \tag{39.31}$$

If the junctions are represented by a scattering matrix and not by a simple matching condition there is an optional procedure for finding the eigenstates. The A and the B vectors are related by

$$B = \boldsymbol{S}\, A \tag{39.32}$$
$$A = \boldsymbol{J}\, \mathrm{e}^{i\boldsymbol{k}\boldsymbol{L}}\, B \tag{39.33}$$

where $\boldsymbol{S}$ is a $2b \times 2b$ matrix that relates the outgoing to the ingoing fluxes, and $\boldsymbol{J}$ is a $2b \times 2b$ permutation matrix that induces the mapping $a \mapsto \tilde{a}$, and $\boldsymbol{L} = \mathrm{diag}\{L_a\}$, and $\boldsymbol{k} = \mathrm{diag}\{k_a\}$. The equation for the eigenstates is

$$\left(\boldsymbol{J} \mathrm{e}^{i\boldsymbol{k}\boldsymbol{L}} \boldsymbol{S} - 1 \right) A = 0 \tag{39.34}$$

We can get from this equation a set of eigenvalues E_n with the corresponding eigenvectors $A^{(n)}$ and the associated amplitudes $B^{(n)} = \boldsymbol{S} A^{(n)}$.

The $\boldsymbol{S}$ matrix of the network (if appropriately ordered) has a block structure, and can be written as $\boldsymbol{S} = \sum_j \boldsymbol{S}^j$, where S^j is the $v_j \times v_j$ block that describes the scattering in the jth vertex. v_j is the number of leads that stretch out of that vertex. A delta function scatterer is regarded as a $v_j = 2$ vertex. Let us construct a simple example. Consider a ring with two delta barriers. Such ring can be regarded as a network with two bonds. The bonds are labeled as $12, 12', 21, 21'$, where the prime distinguishes the second arm. The matrices that define the system are

$$\boldsymbol{S} = \begin{pmatrix} r_1 & t_1 & 0 & 0 \\ t_1 & r_1 & 0 & 0 \\ 0 & 0 & r_2 & t_2 \\ 0 & 0 & t_2 & r_2 \end{pmatrix}, \qquad \boldsymbol{L} = \begin{pmatrix} L & 0 & 0 & 0 \\ 0 & L' & 0 & 0 \\ 0 & 0 & L & 0 \\ 0 & 0 & 0 & L' \end{pmatrix}, \qquad \boldsymbol{J} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{39.35}$$

Finally we note that $\boldsymbol{k} = \sqrt{2mE} + \boldsymbol{\phi}/\boldsymbol{L}$, where the fluxes matrix is $\boldsymbol{\phi} = \mathrm{diag}\{\phi_a\}$. If there is a single flux line ϕ one can write $\boldsymbol{\phi} = \phi \boldsymbol{P}$, where $\boldsymbol{P}$ can be expressed as a linear combination of the channel projectors $\boldsymbol{P}_a$. For example, if only one wire a encloses the flux line, then $\boldsymbol{P} = \boldsymbol{P}_a - \boldsymbol{P}_{\tilde{a}}$ and we get

$$\boldsymbol{k} = \frac{1}{\hbar}\sqrt{2mE} + \phi\frac{\boldsymbol{P}}{\boldsymbol{L}} \tag{39.36}$$

The obvious application of this procedure is for the analysis of a multi-mode Aharonov-Bohm ring, where the "bonds" are the propagation-modes of the ring, and they all enclose the same flux line.

QM in Practice (part II)

[40] Approximation methods for finding eigenstates

===== [40.1] The WKB approximation

In the next sections we discuss the canonical version of perturbation theory. The small parameter is the strength of the perturbation. Another family of methods to find approximate expressions for the eigen-functions is based on treating "$\hbar$" as the small parameter. The $\hbar$ in this context is not the $\hbar$ of Planck but rather its scaled dimensionless version that controls quantum-to-classical correspondence. For a particle in a box the scaled $\hbar$ is the ratio between the De-Broglie wavelength and the linear size of the box. Such approximation methods are known as semi-classical. The most elementary example is known as the WKB (Wentzel, Kramers, Brillouin) approximation [**Messiah p.231**]. It is designed to treat slowly varying potentials in 1D where the wavefunction looks locally like a plane wave (if $V(x) < E$) or as a decaying exponential (in regions where $V(x) > E$). The refined version of WKB, which is known as "uniform approximation", allows also to do the matching at the turning points (where $V(x) \sim E$). The generalization of the $d = 1$ WKB for $d > 1$ dimensions integrable systems is known as the EBK scheme. There is also a different type of generalization for $d > 1$ chaotic systems, via the Wigner Weyl formalism.

Assuming free wave propagation, hence neglecting back reflection, the WKB wavefunction is written as

$$\Psi(x) \quad = \quad \sqrt{\rho(x)}\mathrm{e}^{iS(x)} \tag{40.1}$$

This expression is inserted into the 1D Schrödinger equation. In leading order in $\hbar$ we get a continuity equation for the probability density $\rho(x)$, while the local wavenumber should be as expected

$$\frac{dS(x)}{dx} \quad = \quad p(x) \quad = \quad \sqrt{2\mathsf{m}(E - V(x))} \tag{40.2}$$

Hence (for a right moving wave) one obtains the WKB approximation

$$\psi(x) \quad = \quad \frac{1}{\sqrt{p(x)}}\mathrm{EXP}\Big[i\int_{x_0}^{x} p(x')dx'\Big] \tag{40.3}$$

where x_0 is an arbitrary point. For a standing wave the "EXP" can be replaced by either "sin" or "cos". It should be clear that for a "flat" potential floor this expression becomes exact. Similarly in the "forbidden" region we have a decaying exponential. Namely, the local wavenumber $\pm p(x)$ is replaced by $\pm i\alpha(x)$, where $\alpha(x) = (2\mathsf{m}(V(x) - E))^{1/2}$.

Scattering.– If we have a scattering problem in one dimension we can use the WKB expression (with exp) in order to describe (say) a right moving wave. It should be realized that there is no back-reflection within the WKB framework, but still we can calculate the phase shift for the forward scattering:

$$\begin{aligned} \theta_{\mathrm{WKB}} \quad &= \quad \int_{-\infty}^{\infty} p(x)dx - \int_{-\infty}^{\infty} p_E dx \quad = \quad \int_{-\infty}^{\infty}\Big[\sqrt{2\mathsf{m}(E - V(x))} - \sqrt{2\mathsf{m}E}\Big]\,dx \\ &= \quad \sqrt{2\mathsf{m}E}\int_{-\infty}^{\infty}\Big[\sqrt{1 - \frac{V(x)}{E}} - 1\Big]\,dx \quad \approx \quad -\sqrt{\frac{\mathsf{m}}{2E}}\int_{-\infty}^{\infty} V(x)dx \end{aligned} \tag{40.4}$$

Hence we get

$$\theta_{\mathrm{WKB}} \quad = \quad -\frac{1}{\hbar v_E}\int_{-\infty}^{\infty} V(x)dx \tag{40.5}$$

It should be noted that θ_{1D}^{WKB} is the phase shift in a 1D scattering geometry $(-\infty < x < \infty)$. A similar looking result for semi-1D geometry $(r > 0)$ is known as the Born approximation for the phase shift.

Bound states.– If we have a particle in a well, then there are two turning points x_1 and x_2. On the outer sides of the well we have WKB decaying exponentials, while in the middle we have a WKB standing wave. As mentioned above the WKB scheme can be extended so as to provide matching conditions at the two turning points. Both matching conditions can be satisfied simultaneously if

$$\int_{x_1}^{x_2} p(x)dx = \left(\frac{1}{2} + n\right)\pi\hbar \tag{40.6}$$

where $n = 0, 1, 2, \ldots$ is an integer. Apart from the $1/2$ this is a straightforward generalization of the quantization condition of the wavenumber of a particle in a 1D box with hard walls $(k \times (x_2 - x_1) = n\pi)$. The $(1/2)\pi$ phase shift arise because we assume soft rather than hard walls. This $1/2$ becomes exact in the case of harmonic oscillator.

The WKB quantization condition has an obvious phase space representation, and it coincides with the "Born Oppenheimer quantization condition":

$$\oint p(x)dx = \left(\frac{1}{2} + n\right)2\pi\hbar \tag{40.7}$$

The integral is taken along the energy contour which is formed by the curves $p = \pm p(x)$. This expression implies that the number of states up to energy E is

$$\mathcal{N}(E) = \iint_{H(x,p)<E} \frac{dxdp}{2\pi\hbar} \tag{40.8}$$

The $d > 1$ generalization of this idea is the statement that the number of states up to energy E is equal to the phase space volume divided by $(2\pi\hbar)^d$. The latter statement is known as Weyl law, and best derived using the Wigner-Weyl formalism.

═══════ [40.2] The variational scheme

The variational scheme is an approximation method that is frequently used either as an alternative or in combination with perturbation theory. It is an extremely powerful method for the purpose of finding the ground-state. More generally we can use it to find the lowest energy state within a subspace of states.

The variational scheme is based on the trivial observation that the ground state minimize the energy functional

$$F[\psi] \equiv \langle\psi|\mathcal{H}|\psi\rangle \tag{40.9}$$

If we consider in the variational scheme the most general ψ we simply recover the equation $\mathcal{H}\psi = E\psi$ and hence gain nothing. But in practice we can substitute into $F[]$ a trial function ψ that depends on a set of parameters $X = (X_1, X_2, ...)$. Then we minimize the function $F(X) = F[\psi]$ with respect to X.

The simplest example is to find the ground state on an harmonic oscillator. If we take the trail function as a Gaussian of width σ, then the minimization of the energy functional with respect to σ will give the exact ground state. If we consider an anharmonic oscillator we still can get a very good approximation. A less trivial example is to find bonding orbitals in a molecules using as a trial function a combination of hydrogen-like orbitals.

═══════ [40.3] Perturbation theory - motivation

Let us consider a particle in a two dimensional box. On the left a rectangular box, and on the right a chaotic box.

For a regular box (with straight walls) we found: $E_{n_x,n_y} \propto (n_x/L_x)^2 + (n_y/L_y)^2$, so if we change L_x we get the energy level scheme which is drawn in the left panel of the following figure. But if we consider a chaotic box, we shall get energy level scheme as on the right panel.

The spectrum is a function of a control parameter, which in the example above is the position of a wall. For generality let us call this parameter X. The Hamiltonian is $\mathcal{H}(\hat{Q}, \hat{P}; X)$. Let us assume that we have calculated the levels either analytically or numerically for $X = X_0$. Next we change the control parameter to the value $X = X_0 + \delta X$, and use the notation $\delta X = \lambda$ for the small parameter. Possibly, if λ is small enough, we can linearize the Hamiltonian as follows:

$$\mathcal{H} \;\;=\;\; \mathcal{H}(Q, P; X_0) + \lambda V(Q, P) \;\;=\;\; \mathcal{H}_0 + \lambda V \tag{40.10}$$

With or without this approximation we can try to calculate the new energy levels. But if we do not want or cannot diagonalize $\mathcal{H}$ for the new value of X we can try to use a perturbation theory scheme. Obviously this scheme will work only for small enough λ that do not "mix" the levels too much. There is some "radius of convergence" (in λ) beyond which perturbation theory fails completely. In many practical cases $X = X_0$ is taken as the value for which the Hamiltonian is simple and can be handled analytically. In atomic physics the control parameter X is usually either the prefactor of the spin-orbit term, or an electric field or a magnetic field which are turned on.

There is another context in which perturbation theory is very useful. Given (say) a chaotic system, we would like to predict its response to a small change in one of its parameters. For example we may ask what is the response of the system to an external driving by either an electric or a magnetic field. This response is characterized by a quantity called "susceptibility". In such case, finding the energies without the perturbation is not an easy task (it is actually impossible analytically, so if one insists heavy numerics must be used). Instead of "solving" for the eigenstates it turns out that for any practical purpose it is enough to characterize the spectrum and the eigenstates in a statistical way. Then we can use perturbation theory in order to calculate the "susceptibility" of the system.

═══════ [40.4] Perturbation theory - a mathematical digression

Let us illustrate how the procedure of perturbation theory is applied in order to find the roots of a toy equation. Later we shall apply the same procedure to find the eigenvalues and the eigenstates of a given Hamiltonian. The toy equation that we consider is

$$x + \lambda x^5 = 3 \tag{40.11}$$

We assume that the magnitude of the perturbation (λ) is small. The Taylor expansion of x with respect to λ is:

$$x(\lambda) \ = \ x^{(0)} + x^{(1)}\lambda + x^{(2)}\lambda^2 + x^{(3)}\lambda^3 + \ldots \tag{40.12}$$

The zero-order solution gives us the solution for the case $\lambda = 0$:

$$x^{(0)} \ = \ 3 \tag{40.13}$$

To find the perturbed solution substitute the expansion:

$$\left[x^{(0)} + x^{(1)}\lambda + x^{(2)}\lambda^2 + \ldots\right] \ + \ \lambda\left[x^{(0)} + x^{(1)}\lambda + x^{(2)}\lambda^2 + \ldots\right]^5 \ = \ 3 \tag{40.14}$$

This can be re-arranged as follows:

$$\left[x^{(0)} - 3\right] \ + \ \left[x^{(1)} + (x^{(0)})^5\right]\lambda \ + \ \left[5(x^{(0)})^4 x^{(1)} + x^{(2)}\right]\lambda^2 \ + \ \mathcal{O}(\lambda^3) \ = \ 0 \tag{40.15}$$

By comparing coefficients we get a system of equations that can be solved iteratively order by order:

$$x^{(0)} \ = \ 3 \tag{40.16}$$
$$x^{(1)} \ = \ -(x^{(0)})^5 \ = \ -3^5 \tag{40.17}$$
$$x^{(2)} \ = \ -5(x^{(0)})^4 x^{(1)} \ = \ 5 \times 3^9 \tag{40.18}$$

It is obviously possible to find the corrections for higher orders by continuing in the same way.

[41] Perturbation theory for the eigenstates

===== [41.1] Degenerate perturbation theory (zero-order)

Consider a diagonal Hamiltonian matrix, with a small added perturbation that spoils the diagonalization:

$$\mathcal{H} = \begin{pmatrix} 2 & 0.03 & 0 & 0 & 0 & 0.5 & 0 \\ 0.03 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0.1 & 0.4 & 0 & 0 \\ 0 & 0 & 0.1 & 5 & 0 & 0.02 & 0 \\ 0 & 0 & 0.4 & 0 & 6 & 0 & 0 \\ 0.5 & 0 & 0 & 0.02 & 0 & 8 & 0.3 \\ 0 & 0 & 0 & 0 & 0 & 0.3 & 9 \end{pmatrix} \tag{41.1}$$

The Hamiltonian can be visualized using an energy level diagram:
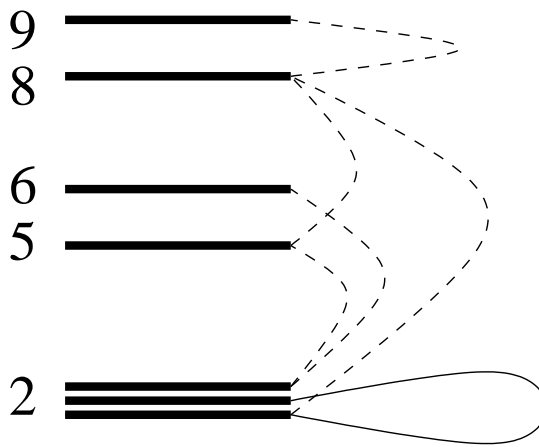
The eigenvectors without the perturbation are:

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \dots \tag{41.2}$$

The perturbation spoils the diagonalization. The question we would like to answer is what are the new eigenvalues and eigenstates of the Hamiltonian. We would like to find them "approximately", without having to diagonalize the Hamiltonian again. First we will take care of the degenerated blocks. The perturbation can remove the existing degeneracy. In the above example we make the following diagonalization:

$$2 \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + 0.03 \cdot \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \rightarrow \quad \begin{pmatrix} 1.97 & 0 & 0 \\ 0 & 2.03 & 0 \\ 0 & 0 & 2 \end{pmatrix} \tag{41.3}$$

We see that the perturbation has removed the degeneracy. At this stage our achievement is that there are no matrix elements that couple degenerate states. This is essential for the next steps: we want to ensure that the perturbative calculation would not diverge.

For the next stage we have to transform the Hamiltonian to the new basis. See the calculation in the Mathematica file "diagonalize.nb". If we diagonalize numerically the new matrix we find that the eigenvector that corresponds to the eigenvalue $E \approx 5.003$ is

$$
|\Psi\rangle \quad \rightarrow \quad
\begin{pmatrix} 0.0008 \\ 0.03 \\ 0.0008 \\ 1 \\ -0.01 \\ -0.007 \\ 0.0005 \end{pmatrix}
=
\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}
+
\begin{pmatrix} 0.0008 \\ 0.03 \\ 0.0008 \\ 0 \\ -0.01 \\ -0.007 \\ 0.0005 \end{pmatrix}
\quad \equiv \quad \Psi_n^{[0]} + \Psi_n^{[1,2,3,\dots]}
\tag{41.4}
$$

We note that within the scheme of perturbation theory it is convenient to normalize the eigenvectors according to the zero order approximation. We also use the convention that all the higher order corrections have zero overlap with the zero order solution. Else the scheme of the solution becomes ill defined.

═════ [41.2] Perturbation theory to arbitrary order

We write the Hamiltonian as $\mathcal{H} = \mathcal{H}_0 + \lambda V$ where V is the perturbation and λ is the control parameter. Note that λ can be "swallowed" in V. We keep it during the derivation in order to have clear indication for the "order" of the terms in the expansion. The Hamiltonian is represented in the unperturbed basis as follows:

$$
\mathcal{H} \;=\; \mathcal{H}_0 + \lambda V \;=\; \sum_n |n\rangle \varepsilon_n \langle n| \;+\; \lambda \sum_{n,m} |n\rangle V_{n,m} \langle m|
\tag{41.5}
$$

which means

$$
\mathcal{H} \quad \rightarrow \quad
\begin{pmatrix} \varepsilon_1 & 0 & 0 & 0 \\ 0 & \varepsilon_2 & 0 & 0 \\ 0 & 0 & \varepsilon_3 & 0 \\ 0 & 0 & 0 & \dots \end{pmatrix}
+ \lambda
\begin{pmatrix} V_{1,1} & V_{1,2} & \dots & \dots \\ V_{2,1} & V_{2,2} & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}
\tag{41.6}
$$

In fact we can assume without loss of generality that $V_{n,m} = 0$ for $n = m$, because these terms can be swallowed into the diagonal part. Most importantly we assume that none of the matrix element couples degenerated states. Such couplings should be treated in the preliminary "zero order" step that has been discussed in the previous section.

We would like to introduce a perturbative scheme for finding the eigenvalues and the eigenstates of the equation

$$
(\mathcal{H}_0 + \lambda V)|\Psi\rangle \;=\; E|\Psi\rangle
\tag{41.7}
$$

The eigenvalues and the eigenvectors are expanded as follows:

$$
\begin{aligned}
E &= E^{[0]} + \lambda E^{[1]} + \lambda^2 E^{[2]} + \cdots \\
\Psi_n &= \Psi_n^{[0]} + \lambda \Psi_n^{[1]} + \lambda^2 \Psi_n^{[2]}
\end{aligned}
\tag{41.8}
$$

where it is implicit that the zero order solution and the normalization are such that

$$
\begin{aligned}
E^{[0]} &= \varepsilon_{n_0} \\
\Psi_n^{[0]} &= \delta_{n,n_0} \\
\Psi_n^{[1,2,3,\dots]} &= 0 \quad \text{for} \quad n = n_0
\end{aligned}
\tag{41.9}
$$

It might be more illuminating to rewrite the expansion of the eigenvector using Dirac notations. For this purpose we label the unperturbed eigenstates as $|\varepsilon_n\rangle$ and the perturbed eigenstates as $|E_n\rangle$. Then the expansion of the latter is

written as

$$|E_{n_0}\rangle \;=\; |E_{n_0}^{[0]}\rangle + \lambda|E_{n_0}^{[1]}\rangle + \lambda^2|E_{n_0}^{[2]}\rangle + \cdots \tag{41.10}$$

hence

$$\langle\varepsilon_n|E_{n_0}\rangle \;=\; \delta_{n,n_0} + \lambda\langle\varepsilon_n|E_{n_0}^{[1]}\rangle + \lambda^2\langle\varepsilon_n|E_{n_0}^{[2]}\rangle + \cdots \tag{41.11}$$

which coincides with the traditional notation. In the next section we introduce a derivation that leads to the following practical results (absorbing λ into the definition of V):

$$
\begin{aligned}
\Psi_n^{[0]} &= \delta_{n,n_0} \\
\Psi_n^{[1]} &= \frac{V_{n,n_0}}{\varepsilon_{n_0} - \varepsilon_n} \\
E^{[0]} &= \varepsilon_{n_0} \\
E^{[1]} &= V_{n_0,n_0} \\
E^{[2]} &= \sum_{m(\neq n_0)} \frac{V_{n_0,m}V_{m,n_0}}{\varepsilon_{n_0} - \varepsilon_m}
\end{aligned}
\tag{41.12}
$$

The calculation can be illustrated graphically using a "Feynman diagram". For the calculation of the second order correction to the energy we should sum all the paths that begin with the state n_0 and also end with the state n_0. We see that the influence of the nearer levels is much greater than the far ones. This clarifies why we cared to treat the couplings between degenerated levels in the zero order stage of the calculation. The closer the level the stronger the influence. This influence is described as "level repulsion". Note that in the absence of first order correction the ground state level always shifts down.

═══════ [41.3] Derivation of the results

The equation we would like to solve is

$$
\begin{pmatrix} \varepsilon_1 & 0 & 0 & 0 \\ 0 & \varepsilon_2 & 0 & 0 \\ 0 & 0 & \varepsilon_3 & 0 \\ 0 & 0 & 0 & \ldots \end{pmatrix}
\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \ldots \end{pmatrix}
+ \lambda
\begin{pmatrix} V_{1,1} & V_{1,2} & \cdots & \cdots \\ V_{2,1} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix}
\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \ldots \end{pmatrix}
= E
\begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \ldots \end{pmatrix}
\tag{41.13}
$$

Or, in index notation:

$$\varepsilon_n \Psi_n + \lambda \sum_m V_{n,m}\Psi_m \;=\; E\Psi_n \tag{41.14}$$

This can be rewritten as

$$(E - \varepsilon_n)\Psi_n \;=\; \lambda \sum_m V_{n,m}\Psi_m \tag{41.15}$$

We substitute the Taylor expansion:

$$
\begin{aligned}
E &= \sum_{k=0} \lambda^k E^{[k]} &=& \; E^{[0]} + \lambda E^{[1]} + \ldots \\
\Psi_n &= \sum_{k=0} \lambda^k \Psi_n^{[k]} &=& \; \Psi_n^{[0]} + \lambda \Psi_n^{[1]} + \ldots
\end{aligned}
\tag{41.16}
$$

We recall that $E^{[0]} = \varepsilon_{n_0}$, and

$$\Psi_n^{(0)} = \delta_{n,n_0} \to \begin{pmatrix} \ldots \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ \ldots \end{pmatrix}, \qquad \Psi_n^{[k \neq 0]} \to \begin{pmatrix} \ldots \\ ? \\ ? \\ 0 \\ ? \\ ? \\ \ldots \end{pmatrix} \tag{41.17}$$

After substitution of the expansion we use on the left side the identity

$$(a_0 + \lambda a_1 + \lambda^2 a_2 + \ldots)(b_0 + \lambda b_1 + \lambda^2 b_2 + \ldots) = \sum_k \lambda^k \sum_{k'=0}^{k} a_{k'} b_{k-k'} \tag{41.18}$$

Comparing the coefficients of λ^k we get a system of equations $k = 1, 2, 3...$

$$\sum_{k'=0}^{k} E^{[k']} \Psi_n^{[k-k']} - \varepsilon_n \Psi_n^{[k]} = \sum_m V_{n,m} \Psi_m^{[k-1]} \tag{41.19}$$

We write the kth equation in a more expanded way:

$$(E^{[0]} - \varepsilon_n)\Psi_n^{(k)} + E^{[1]}\Psi_n^{[k-1]} + E^{[2]}\Psi_n^{[k-2]} + \cdots + E^{[k]}\Psi_n^{[0]} = \sum_m V_{n,m}\Psi_m^{[k-1]} \tag{41.20}$$

If we substitute $n = n_0$ in this equation we get:

$$0 \; + \; 0 \; + \cdots + E^{[k]} \;=\; \sum_m V_{n_0,m}\Psi_m^{[k-1]} \tag{41.21}$$

If we substitute $n \neq n_0$ in this equation we get:

$$(\varepsilon_{n_0} - \varepsilon_n)\Psi_n^{[k]} \;=\; \sum_m V_{n,m}\Psi_m^{[k-1]} - \sum_{k'=1}^{k-1} E^{[k']}\Psi_n^{[k-k']} \tag{41.22}$$

Now we see that we can solve the system of equations that we got in the following order:

$$\Psi^{[0]} \;\to\; E^{[1]} \;,\; \Psi^{[1]} \;\to\; E^{[2]} \;,\; \Psi^{[2]} \;\to\; E^{[3]} \;,\; \Psi^{[3]} \;\to\; \ldots \tag{41.23}$$

where:

$$E^{[k]} \;=\; \sum_m V_{n_0,m}\Psi_m^{[k-1]} \tag{41.24}$$

$$\Psi_n^{[k]} \;=\; \frac{1}{(\varepsilon_{n_0} - \varepsilon_n)}\left[\sum_m V_{n,m}\Psi_m^{[k-1]} - \sum_{k'=1}^{k-1} E^{[k']}\Psi_n^{[k-k']} \right]$$

The practical results that were cited in the previous sections are easily obtained from this iteration scheme.

══════ [41.4] Delta scatterer in a box

Possibly the simplest non-trivial example for the demonstration of perturbation theory and its limitations is to find the effect of introducing a delta scatterer $V(r) = \delta(r)$ in a box. We consider first the exact solution in the one dimensional ($d = 1$) case, where the delta is placed in the centre of segment $|r| < R$, and the $d = 3$ case, where the delta is placed in the centre of sphere $|r| < R$. Later we consider the case of a delta in the centre of a rectangular box $[-R, R]^d$. Below we use units such that the mass is unity, and also $R = 1$.

In the one dimensional case the wavefunction has to satisfy Dirichlet boundary conditions at the walls, and the matching condition across the delta barrier at the origin, leading to the eigenvalue equation $k \cot(k) = u$ for $E > 0$ and $k \coth(k) = u$ for $E < 0$ where $k = \sqrt{2E}$. One observes that for $u < -1$ the ground state become bounded ($E_0 < 0$), while all the other states are extended (with $E > 0$). For very negative u we get $E_0 \approx -u^2/2$ and $E_{n,-} = (\pi n)^2/2$ and $E_{n,+} \approx E_{n,-}$ that are slightly shifted downwards.

For $d \geq 2$ the effect of introducing a delta scatterer is zero. This is complementary to the statement that a delta function has zero scattering cross-section. In order to have a non-zero effect the scatterer should have a finite size. To clarify the "zero" effect of a point scatterer let us consider the eigenfunctions of a $d = 3$ sphere that has an infinite barrier V_0 of radius a in its centre. The zero angular momentum wavefuntions in the extreme case of an infinite barrier are

$$\Psi(r, \theta, \varphi) = \text{const} \frac{\sin(k|r - a|)}{r} \tag{41.25}$$

The healing length is of order a and in the limit $a \to 0$ the "hole" in the wavefunction disappears irrespective of whether $V_0 a^3$ is kept constant or becomes infinite.

Now we would like to see how/whether the above results can be obtained formally via perturbation theory. For this purpose it is most convenient to consider a delta function in a centre of a rectangular box (segment if $d = 1$, square if $d = 2$). Excluding all the states that have node at the centre the Hamiltonian matrix takes the following form:

$$H = \begin{pmatrix} \varepsilon_1 & 0 & 0 & 0 & ... \\ 0 & \varepsilon_2 & 0 & 0 & ... \\ 0 & 0 & \varepsilon_3 & 0 & ... \\ 0 & 0 & 0 & \varepsilon_4 & ... \\ ... & ... & ... & ... & ... \end{pmatrix} + u \begin{pmatrix} 1 & 1 & 1 & 1 & ... \\ 1 & 1 & 1 & 1 & ... \\ 1 & 1 & 1 & 1 & ... \\ 1 & 1 & 1 & 1 & ... \\ ... & ... & ... & ... & ... \end{pmatrix} \tag{41.26}$$

We note that the same Hamiltonian (with $u < 0$) emerges in the analysis of the *Copper pair problem*, which has inspired the BCS theory of superconductivity. In turns out (see below) that the important information for the analysis is the density of states $\varrho \propto \varepsilon^\alpha$, where $\alpha = (d/2) - 1$ with $d = 1, 2, 3$. If we introduce a cutoff and consider the finite-size Hamiltonian that consists of the levels $\varepsilon_n < \omega_c$, it is like to give the scatterer a finite width $a \sim (2\mathsf{m}\omega_c)^{-1/2}$.

The ground state energy using second order perturbation is

$$E_0 = \varepsilon_1 + u + \sum_n \frac{u^2}{E_0 - \varepsilon_n} \quad \sim \quad -\sum_n \frac{u^2}{E_n} \tag{41.27}$$

In the one dimensional case this expression is finite and give a meaningful result if $u \ll 1$. But if $\alpha \geq 1$ this sum diverges in the $\omega_c \to \infty$ limit:

$$E_0 \quad \sim \quad -\sum_n \frac{u^2}{E_n} \quad \sim \quad -\infty \tag{41.28}$$

This divergence obviously applies to all the levels, and to all orders of perturbation theory (we consider above the ground state just as an example). It turns out from the exact analysis (below) that the this divergence indicates that the perturbation in an infinite order (exact) calculation has a zero effect. One way to think about this puzzling observation is to realize that the geometric sum $1 + x + x^2 + x^3 + ...$ is formally zero (and not infinite) in the limit $x \to \infty$ because it equals $1/(1 - x)$.

The exact solution of the eigenvalue problem requires to solve the matrix equation $H\Psi = E\Psi$, namely

$$\varepsilon_n \Psi_n - u \sum_m \Psi_m = E\Psi_n \tag{41.29}$$

Introduction the notation $C = \sum_m \Psi_m$, which later will be determined via normalization, we can solve for the wavefunction:

$$\Psi_n = C\frac{u}{E - \varepsilon_n} \tag{41.30}$$

From the definition of C it follows that the eigenvalues should be the solution of the following equation:

$$\sum \frac{u}{E - \varepsilon_n} = 1 \tag{41.31}$$

The equation has a nice graphical visualization, and one can easily be convinced that in the limit $\omega_c \to \infty$ the perturbed eigenvalues approach the unperturbed values.

In view of the interest in the Cooper pair problem it is of interest to see what happens if we have constant density of states ϱ with finite cutoff ω_c and negative u. The graphical visualization implies that the ground state separates from the quasi-continuum and forms a bound state of energy $E_0 = -\Delta$, as in the familiar $d = 1$ case. In order to estimate Δ we approximate the sum by an integral and get the equation

$$|u|\varrho \ln\left(\frac{\Delta + \omega_c}{\Delta}\right) = 1 \tag{41.32}$$

leading to

$$\Delta = \frac{\omega_c}{\exp\left(\frac{1}{|u|\varrho}\right) - 1} \tag{41.33}$$

In the limit of small u we have the BCS-like result $\Delta = \exp(-1/(|u|\varrho))$, while in the other extreme of very strong u we get $\Delta = Nu$ where $N = \varrho\omega_c$ is the number of levels in the quasi-degenerated band. The latter result is easily verified by direct diagonalization of of the Hamiltonian. Namely, if the unperturbed energies were degenerated the Hamiltonian would become diagonal in the "momentum" representation, where only the zero momentum state is affected.

[42] Beyond perturbation theory

═══════ [42.1] The overlap between the old and the new states

We have found that the perturbed eigenstates to first-order are given by the expression

$$|E_n\rangle \quad \approx \quad |\varepsilon_n\rangle + \sum_m \frac{V_{m,n}}{\varepsilon_n - \varepsilon_m} |\varepsilon_m\rangle \tag{42.1}$$

So, it is possible to write:

$$\langle \varepsilon_m | E_n \rangle \quad \approx \quad \frac{V_{mn}}{\varepsilon_n - \varepsilon_m} \qquad \text{for } m \neq n \tag{42.2}$$

which implies

$$P(m|n) \quad \equiv \quad |\langle \varepsilon_m | E_n \rangle|^2 \quad \approx \quad \frac{|V_{mn}|^2}{(E_m - E_n)^2} \qquad \text{for } m \neq n \tag{42.3}$$

In the latter expression we have replaced in the denominator the unperturbed energies by the perturbed energies. This is OK in leading order treatment. The validity condition is

$$|V| \quad \ll \quad \Delta \tag{42.4}$$

In other words, the perturbation must be much smaller than the mean level spacing. We observe that once this condition breaks down the sum $\sum_m P(m|n)$ becomes much larger than one, whereas the exact value should have unit normalization. This means that if $|V| \gg \Delta$ the above first order expression cannot be trusted.

Can we do better? In principle we have to go to higher orders of perturbation theory, which might be very complicated. But in fact the generic result that comes out is quite simple:

$$P(m|n) \quad \approx \quad \frac{|V_{m,n}|^2}{(E_m - E_n)^2 + (\Gamma/2)^2} \tag{42.5}$$

This is called "Wigner Lorentzian". As we shall see later it is related to an exponential decay law that is called "Wigner decay". The expression for the "width" of this Lorentzian is implied by normalization:

$$\Gamma \quad = \quad \frac{2\pi}{\Delta} |V|^2 \tag{42.6}$$

The Lorentzian expression is not exact. It is implicit that we assume a dense spectrum (high density of states). We also assume that all the matrix elements are of the same order of magnitude. Such assumption can be justified e.g. in the case of a chaotic system. In order to show that $\sum_m P(m|n) = \sum_n P(m|n) = 1$ one use the recipe:

$$\sum_n f(E_n) \quad \approx \quad \int \frac{dE}{\Delta} f(E) \tag{42.7}$$

where Δ is the mean level spacing. In the following we shall discuss further the notion Density of States (DOS) and Local Density of States (LDOS) which are helpful in further clarifying the significance of the Wigner Lorentzian.

════════ [42.2] Bandprofile of the perturbation

At this point it is important to provide some insights (following Feingold and Peres) regarding the bandprofile of the perturbation matrix. We assume that energy basis $|n\rangle$ is determined by Hamiltonian $\mathcal{H}$ that generates chaotic dynamics, and we look for the matrix representation V_{nm} of some observable V. We define $V(t) = e^{i\mathcal{H}t}Ve^{-i\mathcal{H}t}$ and the correlator $C(t) = \langle V(t)V(0)\rangle$. It is implicit that a constant has been subtracted such that $\langle V \rangle = 0$. The expectation value is calculated for a stationary state $|n\rangle$ that has an energy $E_n \sim E$. The numerical practice is to average over states that occupy a narrow window around E, in order to get a smooth result. The chaos assumption implies that the correlator decays after a finite time τ_c. The Fourier transform of $C(t)$ is real, aka power spectrum of $V(t)$. The following identity is implied by definition:

$$\tilde{C}(\omega) \;=\; \int_{-\infty}^{\infty} C(t)\,e^{i\omega t}dt \;=\; \sum_m |V_{mn}|^2 \, 2\pi\delta\left(\omega - (E_m - E_n)\right) \;=\; \frac{2\pi}{\Delta_0}\,\overline{|V|_\omega^2} \tag{42.8}$$

where Δ_0 is the mean level spacing. The last equality defined the notion of bandprofile. Namely, $\overline{|V|_\omega^2}$ is the variance of the matrix elements along the diagonal $(E_m - E_n) \sim \omega$. We can use this relation in reverse in order to get a semi-classical estimate for the bandprofile. In particular the bandwidth is related to the correlation time, namely $\Delta_b = 2\pi/\tau_c$. The dimensionless bandwidth is $b \equiv \Delta_b/\Delta_0$. If we assume that the in-band elements are uniformly distributed with dispersion λ, then it follows that $\mathrm{Var}(V) = C(0) = b\lambda^2$.

════════ [42.3] Lineshape of the local spectrum

When we discussed perturbation theory it was convenient to ask what is the representation of a new (perturbed) eigenstate $|E_n\rangle$ in the old (unperturbed) basis $|m\rangle$. But in practice, for the purpose of studying time-evolution, it is more useful to ask for the expansion of the prepared state $|m\rangle$ in the energy basis $|E_n\rangle$. Accordingly we define $P(n) = |\langle E_n|m\rangle|^2$. We ask what is the lineshape if we plot $P(n)$ versus E_n. We shall refer to this lineshape as the local spectrum for the preparation under consideration. We would like to know how the lineshape depends on the strength λ of the perturbation. First order perturbation theory implies a "delta+tail" structure. Wigner approximation implies a "core-tail" Lorentzian lineshape: the core is of width $\Gamma(\lambda) = (2\pi/\Delta_0)\lambda^2$, while the tail is determined by first-order perturbation theory. Clearly the Wigner Lorentzian approximation makes sense provided $\Gamma(\lambda) < \Delta_b$. This condition breaks down if $\lambda > b^{1/2}\Delta_0$. In the latter case we expect a semiclassical lineshape as explained below.
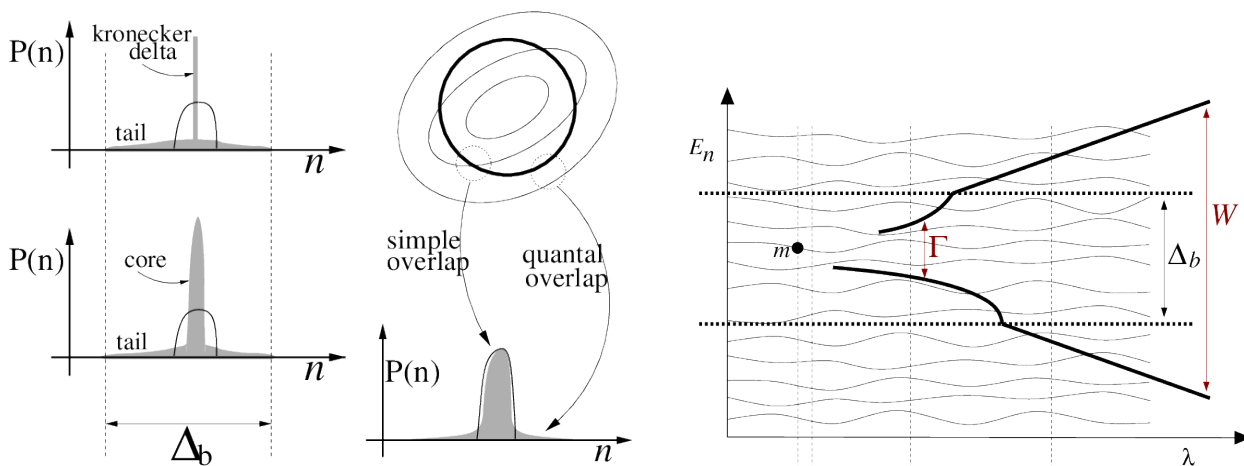
It is important to realize that the definition of $P(n)$ can be written is a way that reflects its classical limit. Namely $P(n) = \mathsf{trace}[\rho^{(n)}\rho^{(m)}]$, where ρ is the probability matrix. For a canonical quantized system the trace can be evaluated using a phase space integral (see lecture regarding the Wigner-Wyle formalism). It is the overlap of microcanonical-like Wigner functions $\rho^{(m)}(X,P)$ and $\rho^{(n)}(X,P)$ that are represented in the figure above by a circle and ellipses respectively. Accordingly, for large λ the result for $P(n)$ reflects the intersection of perturbed energy surfaces with the unperturbed energy surface. The width of classical lineshape is $W(\lambda) = [\mathrm{Var}(V)]^{1/2} = \sqrt{b}\lambda$.

RMT perspective.– The $P(n)$ can be determined analytically for an artificial random-matrix-theory (RMT) model. The so-called Wigner model is defined by the Hamiltonian matrix $\boldsymbol{H} = \boldsymbol{H}_0 + \boldsymbol{V}$, where $\boldsymbol{H}_0 = \text{diag}\{E_n\}$ is diagonal with energies that have spacing Δ_0, while $\boldsymbol{V}$ has bandwidth b. The non-zero in-band elements of $\boldsymbol{V}$ are random numbers that have zero average and dispersion λ. The lineshape of $P(n)$ is indeed "delta+tail" for $\lambda < \Delta_0$, and Lorentzian for $\Delta_0 < \lambda < b^{1/2}\Delta_0$. For larger λ the Lorentzian is not valid, and instead we get a semicircle of width $W(\lambda) = \sqrt{b}\lambda$. However, in contrast with the semiclassical case there is a twist in the story: once $\lambda > b^{3/2}\Delta_0$ the eigenstates become exponentially localized with localization length $\xi \sim b^2$. In this latter regime $\boldsymbol{H} \approx \boldsymbol{V}$ is known as the Anderson-model with off-diagonal disorder.

════════ [42.4] The DOS and the LDOS

Assuming that the spectrum is dense, we can characterize it with a density of states (DOS) function:

$$\varrho(E) \;=\; \sum_n \delta(E - E_n) \tag{42.9}$$

We notice that according to this definition:

$$\int_E^{E+dE} \varrho(E')dE' \;=\; \text{number of states with energy } E < E_n < E + dE \tag{42.10}$$

If the mean level spacing Δ is approximately constant within some energy interval then $\varrho(E) = 1/\Delta$.

The local density of states (LDOS) is a weighted version of the DOS. Each level has a weight which is proportional to its overlap with a reference state:
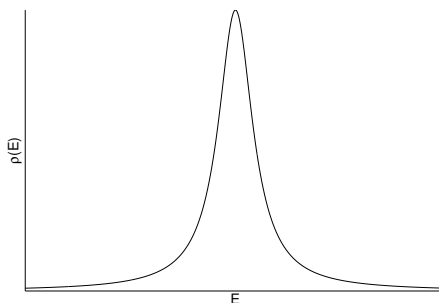
$$\rho(E) \;=\; \sum_n |\langle \Psi | n \rangle|^2 \delta(E - E_n) \tag{42.11}$$

The index n labels as before the eigenstates of the Hamiltonian, while Ψ is the reference state. In particular Ψ can be an eigenstates $|\varepsilon_0\rangle$ of the unperturbed Hamiltonian. In such case the Wigner Lorentzian approximation implies

$$\rho(E) \;=\; \frac{1}{\pi} \frac{(\Gamma/2)}{(E - \varepsilon_0)^2 + (\Gamma/2)^2} \tag{42.12}$$

It should be clear that by definition we have

$$\int_{-\infty}^{\infty} \rho(E)dE \;=\; \sum_n |\langle \Psi | n \rangle|^2 \;=\; 1 \tag{42.13}$$

We have defined $\rho(E)$ such that it is normalized with respect to the measure dE. In the next section we use it inside a Fourier integral, and use ω instead of E. We note that sometimes $\rho(\omega)$ is conveniently re-defined such that it is normalized with respect to the measure $d\omega/(2\pi)$. We recall the common convention which is used for time-frequency Fourier transform in this course:

$$
\begin{aligned}
F(\omega) &= \int f(t)\mathrm{e}^{i\omega t}dt \\
f(t) &= \int \frac{d\omega}{2\pi}F(\omega)\mathrm{e}^{-i\omega t}
\end{aligned}
\tag{42.14}
$$

====== [42.5] Wigner decay and its connection to the LDOS

Let us assume that we have a system with many energy states. We prepare the system in the state $|\Psi\rangle$. Now we apply a field for a certain amount of time, and then turn it off. What is the probability $P(t)$ that the system will remain in the same state? This probability is called the survival probability. By definition:

$$
P(t) = |\langle\Psi(0)|\Psi(t)\rangle|^2
\tag{42.15}
$$

Let $\mathcal{H}_0$ be the unperturbed Hamiltonian, while $\mathcal{H}$ is the perturbed Hamiltonian (while the field is "on"). In what follows the index n labels the eigenstates of the perturbed Hamiltonian $\mathcal{H}$. We would like to calculate the survival amplitude:

$$
\langle\Psi(0)|\Psi(t)\rangle = \langle\Psi|U(t)|\Psi\rangle = \sum_n |\langle n|\Psi\rangle|^2\, \mathrm{e}^{-iE_n t}
\tag{42.16}
$$

We notice that:

$$
\langle\Psi(0)|\Psi(t)\rangle = \mathrm{FT}\left[\sum_n \langle n|\Psi\rangle|^2 2\pi\delta(\omega - E_n)\right] = \mathrm{FT}\left[2\pi\rho(\omega)\right]
\tag{42.17}
$$

If we assume that the LDOS is given by Wigner Lorentzian then:

$$
P(t) = \left|\mathrm{FT}\left[2\pi\rho(E)\right]\right|^2 = \mathrm{e}^{-\Gamma t}
\tag{42.18}
$$

The Wigner decay appears when we "break" first-order perturbation theory. The perturbation should be strong enough to create transitions to other levels. Else the system stays essentially at the same level all the time ($P(t) \approx 1$).

[43] Decay into a continuum

═════ [43.1] Definition of the model

In the problem of a particle in a two-site system, we saw that the particle oscillates between the two sites. We now turn to solve a more complicated problem, where there is one site on one side of the barrier, and on the other side there is a very large number of energy levels (a "continuum").
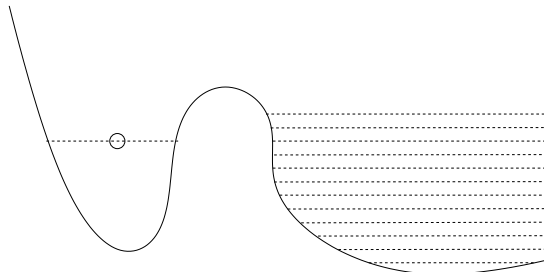
We shall find that the particle decays into the continuum. In the two site problem, the Hamiltonian was:

$$\mathcal{H} = \begin{pmatrix} \epsilon_0 & \sigma \\ \sigma & \epsilon_1 \end{pmatrix} \tag{43.1}$$

where σ is the transition amplitude through the barrier. In the new problem the Hamiltonian is:

$$\mathcal{H} = \begin{pmatrix} \epsilon_0 & \sigma_1 & \sigma_2 & \sigma_3 & . & . & . \\ \sigma_1 & \epsilon_1 & 0 & 0 & . & . & . \\ \sigma_2 & 0 & \epsilon_2 & 0 & . & . & . \\ \sigma_3 & 0 & 0 & \epsilon_3 & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \end{pmatrix} = \mathcal{H}_0 + V \tag{43.2}$$

where the perturbation term V includes the coupling elements σ_k. Without loss of generality we use gauge such that σ_k are real numbers. We assume that the mean level spacing between the continuum states is Δ. If the continuum states are of a one-dimensional box with length L, the quantization of the wavenumber is π/L, and from the dispersion relation $dE = v_E dp$ we get:

$$\Delta = v_E \frac{\pi}{L} \tag{43.3}$$

From the Fermi golden rule (FGR) we expect a decay constant

$$\Gamma\,[\text{FGR}] = 2\pi \frac{1}{\Delta} \sigma^2 \tag{43.4}$$

Below we shall see that this result is exact. We are going to solve both the eigenstate equation $\mathcal{H}\Psi = E\Psi$, and the time dependent Schrödinger's equation. Later we are going to derive the Gamow formula

$$\Gamma\,[\text{Gamow}] = \text{AttemptFrequency} \times \text{BarrierTransmission} \tag{43.5}$$

By comparing with the FGR expression we shall deduce what is the coupling σ between states that touch each other at the barrier. We shall use this result in order to get an expression for the Rabi frequency Ω of oscillations in a double well system.

===== [43.2] An exact solution - the eigenstates

The unperturbed basis is $|0\rangle, |k\rangle$ with energies ϵ_0 and ϵ_k. The level spacing of the quasi continuum states is Δ. The couplings between the discrete state and the quasi-continuum levels are σ_k. The set of equations for the eigenstates $|E_n\rangle$ is

$$\epsilon_0 \Psi_0 + \sum_{k'} \sigma_{k'} \Psi_{k'} = E\Psi_0 \tag{43.6}$$

$$\epsilon_k \Psi_k + \sigma_k \Psi_0 = E\Psi_k, \quad k = 1, 2, 3, ... \tag{43.7}$$

From the kth equation we deduce that

$$\Psi_k = \frac{\sigma_k}{E - \epsilon_k} \Psi_0 \tag{43.8}$$

Hence the expression for the eigenstates is

$$|\Psi\rangle = \sqrt{p}\,|0\rangle + \sqrt{p} \sum_k \frac{\sigma_k}{E - \epsilon_k} |k\rangle \tag{43.9}$$

where $p \equiv |\Psi_0|^2$ is determined by normalization. Substitution of Ψ_k into the 0th equation leads to the secular equation for the eigenenergies

$$\sum_k \frac{\sigma_k^2}{E - \epsilon_k} = E - \epsilon_0 \tag{43.10}$$

This equation can be illustrated graphically. Clearly the roots E_n interlace the the unperturbed values ϵ_k. For equal spacing Δ and equal couplings σ the secular equation can be written as

$$\cot\left(\pi \frac{E}{\Delta}\right) = \frac{1}{\pi} \frac{\Delta}{\sigma^2}(E - \epsilon_0) \qquad \rightsquigarrow \qquad E_n = \left(n + \frac{1}{\pi}\varphi_n\right)\Delta \tag{43.11}$$

where φ changes monotonically from π to 0. Above and below we use the following identities:

$$\sum_{n=-\infty}^{\infty} \frac{1}{x - \pi n} = \cot(x) \equiv S, \qquad \sum_{n=-\infty}^{\infty} \frac{1}{(x - \pi n)^2} = \frac{1}{\sin^2(x)} = 1 + S^2 \tag{43.12}$$

Using the second identity and the secular equation one obtains a compact expression for the normalization constant

$$p = |\Psi_0|^2 = |\langle 0|E_n\rangle|^2 = \frac{\sigma^2}{(E_n - \epsilon_0)^2 + (\Gamma/2)^2} \tag{43.13}$$

where

$$\frac{\Gamma}{2} = \sqrt{\sigma^2 + \left(\frac{\pi}{\Delta}\sigma^2\right)^2} \tag{43.14}$$

The plot of $|\Psi_0|^2$ versus E_n is the Wigner Lorentzian. It gives the overlap of the eigenstates with the unperturbed discrete state.

===== [43.3] An exact solution - the time dependent decay

We switch to the interaction picture:

$$\Psi_k(t) \;=\; c_k(t)\mathrm{e}^{-i\epsilon_k t}, \qquad k = 0, 1, 2, 3, ... \tag{43.15}$$

We distinguish between c_k and c_0. From here on the index runs over the values $k = 1, 2, 3, ...$, and we use the notation $V_{k,0} = \sigma_k$ for the couplings. We get the system of equations:

$$i\frac{dc_0}{dt} \;=\; \sum_k \mathrm{e}^{i(\epsilon_0 - \epsilon_k)t}\, V_{0,k}\, c_k(t) \tag{43.16}$$

$$i\frac{dc_k}{dt} \;=\; \mathrm{e}^{i(\epsilon_k - \epsilon_0)t}\, V_{k,0}\, c_0(t), \qquad k = 1, 2, 3, ...$$

From the second equation we get:

$$c_k(t) \;=\; 0 \;-\; i \int_0^t \mathrm{e}^{i(\epsilon_k - \epsilon_0)t'}\, V_{k,0}\, c_0(t')\, dt' \tag{43.17}$$

By substituting into the first equation we get:

$$\frac{dc_0}{dt} \;=\; -\int_0^t C(t - t')\, c_0(t')\, dt' \tag{43.18}$$

where

$$C(t - t') \;=\; \sum_k |V_{k,0}|^2\, \mathrm{e}^{-i(\epsilon_k - \epsilon_0)(t - t')} \tag{43.19}$$

The Fourier transform of this function is:

$$\tilde{C}(\omega) \;=\; \sum_k |V_{k,0}|^2\, 2\pi\delta(\omega - (\epsilon_k - \epsilon_0)) \;\approx\; \frac{2\pi}{\Delta}\sigma^2 \tag{43.20}$$

Accordingly

$$C(t - t') \;\approx\; \left[\frac{2\pi}{\Delta}\sigma^2\right]\delta(t - t') \;=\; \Gamma\delta(t - t') \tag{43.21}$$

We notice that the time integration only "catches" half of the area of this function. Therefore, the equation for c_0 is:

$$\frac{dc_0}{dt} \;=\; -\frac{\Gamma}{2}c_0(t) \tag{43.22}$$

This leads us to the solution:

$$P(t) \;=\; |c_0(t)|^2 \;=\; \mathrm{e}^{-\Gamma t} \tag{43.23}$$

====== [43.4] An exact solution - the rezolvent and its pole

Using the "P+Q" formalism we can eliminate the continuum and find an explicit expression for the rezolvent of the decaying state:

$$G(z) = \left[\frac{1}{z - \mathcal{H}}\right]_{0,0} = \frac{1}{z - \epsilon_0 - g(z)} \tag{43.24}$$

where

$$g(z) = \sum_k \frac{|V_{k,0}|^2}{z - \epsilon_k} \tag{43.25}$$

The equation for the pole of the rezolvent takes the from $z - \epsilon_0 = g(z)$. This equation has a simple visualization. In the upper complex-plane perspective ($z > 0$) one can regard $g(z)$ as an "electric field" that originates from an "image charge" at $z = -i\infty$. This electric field pushes the zero at $z = \epsilon_0$ into the lower plane a distance Γ_0. If the weighted density of ϵ_k is non-uniform, it is like having a tilted "electric field", hence there is an additional shift Δ_0 in the location of the zero. This correction, that arises due to the interaction of the discrete level with the continuum, is known as the Lamb shift. Accordingly, for the pole that appears in the analytic continuation of $G(z)$ from the upper sheet we write

$$z_{\text{pole}} = \epsilon_0 + \Delta_0 - i\frac{\Gamma_0}{2} \tag{43.26}$$

Using leading order perturbation theory the expressions for the decay rate Γ_0 and for the Lamb shift Δ_0 are:

$$\Gamma_0 = \sum_k 2\pi\delta(\epsilon_0 - \epsilon_k)\,|V_{k,0}|^2 \tag{43.27}$$

$$\Delta_0 = \sum_k \frac{|V_{k,0}|^2}{\epsilon_0 - \epsilon_k} \tag{43.28}$$

The solution above is appealing, but still it does not illuminate the relation to the characteristics of the barrier. We therefore turn in the next section to consider a less artificial example.

====== [43.5] The calculation of the coupling - Bardeen formula

We have discussed a 2×2 matrix model for Rabi oscillations, for which we found

$$\Omega = \sqrt{|2V_{R,L}|^2 + (\epsilon_L - \epsilon_R)^2} \tag{43.29}$$

where $V_{\text{R,L}}$ is the coupling between the "left" and the "right" eigenstates. Above we have discussed the decay of a discrete "left" state into a continuum of "right" states, getting

$$\Gamma = 2\pi\varrho_R\,|V_{R,L}|^2 \tag{43.30}$$

where ϱ_R is the density of states. The question arises how $V_{R,L}$ is estimated for a barrier that is described by a potential $V(x)$.

Consider a 1D Hamiltonian with a potential $V(x)$ that describes free "left" and "right" regions that are separated by a "barrier". In practice one one would like to be able to represent it by a matrix-type model that involves a "junction":

$$\mathcal{H} = \frac{p^2}{2\mathsf{m}} + V(x) \;\mapsto\; \mathcal{H}_L + \mathcal{H}_J + \mathcal{H}_R \tag{43.31}$$

Namely, the unperturbed Hamiltonian is the sum of "left" and "right" segments, and the perturbation is the coupling at a "junction" that couples the two segments. This approach is most popular in STM applications. The question arises how exactly to define the 3 terms in the Hamiltonian. Apparently we have to selects a good basis that is composed of "left" and "right" eigenstates, and figure out how they are coupled at the junction. If the a "point contact" junction is modelled as a delta function $u\delta(x-x_0)$ it is most natural to define the "left" and "right" eigenstates as $\varphi(x) = \sin(k(x-x_0))$, and one can show that the couplings at the energy of interest are given by the formula

$$V_{R,L} \;\; = \;\; \frac{1}{4\mathsf{m}^2 u}(\partial\varphi^R)(\partial\varphi^L) \tag{43.32}$$

where the derivative ∂ is taken at the point $x = x_0$. See derivation at the delta junction subsection. Bardeen has found that for a wide barrier it is possible to use the following approximation:

$$V_{R,L} \;\; = \;\; \frac{1}{2\mathsf{m}}\left[\varphi^R(\partial\varphi^L) - (\partial\varphi^R)\varphi^L\right]_{x_0} \tag{43.33}$$

where $x = x_0$ is an arbitrary point within the barrier region. Note that the point-contact junction formula can be regarded as a limit of the latter. It should be clear that the implied matrix representation of the Hamiltonian is somewhat problematic. Effectively we consider a smaller Hilbert space, from which all the high lying states and the barrier region are truncated. This is possibly not very important for transmission or decay rate calculation, but might be disastrous for Lamb shift calculation. We note that within the matrix model analysis the Lamb shift is

$$\Delta \;\; \approx \;\; \sum_k \frac{|V_{k,0}|^2}{\epsilon_0 - \epsilon_k} \;\; = \;\; \text{prefactor} \times \Gamma \tag{43.34}$$

where the prefactor depends on the cutoff of the dk integration. Thus Δ, unlike Γ depends not only on the transmission g of the junction but also on the k dependence and on the global variation of the density of states.

======= [43.6] The calculation of the coupling - Scattering formalism

Optionally one can relate $|V_{R,L}|^2$ to the transmission g of the barrier. Consider a scattering problem that involves a junction that has two attached leads. The transmission can be calculated using the T-matrix formalism. In leading order the result is

$$g \;\; = \;\; |T_{L,R}|^2 \;\; \approx \;\; (2\pi\varrho_L)(2\pi\varrho_R)|V_{R,L}|^2 \tag{43.35}$$

where the density of states for a lead of length L is $\varrho = L/(\pi v_E)$, and v_E is the velocity at the energy of interest. In order to obtain this result notice that the matrix elements of the T matrix should be taken with flux-normalized states $(2/\sqrt{v_E})\sin(kx)$, while the matrix elements of V are defined with standard normalized states $(2/L)^{1/2}\sin(kx)$. If g is large, one should include higher orders in the T matrix calculation. Accordingly the result depends on the details of the junction. For a simple point-contact junction the result of the geometric summation implies $g \mapsto g/(1+g)$, as expected from the delta-barrier expression.

It is illuminating to realize that $(2\pi\varrho)^{-1}$ can be interpreted as the attempt frequency: the number of collisions with the barrier per units time. For a lead of length L it equals $v_E/2L$. By the above analysis one can deduce that the decay constant can be calculated using the Gamow formula:

$$\Gamma \;\; = \;\; \frac{1}{2\pi\varrho_R}\, g \;\; = \;\; \frac{v_E}{2a}\, g \tag{43.36}$$

where a is the length of the "left" lead, and $v_E/(2a)$ is the attempt frequency. In fact this semi-classically expected result is quite general, as discussed in the following sections.

===== [43.7] Decay out of a square well

A particle of mass m in 1D is confined from the left by an infinite potential wall and from the right by a delta barrier $U(x) = u\delta(x - a)$. We assume large u such that the two regions are weakly coupled. In this section we shall derive an expression for the decay constant Γ. We shall prove that it equals the "attempt frequency" multiplied by the transmission of the barrier. This is called Gamow formula.
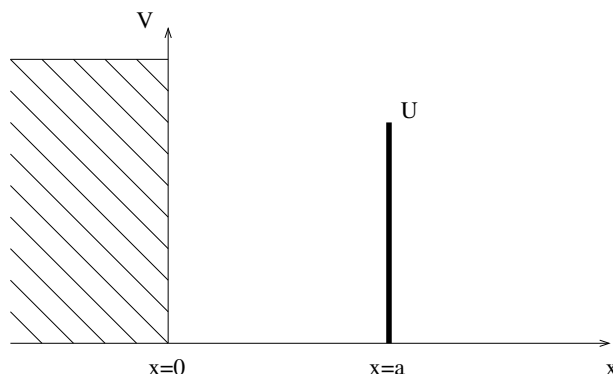
We look for the complex poles of the rezolvent. We therefore look for stationary solutions of the equation $\mathcal{H}\psi = E\psi$ that satisfy "outgoing wave" boundary conditions. The wavenumber of the outgoing wave is written as

$$k \quad = \quad k_n - i\gamma_n \tag{43.37}$$

which implies complex energies

$$E \quad = \quad \frac{k^2}{2\mathsf{m}} \quad = \quad E_n - i\frac{\Gamma_n}{2}, \qquad n = 0, 1, 2, 3... \tag{43.38}$$

$$E_n \quad = \quad \frac{1}{2\mathsf{m}}(k_n^2 - \gamma_n^2) \tag{43.39}$$

$$\Gamma_n \quad = \quad \frac{2}{\mathsf{m}}k_n\gamma_n \quad \equiv \quad 2v_n\gamma_n \tag{43.40}$$

Within the well the most general stationary solution is $\psi(x) = Ae^{ikx} + Be^{-ikx}$. Taking into account the boundary condition $\psi(0) = 0$ at the hard wall, and the outgoing wave boundary condition at infinity we write the wavefunction as

$$\psi(x) \quad = \quad C\sin(kx) \qquad \text{for } 0 < x < a \tag{43.41}$$
$$\psi(x) \quad = \quad De^{ikx} \qquad \text{for } x > a$$

The matching conditions across the delta barrier are:

$$\psi(a + 0) - \psi(a - 0) \quad = \quad 0 \tag{43.42}$$
$$\psi'(a + 0) - \psi'(a - 0) \quad = \quad 2\mathsf{m}u\ \psi(a) \tag{43.43}$$

Thus at $x = a$ the logarithmic derivative should have a jump:

$$\left.\frac{\psi'}{\psi}\right|_{+} - \left.\frac{\psi'}{\psi}\right|_{-} \quad = \quad 2\mathsf{m}u \tag{43.44}$$

leading to the equation

$$ik - k\cot(ka) \quad = \quad 2\mathsf{m}u \tag{43.45}$$

We can write the last equation as:

$$\tan(ka) = -\frac{\frac{k}{2\mathrm{m}u}}{1 - i\frac{k}{2\mathrm{m}u}} \tag{43.46}$$

The zero order solution in the coupling ($u = \infty$) are the energies of an isolated well corresponding to

$$k_n^{(0)} = \frac{\pi}{a}n \qquad \text{[zero order solution]} \tag{43.47}$$

We assume small $k_n/(2\mathrm{m}u)$, and expand both sides of the equation around k_n. Namely we set $k = (k_n + \delta k) - i\gamma$ where δk and γ are small corrections to the unperturbed energy of the isolated state. To leading order the equation takes the form

$$a\delta k - ia\gamma = -\left(\frac{k_n}{2\mathrm{m}u}\right) - i\left(\frac{k_n}{2\mathrm{m}u}\right)^2 \tag{43.48}$$

Hence we get in leading order

$$k_n = k_n^{(0)} - \frac{1}{a}\left(\frac{k_n^{(0)}}{2\mathrm{m}u}\right) \tag{43.49}$$

$$\gamma_n = \frac{1}{a}\left(\frac{k_n^{(0)}}{2\mathrm{m}u}\right)^2 \tag{43.50}$$

From here we can calculate both the shift and the "width" of the energy. To write the result in a more attractive way we recall that the transmission of the delta barrier at the energy $E = E_n$ is

$$g = \frac{1}{1 + (u/v_n)^2} \approx \left(\frac{v_n}{u}\right)^2 \tag{43.51}$$

hence

$$\Gamma_n = 2v_n\gamma_n \approx \frac{v_n}{2a}g \tag{43.52}$$

This is called Gamow formula. It reflects the following semiclassical picture: The particle oscillates with velocity v_n inside the well, hence $v_n/(2a)$ is the number of collisions that it has with the barrier per unit time. The Gamow formula expresses the decay rate as a product of this "attempt frequency" with the transmission of the barrier. It is easy to show that the assumption of weak coupling can be written as $g \ll 1$.

===== [43.8] The Gamow Formula

We consider a particle in a well of width a that can decay to the continuum through a general barrier that has transmission g and reflection amplitude

$$\text{reflection amplitude} \quad = \quad -\sqrt{1-g}\, e^{i\theta_0} \tag{43.53}$$

where both g and the phase shift θ_0 can depend on energy. We would like to derive the Gamow Formula in this more general setup. Our starting point as before is the zero order solution of an isolated square well ($g=0$) for which the unperturbed eigenstates are $\psi(x) = \sin(k_n x)$ with

$$k_n^{(0)} \quad = \quad \left[n - \frac{\theta_0}{2\pi}\right]\frac{\pi}{a} \qquad \text{[zero order solution]} \tag{43.54}$$

But for finite barrier ($g > 0$) the poles of the rezolvent become complex. The equation that determines these poles is obtained by matching of the inside solution $\exp(ikx) - \exp(-ikx)$ with the barrier at $x = a$. Namely, the reflected amplitude $B = -e^{-ika}$ should match the incident amplitude $A = e^{ika}$ as follows:

$$B \quad = \quad -\sqrt{1-g}\, e^{i\theta_0}\, A \tag{43.55}$$

This leads to the equation

$$\exp\left[-i(2ka + \theta_0)\right] \quad = \quad \sqrt{1-g} \tag{43.56}$$

Assuming that the real part k_n of the solution is known we solve for γ_n which is assumed to be small. In leading order the solution is

$$\gamma_n \quad = \quad \frac{1}{4a_n}\ln\left[\frac{1}{1-g}\right] \tag{43.57}$$

In the latter expression we have taken into account that the phase shift might depend on energy, defining the effective width of the well as

$$a_n \quad = \quad a \ + \ \frac{1}{2}\frac{d}{dk}\theta_0(k) \tag{43.58}$$

From here we get

$$\Gamma_n \quad \approx \quad \frac{v_n}{2a_n}\, g \tag{43.59}$$

This is the Gamow formula, and it is in agreement with the semi-classical expectation. Namely, the interpretation of the prefactor as the attempt frequency is consistent with the definition of the Wigner delay time: the period of the oscillations within the well is

$$\text{TimePeriod} \quad = \quad \frac{2a}{v_n} + \frac{d}{dE}\theta_0(E) \quad = \quad \frac{2a_n}{v_n} \tag{43.60}$$

[43.9] From Gamow to the double well problem

Assume a double well which is divided by the same delta function as in the Gamow decay problem. Let us use the solution of the Gamow decay problem in order to deduce the oscillation frequency in the double well.
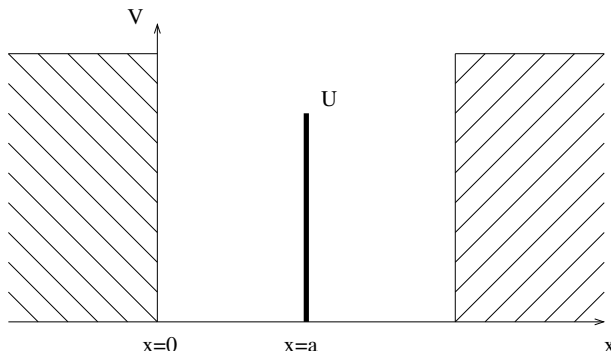
Re-considering the Gamow problem we assume that the region outside of the well is very large, namely it has some length L much larger than a. The k states form a quasi-continuum with mean level spacing Δ_L. By Fermi golden rule the decay rate is

$$\Gamma \;=\; \frac{2\pi}{\Delta_L}\,|V_{nk}|^2 \;=\; \frac{2L}{v_E}\,|V_{nk}|^2 \tag{43.61}$$

where V_{nk} is the probability amplitude per unit time to make a transitions form level n inside the well to any of the k states outside of the well. This expression should be compared with the Gamow formula, which we write as

$$\Gamma \;=\; \frac{v_E}{2a}\,g \tag{43.62}$$

where g is the transmission of the barrier, The Gamow formula should agree with the Fermi golden rule. Hence we deduce that the over-the-barrier coupling is

$$|V_{nk}|^2 \;=\; \left(\frac{v_E}{2L}\right)\left(\frac{v_E}{2a}\right) g \tag{43.63}$$

One can verify that this is consistent with the formula for the coupling between two wavefunctions at the point of a delta junction [see Section 34]:

$$V_{nk} \;=\; -\frac{1}{4\mathsf{m}^2 u}[\partial\psi^{(n)}][\partial\psi^{(k)}] \tag{43.64}$$

where $\partial\psi$ is the radial derivative at the point of the junction. This formula works also if both functions are on the same side of the barrier.

Now we can come back to the double well problem. For simplicity assume a symmetric double well. In the two level approximation n and k are "left" and "right" states with the same unperturbed energy. Due to the coupling we have coherent Bloch oscillation whose frequency is

$$\Omega \;=\; 2|V_{nk}| \;=\; \frac{v_E}{a}\,\sqrt{g} \tag{43.65}$$

[44] Scattering resonances

━━━━━ [44.1] Fabry Perrot interference / transmission resonance

The Fabry-Perrot problem is to find the transmission of a double barrier given the transmission of each barrier and their "optical distance" ϕ (see definition below). We could assume that the barriers are represented by delta functions $u\delta(x \pm (a/2))$. The conventional way of solving this problem is to match together the solutions in the three segments. This procedure is quite lengthy and better to do it with Mathematica. The optional (short) way of solving this problem is to "sum over paths", similar to the way one solves the interference problem in the two slit geometry.
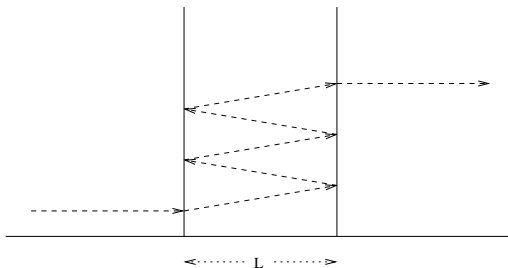
We take as given the transmission coefficient $T = |t|^2$, and the reflection coefficient $R = |r|^2 = 1 - T$. If the distance between the two barriers is a, then a wave accumulates a phase ka when going from the one barrier to the other. The transmission of both barriers together is:

$$\text{transmission} = |t \times \mathrm{e}^{ika} \times (1 + (r\mathrm{e}^{ika})^2 + (r\mathrm{e}^{ika})^4 + \dots) \times t|^2 \tag{44.1}$$

Every round trip between the barriers includes two reflections, so the wave accumulates a phase factor $(\mathrm{e}^{i\phi})^2$, where

$$\phi \quad = \quad ka + \text{phase}(r) \tag{44.2}$$

We have a geometric series, and its sum is:

$$\text{transmission} \quad = \quad \left| t \times \frac{\mathrm{e}^{ika}}{1 - (|r|\mathrm{e}^{i\phi})^2} \times t \right|^2 \tag{44.3}$$

After some algebra we find the Fabry Perrot expression:

$$\text{transmission} \quad = \quad \frac{|t|^4}{1 + |r|^4 - 2|r|^2 \cos(2\phi)} \quad = \quad \frac{1}{1 + 4[R/T^2](\sin(\phi))^2} \tag{44.4}$$

We notice that this is a very "dramatic" result. If we have two barriers that are almost absolutely opaque $R \sim 1$, then as expected for most energies we get a very low transmission of the order of magnitude of T^2. But there are energies for which $\phi = \pi \times$ integer and then we find that the total transmission is 100%! In the following figure we compare the two slit interference pattern (left) to the Fabry Perrot result (right):
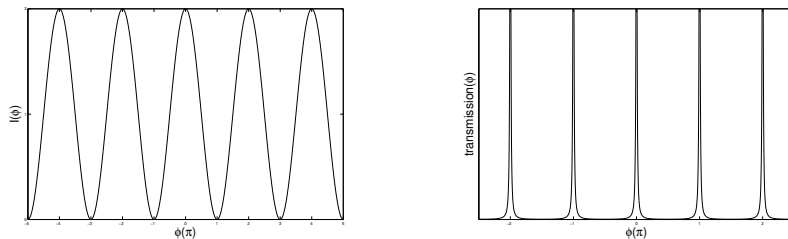
═══════ [44.2] Scattering on a single level system

The most elementary example for a resonance is when the scattering region contains only one level. This can be regarded as a simplified version of the Fabry-Perrot double barrier problem, or it can be regarded as simplified version of scattering on a shielded well which we discuss later on.

We assume, as in the Wigner decay problem that we had been analyzed in a previous lecture, that the scattering region contains a single level of energy E_0. Due to the coupling with the continuum states of the lead, this level acquire width Γ_0. This width would determine the Wigner decay rate if initially the particle were prepared in this level. But we would like to explore a different scenario in which the particle is scattered from the outside. Then we shall see that Γ_0 determines the Wigner delay time of the scattering.

In order to perform the analysis using the a formal scattering approach we need a better characterization of the lead states $|k\rangle$. For simplicity of presentation it is best to imagine the leas as a 1D segment of length L (later we take L to be infinite). The density of states in the energy range of interest is $L/(\pi v_E)$. The volume-normalized free waves of the lead are $|k\rangle \mapsto (2/L)^{1/2}\sin(kx)$. The coupling between the E_0 state of the dot and any of the lead states is $V_{0,k} = w/\sqrt{L}$. The coupling parameter w can be calculated if the form the barrier or its transmission are known (see appropriate "QM is practice I" sections). Consequently we get that the FGR width of the dot level is $\Gamma_0 = (2/v_E)w^2$. Using a formal language it means that the resolvent of the E_0 subsystem is $G = |0\rangle G_{0,0}\langle 0|$, where

$$G_{0,0}(E) \;\;=\;\; \frac{1}{E - E_0 + i(\Gamma_0/2)} \tag{44.5}$$

In order to find the S matrix, the element(s) of the T matrix should be calculated in a properly normalized basis. The relation between the flux-normalized states and the volume-normalized states is:

$$|\phi^{E,a}\rangle \;\;=\;\; \sqrt{\frac{2L}{v_E}}|k\rangle \;\;\longmapsto\;\; \frac{1}{\sqrt{v_E}}e^{-ikx} - \frac{1}{\sqrt{v_E}}e^{+ikx} \tag{44.6}$$

Here the channel index has just one value ($a = 1$). Below we consider also a two-lead system where $a = 1, 2$. Consequently, for the single lead system, we get a 1×1 scattering matrix:

$$S_{aa}(E) \;\;=\;\; 1 - iT_{aa} \;\;=\;\; 1 - i\langle\phi^{E,a}|V|0\rangle G_{0,0}(E)\langle 0|V|\phi^{E,a}\rangle \;\;=\;\; 1 - i\frac{\Gamma_0}{E - E_0 + i(\Gamma_0/2)} \tag{44.7}$$

which implies a phase shift

$$\delta_0 \;\;=\;\; \arctan\left[-\frac{\Gamma_0/2}{E - E_0}\right] \tag{44.8}$$

and accordingly the time delay is

$$\tau_0 \;\;=\;\; \frac{\Gamma_0}{(E - E_0)^2 + (\Gamma_0/2)^2} \tag{44.9}$$

Note that at resonance the time delay is of order $1/\Gamma_0$.

The procedure is easily generalized in order to handle several leads, say two leads as in the double barrier problem. Now we have to use an index $a = 1, 2$ in order to distingush the left and right channels. The width of the E_0 levels is $\Gamma_0 = (2/v_E)[w_1^2 + w_2^2]$. The freewaves solution is the leads are labled as $|\phi^{E,a}\rangle$, and the S matrix comes out

$$S_{ab}(E) \;\;=\;\; \delta_{a,b} - iT_{ab} \;\;=\;\; \delta_{a,b} - i\frac{\Gamma_0/2}{E - E_0 + i(\Gamma_0/2)}\left[\frac{2w_a w_b}{w_1^2 + w_2^2}\right] \tag{44.10}$$

We see that the maximum transmission is for scattering with $E = E_0$, namely $|2w_a w_b/(w_1^2 + w_2^2)|^2$, which becomes 100% transmission if $w_1 = w_2$ as expected from the Fabry-Perrot analysis.

══════ [44.3] Scattering resonance of a shielded 1D well

A shielded 1D well is defined by

$$V(r) = V\Theta(a - r) + u\delta(r - a) \tag{44.11}$$

where V is the potential floor inside the scattering region $0 < r < a$, and u is a shielding potential barrier at the boundary $r = a$ of the scattering region. We add the shield in order to have the option for demonstrating distinct narrow resonances. The interior wave function is

$$\psi(r) = \text{SIN}(\alpha r) \tag{44.12}$$

where $\alpha = \sqrt{2\mathsf{m}|E - V|}$, and SIN is either sin or sinh depending on whether E is larger or smaller than V. Taking the logarithmic derivative at $r = a$ and realizing that the effect of the shield u is simply to boost the result we get:

$$\tilde{k}_0(E; V, u) \equiv \left[\frac{1}{\psi(r)}\frac{d\psi(r)}{dr}\right]_{r=a+0} = \alpha\text{COT}(\alpha a) + 2\mathsf{m}u \tag{44.13}$$

where COT is either cot or coth depending on the energy E. It should be realized that $\tilde{k}_0$ depends on the energy as well as on V and on u. For some of the discussions below, and also for some experimental application it is convenient to regard E as fixed (for example it can be the Fermi energy of an electron in a metal), while V is assumed to be controlled (say by some gate voltage). The dependence of $\tilde{k}_0$ on V is illustrated in the following figure.
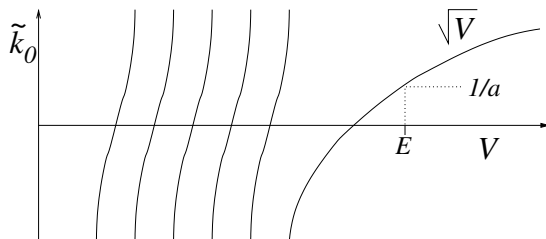
At $V = E$ there is a smooth crossover from the "cot" region to the "coth" region. If V is very large then $\tilde{k}_0 = \infty$. This means that the wavefunction has to satisfy Dirichlet (zero) boundary conditions at $r = a$. This case is called "hard sphere scattering": the particle cannot penetrate the scattering region. For negative V we have values $V = V_r$ at which $\tilde{k}_0 = 0$. We call such locations resonances for a reason that becomes obvious from the discussion below.

One realizes that for $u = 0$ the locations of the resonances are determined by the equation $\cot(\alpha a) = 0$, which corresponds to bounds states of the well if we had at $r = a$ Neumann boundary conditions (derivative of the wavefunction equals zero). In contrast for very large u the zeros are where $\cot(\alpha a) \to \infty$, which corresponds to bounds states of the well if we had Dirichlet boundary conditions.

The scattering phase is determined from the matching condition $k\cot(ka + \delta_0) = \tilde{k}_0$. At resonances we can linearize $\tilde{k}_0$ with respect to the control parameter V, namely, $\tilde{k}_0(V) \approx (V - V_r)/v_r$, where the definitions of v_r is implied by the linearization procedure. Then we get the following approximation

$$\delta_0 = \delta_0^\infty + \arctan\left[\frac{k}{\tilde{k}_0(V)}\right] \approx -ka + \arctan\left[\frac{\Gamma_r/2}{V - V_r}\right] \tag{44.14}$$

with $\Gamma_r = 2v_r k$. The approximation above assumes well separated resonances. The distance between the locations V_r of the resonances is simply the distance between the metastable states of the well. Let us call this level spacing Δ_0. The condition for having a narrow resonance is $\Gamma_r < \Delta_0$. By inspection of the plot it should be clear that shielding (large u) shifts the plot upwards, and consequently v_r and hence Γ_r become smaller. Thus by making u large enough we can ensure the validity of the above approximation.

Optionally if V is fixed, we can plot $k_0(E)$ as a function of E. This plot looks locally the same as the $\tilde{k}_0(V)$ plot, with $E \leftrightarrow -V$. We can determined location of resonances with respect to the energy E, and we can use the approximation $\tilde{k}_0(E) \approx -(E - E_r)/v_r$, where the definitions of E_r and v_r are implied by the linearization procedure. Then we can obtain $\delta_0(E)$ as a function of E, which is illustrated in the figure below.
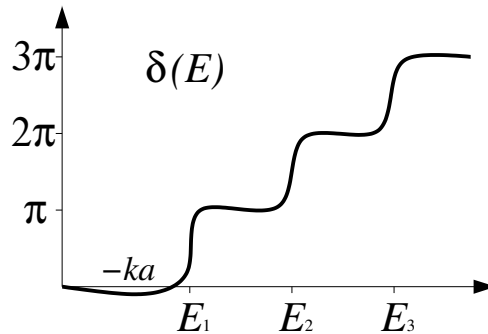
The phase shift is defined modulo π, but in the figure it is convenient not to take the modulo so as to have a continuous plot. The Wigner time delay is obtained by taking the derivative with respect to E. At low energies the s-scattering phase shift is $\delta_0(E) = -ka$ and the time delay is $\tau \approx -2a/v_E$. As the energy is raised there is an extra π shift each time that E goes through a resonance, and the corresponding result for the time delay features a Lorentzian peak. In order to ensure narrow resonance one should assume that the well is shielded by a large barrier. At the center of a resonance the time delay is of order $1/\Gamma_r$.

===== [44.4] Scattering resonance of a spherical shielded well

The solution of the $\ell > 1$ version of the shielded well scattering problem goes along the same lines as in the $\ell = 0$ case that has been discussed above. The only modification is a change of convention: we work below with the radial functions $R(r) = u(r)/r$ and not with $u(r)$. Accordingly for the logarithmic derivative on the boundary of the scattering region we use the notation k_ℓ instead of $\tilde{k}_\ell$. Once we know the $\tilde{k}_\ell$ the phase shift can be calculated using the formula

$$
e^{i2\delta_\ell} = \left. \left(\frac{h_\ell^-}{h_\ell^+} \right) \frac{k_\ell(V) - (h_\ell'^-/h_\ell^-)k}{k_\ell(V) - (h_\ell'^+/h_\ell^+)k} \right|_{r=a} \tag{44.15}
$$

In what follows we fix the energy E of the scattered particle, and discuss the behavior of the phase shift and the cross section as a function of V. In physical applications V can be interpreted as some "gate voltage". Note that in most textbooks it is customary to fix V and to change E. We prefer to change V because then the expansions are better controlled. In any case our strategy gives literally equivalent results. Following Messiah p.391 and using the notations

$$
\left(\frac{h_\ell^-}{h_\ell^+} \right) \equiv e^{i2\delta_\ell^\infty}, \qquad k \left(\frac{h_\ell'^+}{h_\ell^+} \right)_{r=a} \equiv \kappa + i k_{\text{eff}} \tag{44.16}
$$

consequently

$$
e^{i2\delta_\ell} = \left(e^{i2\delta_\ell^\infty} \right) \frac{k_\ell(V) - \kappa + i k_{\text{eff}}}{k_\ell(V) - \kappa - i k_{\text{eff}}} \tag{44.17}
$$

$$
\delta_\ell = \delta_\ell^\infty + \arctan\left[\frac{k_{\text{eff}}}{k_\ell(V) - \kappa} \right] \tag{44.18}
$$

We can plot the right hand side of the last equation as a function of V. If the shielding is large we get typically $\delta_\ell \approx \delta_\ell^\infty$ as for a hard sphere. But if V is smaller than E we can find narrow resonances as in the $\ell = 0$ quasi 1D problem. The analysis of these resonances is carried out exactly in the same way. Note that for $\ell > 0$ we might have distinct resonances even without shielding thanks to the centrifugal barrier.

QM in Practice (part III)

[45] The Aharonov-Bohm effect

========= [45.1] The Aharonov-Bohm geometry

In the quantum theory it is natural to describe the electromagnetic field using the potentials V, A and regard $\mathcal{E}, \mathcal{B}$ as associated observables. Below we discuss the case in which $\mathcal{E} = \mathcal{B} = 0$ in the region where the particle is moving. According to the classical theory one expects that the motion of the particle would not be affected by the field, since the Lorentz force is zero. However, we shall see that according to the quantum theory the particle is affected due to the non-zero circulation of A. This is a topological effect that we are going to clarify. Specifically we consider ring that is penetrated by a magnetic flux Φ through its center. This is the so-called Aharonov-Bohm geometry. To have a flux through the ring means that:

$$\oint \vec{A} \cdot d\vec{l} \;\; = \;\; \iint \mathcal{B} \cdot d\vec{s} \;\; = \;\; \Phi \tag{45.1}$$

The simplest gauge choice for the vector potential is

$$A \;\; = \;\; \frac{\Phi}{L} \qquad \text{[tangential]} \tag{45.2}$$

where L is the length of the ring. Below we treat the ring as a 1D segment $0 < x < L$ with periodic boundary conditions. The Hamiltonian is

$$\mathcal{H} \;\; = \;\; \frac{1}{2\mathsf{m}} \left(\hat{p} - \frac{e\Phi}{cL} \right)^2 \tag{45.3}$$

The eigenstates of $\mathcal{H}$ are the momentum states $|k_n\rangle$ where:

$$k_n \;\; = \;\; \frac{2\pi}{L} n, \qquad n = 0, \pm 1, \pm 2, ... \tag{45.4}$$

The eigenvalues are (written with $\hbar$ for historical reasons):

$$E_n \;\; = \;\; \frac{1}{2\mathsf{m}} \left(\frac{2\pi\hbar}{L} n - \frac{e\Phi}{cL} \right)^2 \;\; = \;\; \frac{1}{2\mathsf{m}} \left(\frac{2\pi\hbar}{L} \right)^2 \left(n - \frac{e\Phi}{2\pi\hbar c} \right)^2 \tag{45.5}$$

The unit $2\pi\hbar c/e$ is called "fluxon". It is the basic unit of flux in nature. We see that the energy spectrum is influenced by the presence of the magnetic flux. On the other hand, if we draw a plot of the energies as a function of the flux we see that the energy spectrum repeats itself every time the change in the flux is an integer multiple of a fluxon. (To guide the eye we draw the ground state energy with thick line).

The fact that the electron is located in an area where there is no Lorentz force $\mathcal{E} = \mathcal{B} = 0$, but is still influenced by the vector potential is called the Aharonov-Bohm Effect. This is an example of a topological effect.
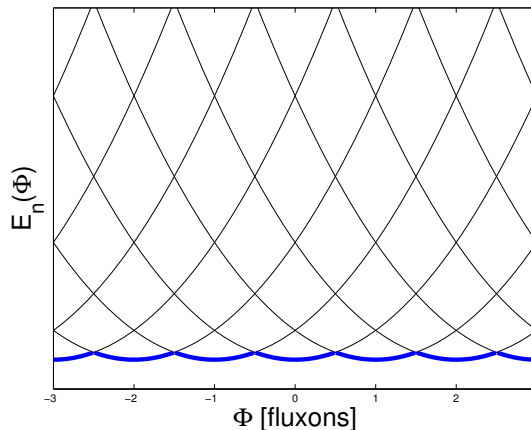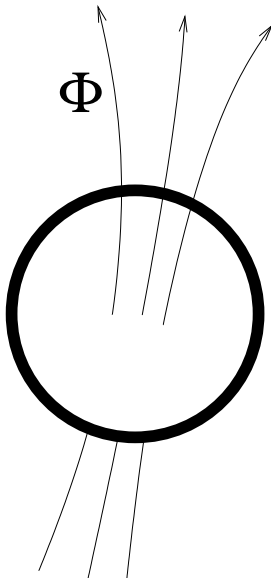
═══════ [45.2] The energy levels of a ring with a scatterer

Consider an Aharonov-Bohm ring with (say) a delta scatterer:

$$\mathcal{H} \;\; = \;\; \frac{1}{2\mathsf{m}}\left(p - \frac{e\Phi}{L}\right)^2 + u\delta(x) \tag{45.6}$$

We would like to find the eigenenergies of the ring. The standard approach is to write the general solution in the empty segment, and then to impose the matching condition over the delta scatterer. An elegant procedure for solution is based on the scattering formalism. In order to characterize the scattering within the system, the ring is cut at some arbitrary point and the S matrix of the open segment is specified. It is more convenient to use the row-swapped matrix, such that the transmission amplitudes are along the diagonal:

$$\tilde{\mathbf{S}} \;\; = \;\; \mathrm{e}^{i\gamma}\begin{pmatrix} \sqrt{g}\mathrm{e}^{i\phi} & -i\sqrt{1-g}\mathrm{e}^{-i\alpha} \\ -i\sqrt{1-g}\mathrm{e}^{i\alpha} & \sqrt{g}\mathrm{e}^{-i\phi} \end{pmatrix} \tag{45.7}$$

The transmision amplitude for a delta scatter is $t = [1 + i(u/v_E)]^{-1}$, hence the transmission is

$$g(E) = \left[1 + \left(\frac{u}{v_E}\right)^2\right]^{-1}, \qquad\qquad v_E = \text{velocity at energy } E \tag{45.8}$$

We include "legs" to the delta scatterer, hence the total transmission phase is

$$\gamma(E) \;\; = \;\; k_E L - \arctan\left(\frac{u}{v_E}\right) \tag{45.9}$$

More precisely, with added flux the transmission phases are $\gamma \pm \phi$ where $\phi = e\Phi/\hbar$. The reflection phases are $\gamma - (\pi/2) \pm \alpha$, where $\alpha = 0$ if we cut the ring symmetrically, such that the two legs have the same length.

The periodic boundary conditions imply the "matching condition"

$$\begin{pmatrix} A \\ B \end{pmatrix} \;\; = \;\; \tilde{\mathbf{S}}\begin{pmatrix} A \\ B \end{pmatrix} \tag{45.10}$$

This equation has a non-trivial solution if and only if

$$\det(\tilde{\mathbf{S}}(E) - \mathbf{1}) = 0 \tag{45.11}$$

For the calculation is is useful to note that

$$\det(\tilde{\mathbf{S}} - \mathbf{1}) = \det(\tilde{\mathbf{S}}) - \mathsf{trace}(\tilde{\mathbf{S}}) + 1 \tag{45.12}$$
$$\det(\tilde{\mathbf{S}}) = (e^{i\gamma})^2 \tag{45.13}$$
$$\mathsf{trace}(\tilde{\mathbf{S}}) = 2\sqrt{g}e^{i\gamma}\cos\phi \tag{45.14}$$

Hence we get an equation for the eigen-energies:

$$\cos(\gamma(E)) = \sqrt{g(E)}\cos(\phi) \tag{45.15}$$

In order to find the eigen-energies we plot both sides as a function of E. The left hand side oscillates between -1 and $+1$, while the right hand side is slowly varying monotonically. It is easily verified that the expected results are obtained for clean ring ($g = 1$) and for infinite well ($g = 0$).

══════ [45.3] Perturbation theory for a ring + scatterer

Let us consider a particle with mass m on a 1D ring. A flux Φ goes through the ring. In addition, there is a scatterer that is described by a delta function. The Hamiltonian that describes the system is:

$$\mathcal{H} = \frac{1}{2\mathsf{m}}\left(p - \frac{\Phi}{L}\right)^2 + u\delta(x) \tag{45.16}$$

For $\Phi = u = 0$ the symmetry group of this Hamiltonian is $O(2)$. This means symmetry with respect to rotations and reflections. Note that in one-dimension ring = circle = torus, hence rotations and displacements are the same. Only in higher dimensions they are different (torus $\neq$ sphere).

Degeneracies are an indication for symmetries of the Hamiltonian. If the eigenstate has a lower symmetry than the Hamiltonian, a degeneracy appears. Rotations and reflections do not commute, that is why we have degeneracies. When we add flux or a scatterer, the degeneracies open up. Adding flux breaks the reflection symmetry, and adding a scatterer breaks the rotation symmetry. Accordingly, depending on the perturbation, it would be wise to use one of the following two bases:

The first basis: The first basis complies with the rotation (=translations) symmetry:

$$|n = 0\rangle = \frac{1}{\sqrt{L}} \tag{45.17}$$
$$|n, \text{anticlockwise}\rangle = \frac{1}{\sqrt{L}}e^{+ik_n x}, \qquad n = 1, 2, ...$$
$$|n, \text{clockwise}\rangle = \frac{1}{\sqrt{L}}e^{-ik_n x}, \qquad n = 1, 2, ...$$

The degenerate states are different under reflection. Only the ground state $|n = 0\rangle$ is symmetric under both reflections and rotations, and therefore it does not have to be degenerate. It is very easy to calculate the perturbation matrix elements in this basis:

$$\langle n|\delta(x)|m\rangle = \int \Psi^n(x)^*\delta(x)\Psi^m(x)dx = \Psi^n(0)\Psi^m(0) = \frac{1}{L} \tag{45.18}$$

so we get:

$$V_{nm} = \frac{u}{L} \begin{pmatrix} 1 & 1 & 1 & 1 & \dots \\ 1 & 1 & 1 & 1 & \dots \\ 1 & 1 & 1 & 1 & \dots \\ 1 & 1 & 1 & 1 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} \tag{45.19}$$

The second basis: The second basis complies with the reflection symmetry:

$$|n = 0\rangle = \frac{1}{\sqrt{L}} \tag{45.20}$$

$$|n, +\rangle = \sqrt{\frac{2}{L}} \cos(k_n x), \qquad n = 1, 2, \dots$$

$$|n, -\rangle = \sqrt{\frac{2}{L}} \sin(k_n x), \qquad n = 1, 2, \dots$$

The degeneracy is between the even states and the odd states that are displaced by half a wavelength with respect to each other. If the perturbation is not the flux but rather the scatterer, then it is better to work with the second basis, which complies with the potential's symmetry. The odd states are not influenced by the delta function, and they are also not "coupled" to the even states. The reason is that:

$$\langle m|\delta(x)|n\rangle = \int \Psi^m(x)^* \delta(x) \Psi^n(x) dx = 0, \qquad \text{if } n \text{ or } m \text{ are "sin"} \tag{45.21}$$

Consequently the subspace of odd states is not influenced by the perturbation, i.e. $V_{nm}^{(-)} = \mathbf{0}$, and we only need to diagonalize the block that belongs to the even states. It is very easy to write the perturbation matrix for this block:

$$V_{nm}^{(+)} = \frac{u}{L} \begin{pmatrix} 1 & \sqrt{2} & \sqrt{2} & \sqrt{2} & \dots \\ \sqrt{2} & 2 & 2 & 2 & \dots \\ \sqrt{2} & 2 & 2 & 2 & \dots \\ \sqrt{2} & 2 & 2 & 2 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} \tag{45.22}$$

Energy levels: Without a scatterer the eigenenergies are:

$$E_n(\Phi, u{=}0) = \frac{1}{2\mathsf{m}} \left(\frac{2\pi}{L} \times \text{integer} - \frac{\Phi}{L} \right)^2, \qquad \text{integer} = 0, \pm 1, \pm 2, \dots \tag{45.23}$$

On the other hand, in the limit $u \to \infty$ the system does not "feel" the flux, and the ring becomes a one-dimensional box. The eigenenergies in this limit are:

$$E_n(\Phi, u{=}\infty) = \frac{1}{2\mathsf{m}} \left(\frac{\pi}{L} \times \text{integer} \right)^2, \qquad \text{integer} = 1, 2, \dots \tag{45.24}$$

As one increases u the number of the energy levels does not change, they just move. See figure below. We would like to use perturbation theory in order to find corrections to the above expressions. We consider how we do perturbation theory with respect to the $u{=}0$ Hamiltonian. It is also possible to carry out perturbation theory with respect to the $u{=}\infty$ Hamiltonian (for that one should use the formula for the interaction at a junction).
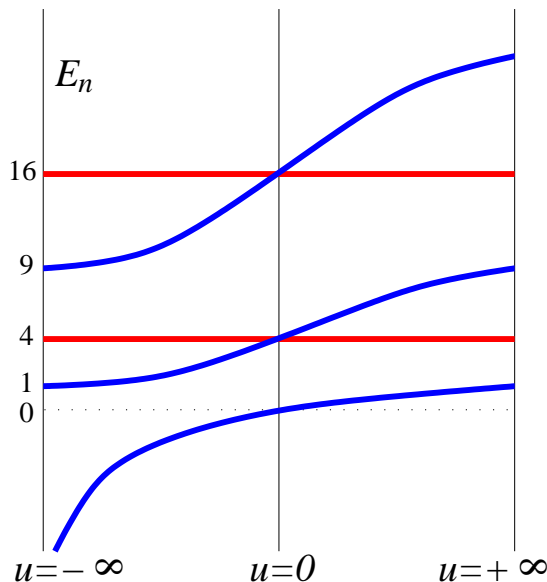
The corrections to the energy: Let us evaluate the first-order correction to the energy of the eigenstates in the absence of an external flux.

$$
\begin{aligned}
E_{n=0} &= E_{n=0}^{[0]} + \frac{u}{L} \\
E_{n=1,2,3,\ldots} &= E_n^{[0]} + \frac{2u}{L}
\end{aligned}
\tag{45.25}
$$

The correction to the ground state energy, up to the second order is:

$$
E_{n=0} \;=\; 0 + \frac{u}{L} + \left(\frac{u}{L}\right)^2 \sum_{k=1}^{\infty} \frac{(\sqrt{2})^2}{0 - \frac{1}{2\mathsf{m}}\left(\frac{2\pi}{L}k\right)^2} \;=\; \frac{u}{L}\left(1 - \frac{1}{6}u\mathsf{m}L\right)
\tag{45.26}
$$

where we have used the identity:

$$
\sum_{k=1}^{\infty} \frac{1}{k^2} \;=\; \frac{\pi^2}{6}
\tag{45.27}
$$

Optional calculation: We will now assume that we did not notice the symmetry of the problem, and we chose to work with the first basis. Using perturbation theory on the ground state energy is simple in this basis:

$$
E_{n=0} \;=\; 0 + \frac{u}{L} + \left(\frac{u}{L}\right)^2 2\sum_{k=1}^{\infty} \frac{(1)^2}{0 - \frac{1}{2\mathsf{m}}\left(\frac{2\pi}{L}k\right)^2} \;=\; \frac{u}{L}\left(1 - \frac{1}{6}u\mathsf{m}L\right)
\tag{45.28}
$$

But using perturbation theory on the rest of the states is difficult because there are degeneracies. The first thing we must do is "degenerate perturbation theory". The diagonalization of each degenerate energy level is:

$$
\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \;\rightarrow\; \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}
\tag{45.29}
$$

Now we should transform to a new basis, where the degeneracy is removed. This is exactly the basis that we chose to work with due to symmetry considerations. The moral lesson is: understanding the symmetries in the system can save us work in the calculations of perturbation theory.

═══════ [45.4] The AB effect in a closed geometry

The eigen-energies of a particle in a closed ring are periodic functions of the flux. In particular in the absence of scattering

$$E_n \;=\; \frac{1}{2\mathsf{m}}\left(\frac{2\pi\hbar}{L}\right)^2\left(n-\frac{e\Phi}{2\pi\hbar c}\right)^2 \;=\; \frac{1}{2}\mathsf{m}v_n^2 \tag{45.30}$$

That is in contrast with classical mechanics, where the energy can have any positive value:

$$E_{\text{classical}} \;=\; \frac{1}{2}\mathsf{m}v^2 \tag{45.31}$$

According to classical mechanics the lowest energy of a particle in a magnetic field is zero, with velocity zero. This is not true in the quantum case. It follows that an added magnetic flux has an detectable effect on the system. The effect can be described in one of the following ways:

- The spectrum of the system changes (it can be measured using spectroscopy)
- For flux that is not an integer or half integer number there are persistent currents in the system.
- The system has either a diamagnetic or a paramagnetic response (according to the occupancy).

We already have discussed the spectrum of the system. So the next thing is to derive an expression for the current in the ring. The current operator is

$$\hat{I} \;\equiv\; -\frac{\partial \mathcal{H}}{\partial \Phi} \;=\; \frac{e}{L}\left[\frac{1}{\mathsf{m}}\left(\hat{p}-\frac{e\Phi}{L}\right)\right] \;=\; \frac{e}{L}\hat{v} \tag{45.32}$$

It follows that the current which is created by an electron that occupies the nth level is:

$$I_n \;=\; \left\langle n\left|\left(-\frac{\partial \mathcal{H}}{\partial \Phi}\right)\right|n\right\rangle \;=\; -\frac{dE_n}{d\Phi} \tag{45.33}$$

The proof of the second equality is one line of algebra. If follows that by looking at the plot of the energies $E_n(\Phi)$ as a function of the flux, one can determine (according to the slope) what is the current that flows in each occupied energy level. If the flux is neither integer nor half integer, all the states "carry current" so that in equilibrium the net current is not zero. This phenomenon is called "persistent currents". The equilibrium current in such case cannot relax to zero, even if the temperature of the system is zero.

There is a statement in classical statistical mechanics that the equilibrium state of a system is not affected by magnetic fields. The magnetic response of any system is a quantum mechanical effect that has to do with the quantization of the energy levels (Landau magnetism) or with the spins (Pauly magnetism). Definitions:

- Diamagnetic System - in a magnetic field, the system energy increases.
- Paramagnetic System - in a magnetic field, the system energy decreases.

The Aharonov Bohm geometry provides the simplest example for magnetic response. If we place one electron in a ring, and add a weak magnetic flux, the system energy increases. Accordingly we say that the response is "diamagnetic". The electron cannot "get rid" of its kinetic energy, because of the quantization of the momentum.

========= [45.5] Dirac Monopoles

Yet another consequence of the "Aharonov Bohm" effect is the quantization of the magnetic charge. Dirac has claimed that if magnetic monopoles exist, then there must be an elementary magnetic charge. The formal argument can be phrased as follows: If a magnetic monopole exists, it creates a vector potential field in space ($A(x)$). The effect of the field of the monopole on an electron close by is given by the line integral $\oint \vec{A} \cdot d\vec{r}$. We can evaluate the integral by calculating the magnetic flux Φ through a Stokes surface. The result should not depend on the choice of the surface, otherwise the phase is not be well defined. In particular we can choose Stokes surfaces that pass above and below the monopole, and deduce that the phase difference $\phi = e\Phi/\hbar c$ should be zero modulo 2π. Hence the flux Φ should be an integer multiple of $2\pi\hbar c/e$. Using "Gauss law" we conclude that the monopole must have a magnetic charge that is quantized in units of $\hbar c/2e$.

Dirac's original reasoning was somewhat more constructive. Let us assume that a magnetic monopole exist. The magnetic field that would be created by this monopole would be like that of a tip of a solenoid. But we have to *exclude* the region in space where we have the magnetic flux that goes through the solenoid. If we want this "flux line" to be unobservable then it should be quantized in units of $2\pi\hbar c/e$. This shows that Dirac "heard" about the Aharonov Bohm effect, but more importantly this implies that the "tip" would have a charge which equals an integer multiple of $\hbar c/2e$.

========= [45.6] The AB effect: path integral formulation

We can optionally illustrate the Aharonov-Bohm Effect by considering an open geometry. In an open geometry the energy is not quantized: it is determined by scattering arrangement. If the energy potential floor is taken as a reference - the energy E can be any positive value. We are looking for stationary states that solve the Schrödinger equation for a given energy. These states are called "scattering states". Below we discuss the Aharonov-Bohm effect in a "two slit" geometry, and later refer to a "ring" geometry (with leads).

First we notice the following rule: if we have a planar wave $\psi(x) \propto e^{ikx}$, and if the amplitude at the point $x = x_1$ is $\psi(x_1) = C$, then at another point $x = x_2$ the amplitude is $\psi(x_2) = Ce^{ik(x_2 - x_1)}$.

Now we generalize this rule for the case in which there is a vector potential A. For simplicity, we assume that the motion is in one-dimension. The eigenstates of the Hamiltonian are the momentum states. If the energy of the particle is E then the wavefunctions that solve the Schrödinger's equation are $\psi(x) \propto e^{ik_\pm x}$, where

$$k_\pm = \pm\sqrt{2\mathsf{m}E} + A \equiv \pm k_E + A \tag{45.34}$$

Below we refer to the advancing wave: if at point $x = x_1$ the amplitude is $\psi(x_1) = C$, then at another point $x = x_2$ the amplitude is $\psi(x_2) = Ce^{ik_E(x_2 - x_1) + A \cdot (x_2 - x_1)}$. It is possible to generalize the idea to three dimensions: if a wave advances along a certain path from point x_1 to point x_2, then the accumulated phase is:

$$\phi = k_E L + \int_{x_1}^{x_2} A \cdot dx, \qquad L = \text{length of the path} \tag{45.35}$$

If there are two different paths that connect the points x_1 and x_2, then the phase difference is:

$$\Delta\phi = k_E \Delta L + \int_{L_2} A \cdot dx - \int_{L_1} A \cdot dx = k_E \Delta L + \oint A \cdot dx = k_E \Delta L + \frac{e}{\hbar c}\Phi \tag{45.36}$$

where in the last term we "bring back" the standard physical units. The approach which was presented above for calculating the probability of the particle to go from one point to another is called "path integrals". This approach was developed by Feynman, and it leads to what is called "path integral formalism" - an optional approach to do calculations in quantum mechanics. The conventional method is to solve the Schrödinger's equation with the appropriate boundary conditions.

══════ [45.7] The AB effect in a two slits geometry

We can use the path integral point of view in order to analyze the interference in the two slit experiment. A particle that passes through two slits, splits into two partial waves that unite at the detector. Each of these partial waves passes a different optical path. Hence the probability of reaching the detector, and consequently the measured intensity of the beam is

$$\text{Intensity} \quad = \quad \left|1 \times e^{ikr_1} + 1 \times e^{ikr_2}\right|^2 \quad \propto \quad 1 + \cos(k(r_2 - r_1)) \tag{45.37}$$

Marking the length difference as ΔL, and the associated phase difference as $\Delta \phi$, we rewrite this expression as:

$$\text{Intensity} \quad \propto \quad 1 + \cos(\Delta \phi), \tag{45.38}$$

Changing the location of the detector results in a change in the phase difference ϕ. The "intensity", or more precisely the probability that the particle will reach the detector, as a function of the phase difference ϕ, is called "interference pattern". If we place a solenoid between the slits, then the formula for the phase difference becomes:

$$\Delta \phi \quad = \quad k\Delta L + \frac{e}{\hbar c}\Phi \tag{45.39}$$

If we draw a plot of the "intensity" as a function of the flux we get the same "interference pattern".
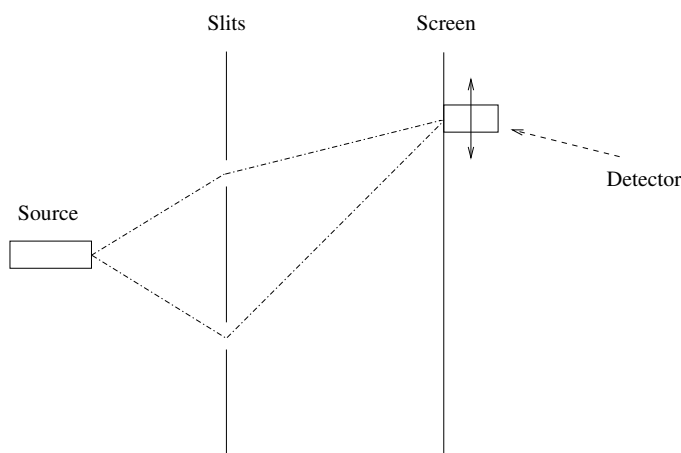
If we want to find the transmission of an Aharonov-Bohm device (a ring with two leads) then we must sum all the paths going from the first lead to the second lead. If we only take into account the two shortest paths (the particle can pass through one arm or the other arm), then we get a result that is formally identical to the result for the two slit geometry. In reality we must take into account all the possible paths. That is a very long calculation, leading to a Fabry-Perrot type result (see previous lecture). In the latter case the transmission is an even function of Φ, even if the arms do not have the same length. Having the same transmission for $\pm\Phi$ in the case of a closed device is implied by time reversal symmetry.

[46] Motion in uniform magnetic field (Landau, Hall)

======= [46.1] The two-dimensional ring geometry

Let us consider a three-dimensional box with periodic boundary conditions in the x direction, and zero boundary conditions on the other sides. In the absence of magnetic field we assume that the Hamiltonian is:

$$\mathcal{H} \quad = \quad \frac{1}{2\mathsf{m}}\hat{p}_x^2 + \left[\frac{1}{2\mathsf{m}}\hat{p}_y^2 + V(y)\right] + \left[\frac{1}{2\mathsf{m}}\hat{p}_z^2 + V_{\text{box}}(z)\right] \tag{46.1}$$

The eigenstates of a particle in such box can be labeled as follows:

$$|k, \nu, n\rangle \quad \mapsto \quad \frac{1}{\sqrt{L_x}}e^{ikx} \times \varphi^{(\nu)}(y) \times \frac{2}{\sqrt{L_z}}\sin\left(\frac{\pi n}{L_z}z\right) \tag{46.2}$$

$$k = \frac{2\pi}{L_x} \times \text{integer}$$

$$\nu = 0, 1, 2, \dots \quad n = 1, 2, 3, \dots \dots .$$

The eigenenergies are:

$$E_{k,\nu,n} \quad = \quad \frac{k^2}{2\mathsf{m}} + \varepsilon_\nu + \frac{1}{2\mathsf{m}}\left(\frac{\pi}{L_z}n\right)^2 \tag{46.3}$$

We assume L_z to be very small compared to the other dimensions. We shall discuss what happens when the system is prepared in low energies such that only $n = 1$ states are relevant. So we can ignore the z axis.

======= [46.2] Classical Motion in a uniform magnetic field

Consider the motion of an electron in a two-dimensional ring. We assume that the vertical dimension is "narrow", so that we can safely ignore it, as was explained in the previous section. For convenience we "spread out" the ring susch that it forms a rectangle with periodic boundary conditions over $0 < x < L_x$, and an arbitrary confining potential $V(y)$ in the perpendicular direction. Additionally we assume that there is a uniform magnetic field $\mathcal{B}$ along the z axis. Therefore the electron is affected by a Lorentz force $F = -(e/c)\mathcal{B} \times v$. If there is no electrical potential, the electron performs a circular motion with the cyclotron frequency:

$$\omega_B \quad = \quad \frac{e\mathcal{B}}{\mathsf{m}c} \tag{46.4}$$

If the electron has a kinetic energy E, its velocity is:

$$v_E \quad = \quad \sqrt{\frac{2E}{\mathsf{m}}} \tag{46.5}$$

Consequently it moves along a circle of radius

$$r_E \quad = \quad \frac{v_E}{\omega_B} \quad = \quad \frac{\mathsf{m}c}{e\mathcal{B}}v_E \tag{46.6}$$

If we take into account a non-zero electric field

$$\mathcal{E}_y \quad = \quad -\frac{dV}{dy} \tag{46.7}$$

we get a motion along a cycloid with the drift velocity (see derivation below):

$$v_{\text{drift}} = c\frac{\mathcal{E}_y}{\mathcal{B}} \tag{46.8}$$

Let us remind ourselves why the motion is along a cycloid. The Lorentz force in the laboratory reference frame is (from now on we absorb the (e/c) of the electron into the definition of the field):

$$F = \mathcal{E} - \mathcal{B} \times v \tag{46.9}$$

If we transform to a reference frame that is moving at a velocity v_0 we get:

$$F = \mathcal{E} - \mathcal{B} \times (v_0 + v') = (\mathcal{E} + v_0 \times \mathcal{B}) - \mathcal{B} \times v' \tag{46.10}$$

Therefore, the non-relativistic transformation of the electromagnetic field is:

$$\mathcal{E}' = \mathcal{E} + v_0 \times \mathcal{B} \tag{46.11}$$
$$\mathcal{B}' = \mathcal{B}$$

If there is a field in the y direction in the laboratory reference frame, we can transform to a new reference frame where the field is zero. From the transformation above we conclude that in order to have a zero electrical field, the velocity of the "new" frame of reference should be:

$$v_0 = \frac{\mathcal{E}}{\mathcal{B}}c \qquad [\text{restoring CGS units for clarity}] \tag{46.12}$$

In the new reference frame the particle moves along a circle. Therefore, in the laboratory reference frame it moves along a cycloid.
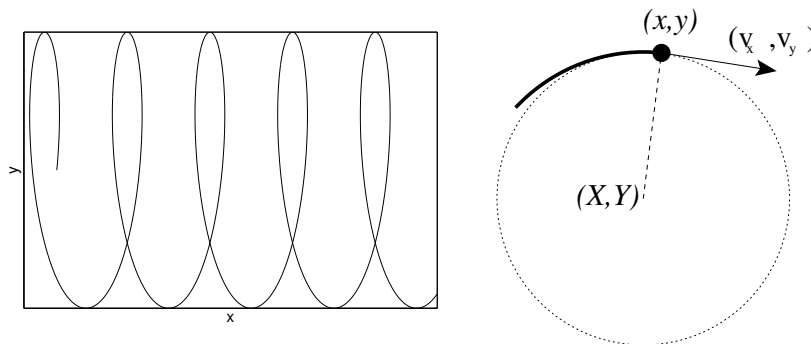
Conventionally the classical state of the particle is described by the coordinates $r = (x, y)$ and $v = (v_x, v_y)$. But from the above discussion it follows that a simpler description of the trajectory is obtained if we follow the motion of the moving circle. The center of the circle $R = (X, Y)$ is moving along a straight line, and its velocity is v_{drift}. The transformation that relates R to r and v is

$$\vec{R} = \vec{r} - \vec{e}_z \times \frac{1}{\omega_B}\vec{v} \tag{46.13}$$

where $\vec{e}_z$ is a unit vector in the z direction. The second term in the right hand side is a vector of length r_E in the radial direction (perpendicular to the velocity). Thus instead of describing the motion with the canonical coordinates (x, y, v_x, v_y), we can use the new coordinated (X, Y, v_x, v_y).

═══════ [46.3] The Hall Effect

If we have particles spread out in a uniform density ρ per unit area, then the current density per unit length is:

$$J_x \;=\; e\rho v_{\text{drift}} \;=\; \rho\frac{ec}{\mathcal{B}}\mathcal{E}_y \;=\; -\rho\frac{ec}{\mathcal{B}}\frac{dV}{dy} \tag{46.14}$$

where we keep CGS units and V is the electrical potential (measured in Volts). The total current is:

$$I_x \;=\; \int_{y_1}^{y_2} J_x\,dy \;=\; -\rho\frac{ec}{\mathcal{B}}(V(y_2) - V(y_1)) \;=\; -\rho\frac{c}{\mathcal{B}}(\mu_2 - \mu_1) \tag{46.15}$$

Here $\mu = eV$ is the chemical potential. Accordingly the Hall conductance is:

$$G_{\text{Hall}} \;=\; -\rho\frac{ec}{\mathcal{B}} \tag{46.16}$$

In the quantum analysis we shall see that the electrons occupy "Landau levels". The density of electrons in each Landau Level is $e\mathcal{B}/2\pi\hbar c$. From this it follows that the Hall conductance is quantized in units of $e^2/2\pi\hbar$, which is the universal unit of conductance in quantum mechanics. The experimental observation is illustrated in the figure below [taken from the web]. The right panels shows that for very large field fractional values are observed. The explanation of this fraction quantum Hall effect (FQHE) requires to taken into account the interactions between the electrons.
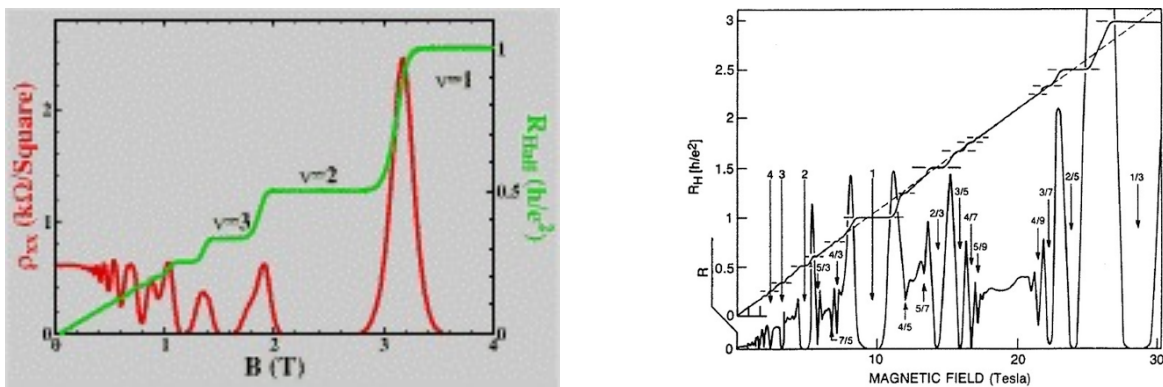
We note that both Ohm law and Hall law should be written as:

$$I \;=\; G \times \frac{1}{e}(\mu_2 - \mu_1) \tag{46.17}$$

and not as:

$$I \;=\; G \times (V_2 - V_1) \tag{46.18}$$

where μ is the electrochemical potential. If the electrical force is the only cause for the current, then the electrochemical potential is simply the electrical potential (multiplied by the charge of the electron). At zero absolute temperature μ can be identified with the Fermi energy. In metals in equilibrium, according to classical mechanics, there are no currents inside the metal. This means that the electrochemical potential must be uniform. This does not mean that the electrical potential is uniform! For example: when there is a difference in concentrations of the electrons (e.g. different metals) then there should be a "contact potential" to balance the concentration gradient, so as to have a uniform electrochemical potential. Another example: in order to balance the gravitation force in equilibrium, there must be an electrical force such that the total potential is uniform. In general, the electrical field in a metal in equilibrium cannot be zero.

═══════ [46.4] Electron in Hall geometry: Landau levels

In this section we show that there is an elegant formal way of treating the problem of an electron in Hall geometry using a canonical transformation. This method of solution is valid both in classical mechanics and in quantum mechanics (all one has to do is to replace the Poisson brackets with commutators). In the next lecture we solve the quantum problem again, using the conventional method of "separation of variables". Here and later we use the Landau gauge:

$$
\begin{aligned}
\vec{A} &= (-\mathcal{B}y, 0, 0) \\
\mathcal{B} &= \nabla \times \vec{A} = (0, 0, \mathcal{B})
\end{aligned}
\tag{46.19}
$$

Recall that we absorb the charge of the electron in the definition of the fields. Consequently the Hamiltonian is

$$
\mathcal{H} = \frac{1}{2\mathsf{m}}(\hat{p}_x + \mathcal{B}y)^2 + \frac{1}{2\mathsf{m}}(\hat{p}_y)^2 + V(y)
\tag{46.20}
$$

We define a new set of operators:

$$
\begin{aligned}
v_x &= \frac{1}{\mathsf{m}}(p_x + \mathcal{B}y) \\
v_y &= \frac{1}{\mathsf{m}}p_y \\
X &= x + \frac{1}{\omega_B}v_y = x + \frac{1}{\mathcal{B}}p_y \\
Y &= y - \frac{1}{\omega_B}v_x = -\frac{1}{\mathcal{B}}p_x
\end{aligned}
\tag{46.21}
$$

Recall that from a geometrical perspective, (X, Y) represent the center of the circle along which the particle is moving. Note also that the operators X, Y commute with v_x, v_y. On the other hand:

$$
\begin{aligned}
[X, Y] &= -i\mathcal{B}^{-1} \\
[v_x, v_y] &= i\frac{1}{\mathsf{m}^2}\mathcal{B}
\end{aligned}
\tag{46.22}
$$

Consequently we can define a new set of canonical coordinates:

$$
Q_1 = \frac{\mathsf{m}}{\mathcal{B}}v_x, \qquad P_1 = \mathsf{m}v_y, \qquad Q_2 = Y, \qquad P_2 = \mathcal{B}X
\tag{46.23}
$$

The Hamiltonian takes the form

$$
\mathcal{H}(Q_1, P_1, Q_2, P_2) = \frac{1}{2\mathsf{m}}P_1^2 + \frac{1}{2}\mathsf{m}\omega_B^2 Q_1^2 + V(Q_1 + Q_2)
\tag{46.24}
$$

We see, as expected, that $Q_2 = Y$ is a constant of motion. Let us further assume that the potential $V(y)$ is zero within a large box of area $L_x L_y$. Then also $P_2 \propto X$ is a constant of motion. The coordinates (X, Y) are conjugate with $\hbar_B = B^{-1}$ and therefore we deduce that there are g_{Landau} states that have the same energy, where

$$
g_{\text{Landau}} = \frac{L_x L_y}{2\pi\hbar_B} = \frac{L_x L_y}{2\pi}\mathcal{B}
\tag{46.25}
$$

Later we shall explain that it leads to the $e^2/(2\pi\hbar)$ quantization of the Hall conductance. Beside the (X, Y) degree of freedom we have of course the kinetic (v_x, v_y) degree of freedom. Form the transformed Hamiltonian in the new coordinates we clearly see that the kinetic energy is quantized in units of ω_B. Therefore, it is natural to label the

eigenstates as $|\ell, \nu\rangle$, where: $\nu = 0, 1, 2, 3 \ldots$, is the kinetic energy index, and ℓ labels the possible values of the constant of motion Y.

======= [46.5] Electron in Hall geometry: The Landau states

We go back to the Hamiltonian that describes the motion of a particle in the Hall bar geometry (see beginning of previous section). Recall that we have periodic boundary conditions in the x axis, and an arbitrary confining potential $V(y)$ in the y direction. We would like to find the eigenstates and the eigenvalues of the Hamiltonian. The key observation is that in the Landau gauge the momentum operator p_x is a constant of motion. It is more physical to re-phrase this statement in a gauge independent way. Namely, the constant of motion is in fact

$$
Y \quad = \quad \hat{y} - \frac{1}{\omega_B}\hat{v}_x \quad = \quad -\frac{1}{\mathcal{B}}\hat{p}_x
\tag{46.26}
$$

which represents the y location of the classical cycloid. In fact the eigenstates that we are going to find are the quantum mechanical analogue of the classical cycloids. The eigenvalues of $\hat{p}_x$ are $2\pi/L_x \times$ integer. Equivalently, we may write that the eigenvalues of $\hat{Y}$ are:

$$
Y_\ell \quad = \quad \frac{2\pi}{\mathcal{B}L_x}\ell, \qquad [\ell = \text{integer}]
\tag{46.27}
$$

That means that the y distance between the eigenstates is quantized. According to the "separation of variables theorem" the Hamiltonian matrix is a block diagonal matrix in the basis in which the $\hat{Y}$ matrix is diagonal. It is natural to choose the basis $|\ell, y\rangle$ which is determined by the operators $\hat{p}_x, \quad \hat{y}$.

$$
\langle \ell, y | \mathcal{H} | \ell', y' \rangle \quad = \quad \delta_{\ell, \ell'} \, \mathcal{H}^\ell_{yy'}
\tag{46.28}
$$

It is convenient to write the Hamiltonian of the block ℓ in abstract notation (without indexes):

$$
\mathcal{H}^\ell \quad = \quad \frac{1}{2\mathsf{m}}\hat{p}_y^2 + \frac{\mathcal{B}^2}{2\mathsf{m}}(\hat{y} - Y_\ell)^2 + V(\hat{y})
\tag{46.29}
$$

Or, in another notation:

$$
\mathcal{H}^\ell \quad = \quad \frac{1}{2\mathsf{m}}\hat{p}_y^2 + V_\ell(\hat{y})
\tag{46.30}
$$

where the effective potential is:

$$
V_\ell(y) \quad = \quad V(y) + \frac{1}{2}\mathsf{m}\omega_\mathcal{B}^2(y - Y_\ell)^2
\tag{46.31}
$$

For a given ℓ, we find the eigenvalues $|\ell, \nu\rangle$ of the one-dimensional Hamiltonian $\mathcal{H}^\ell$. The running index $\nu = 0, 1, 2, 3, \ldots$ indicates the quantized values of the kinetic energy.

For a constant electric field we notice that this is the Schrödinger equation of a displaced harmonic oscillator. More generally, the harmonic approximation for the effective potential is valid if the potential $V(y)$ is wide compared to the quadratic potential which is contributed by the magnetic field. In other words, we assume that the magnetic field is strong. We write the wave functions as:

$$
|\ell, \nu\rangle \quad \rightarrow \quad \frac{1}{\sqrt{L_x}} \, e^{-i(\mathcal{B}Y_\ell)x} \, \varphi^{(\nu)}(y - Y_\ell)
\tag{46.32}
$$

We notice that $\mathcal{B}Y_\ell$ are the eigenvalues of the momentum operator. If there is no electrical field then the harmonic approximation is exact, and then $\varphi^{(\nu)}$ are the eigenfunctions of a harmonic oscillator. In the general case, we must

"correct" them (in case of a constant electric field they are simply shifted). If we use the harmonic approximation then the energies are:

$$E_{\ell,\nu} \;\approx\; V(Y_\ell) \;+\; \left(\frac{1}{2} + \nu\right)\omega_B \tag{46.33}$$
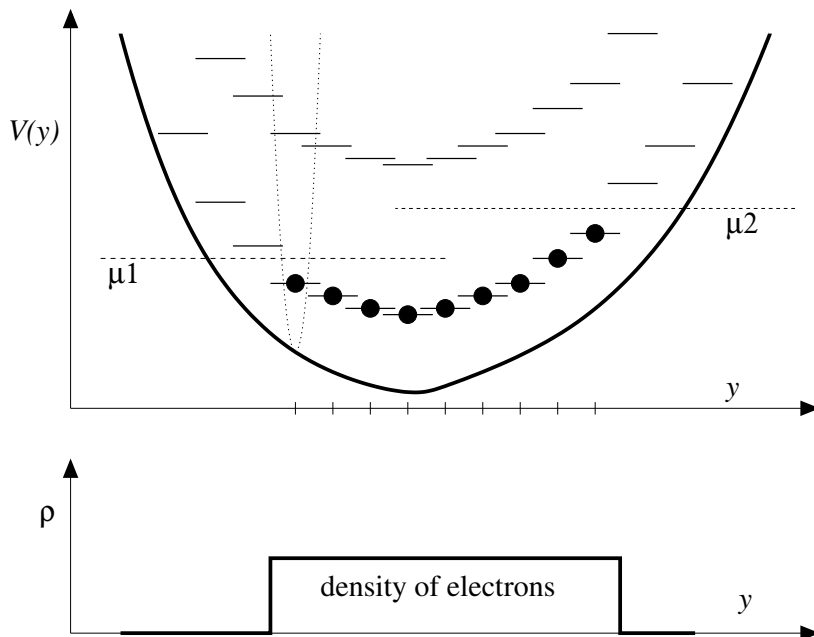
Plotting $E_{\ell,\nu}$ against Y_ℓ we get a picture of "energy levels" that are called "Landau levels" (or more precisely they should be called "energy bands"). The first Landau level is the collection of states with $\nu = 0$. We notice that the physical significance of the term with ν is kinetic energy. The Landau levels are "parallel" to the bottom of the potential $V(y)$. If there is a region of width L_y where the electric potential is flat (no electric field), then the eigenstates in that region (for a given ν) would be degenerate in the energy (they would have the same energy). Because of the quantization of Y_ℓ the number of particles that can occupy a Hall-bar of width L_y in each Landau level is $g_{\text{Landau}} = L_y/\Delta Y$, leading to the same result that we deduced earlier. In different phrasing, and restoring CGS units, the density of electrons in each Landau level is

$$\rho_{\text{Landau}} \;=\; \frac{g_{\text{Landau}}}{L_x L_y} \;=\; \frac{e}{2\pi\hbar c}\mathcal{B} \tag{46.34}$$

This leads to the $e^2/(2\pi\hbar)$ quantization of the Hall conductance.

===== [46.6] Hall geometry with AB flux

Here we discuss a trivial generalization of the above solution that helps later (next section) to calculate the Hall current. Let us assume that we add a magnetic flux Φ through the ring, as in the case of Aharonov-Bohm geometry. In this case, the vector potential is:

$$\vec{A} \;=\; \left(\frac{\Phi}{L_x} - \mathcal{B}y, 0, 0\right) \tag{46.35}$$

We can separate the variables in the same way, and get:

$$E_{\ell,\nu} \;\approx\; V\left(Y_\ell + \frac{1}{\mathcal{B}L_x}\Phi\right) \;+\; \left[\frac{1}{2} + \nu\right]\omega_B \tag{46.36}$$

══════ [46.7] The Quantum Hall current

We would like to calculate the current for an electron that occupies a Landau state $|\ell, \nu\rangle$:

$$
\hat{J}_x(x,y) = \frac{1}{2}(v_x \delta(\hat{x} - x)\delta(\hat{y} - y) + h.c.) \tag{46.37}
$$

$$
\hat{J}_x(y) = \frac{1}{L_x}\int \hat{J}_x(x,y)dx = \frac{1}{L_x}\hat{v}_x \delta(\hat{y} - y)
$$

$$
\hat{I}_x = -\frac{\partial\mathcal{H}}{\partial\Phi} = \frac{1}{L_x}v_x = \int \hat{J}_x(y)dy
$$

Recall that $v_x = (\mathcal{B}/\mathsf{m})(\hat{y} - \hat{Y})$, and that the Landau states are eigenstates of $\hat{Y}$. Therefore, the current density of an occupied state is given by:

$$
J_x^{\nu\ell}(y) = \langle \ell\nu|\hat{J}_x(y)|\ell\nu\rangle = \frac{\mathcal{B}}{L_x \mathsf{m}}\left\langle (\hat{y} - \hat{Y})\,\delta(\hat{y} - y)\right\rangle = \frac{\mathcal{B}}{\mathsf{m}L_x}(y - Y_\ell)\,|\varphi^\nu(y - Y_\ell)|^2 \tag{46.38}
$$

If we are in the region $(Y_\ell < y)$ we observe current that flows to the right (in the direction of the positive x axis), and the opposite if we are on the other side. This is consistent with the classical picture of a particle moving clockwise in a circle. If there is no electric field, the wave function is symmetric around Y_ℓ, so we get zero net current. If there is a non-zero electric field, it shifts the wave function and then we get a net current that is not zero. The current is given by:

$$
I_x^{\ell\nu} = \int J_x^{\ell\nu}(y)dy = -\frac{\partial E_{\ell\nu}}{\partial\Phi} = -\frac{1}{\mathcal{B}L_x}\frac{dV(y)}{dy}\bigg|_{y=Y_\ell} \tag{46.39}
$$

For a Fermi occupation of the Landau level we get:

$$
I_x = \sum_\ell I_x^{\ell\nu} = \int_{y_1}^{y_2}\frac{dy}{2\pi/(BL_x)}\left(-\frac{1}{\mathcal{B}L_x}\frac{dV(y)}{dy}\right) \tag{46.40}
$$

$$
= -\frac{1}{2\pi}(V(y_2) - V(y_1)) = -\frac{e}{2\pi\hbar}(\mu_2 - \mu_1)
$$

In the last equation we have restored the standard physical units. We see that if there is a chemical potential difference we get a current I_x. Writing $\mu = eV$, the Hall coefficient is $e^2/(2\pi\hbar)$ times the number of full Landau levels.

══════ [46.8] Hall effect and adiabtic transport

The calculation of the Hall conductance is possibly the simplest non-trivial example for adiabatic non-dissipative response. The standard geometry is the 2D "hall bar" of dimension $L_x \times L_y$. We have considered what happens if the electrons are confined in the transverse direction by a potential $V(y)$. Adopting the Landauer approach it is assumed that the edges are connected to leads that maintain a chemical potential difference. Consequently there is a net current in the x direction. From the "Landau level" picture it is clear that the Hall conductance G_{xy} is quantized in units $e^2/(2\pi\hbar)$. The problem with this approach is that the more complicated case of disordered $V(x,y)$ is difficult for handling. We therefore turn to a formal linear response approach [see section 22]. From now on we use units such that $e = \hbar = 1$.

We still consider a Hall bar $L_x \times L_y$, but now we impose periodic boundary condition such that $\psi(L_x, y) = e^{i\phi_x}\psi(0, y)$ and $\psi(x, L_y) = e^{i\phi_y}\psi(x, 0)$. Accordingly the Hamiltonian depends on the parameters (ϕ_x, ϕ_y, Φ_B), where Φ_B is the uniform magnetic flux through the Hall bar in the z direction. The currents $I_x = (e/L_x)v_x$ and $I_y = (e/L_y)v_y$ are conjugate to ϕ_x and ϕ_y. We consider the linear response relation $I_y = -G_{yx}\dot{\phi}_x$. This relation can be written as $dQ_y = -G_{yx}d\phi_x$. The Hall conductance quantization means that a 2π variation of ϕ_x leads to one particle transported in the y direction. The physical picture is very clear in the standard $V(y)$ geometry: the net effect is to displace all the filled Landau level "one step" in the y direction.

We now proceed with a formal analysis to show that the Hall conductance is quantized for general $V(x,y)$ potential. We can define a "vector potential" A_n on the (ϕ_x, ϕ_y) manifold. If we performed an adiabatic cycle the Berry phase would be a line integral over A_n. By Stokes theorem this can be converted into a $d\phi_x d\phi_y$ integral over B_n. However there are two complementary domains over which the surface integral can be done. Consistency requires that the result for the Berry phase would come out the same modulo 2π. It follows that

$$\frac{1}{2\pi} \int_0^{2\pi} \int_0^{2\pi} B_n d\phi_x d\phi_y = \text{integer} \quad \text{[Chern number]} \tag{46.41}$$

This means that the ϕ averaged B_n is quantized in units of $1/(2\pi)$. If we fill several levels the Hall conductance is the sum $\sum_n B_n$ over the occupied levels, namely

$$G_{yx} = \sum_{n \in \text{band}} \sum_m \frac{2\text{Im}[I_{nm}^y I_{mn}^x]}{(E_m - E_n)^2} \tag{46.42}$$

If we have a quasi-continuum it is allowed to average this expression over (ϕ_x, ϕ_y). Then we deduce that the Hall conductance of a filled band is quantized. The result is of physical relevance if non-adiabatic transitions over the gap can be neglected.

======== [46.9] The Hofstadter butterfly

Let us consider the same Hall geometry but assume that the motion of the electron is bounded to a periodic lattice, such that the x and y spacings between sites are a and b respectively. In the absence of magnetic field the Hamiltonian is $H = -2\cos(ap_x) - 2\cos(bp_y)$ where the units of times are chosen such that the hopping coefficient is unity. The eigenenergies occupy a single band $E \in [-4, +4]$. We now turn on a magnetic field. Evidently if the flux Φ through a unit-cell is increases by 2π the spectrum remains the same, accordingly it is enough to consider $0 < \Phi \leq 2\pi$. It is convenient to write the flux per unit cell as $\Phi = 2\pi \times (p/q)$. Given q we can define a super-cell that consists of q unit cells, such that the Hamiltonian is periodic with respect to it. It follows from Bloch theorem that the spectrum consists of q bands. Plotting the bands as a function of Φ we get the Hofstadter butterfly [Hofstadter, PRB 1976]. See figure [taken from the homepage of Daniel Osadchy]: the horizontal axis is the flux and the vertical axis is the energy. Note that for $q = 2$ the two bands are touching with zero gap at $E = 0$, and therefore cannot be resolved. One can see how for intermediate values of Φ the Landau bands become distinct as expected from the standard analysis.
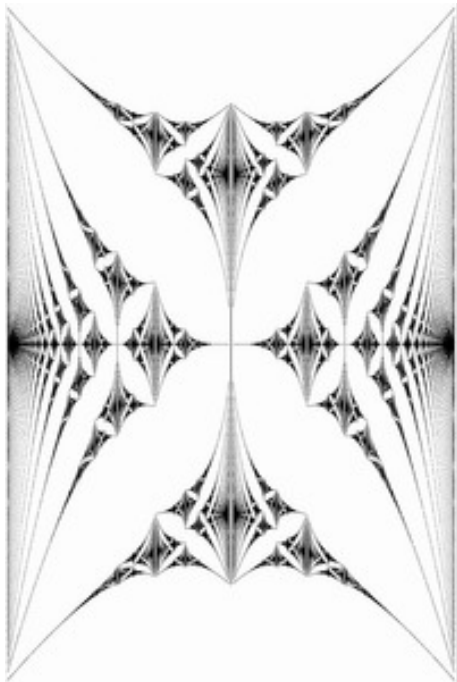
══════ [46.10] The fractional Hall effect

Instead of using rectangular geometry let us assume that we have a circular geometry. Using the symmetric gauge one observes that $L_z = m$ is a good quantum number. Hence the eigenstates can be written as $\psi(x, y) = R(r)\mathrm{e}^{im\varphi}$, where m is integer, and $R(r)$ is a radial function. Given m the lowest energy is found to be $E = (1/2)\omega_B$, and for the radial function one obtains $R^{(m)}(r) \propto r^m \exp(-(1/4)[r/r_B]^2)$, where $r_B = (eB)^{-1/2}$ is identified as the cyclotron radius in the lower Landau level. This radial function is picked at $r \approx (2m)^{1/2} r_B$. If the electrons are confined in a disc of radius R, then m is allowed to range from zero to $(1/2)[R/r_B]^2$, which is the expected degeneracy of the first Landau level. Using the notation $z = x + iy$ and working with length units such that $r_B = 1$, the degenerate set of orbitals in the lowest Landau level can be written compactly as $\psi^{(m)}(z) \propto z^m \exp(-(1/4)z^2)$.

If the potential looks like a shallow bowl, then N non-interacting Fermions would occupy at zero temperature the lowest orbitals $m = 1, 2, ..., N$. The many body wavefunction of N fermions is a Slater determinant

$$\Psi(z_1, z_2, ..., z_N) = f(z_1, z_2, ..., z_N) \exp\left[-\frac{1}{4}\sum_i z_i^2\right] = \left(\prod_{\langle ij\rangle}(z_i - z_j)^q\right) \exp\left[-\frac{1}{4}\sum_i z_i^2\right] \tag{46.43}$$

with $q = 1$. Let us take into account that the electrons repel each other. In such a case it might be advantageous to have a more dilute population of the m orbitals. We first note that if we make a Slater determinant out of states that have total angular momentum $M = m_1 + m_2 + ... + m_N$ the result would be with a polynomial f that all his terms are of degree M. Obviously M is a good quantum number, and there are many ways to form an M states. So a general M state is possibly a superposition of all possible Slater determinants. Laughlin [PRL 1983] has made an educated guess that odd values of q, that are consistent with the anti-symmetry requirement, would minimize the cost of the repulsion. His guess turns out to be both a good approximation and an exact result for a delta repulsion. In such states the occupation extends up to the orbital $m = Nq$. It corresponds to filling fraction $\nu = 1/q$. Indeed Hall plateaus have been observed for such values. This is known as the fractional Hall effect.

══════ [46.11] The spin Hall effect

Consider an electron that is constraint to move in a 2D sample, experiencing an in-plane electric field $\mathcal{E}$ that is exerted by the confining potential $V(x, y)$. There is no magnetic field, yet there is always a spin-orbit interaction:

$$H_{\text{SO}} = C\,\boldsymbol{\mathcal{E}} \times \boldsymbol{p} \cdot \boldsymbol{\sigma} = C\,\sigma_z\,(\boldsymbol{n} \times \boldsymbol{\mathcal{E}}) \cdot \boldsymbol{p} \tag{46.44}$$

where C is a constant, and n is a unit vector in the z direction. Note that in this geometry only the z component of the spin is involved, hence $\sigma_z = \pm 1$ is a good quantum number. One observes that the "down" electrons experience a vector potential $\boldsymbol{A} = C\boldsymbol{n} \times \boldsymbol{\mathcal{E}}$, that looks like a rotated version of $\mathcal{E}$. This has formally the same effect as that of a perpendicular magnetic field. The "up" electrons experience the same field with an opposite sign.
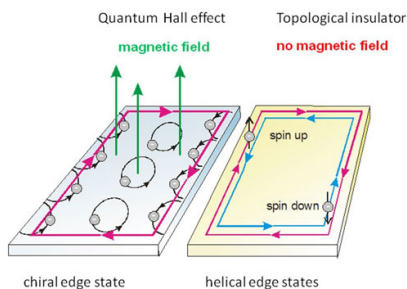
Considering an electron that has an "up" or "down" spin one observes that its direction of motion along the edge of a potential wall is clockwise or anticlockwise respectively. The spin is "locked" to the direction of the motion. This implies that it is very difficult to back-scattered such an electron: If there is a bump in the potential along the wall it can reverse the direction, but not the spin, hence there is a zero matrix element for back-scattering from $k\uparrow$ to $-k\downarrow$. In order to have a non-zero matrix element one has to add magnetic field or magnetic impurities, breaking the time reversal symmetry that "protected" the undisturbed motion of the electron.

[47] Motion in a central potential

═══════ [47.1] The Hamiltonian

Consider the motion of a particle under the influence of a spherically symmetric potential that depends only on the distance from the origin. We can write the Hamiltonian in "spherical coordinates" as a sum of radial term and an additional azimuthal term that involves the generators $\vec{L} = \vec{r} \times \vec{p}$. Namely,

$$\mathcal{H} = \frac{1}{2\mathsf{m}}p^2 + eV(r) = \frac{1}{2\mathsf{m}}\left(p_r^2 + \frac{1}{r^2}L^2\right) + eV(r) \tag{47.1}$$

In order to go form the first to the second expression we have used the vector style version of $1 = \cos^2 + \sin^2$, which is $A^2B^2 = (A \cdot B)^2 + (A \times B)^2$, with $A = r$ and $B = p$. One should be careful about operator ordering. Optionally we can regard this identity as the differential representation of the Laplacian in spherical coordinates, with

$$p_r^2 \rightarrow -\frac{1}{r}\frac{\partial^2}{\partial r^2}r \tag{47.2}$$

The Hamiltonian commutes with rotations:

$$[\mathcal{H}, \hat{R}] = 0 \tag{47.3}$$

And in particular:

$$\begin{aligned} [\mathcal{H}, L^2] &= 0 \\ [\mathcal{H}, L_z] &= 0 \end{aligned} \tag{47.4}$$

According to the separation of variables theorem the Hamiltonian becomes block diagonal in the basis which is determined by L^2 and L_z. The states that have definite ℓ and m quantum numbers are of the form $\psi(x, y, z) = R(r)Y^{\ell m}(\theta, \varphi)$, so there is some freedom in the choice of this basis. The natural choice is $|r, \ell, m\rangle$

$$\langle r, \theta, \varphi | r_0, \ell_0, m_0 \rangle = Y^{\ell_0, m_0}(\theta, \varphi)\frac{1}{r}\delta(r - r_0) \tag{47.5}$$

These are states that "live" on spherical shells. Any wavefunction can be written as a linear combination of the states of this basis. Note that the normalization is correct (the volume element in spherical coordinates includes r^2). The Hamiltonian becomes

$$\langle r, \ell, m | \mathcal{H} | r', \ell', m' \rangle = \delta_{\ell, \ell'}\delta_{m, m'}\mathcal{H}_{r, r'}^{(\ell, m)} \tag{47.6}$$

$$\mathcal{H}^{(\ell, m)} = \frac{1}{2\mathsf{m}}\hat{p}^2 + \left(\frac{\ell(\ell + 1)}{2\mathsf{m}r^2} + V(r)\right) = \frac{1}{2\mathsf{m}}p^2 + V^{(\ell)}(r) \tag{47.7}$$

where $p \rightarrow -i(d/dr)$. The wavefunction in the basis which has been defined above are written as

$$|\psi\rangle = \sum_{r, \ell, m} u_{\ell m}(r)\,|r, \ell, m\rangle \longmapsto \sum_{\ell m}\frac{u_{\ell m}(r)}{r}Y^{\ell, m}(\theta, \varphi) \tag{47.8}$$

In the derivation above we have made a "shortcut". In the approach which is popular in textbooks the basis is not properly normalized, and the wave function is written as $\psi(x, y, z) = \psi(r, \theta, \varphi) = R(r)Y^{\ell, m}(\theta, \varphi)$, without taking the correct normalization measure into account. Only in a later stage they define $u(r) = rR(r)$. Eventually they get the same result. By using the right normalization of the basis we have saved an algebraic stage.

By separation of variables the Hamiltonian has been reduced to a semi-one-dimensional Schrödinger operator acting on the wave function $u(r)$. By "semi-one-dimensional" we mean that $0 < r < \infty$. In order to get a wave function $\psi(x, y, z)$ that is continuous at the origin, we must require the radial function $R(r)$ to be finite, or alternatively the function $u(r)$ has to be zero at $r = 0$.

====== [47.2] Eigenstates of a particle on a spherical surface

The simplest central potential that we can consider is such that confine the particle to move within a spherical shell of radius R. Such potential can be modeled as $V(r) = -\lambda\delta(r - R)$. For $\ell = 0$ we know that a narrow deep well has only one bound state. We fix the energy of this state as the reference. The centrifugal potential for $\ell > 0$ simply lifts the potential floor upwards. Hence the eigen-energies are

$$E_{\ell m} \quad = \quad \frac{1}{2\mathsf{m}R^2}\ell(\ell + 1) \tag{47.9}$$

We remind ourselves of the considerations leading to the degeneracies. The ground state Y^{00}, has the same symmetry as that of the Hamiltonian: both invariant under rotations. This state has no degeneracy. On the other hand, the state Y^{10} has a lower symmetry and by rotating it we get 3 orthogonal states with the same energy. The degeneracy is a "compensation" for the low symmetry of the eigenstates: the symmetry of the energy level as a whole (i.e. as a subspace) is maintained.

The number of states $N(E)$ up to energy E, that satisfy $E_{\ell m} < E$, is easily found. The density of states turns out to be constant:

$$\frac{dN}{dE} \quad \approx \quad \frac{\mathsf{m}}{2\pi\hbar^2}\mathsf{A}, \qquad \mathsf{A} = 4\pi R^2 \tag{47.10}$$

It can be proved that this formula is valid also for other surfaces: to leading order only the surface area A is important. The most trivial example is obviously a square for which

$$E_{n,m} \quad = \quad \frac{\pi^2}{2\mathsf{m}L^2}(n^2 + m^2) \tag{47.11}$$

The difference between the $E_{\ell m}$ spectrum of a particle on a sphere, and the $E_{n,m}$ spectrum of a particle on a square, is in the way that the eigenvalues are spaced, not in their average density. The degeneracies of the spectrum are determined by the symmetry group of the surface on which the motion is bounded. If this surface has no special symmetries the spectrum is expected to be lacking systematic degeneracies.

====== [47.3] The Hydrogen Atom

The effective potential $V^\ell(r)$ that appears in the semi-one-dimensional problem includes the original potential plus a centrifugal potential (for $\ell \neq 0$). Typically, the centrifugal potential $+1/r^2$ leads to the appearance of a potential barrier. Consequently there are "resonance states" in the range $E > 0$, that can "leak" out through the centrifugal barrier (by tunnelling) into the outside continuum. But in the case of the Hydrogen atom the attractive potential $-1/r$ wins over the centrifugal potential, and there is no such barrier. Moreover, unlike typical short range potentials, there are infinite number of bound states in the $E < 0$ range. Another special property of the Hydrogen atom is the high degree of symmetry: the Hamiltonian commutes with the Runge-Lentz operators. This is manifested in the degeneracy of energy levels, which is much greater than expected from SO(3).

For sake of later reference we write the potential as:

$$V(r) \quad = \quad -\frac{\alpha c}{r}, \qquad \alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137} \tag{47.12}$$

Below we use as usual $\hbar = 1$ units. Solving the radial equation (for each ℓ separately) one obtains:

$$E_{\ell,m,\nu} \;\;=\;\; [\mathsf{m}c^2] \;-\; \frac{\alpha^2 \mathsf{m}c^2}{2(\ell + \nu)^2} \tag{47.13}$$

where $\nu = 1, 2, 3, \ldots$. The rest-mass of the atom has been added here in square brackets as a reminder that from a relativistic point of view we are dealing here with an expansion with respect to the fine structure constant α. In the non-relativistic treatment this term is omitted. The energy levels are illustrated in the diagram below. It is customary in text books to use the quantum number $n = \ell + \nu$ in order to label the levels. One should bare in mind that the n quantum number has significance only for the $1/r$ potential due to its high symmetry: it has no meaning if we have say $1/r^5$ potential.
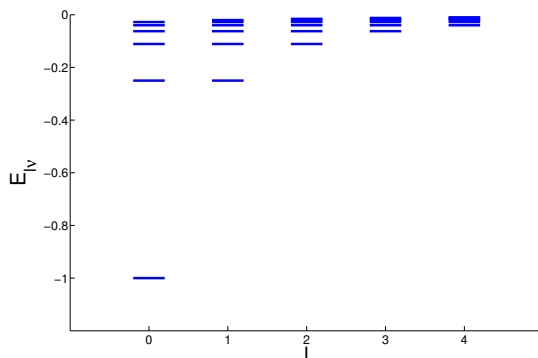

Degeneracies.– We would like to remind the reader why there are degeneracies in the energy spectrum (this issue has been discussed in general in the section about symmetries and their implications). If the Hamiltonian has a single constant of motion, there will usually not be a degeneracy. According to the separation of variables theorem it is possible to transform to a basis in which the Hamiltonian has a block structure, and then diagonalize each block separately. There is no reason for a conspiracy amongst the blocks. Therefore there is no reason for a degeneracy. If we still get a degeneracy it is called an accidental degeneracy.

But, if the Hamiltonian commutes with a "non-commutative group" then there are necessarily degeneracies that are determined by the dimensions of the irreducible representations. In the case of a central potential, the symmetry group is the "rotation group". In the special case of the potential $-1/r$ a larger symmetry group exists.

A degeneracy is a compensation for having eigenstates with lower symmetry compared with the Hamiltonian. The degree of degeneracy is determined by the dimensions of the irreducible representations. These statements were discussed in the Fundamentals II section. Let us paraphrase the argument in the present context: Assume that we have found an eigenstate of the Hamiltonian. If it has full spherical symmetry then there is no reason for degeneracy. These are the states with $\ell = 0$. But, if we have found a state with a lower symmetry (the states with $\ell \neq 0$) then we can rotate it and get another state with the same energy level. Therefore, in this case there must be a degeneracy.

Instead of "rotating" an eigenstate, it is simpler (technically) to find other states with the same energy by using ladder operators. This already gives an explanation why the degree of the degeneracy is determined by the dimension of the irreducible representations. Let us paraphrase the standard argument for this statements in the present context: The Hamiltonian $\mathcal{H}$ commutes with all the rotations, and therefore it also commutes with all their generators and also with L^2. We choose a basis $|n, \ell, \mu\rangle$ in which both $\mathcal{H}$ and L^2 are diagonal. The index of the energy levels n is determined by $\mathcal{H}$, while the index ℓ is determined by L^2. The index μ differentiates states with the same energy and the same ℓ. According to the "separation of variables theorem" every rotation matrix will have a "block structure" in this basis: each level that is determined by the quantum numbers (n, ℓ) is an invariant subspace under rotations. In other words, $\mathcal{H}$ together with L^2 induce a decomposition of the group representation. Now we can apply the standard procedure in order to conclude that the dimension of the (sub) representation which is characterized by the quantum number ℓ, is $2\ell + 1$. In other words, we have "discovered" that the degree of the degeneracy must be $2\ell + 1$ (or a multiple of this number).

Relativistic solution.– In order to explain the spectroscopy of the Hydrogen atom, Pauli has suggested that the electron has an extra spin 1/2 degree of freedom. The system as whole has a symmetry with respect to rotations, and therefore the primary good quantum number for classification of eigenstates is not ℓ but the total angular momentum j. The $\ell = 0$ orbitals become $j = 1/2$ multiplets, and each $\ell \neq 0$ sub-level splits into $j = \ell + (1/2)$ and $j = \ell - (1/2)$ multiplets, as illustrated in the figure below for the $n = 2$ level. We shall see that due to a spin-orbit interaction the two j sub-levels also split "vertically" in energy, which explains the experimentally observed *fine structure* of the spectrum.
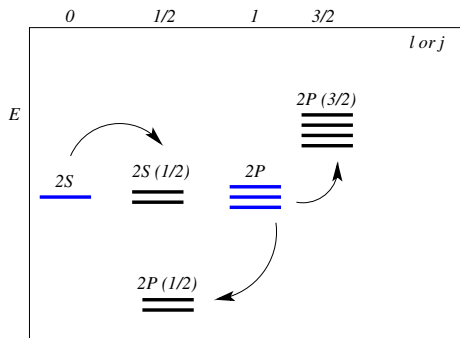
The full relativistic treatment is based on the Dirac Hamiltonian. As pointed out, the primary good quantum number for classification of eigenstates is j. Within the j-th subspace it is natural to number the eigenstated using a radial quantum number $n_r = 0, 1, 2, ...$ This quantum number comes instead of ν, and should not to be confused with n. In fact we need an additional quantum number $\kappa = \pm$ to distinguish the two same-j multiplets that we have in each level. For example, we should distingush between the $2S_{1/2}$ and the $2P_{1/2}$ multiplets (see figure) that are associated with the non-relativistic orbital $\ell = 0$ and $\ell = 1$, respectively. The κ quantum number corresponds to the sign in $j = \ell \pm (1/2)$. Note however that ℓ by itself is not a good quantum number in the full relativistic treatment. The explicit expression for the eigenenrgies is

$$ E_{\kappa,j,m,n_r} \;\;=\;\; \frac{\mathsf{m}c^2}{\sqrt{1+\dfrac{\alpha^2}{\left[n_r+\sqrt{\left(j+\frac{1}{2}\right)^2-\alpha^2}\right]^2}}} \;\;+\;\; \text{LambShift} \;\;+\;\; \text{HyperFine} \tag{47.14} $$

The first term comes from the exact relativistic solution of the Dirac equation. Surprisingly one observes that this solution exhibits degeneracy with respect to κ. For example the $2S_{1/2}$ and the $2P_{1/2}$ multiplets have the same energy, contrary to the figure that takes into account only the spin-orbit interaction. In reality there is a small splitting between those quasi-degenerate multiplets, known as the Lamb-shift. The theoretical understanding of the Lamb-shift requires to go beyond Dirac equation, as explained in the next paragraph.

The realistic expression for the energy levels of Hydrogen atom contains a term that originates from the relativistic Dirac equation, plus a Lamb-Shift due to the interaction with the fluctuations of the electromagnetic vacuum, plus additional "hyperfine" correction due to the interaction with the nucleus. It is customary to expand the Dirac expression with respect to the the fine-structure constant $\alpha \equiv e^2/(\hbar c)$. The leading α^2 term is the same as that of Bohr, with the identification $n = [j + (1/2))] + n_r$. The next α^4 term can be regarded as the sum of relativistic kinetic p^4 correction, a Darwin term $\delta^3(r)$ that affects s-orbitals, and a spin-orbit term $(1/r^3)L\cdot S$. On top we have the α^5 Lamb-shift correction, that can be approximated as an additional $\delta^3(r)$ term. The Darwin and the Lamb-shift terms can be interpreted as arising from the smearing of the $1/r$ interaction, either due to zitterbewegung or due to the fluctuations that are induced by the electromagnetic field, respectively. The Lamb shift splits the degeneracy of the j sub-levels, e.g. "2s" and "2p". The Lamb shift physics is also responsible for the anomalous value of the spin-orbit coupling ($g \approx 2 + (\alpha/\pi)$).

The spin-related fine-structure will be discussed in the next lectures. It will be regarded as arising from "corrections" to the non-relativistic Schroedinger Hamiltonian. In particular we shall see how the quantum number j arises due to the addition of the angular momentum of the spin, and the presence of the spin-orbit interaction.

[48] The Hamiltonian of a spin 1/2 particle

======= [48.1] The Hamiltonian of a spinless particle

The Hamiltonian of a spinless particle can be written as:

$$\mathcal{H} \;=\; \frac{1}{2\mathsf{m}}(\vec{p} - e\vec{A}(r))^2 + eV(r) \;=\; \frac{p^2}{2\mathsf{m}} - \frac{e}{2\mathsf{m}}(\vec{A}\cdot\vec{p} + \vec{p}\cdot\vec{A}) + \frac{e^2}{2\mathsf{m}}A^2 + eV(r) \tag{48.1}$$

where c=1. We assume that the field is uniform $\mathcal{B} = (0,0,\mathcal{B}_0)$. In the previous lectures we saw that this field can be derived from $\vec{A} = (-\mathcal{B}_0 y, 0, 0)$, but this time we use a different gauge, called "symmetrical gauge":

$$\vec{A} \;=\; \left(-\frac{1}{2}\mathcal{B}_0 y, \frac{1}{2}\mathcal{B}_0 x, 0\right) \;=\; \frac{1}{2}\mathcal{B}\times\vec{r} \tag{48.2}$$

Triple vector multiplication is associative, and therefore we have the following identity:

$$\vec{A}\cdot\vec{p} \;=\; \frac{1}{2}(\mathcal{B}\times\vec{r})\cdot\vec{p} \;=\; \frac{1}{2}\mathcal{B}\cdot(\vec{r}\times\vec{p}) \;=\; \frac{1}{2}\mathcal{B}\cdot\vec{L} \tag{48.3}$$

Substitution into the Hamiltonian gives:

$$\mathcal{H} \;=\; \frac{p^2}{2\mathsf{m}} + eV(r) - \frac{e}{2\mathsf{m}}\mathcal{B}\cdot\vec{L} + \frac{e^2}{8\mathsf{m}}(r^2\mathcal{B}^2 - (\vec{r}\cdot\mathcal{B})^2) \tag{48.4}$$

Specifically for a homogeneous field in the z axis we get

$$\mathcal{H} \;=\; \frac{p^2}{2\mathsf{m}} + eV(r) - \frac{e}{2\mathsf{m}}\mathcal{B}_0 L_z + \frac{e^2}{8\mathsf{m}}\mathcal{B}_0^2(x^2 + y^2) \;\equiv\; \frac{p^2}{2\mathsf{m}} + eV(r) - \Omega_0 L_z + \frac{1}{2}\mathsf{m}\Omega_0^2(x^2 + y^2) \tag{48.5}$$

The two last terms are called the "Zeeman term" and the "diamagnetic term". From a different perspective we recall the the Hamiltonian of a particle in a rotating frame is $\mathcal{H} = [1/(2\mathsf{m})]p^2 - \Omega_0 L_z$. Taking the above procedure in reverse we conclude that it is formally equivalent to the Hamiltonian of a particle in a Coriolis field $e\mathcal{B}_0 = 2\mathsf{m}\Omega_0$ plus a centrifugal potential $-(1/2)\mathsf{m}\Omega_0^2(x^2 + y^2)$.

======= [48.2] The additional Zeeman term for the spin

Spectroscopic measurements on atoms have shown, in the presence of a magnetic field, a double (even) Zeeman splitting of the levels, and not just the expected "orbital" splitting (which is always odd). From this Zeeman has concluded that the electron has another degree of freedom which is called "spin 1/2". The Hamiltonian should include both an orbital Zeeman term and an additional spin term:

$$\mathcal{H}_{\text{Zeeman}} \;=\; -\frac{e}{2\mathsf{m}c}\mathcal{B}\cdot\vec{L} \;-\; g\frac{e}{2\mathsf{m}c}\mathcal{B}\cdot\vec{S} \tag{48.6}$$

The spectroscopic measurements of the splitting make it possible to determine the gyromagnetic coefficient to a high precision. The same measurements were conducted also for protons, neutrons (a neutral particle!) and other particles:

Electron: $g_e = 2.0023$ [with $e = -|e|$ reflecting its negative charge]
Proton: $g_p = 5.5854$ [with $e = +|e|$ reflecting its positive charge]
Neutron: $g_n = 3.8271$ [with $e = -|e|$ as if it were charged negatively]

The implication of the Zeeman term in the Hamiltonian is that the wavefunction of the electron precesses with the frequency

$$\Omega \;=\; -\frac{e}{2\mathsf{m}c}\mathcal{B} \tag{48.7}$$

while the spin of the electron precesses with a twice larger frequency

$$\Omega \;=\; -g_e\frac{e}{2\mathsf{m}c}\mathcal{B}, \qquad \left[g_e \approx 2\right] \tag{48.8}$$

═══════ [48.3] The spin orbit term

The added Zeeman term describes the interaction of the spin with the magnetic field. In fact, the "spin" degree of freedom (and the existence of anti-particles) is inevitable because of relativistic considerations of invariance under the Lorentz transformation. These considerations lead to Dirac's Hamiltonian. There are further "corrections" to the non-relativistic Hamiltonian that are required in order to make it "closer" to Dirac's Hamiltonian. The most important of these corrections is the "spin orbit interaction":

$$\mathcal{H}_{spin-orbit} \;=\; -(g{-}1)\frac{e}{2\mathsf{m}c^2}\,\vec{\mathcal{E}}\times\vec{v}\;\cdot\;\vec{S} \tag{48.9}$$

In other words, the spin interacts with the electric field. This interaction depends on its velocity. This is why the interaction is called spin-orbit interaction. If there is also a magnetic field then we have the additional interaction which is described by the Zeeman term.

We can interpret the "spin-orbit" interaction in the following way: even if there is no magnetic field in the "laboratory" reference frame, still there is a magnetic field in the reference frame of the particle, which is a moving reference frame. This follows from Lorentz transformation:

$$\tilde{\mathcal{B}} \;=\; \mathcal{B} - (1/c)\vec{\mathbf{v}}_{\text{frame}}\times\mathcal{E} \tag{48.10}$$

It looks by this argument that the spin-orbit term should be proportional to g, while in fact it is proportional to $(g{-}1)$. The extra contribution is called "Thomas precession" and has a purely kinematical reason [discussed in the book of Jackson]. The physical picture is as follows: the spin-orbit term originates from the component of the electric field that is perpendicular to the velocity; This leads to a rotated motion; In the rotating rest-frame of the particle one observes precession due to the Zeeman interaction; Going back to the laboratory frame the Lorentz transformation implies that the spin experiences an extra magnetic-like field, analogous to Coriolis. This is because the laboratory frame is rotating with respect to the rest frame of the particle.

We summarize this section by writing the common non-relativistic approximation to the Hamiltonian of a particle with spin 1/2.

$$\mathcal{H} \;=\; \frac{1}{2\mathsf{m}}\left(\vec{p}-\frac{e}{c}\vec{A}(r)\right)^2 + eV(r) \;-\; g\frac{e}{2(\mathsf{m}c)}\mathcal{B}\cdot\vec{S} \;-\; (g{-}1)\frac{e}{2(\mathsf{m}c)^2}(\mathcal{E}\times\vec{p})\cdot\vec{S} \tag{48.11}$$

In the case of spherically symmetric potential $V(r)$ the electric field is

$$\mathcal{E} \;=\; -\frac{V'(r)}{r}\vec{r} \tag{48.12}$$

Consequently the Hamiltonian takes the form (here again $c{=}1$):

$$\mathcal{H} \;=\; \frac{1}{2\mathsf{m}}\left(p_r^2+\frac{1}{r^2}L^2\right) + eV(r) + \frac{e^2}{8\mathsf{m}}\mathcal{B}^2 r_\perp^2 - \frac{e}{2\mathsf{m}}\mathcal{B}\cdot\vec{L} - g\frac{e}{2\mathsf{m}}\mathcal{B}\cdot\vec{S} + (g{-}1)\frac{e}{2\mathsf{m}^2}\frac{V'(r)}{r}\vec{L}\cdot\vec{S} \tag{48.13}$$

══════ [48.4] The Dirac Hamiltonian

In the absence of an external electromagnetic field the Hamiltonian of a free particle should be a function of the momentum operator alone $\mathcal{H} = h(\hat{p})$ where $\hat{p} = (\hat{x}, \hat{y}, \hat{z})$. Thus p is a good quantum number. The reduced Hamiltonian within a p subspace is $\mathcal{H}^{(p)} = h(p)$. If the particle is spineless $h(p)$ is a number and the dispersion relation is $\epsilon = h(p)$. But if the particle has an inner degree of freedom (spin) then $h(p)$ is a matrix. In the case of Pauli Hamiltonian $h(p) = (p^2/(2\mathsf{m}))\hat{1}$ is a 2×2 matrix. We could imagine a more complicated possibility of the type $h(p) = \sigma \cdot p + ...$ In such case p is a good quantum number, but the spin degree of freedom is no longer degenerated: Given p, the spin should be polarized either in the direction of the motion (right handed polarization) or in the opposite direction (left handed polarization). This quantum number is also known as helicity. The helicity might be a good quantum number, but it is a "Lorentz invariant" feature only for a massless particle (like a photon) that travels in the speed of light, else one can always transform to a reference frame where $p = 0$ and the helicity become ill defined.

Dirac has speculated that in order to have a Lorentz invariant Schrodinger equation ($d\psi/dt = ...$) for the evolution, the matrix $h(p)$ has to be linear (rather than quadratic) in p. Namely $h(p) = \alpha \cdot p + \text{const}\beta$. The dispersion relation should be consistent with $\epsilon^2 = \mathsf{m}^2 + p^2$ which implies $h(p)^2 = (\mathsf{m}^2 + p^2)\hat{1}$. It turns out that the only way to satisfy the latter requirement is to assume that α and β are 4×4 matrices:

$$\alpha_j = \begin{bmatrix} \mathbf{0} & \boldsymbol{\sigma}_j \\ \boldsymbol{\sigma}_j & \mathbf{0} \end{bmatrix} \qquad \beta = \begin{bmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{bmatrix} \tag{48.14}$$

Hence the Dirac Hamiltonian is

$$\mathcal{H} \;=\; \alpha \cdot p + \beta \mathsf{m} \tag{48.15}$$

It turns out that the Dirac equation, which is the Schrodinger equation with Dirac's Hamiltonian, is indeed invariant under Lorentz. Given p there are 4 distinct eigenstates which we label as $|p, \lambda\rangle$. The 4 eigenstates are determined via the diagonalization of $h(p)$. Two of them have the dispersion $\epsilon = +\sqrt{p^2 + \mathsf{m}^2}$ and the other two have the dispersion $\epsilon = -\sqrt{p^2 + \mathsf{m}^2}$. It also turns out that the helicity (in a give reference frame) is a good quantum number. The helicity operator is $\Sigma \cdot p$ where

$$\Sigma_j = \begin{bmatrix} \boldsymbol{\sigma}_j & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\sigma}_j \end{bmatrix} \tag{48.16}$$

This operator commutes with Dirac Hamiltonian. Thus the electron can be right or left handed with either positive or negative mass. Dirac's interpretation for this result was that the "vacuum" state of the universe is like that of an intrinsic semiconductor with gap $2\mathsf{m}c^2$. Namely, instead of talking about electrons with negative mass we can talk about holes (positrons) with positive mass. The transition of an electron from an occupied negative energy state to an empty positive energy state is re-interpreted as the creation of an electron positron pair. The reasoning of Dirac has lead to the conclusion that particles like the electron must have a spin as well as antiparticle states.

The consistency with the no-relativistic limit can be demonstrated by considering the equation $\mathcal{H}\Psi = E\Psi$ for the low energy eigenstates ($E \sim \mathsf{m}$). Including the electromagentic field the equation takes the form

$$\begin{pmatrix} \mathsf{m} + eV & \boldsymbol{\sigma} \cdot (\boldsymbol{p} - e\boldsymbol{A}) \\ \boldsymbol{\sigma} \cdot (\boldsymbol{p} - e\boldsymbol{A}) & -\mathsf{m} + eV \end{pmatrix} \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = E \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} \tag{48.17}$$

We define $\psi_+ \equiv \psi$, and $E = \mathsf{m} + \varepsilon$, and assume $\varepsilon \ll \mathsf{m}$. From the second row of this equation we deduce $\psi_- \approx (2\mathsf{m} - eV)^{-1}[\boldsymbol{\sigma} \cdot (\boldsymbol{p} - e\boldsymbol{A})]\psi$. and get from the first line

$$\frac{1}{2\mathsf{m}}[\boldsymbol{\sigma} \cdot (\boldsymbol{p} - e\boldsymbol{A})] \left(1 + \frac{eV}{2\mathsf{m}}\right) [\boldsymbol{\sigma} \cdot (\boldsymbol{p} - e\boldsymbol{A})]\psi + eV\psi \;=\; \varepsilon\psi \tag{48.18}$$

Using the identity $(\sigma \cdot a)(\sigma \cdot b) = (a \cdot b) + i\sigma \cdot (a \times b)$, we get the Pauli Hamiltonian, including the spin-Zeeman term and the spin-orbit term with $g = 2$. The latter originates from the eV in the kinetic part. A more careful treatment using the above procedure provides an additional p^4 correction and a Darwin term.

[49] Implications of having "spin"

════════ [49.1] The Stern-Gerlach effect

We first discuss what effect the Zeeman term has on the dynamics of a "free" particle. We shall see that because of this term, there is a force acting on the particle if the magnetic field is non-homogeneous. For simplicity of presentation we assume that the magnetic field is mainly in the Z direction, and neglect its other components. Defining $r = (x, y, z)$ the Hamiltonian takes the form

$$\mathcal{H} \;=\; \frac{\vec{p}^2}{2\mathsf{m}} - g\frac{e}{2\mathsf{m}}\mathcal{B}_z(r)S_z \tag{49.1}$$

We see that S_z is a constant of motion. If particle is prepared with spin "up" it experiences an effective potential:

$$V_{\text{eff}} \;=\; -\frac{1}{2}g\frac{e}{2\mathsf{m}}\mathcal{B}_z(r) \tag{49.2}$$

A a particle with spin "down" experiences an inverted potential (with the opposite sign). That means that the direction of the force depends on the direction of the spin. We can come to the same conclusion by looking at the equations of motion. The velocity of the particle is

$$\frac{d}{dt}\langle r \rangle \;=\; \langle i[\mathcal{H}, r] \rangle \;=\; \left\langle \frac{1}{\mathsf{m}}\left(\vec{p} - A(r)\right)\right\rangle \tag{49.3}$$

This still holds with no change. But what about the acceleration? We see that there is a new term:

$$\frac{d}{dt}\langle v \rangle \;=\; \langle i[\mathcal{H}, v] \rangle \;=\; \frac{1}{\mathsf{m}}\left\langle \text{Lorentz force} \;+\; g\frac{e}{2\mathsf{m}}(\nabla\mathcal{B}_z)S_z \right\rangle \tag{49.4}$$

The observation that in inhomogeneous magnetic field the force on the particle depends on the spin orientation is used in order to measure the spin using a Stern-Gerlach apparatus.

════════ [49.2] The reduced Hamiltonian in a central potential

We would like to consider the problem of electron in a central potential, say in the Hydrogen atom, taking into account the spin-orbit interaction. This add an $L \cdot S$ term to the Hamiltonian. We first would like to clarify what are the surviving constants of motion. In the absence of magnetic field, the system still has symmetry to rotations, and therefore the full Hamiltonian as well as $L \cdot S$ commutes with $J = L + S$. The J_i generate rotations of the wavefunction and the spin as one "package". The Hamiltonian does not commute with the generators L_x, L_y, L_z separately. For example $[L \cdot S, L_x] \neq 0$. Still the Hamiltonian commutes with L^2. In particular $[L \cdot S, L^2] = 0$. This is clear because L^2 is a Casimir operators (commutes with all the generators). Note also that

$$\vec{L} \cdot \vec{S} \;=\; \frac{1}{2}\left(J^2 - L^2 - S^2\right) \tag{49.5}$$

Form the above we deduce that ℓ is still a good quantum number, as far as the spin-otbit term is concerned. Recall that the standard basis is

$$|\ell, \nu; m_\ell, m_s\rangle \;\rightarrow\; R^{\ell\nu}(r)\,Y^{\ell,m}(\theta, \varphi) \otimes |m_s\rangle \tag{49.6}$$

The Hamiltonian in the ℓ subspace is

$$\mathcal{H}^{(\ell)} \;=\; \mathcal{H}_0^{(\ell)} - \frac{e}{2\mathsf{m}}\mathcal{B}L_z - g\frac{e}{2\mathsf{m}}\mathcal{B}S_z + f(r)L \cdot S \tag{49.7}$$

So far no approximations were involved. If we further assume that the last terms in the Hamiltonian is a weak perturbation that does not "mix" energy levels, then we can make an approximation that reduces further Hamiltonian into the subspace of states that have the same energy:

$$\mathcal{H}^{(\ell,\nu)} \;=\; -hL_z - ghS_z + vL \cdot S + \text{const} \tag{49.8}$$

where the first term with $h = e\mathcal{B}/(2\mathsf{m})$ is responsible for the orbital Zeeman splitting, and the second term with gh is responsible to the spin-related Zeeman splitting. Note that $g = 2.0023$. We also use the notation

$$v \;=\; \langle \ell, \nu | f(r) | \ell, \nu \rangle \tag{49.9}$$

If the spin-orbit interaction did not exist, the dynamics of the spin would become independent of the dynamics of the wave function. But even with the spin-orbit interaction, the situation is not so bad. $L \cdot S$ couples only states with the same ℓ. Furthermore the $\ell = 0$ for which $L \cdot S = 0$ are not affected by the spin-orbit interactions.

════════ [49.3] The Zeeman Hamiltonian

From now we focus on the $\ell = 1$ subspace in the second energy level of the Hydrogen atom. The Hamiltonian matrix is 6×6. The reduced Hamiltonian can be written in the standard basis $|\ell = 1, \nu = 1, m_\ell, m_s\rangle$. It is easy to write the matrices for the Zeeman terms:

$$L_z \;\rightarrow\; \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \;=\; \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix} \tag{49.10}$$

$$S_z \;\rightarrow\; \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \otimes \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \;=\; \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}$$

But the spin-orbit term is not diagonal. The calculation of this term is more demanding:

$$\vec{L} \cdot \vec{S} \;=\; \frac{1}{2}\left(J^2 - L^2 - S^2\right) \;=\; \frac{1}{2}\left(J^2 - \frac{11}{4}\right) \tag{49.11}$$

The calculation of the matrix that represent J^2 in the standard basis is lengthy, though some shortcuts are possible (see lecture regarding "addition of angular momentum"). Doing the calculation, the result for the total Hamiltonian is

$$\mathcal{H} \;\rightarrow\; -h\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix} - gh\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} \end{pmatrix} + v\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{pmatrix} \tag{49.12}$$

At this stage we can diagonalize the Hamiltonian, and find exact results for the eigen-energies. However, we shall see in the next section that it is possible to find some shortcuts that save much of the technical burden.

======= [49.4] The Zeeman energies

We write again the Hamiltonian that we want to diagonalize:

$$\mathcal{H} \;=\; \frac{v}{2}\left(J^2 - \frac{11}{4}\right) \;-\; hL_z \;-\; ghS_z \tag{49.13}$$

There is a relatively simple way to figure out the representation of J^2 using the "addition theorem". Namely, after diagonalization it should become:

$$J^2 \;\to\; \begin{pmatrix} (15/4) & 0 & 0 & 0 & 0 & 0 \\ 0 & (15/4) & 0 & 0 & 0 & 0 \\ 0 & 0 & (15/4) & 0 & 0 & 0 \\ 0 & 0 & 0 & (15/4) & 0 & 0 \\ 0 & 0 & 0 & 0 & (3/4) & 0 \\ 0 & 0 & 0 & 0 & 0 & (3/4) \end{pmatrix} \tag{49.14}$$

It follows that the exact eigenenergies of the Hamiltonian in the absence of a magnetic field are:

$$E_{j=\frac{3}{2}} \;=\; v/2, \qquad \text{[degeneracy = 4]} \tag{49.15}$$
$$E_{j=\frac{1}{2}} \;=\; -v, \qquad \text{[degeneracy = 2]}$$

On the other hand, in a strong magnetic field the spin-orbit term is negligible, and we get:

$$E_{m_\ell, m_s} \;\approx\; -(m_\ell + gm_s)h \tag{49.16}$$

In fact there are two levels that are exact eigensates of the Hamiltonian for any h. These are:

$$E_{j=\frac{3}{2}, m=\pm\frac{3}{2}} \;=\; \frac{v}{2} \mp \left(1 + \frac{g}{2}\right)h \tag{49.17}$$

The spectrum of $\mathcal{H}$ can be found for a range of h values. See the Mathematica file zeeman.nb. The results (in units such that $v = 1$) are illustrated in the following figure:
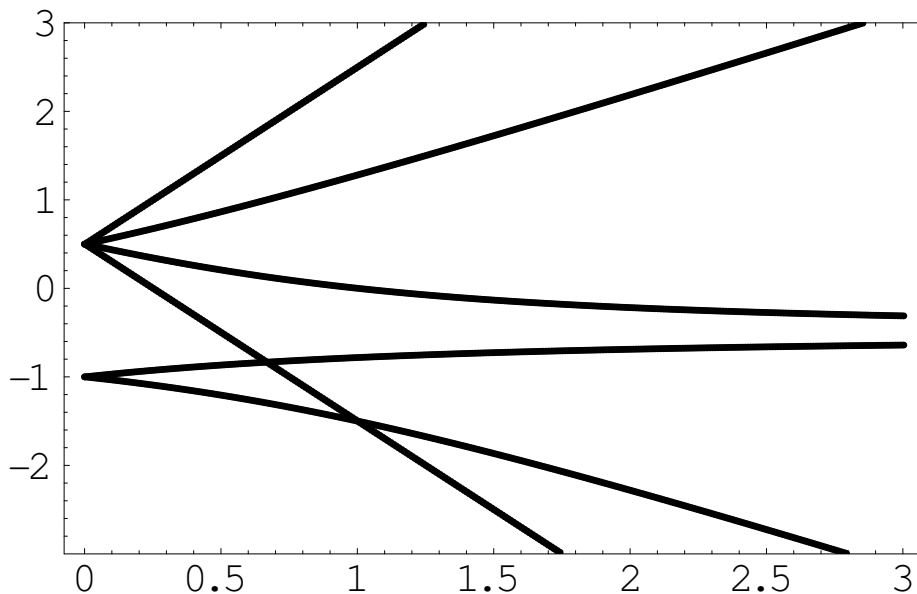
━━━━━ [49.5] Calculation of the Zeeman splitting

For a weak magnetic field it is better to write the Hamiltonian in the $|j, m_j\rangle$ basis, such that $\vec{L} \cdot \vec{S}$ is diagonal, while the Zeeman terms are treated as a perturbation. The calculation, using Mathematica, leads to

$$
\mathcal{H} \to \frac{v}{2}
\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & -2 & 0 \\
0 & 0 & 0 & 0 & 0 & -2
\end{pmatrix}
- \frac{h}{3}
\begin{pmatrix}
3 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & -\sqrt{2} & 0 \\
0 & 0 & -1 & 0 & 0 & -\sqrt{2} \\
0 & 0 & 0 & -3 & 0 & 0 \\
0 & -\sqrt{2} & 0 & 0 & 2 & 0 \\
0 & 0 & -\sqrt{2} & 0 & 0 & -2
\end{pmatrix}
- g\frac{h}{6}
\begin{pmatrix}
3 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 2\sqrt{2} & 0 \\
0 & 0 & -1 & 0 & 0 & 2\sqrt{2} \\
0 & 0 & 0 & -3 & 0 & 0 \\
0 & 2\sqrt{2} & 0 & 0 & 1 & 0 \\
0 & 0 & 2\sqrt{2} & 0 & 0 & -1
\end{pmatrix}
$$

Optionally, if we want to avoid the above numerical task, we can exploit a shortcut. Namely, the splitting of the j-multiplet can be estimated using degenerate perturbation theory. In order to do so we have to find the j blocks of the perturbation terms. For that we can exploit the Wigner Eckart theorem (see lecture regarding algebraic characterization of rotations). The procedure is explained below.

The Wigner Eckart theorem states that the matrix elements of any vector operator $\boldsymbol{A} = (A_x, A_y, A_z)$ within a j subspace are the same as that of $\boldsymbol{J} = (J_x, J_y, J_z)$ up to a prefactor g_A that can be determined easily. This can be summarized concisely by saying the for the j block we have $\boldsymbol{A} = g_A \boldsymbol{J}$. If follows that $\boldsymbol{J} \cdot \boldsymbol{A} = g_A \boldsymbol{J}^2 = g_A j(j+1)$. We therefore deduce that the prefactor can be determined from $g_A = \langle \boldsymbol{J} \cdot \boldsymbol{A} \rangle / [j(j+1)]$. Note that $\boldsymbol{J} \cdot \boldsymbol{A}$ is a scalar operator and therefore has the same expectation value for all the states within the j subspace.

Specifically for L_z we have $\langle m|L_z|m'\rangle = g_L m \delta_{m,m'}$, and for S_z we have $\langle m|S_z|m'\rangle = g_S m \delta_{m,m'}$. Accordingly, for the vector operator $\boldsymbol{M} = \boldsymbol{L} + g\boldsymbol{S}$ we get $\langle m|M_z|m'\rangle = g_M m \delta_{m,m'}$ with $g_M = g_L + g g_S$. Consequently, degenerate perturbation theory implies

$$
E_{j,m} \approx E_j - (g_M m)h \tag{49.18}
$$

The determination of g_L and g_S can be carried out using

$$
g_L = \frac{\langle \vec{J} \cdot \vec{L} \rangle}{j(j+1)} = \frac{j(j+1) + \ell(\ell+1) - s(s+1)}{2j(j+1)} \tag{49.19}
$$

$$
g_S = \frac{\langle \vec{J} \cdot \vec{S} \rangle}{j(j+1)} = \frac{j(j+1) + s(s+1) - \ell(\ell+1)}{2j(j+1)} \tag{49.20}
$$

leading to $g_L = \frac{2}{3}$ and $g_S = \frac{1}{3}$ for $j = \frac{3}{2}$, while $g_L = \frac{4}{3}$ and $g_S = -\frac{1}{3}$ for $j = \frac{1}{2}$. **Note:** In fact we do not need here those formulas. We can deduce by inspection what are g_L and g_S, simply by looking at the *exact* results that we already have for $E_{j,j}$. No further algebra is required!

Special Topics

[50] Quantization of the EM Field

═══════ [50.1] The Classical Equations of Motion

The equations of motion for a system which is composed of non-relativistic classical particles and EM fields are:

$$
\begin{aligned}
\mathsf{m}_i \frac{d^2 \mathbf{x}_i}{dt^2} &= e_i \mathcal{E} - e_i \mathcal{B} \times \dot{\mathbf{x}}_i \\
\nabla \cdot \mathcal{E} &= 4\pi\rho \\
\nabla \times \mathcal{E} &= -\frac{\partial \mathcal{B}}{\partial t} \\
\nabla \cdot \mathcal{B} &= 0 \\
\nabla \times \mathcal{B} &= \frac{\partial \mathcal{E}}{\partial t} + 4\pi\vec{J}
\end{aligned}
\tag{50.1}
$$

where

$$
\begin{aligned}
\rho(x) &= \sum_i e_i \delta(x - \mathbf{x}_i) \\
J(x) &= \sum_i e_i \dot{\mathbf{x}}_i \delta(x - \mathbf{x}_i) \qquad \text{[to be symmetrized in the quantum context]}
\end{aligned}
\tag{50.2}
$$

We also note that there is a continuity equation which is implied by the above definition and also can be regarded as a consistency requirement for the Maxwell equation:

$$
\frac{\partial \rho}{\partial t} = -\nabla \cdot J
\tag{50.3}
$$

It is of course simpler to derive the EM field from a potential (V, A) as follows:

$$
\begin{aligned}
\mathcal{B} &= \nabla \times A \\
\mathcal{E} &= -\frac{\partial A}{\partial t} - \nabla V
\end{aligned}
\tag{50.4}
$$

Then we can write an equivalent system of equations of motion

$$
\begin{aligned}
\mathsf{m}_i \frac{d^2 \mathbf{x}_i}{dt^2} &= e_i \mathcal{E} - e_i \mathcal{B} \times \dot{\mathbf{x}}_i \\
\frac{\partial^2 A}{\partial t^2} &= \nabla^2 \vec{A} - \nabla \left(\nabla \cdot \vec{A} + \frac{\partial}{\partial t} V \right) + 4\pi J \\
\nabla^2 V &= -\frac{\partial}{\partial t} \left(\nabla \cdot \vec{A} \right) - 4\pi\rho
\end{aligned}
\tag{50.5}
$$

═══════ [50.2] The Coulomb Gauge

In order to further simplify the equations we would like to use a convenient gauge which is called the "Coulomb gauge". To fix a gauge is essentially like choosing a reference for the energy. Once we fix the gauge in a given reference frame ("laboratory") the formalism is no longer manifestly Lorentz invariant. Still the treatment is exact.

Any vector field can be written as a sum of two components, one that has zero divergence and another that has zero curl. For the case of the electric field $\mathcal{E}$, the sum can be written as:

$$\mathcal{E} = \mathcal{E}_{\shortparallel} + \mathcal{E}_{\perp} \tag{50.6}$$

where $\nabla \cdot \mathcal{E}_{\perp} = 0$ and $\nabla \times \mathcal{E}_{\shortparallel} = 0$. The field $\mathcal{E}_{\perp}$ is called the transverse or solenoidal or "radiation" component, while the field $\mathcal{E}_{\shortparallel}$ is the longitudinal or irrotational or "Coulomb" component. The same treatment can be done for the magnetic field $\mathcal{B}$ with the observation that from Maxwell's equations $\nabla \cdot \mathcal{B} = 0$ yields $\mathcal{B}_{\shortparallel} = 0$. That means that there is no magnetic charge and hence the magnetic field $\mathcal{B}$ is entirely transverse. So now we have

$$\text{EM field} = (\mathcal{E}_{\shortparallel}, \mathcal{E}_{\perp}, \mathcal{B}) = \text{Coulomb field} + \text{radiation field} \tag{50.7}$$

Without loss of generality we can derive the radiation field from a transverse vector potential. Thus we have:

$$\mathcal{E}_{\shortparallel} = -\nabla V \tag{50.8}$$
$$\mathcal{E}_{\perp} = -\frac{\partial A}{\partial t}$$
$$\mathcal{B} = \nabla \times A$$

This is called the Coulomb gauge, which we use from now on. We can solve the Maxwell equation for V in this gauge, leading to the potential

$$V(x) = \sum_j \frac{e_j}{|x - \mathbf{x}_j|} \tag{50.9}$$

Now we can insert the solution into the equations of motion of the particles. The new system of equations is

$$\mathsf{m}_i \frac{d^2 \mathbf{x}_i}{dt^2} = \left[\sum_j \frac{e_i e_j \, \vec{n}_{ij}}{|\mathbf{x}_i - \mathbf{x}_j|^2} \right] + e_i \mathcal{E}_{\perp} - e_i \mathcal{B} \times \dot{\mathbf{x}}_i \tag{50.10}$$
$$\frac{\partial^2 A}{\partial t^2} = \nabla^2 \vec{A} + 4\pi J_{\perp}$$

It looks as if $J_{\shortparallel}$ is missing in the last equation. In fact it can be easily shown that it cancells with the ∇V term due to the continuity equation that relates $\partial_t \rho$ to $\nabla \cdot J$, and hence $\partial_t \nabla V$ to $J_{\shortparallel}$ respectively.

══════ [50.3] Hamiltonian for the Particles

We already know from the course in classical mechanics that the Hamiltonian, from which the equations of motion of *one* particles in EM field are derived, is

$$\mathcal{H}^{(i)} = \frac{1}{2\mathsf{m}_i} (\mathbf{p}_i - e_i A(\mathbf{x}_i))^2 + e_i V(\mathbf{x}_i) \tag{50.11}$$

This Hamiltonian assumes the presence of A while V is potential which is created by all the other particles. Once we consider the many body system, the potential V is replaced by a mutual Coulomb interaction term, from which the forces on any of the particles are derived:

$$\mathcal{H} = \sum_i \frac{1}{2\mathsf{m}_i} (\mathbf{p}_i - e_i A(\mathbf{x}_i))^2 + \frac{1}{2} \sum_{i,j} \frac{e_i e_j}{|\mathbf{x}_i - \mathbf{x}_j|} \tag{50.12}$$

By itself the *direct Coulomb interaction* between the particles seems to contradict relativity. This is due to the non-invariant way that we had separated the electric field into components. In fact our treatment is exact: as a whole the Hamiltonian that we got is Lorentz invariant, as far as the EM field is concerned.

The factor $1/2$ in the Coulomb interaction is there in order to compensate for the double counting of the interactions. What about the diagonal terms $i = j$? We can keep them if we want because they add just a finite constant term to the Hamiltonian. The "self interaction" infinite term can be regularized by assuming that each particle has a very small radius. To drop this constant from the Hamiltonian means that "infinite distance" between the particles is taken as the reference state for the energy. However, it is more convenient to keep this infinite constant in the Hamiltonian, because then we can write:

$$\mathcal{H} = \sum_i \frac{1}{2\mathsf{m}_i}(\mathbf{p}_i - e_i A(\mathbf{x}_i))^2 + \frac{1}{8\pi} \int \mathcal{E}_{\shortparallel}^2 d^3x \tag{50.13}$$

In order to get the latter expression we have used the following identity:

$$\frac{1}{2} \int \frac{\rho(x)\rho(x')}{|x - x'|} d^3x d^3x' \quad = \quad \frac{1}{8\pi} \int \mathcal{E}_{\shortparallel}^2 d^3x \tag{50.14}$$

The derivation of this identity is based on Gauss law, integration by parts, and using the fact that the Laplacian of $1/|x - x'|$ is a delta function. Again we emphasize that the integral diverges unless we regularize the physical size of the particles, or else we have to subtract an infinite constant that represents the "self interaction".

The above Hamiltonian contains the interaction with the radiation field, namely,

$$\mathcal{H}_{\text{interaction}} \quad = \quad \sum_i \frac{e_i}{2} \left[v_i \cdot A(\mathbf{x}_i) + A(\mathbf{x}_i) \cdot v_i\right] \quad = \quad -\int \vec{J}(x) \cdot \vec{A}(x) \; d^3x \tag{50.15}$$

In Fourier components the latter expressions can be written schematically, as $\sum_k J_k A_k$. The precise way to define the Fourier components will be elaborated in the next section, where we discuss the way to write the radiation field Hamiltonian. A key point is to realize that the the interaction term has a dual role. It is the *same* interaction term that drives the particles by the field, and that drives the field by the particles...

══════ [50.4] Hamiltonian for the Radiation Field

So now we need another term in the Hamiltonian from which the second equation of motion is derived

$$\frac{\partial^2 A}{\partial t^2} - \nabla^2 \vec{A} = 4\pi \vec{J}_\perp \tag{50.16}$$

In order to decouple the above equations into "normal modes" we write $\vec{A}$ in a Fourier series:

$$\vec{A}(x) = \frac{1}{\sqrt{\text{volume}}} \sum_k \vec{A}_k \; \mathrm{e}^{ikx} = \frac{1}{\sqrt{\text{volume}}} \sum_{k,\alpha} A_{k,\alpha} \; \varepsilon^{k,\alpha} \mathrm{e}^{ikx} \tag{50.17}$$

where $\varepsilon^{k,\alpha}$ for a given k is a set of two orthogonal unit vectors. If A were a general vector field rather than a transverse field, then we would have to include a third unit vector. Note that $\nabla \cdot A = 0$ is like $k \cdot \vec{A}_k = 0$. Now we can rewrite the equation of motion as

$$\ddot{A}_{k,\alpha} + \omega_k^2 A_{k,\alpha} = 4\pi J_{k,\alpha} \tag{50.18}$$

where $\omega_k = |k|$. For pedagogical clarity, let us ignore for a moment the α index, and regard $Q_k \equiv A_k$ as independent real (rather than complex) coordinates. This would allow to regard each mode as Harmonic oscillator, that is driven

by a field of force J_k, derived from an interaction term $-J_k Q_k$ that resides in the total Hamiltonian. By inspection of the equation of motion we see that each mode has "mass" that equals $1/(4\pi)$ [CGS!!!], So we write schematically

$$\text{mass}\,\frac{d^2}{dt^2}Q_k \;\; = \;\; -[\text{mass}\,\omega_k^2]\,Q_k \; + \; J_k \tag{50.19}$$

It follows that the conjugate coordinate is $P_k = [1/(4\pi)]\dot{A}_k$. This conjugate coordinate, up to a factor, is just the k-th Fourier component of the electric field. The equations of motion can be derived from an Hamiltonian that contains the terms $(1/2)[4\pi]P_k^2$ and $(1/2)[1/(4\pi)]\omega_k^2 A_k^2$. This leads in real space to an integral over $(\mathcal{E}^2 + \mathcal{B}^2)$, multiplied by the "mass" factor $1/(8\pi)$.

The disadvantage of the above Fourier expansion is that it does not reflect that $A(x)$ is a real field. In fact the $A_{k,\alpha}$ should satisfy $A_{-k,\alpha} = (A_{k,\alpha})^*$. In order to have proper "normal mode" coordinates we have to replace each pair of complex $A_{k,\alpha}$ and $A_{-k,\alpha}$ by a pair of real coordinates $A'_{k,\alpha}$ and $A''_{k,\alpha}$. Namely

$$A_{k,\alpha} = \frac{1}{\sqrt{2}}[A'_{k,\alpha} + iA''_{k,\alpha}] \tag{50.20}$$

We also use a similar decomposition for $J_{k,\alpha}$. We choose the $1/\sqrt{2}$ normalization so as to have the following identity:

$$\int J(x) \cdot A(x)\; dx \;\; = \;\; \sum_{k,\alpha} J^*_{k,\alpha} A_{k,\alpha} = \sum_{[k],\alpha} (J'_{k,\alpha} A'_{k,\alpha} + J''_{k,\alpha} A''_{k,\alpha}) \;\; \equiv \;\; \sum_r J_r Q_r \tag{50.21}$$

In the sum over degrees of freedom r we must remember to avoid double counting. The vectors k and $-k$ represent the same direction which we denote as $[k]$. The variable $A'_{-k,\alpha}$ is the same variable as $A'_{k,\alpha}$, and the variable $A''_{-k,\alpha}$ is the same variable as $-A''_{k,\alpha}$. We denote this set of coordinates Q_r, and the conjugate momenta as P_r. We see that each of the normal coordinates Q_r has a "mass" that equals $1/(4\pi)$, Therefore the conjugate "momenta" are $P_r = [1/(4\pi)]\dot{Q}_r$, which up to a factor are just the Fourier components of the electric field. Now we can write the Hamiltonian as

$$\mathcal{H} \;\; = \;\; \sum_r \left[\frac{1}{2\cdot\text{mass}} P_r^2 + \frac{1}{2}\text{mass}\cdot\omega_r^2\, Q_r^2 - J_r Q_r \right] \tag{50.22}$$

where r is the sum over all the degrees of freedom: two independent modes for each direction and polarization. By straightforward algebra the sum can be written as

$$\mathcal{H} \;\; = \;\; \frac{1}{8\pi}\int (\mathcal{E}_\perp^2 + \mathcal{B}^2)d^3x - \int \vec{J}\cdot A d^3x \tag{50.23}$$

More generally, if we want to write the total Hamiltonian for the particle and the EM field we have to ensure that $-\partial\mathcal{H}/\partial A(x) = J(x)$. It is not difficult to figure out the the following Hamiltonian is doing the job:

$$\mathcal{H} = \mathcal{H}_{\text{particles}} + \mathcal{H}_{\text{interaction}} + \mathcal{H}_{\text{radiation}} = \sum_i \frac{1}{2\mathsf{m}_i}(\mathbf{p}_i - e_i A(\mathbf{x}_i))^2 + \frac{1}{8\pi}\int (\mathcal{E}^2 + \mathcal{B}^2)d^3x \tag{50.24}$$

The term that corresponds to $\vec{J}\cdot A$ is present in the first term of the Hamiltonian. As expected this terms has a dual role: on the one hand it gives the Lorentz force on the particle, while on the other hand it provides the source term that drives the EM field. I should be emphasized that the way we write the Hamiltonian is somewhat misleading: The Coulomb potential term (which involves $\mathcal{E}_\parallel^2$) is combined with the "kinetic" term of the radiation field (which involves $\mathcal{E}_\perp^2$).

═══════ [50.5] Quantization of the EM Field

Now that we know the "normal coordinates" of the EM field the quantization is trivial. For each "oscillator" of "mass" $1/(4\pi)$ we can define a and $a^\dagger$ operators such that $Q_r = (2\pi/\omega)^{1/2}(a_r + a_r^\dagger)$. Since we have two distinct variables for each direction, we use the notations $(b, b^\dagger)$ and $(c, c^\dagger)$ respectively:

$$Q_{[k]'\alpha} = A'_{k\alpha} = A'_{-k\alpha} = \sqrt{\frac{2\pi}{\omega_k}} \left(b_{[k]\alpha} + b^\dagger_{[k]\alpha} \right) \tag{50.25}$$

$$Q_{[k]''\alpha} = A''_{k\alpha} = -A''_{-k\alpha} = \sqrt{\frac{2\pi}{\omega_k}} \left(c_{[k]\alpha} + c^\dagger_{[k]\alpha} \right) \tag{50.26}$$

In order to make the final expressions look more elegant we use the following canonical transformation:

$$a_+ = \frac{1}{\sqrt{2}}(b + ic) \tag{50.27}$$

$$a_- = \frac{1}{\sqrt{2}}(b - ic)$$

It can be easily verified by calculating the commutators that the transformation from (b, c) to (a_+, a_-) is canonical. Also note that $b^\dagger b + c^\dagger c = a_+^\dagger a_+ + a_-^\dagger a_-$. Since the oscillators (normal modes) are uncoupled the total Hamiltonian is a simple sum over all the modes:

$$\mathcal{H} = \sum_{[k],\alpha} (\omega_k b^\dagger_{k,\alpha} b_{k,\alpha} + \omega_k c^\dagger_{k,\alpha} c_{k,\alpha}) = \sum_{k,\alpha} \omega_k a^\dagger_{k,\alpha} a_{k,\alpha} \tag{50.28}$$

For completeness we also write the expression for the field operators:

$$A_{k,\alpha} = \frac{1}{\sqrt{2}}(A' + iA'') = \frac{1}{\sqrt{2}} \left[\sqrt{\frac{2\pi}{\omega_k}}(b + b^\dagger) + i\sqrt{\frac{2\pi}{\omega_k}}(c + c^\dagger) \right] = \sqrt{\frac{2\pi}{\omega_k}}(a_{k,\alpha} + a^\dagger_{-k,\alpha}) \tag{50.29}$$

and hence (restoring CGS units)

$$\frac{1}{c}\vec{A}(x) = \frac{1}{\sqrt{\text{volume}}} \sum_{k,\alpha} \sqrt{\frac{2\pi}{\omega_k}}(a_{k,\alpha} + a^\dagger_{-k,\alpha}) \, \varepsilon^{k,\alpha} e^{ikx} \tag{50.30}$$

The eigenstates of the EM field are

$$|n_1, n_2, n_3, \ldots, n_{k,\alpha}, \ldots\rangle \tag{50.31}$$

We refer to the ground state as the vacuum state, and we can define e.g. one-photon and two-photon states as follows:

$$|\text{vacuum}\rangle = |0, 0, 0, 0, \ldots\rangle \tag{50.32}$$

$$|\text{one photon state}\rangle = \hat{a}^\dagger_{k\alpha} |\text{vacuum}\rangle \tag{50.33}$$

$$|\text{two photon state}\rangle = \hat{a}^\dagger_{k_2\alpha_2} \hat{a}^\dagger_{k_1\alpha_1} |\text{vacuum}\rangle \tag{50.34}$$

$$|\text{two photon state}\rangle = \frac{1}{\sqrt{2}}(\hat{a}^\dagger_{k_1\alpha_1})^2 |\text{vacuum}\rangle \tag{50.35}$$

and in general we can have N photon states or any superposition of such states.

An important application of the above formalism is for the calculation of spontaneous emission. Let us assume that the atom has an excited level E_B and a ground state E_A. The atom is prepared in the excited state, and the electromagnetic field is assume to be initially in a vacuum state. According to Fermi Golden Rule the system decays into final states with one photon $\omega_k = (E_B - E_A)$. Regarding the atom as a point-like object the interaction term is

$$\mathcal{H}_{\text{interaction}} \quad \approx \quad -\frac{e}{c} A(0) \cdot \hat{v} \tag{50.36}$$

where $\hat{v} = \hat{p}/\mathsf{m}$ is the velocity operator. It is useful to realize that $\hat{v}_{AB} = i(E_B - E_A)\hat{x}_{AB}$. The vector $\vec{D} = \hat{x}_{AB}$ is known as the dipole matrix element. It follows that matrix element for the decay is

$$|\langle n_{k\alpha} = 1, A|\mathcal{H}_{\text{interaction}}|\text{vacuum}, B\rangle|^2 = \frac{e^2}{\text{volume}} 2\pi\omega_k |\varepsilon^{k,\alpha} \cdot D|^2 \tag{50.37}$$

In order to calculate the decay rate using FGR we have to multiply this expression by 2π, and by the density of the final states $[\text{volume}/(2\pi)^3] (\omega^2/c^3)d\Omega$, and by an additional factor $8\pi/3$ that comes from the integration ($d\Omega$) over all the possible directions and polarizations. This gives $\Gamma = (4/3)(e^2/c^3)\omega^3|D|^2$.

[51] Quantization of a many body system

═══════ [51.1] Second Quantization

If we regard the electromagnetic field as a collection of oscillators then we call $a^\dagger$ and a raising and lowering operators. This is "first quantization" language. But we can also call $a^\dagger$ and a creation and destruction operators. Then it is "second quantization" language. So for the electromagnetic field the distinction between "first quantization" and "second quantization" is merely a linguistic issue. Rather than talking about "exciting" an oscillator we talk about "occupying" a mode.

For particles the distinction between "first quantization" and "second quantization" is not merely a linguistic issue. The quantization of *one* particle is called "first quantization". If we treat several distinct particles (say a proton and an electron) using the same formalism then it is still "first quantization".

If we have many (identical) electrons then a problem arises. The Hamiltonian commutes with "transpositions" of particles, and therefore its eigenstates can be categorized by their symmetry under permutations. In particular there are two special subspaces: those of states that are symmetric for *any* transposition, and those that are antisymmetric for *any* transposition. It turns out that in nature there is a "super-selection" rule that allows only one of these two symmetries, depending on the type of particle. Accordingly we distinguish between Fermions and Bosons. All other sub-spaces are excluded as "non-physical".

We would like to argue that the "first quantization" approach, is simply the wrong language to describe a system of identical particles. We shall show that if we use the "correct" language, then the distinction between Fermions and Bosons comes out in a natural way. Moreover, there is no need for the super-selection rule!

The key observation is related to the definition of Hilbert space. If the particles are distinct it makes sense to ask "where is each particle". But if the particles are identical this question is meaningless. The correct question is "how many particles are in each site". The space of all possible occupations is called "Fock space". Using mathematical language we can say that in "first quantization", Hilbert space is the external product of "one-particle spaces". In contrast to that, Fock space is the external product of "one site spaces".

When we say "site" we mean any "point" in space. Obviously we are going to demand at a later stage "invariance" of the formalism with respect to the choice of one-particle basis. The formalism should look the same if we talk about occupation of "position states" or if we talk about occupation of "momentum states". Depending on the context we talk about occupation of *"sites"* or of *"orbitals"* or of *"modes"* or we can simply use the term *"one particle states"*.

Given a set of orbitals $|r\rangle$ the Fock space is spanned by the basis $\{|...,n_r,...,n_s,...\rangle\}$. We can define a subspace of all N particles states

$$\text{span}_N\{|...,n_r,...,n_s,...\rangle\} \tag{51.1}$$

that includes all the superpositions of basis states with $\sum_r n_r = N$ particles. On the other hand, if we use the first quantization approach, we can define Hilbert subspaces that contains only totally symmetric or totally anti-symmetric states:

$$\text{span}_S\{|r_1,r_2,...,r_N\rangle\} \tag{51.2}$$
$$\text{span}_A\{|r_1,r_2,...,r_N\rangle\}$$

The mathematical claim is that there is a one-to-one correspondence between Fock span_N states and Hilbert span_S or span_A states for Bosons and Fermions respectively. The identification is expressed as follows:

$$|\Psi\rangle = |...,n_r,...,n_s,...\rangle \iff \frac{1}{N!}\sqrt{C_N^n}\sum_P \xi^P\, P|r_1,r_2,...,r_N\rangle \tag{51.3}$$

where $r_1,...,r_N$ label the occupied orbitals, P is an arbitrary permutation operator, ξ is $+1$ for Bosons and -1 for Fermions, and $C_N^n = N!/(n_r!n_s!...)$. We note that in the case of Fermions the formula above can be written as a Slater

determinant. In order to adhere to the common notations we use the standard representation:

$$\langle x_1, ..., x_N | \Psi \rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} \langle x_1 | r_1 \rangle & \cdots & \langle x_1 | r_N \rangle \\ \vdots & & \vdots \\ \langle x_N | r_1 \rangle & \cdots & \langle x_N | r_N \rangle \end{vmatrix} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi^{(1)}(x_1) & \cdots & \varphi^{(N)}(x_1) \\ \vdots & & \vdots \\ \varphi^{(1)}(x_N) & \cdots & \varphi^{(N)}(x_N) \end{vmatrix} \tag{51.4}$$

In particular for occupation of $N = 2$ particles in orbitals r and s we get

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}} \Big(\varphi^r(x_1)\varphi^s(x_2) - \varphi^s(x_1)\varphi^r(x_2) \Big) \tag{51.5}$$

In the following section we discuss only the Fock space formalism. Nowadays the first quantization Hilbert space approach is used mainly for the analysis of two particle systems. For larger number of particles the Fock formalism is much more convenient, and all the issue of "symmetrization" is avoided.

===== [51.2] Raising and Lowering Operators

First we would like to discuss the mathematics of a single "site". The basis states $|n\rangle$ can be regarded as the eigenstates of a number operator:

$$\hat{n}|n\rangle = n|n\rangle \tag{51.6}$$

$$\hat{n} \longrightarrow \begin{pmatrix} 0 & & & 0 \\ & 1 & & \\ & & 2 & \\ 0 & & & \ddots \end{pmatrix}$$

In general the action of the lowering operator, and accordingly its adjoint raising operator, can be written in terms of a function $f(n)$ as follows:

$$\hat{a}\,|n\rangle = f(n)\,|n-1\rangle \tag{51.7}$$
$$\hat{a}^\dagger\,|n\rangle = f(n+1)\,|n+1\rangle \tag{51.8}$$

The associated matrix representation is:

$$\hat{a} \longrightarrow \begin{pmatrix} 0 & * & & \\ & \ddots & \ddots & \\ & & \ddots & * \\ 0 & & & 0 \end{pmatrix}, \qquad \hat{a}^\dagger \longrightarrow \begin{pmatrix} 0 & & & 0 \\ * & \ddots & & \\ & \ddots & \ddots & \\ & & * & 0 \end{pmatrix} \tag{51.9}$$

By appropriate gauge we can assume without loss of generality that $f(n)$ is real and non-negative. so we can write

$$f(n) = \sqrt{g(n)} \tag{51.10}$$

From the definition of $\hat{a}$ it follows that

$$\hat{a}^\dagger \hat{a}|n\rangle = g(n)|n\rangle \tag{51.11}$$

and therefore

$$\hat{a}^\dagger \hat{a} = g(\hat{n}) \tag{51.12}$$

There are 3 cases of interest

- The raising/lowering is unbounded $(-\infty < n < \infty)$
- The raising/lowering is bounded from one side (say $0 \leq n < \infty$)
- The raising/lowering is bounded from both sides (say $0 \leq n < \mathcal{N}$)

The simplest choices for $g(n)$ in the 3 cases are respectively

$$g(n) = 1 \tag{51.13}$$
$$g(n) = n \tag{51.14}$$
$$g(n) = (\mathcal{N} - n)n \tag{51.15}$$

In the 1st case $\hat{a}$ becomes the translation operator, and the spectrum of n stretches from $-\infty$ to ∞. In the 2nd case we get the same algebra as in the case of an harmonic oscillator. In the 3rd case the algebra is the same as that for angular momentum. In the latter case once can define

$$m = n - \frac{\mathcal{N} - 1}{2} = -s, \ldots, +s \tag{51.16}$$

where $s = (\mathcal{N} - 1)/2$. Then it is possible to write

$$g(m) = s(s+1) - m(m+1) \tag{51.17}$$

In the next sections we are going to discuss the "Bosonic" case $\mathcal{N} = \infty$ with $g(n) = n$, and the "Fermionic" case $\mathcal{N} = 2$ with $g(n) = n(1-n)$. Later we are going to argue that these are the only two possibilities that are relevant to the description of many body occupation.
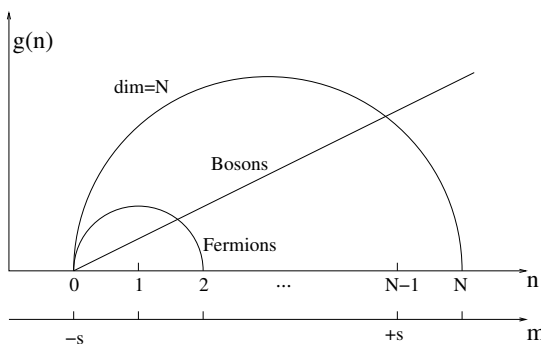
It is worthwhile to note that the algebra of "angular momentum" can be formally obtained from the Bosonic algebra using a trick due to Schwinger. Let us define two Bosonic operators a_1 and a_2, and

$$c^{\dagger} = a_2^{\dagger} a_1 \tag{51.18}$$

The $c^{\dagger}$ operator moves a particle from site 1 to site 2. Consider how c and $c^{\dagger}$ operate within the subspace of $(N-1)$ particle states. It is clear that c and $c^{\dagger}$ act like lowering/raising operators with respect to $\hat{m} = (a_2^{\dagger} a_2 - a_1^{\dagger} a_1)/2$. Obviously the lowering/raising operation in bounded from both ends. In fact it is easy to verify that c and $c^{\dagger}$ have the same algebra as that of "angular momentum".

══════ [51.3] Creation Operators for Bosons

For a "Bosonic" site we define field operators such that

$$\hat{a} \left| n \right\rangle = \sqrt{n} \left| n-1 \right\rangle \tag{51.19}$$
$$\hat{a}^{\dagger} \left| n \right\rangle = \sqrt{n+1} \left| n+1 \right\rangle \tag{51.20}$$

hence

$$\left[\hat{a}, \hat{a}^{\dagger}\right] = \hat{a}\hat{a}^{\dagger} - \hat{a}^{\dagger}\hat{a} = 1 \tag{51.21}$$

If we have many sites then we define

$$\hat{a}_r^{\dagger} = 1 \otimes 1 \otimes \cdots \otimes \hat{a}^{\dagger} \otimes \cdots \otimes 1 \tag{51.22}$$

which means

$$\hat{a}_r^{\dagger} \left| n_1, n_2, \ldots, n_r, \ldots \right\rangle = \sqrt{n_r + 1} \left| n_1, n_2, \ldots, n_r + 1, \ldots \right\rangle \tag{51.23}$$

and hence

$$[\hat{a}_r, \hat{a}_s] = 0 \tag{51.24}$$

and

$$\left[\hat{a}_r, \hat{a}_s^{\dagger}\right] = \delta_{r,s} \tag{51.25}$$

We have defined our set of creation operators using a particular one-particle basis. What will happen if we switch to a different basis? Say from the position basis to the momentum basis? In the new basis we would like to have the same type of *occupation rules*. As further discuss in the next section the occupation rules are dictated by the *algebra* of the field operator. Here we would like to have

$$\left[\hat{a}_{\alpha}, \hat{a}_{\beta}^{\dagger}\right] = \delta_{\alpha\beta} \tag{51.26}$$

Let us see that indeed this is the case. The unitary transformation matrix from the original $|r\rangle$ basis to the new $|\alpha\rangle$ basis is

$$T_{r,\alpha} = \langle r|\alpha \rangle \tag{51.27}$$

Then we have the relation

$$|\alpha\rangle = \sum_r |r\rangle \langle r|\alpha\rangle = \sum_r T_{r,\alpha} |r\rangle \tag{51.28}$$

and therefore

$$\hat{a}_{\alpha}^{\dagger} = \sum_r T_{r,\alpha} \hat{a}_r^{\dagger} \tag{51.29}$$

Taking the adjoint we also have

$$\hat{a}_{\alpha} = \sum_r T_{r,\alpha}^* \hat{a}_r \tag{51.30}$$

Now we find that

$$\left[\hat{a}_{\alpha}, \hat{a}_{\beta}^{\dagger}\right] = \sum_{r,s} \left[T_{r\alpha}^* \hat{a}_r, T_{s\beta} \hat{a}_s^{\dagger}\right] = T_{r\alpha}^* T_{s\beta} \delta_{rs} = \left(T^{\dagger}\right)_{\alpha r} T_{r\beta} = \left(T^{\dagger}T\right)_{\alpha\beta} = \delta_{\alpha\beta} \tag{51.31}$$

This result shows that $\hat{a}_\alpha$ and $\hat{a}_\beta^\dagger$ are indeed destruction and creation operators of the same "type" as $\hat{a}_r$ and $\hat{a}_r^\dagger$. Can we have the same type of invariance for other types of occupation? We shall see that the only other possibility that allows *invariant description* is $\mathcal{N} = 2$.

════ [51.4] Creation Operators for Fermions

In analogy with the case of a "Boson site" we define a "Fermion site". The field operators satisfy

$$\hat{a}\,|n\rangle \;=\; \sqrt{n}\,|n-1\rangle \tag{51.32}$$
$$\hat{a}^\dagger\,|n\rangle \;=\; \sqrt{n+1}\,|n+1\rangle \qquad \text{with mod(2) plus operation} \tag{51.33}$$

The representation of the operators using Pauli matrices is:

$$\hat{n} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}\left(\hat{1} + \sigma_3\right) \tag{51.34}$$

$$\hat{a} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}\left(\sigma_1 - i\sigma_2\right)$$

$$\hat{a}^\dagger = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}\left(\sigma_1 + i\sigma_2\right)$$

and we have the relations

$$\hat{a}^\dagger \hat{a} = \hat{n} \tag{51.35}$$
$$\hat{a}\hat{a}^\dagger = \hat{1} - \hat{n}$$
$$\left[\hat{a}, \hat{a}^\dagger\right]_+ = \hat{a}\hat{a}^\dagger + \hat{a}^\dagger \hat{a} = 1$$
$$\left[\hat{a}, \hat{a}^\dagger\right] = 1 - 2\hat{n}$$

Now we would like to proceed with the many-site system as in the case of "Bosonic sites". But the problem is that the algebra

$$\left[\hat{a}_r, \hat{a}_s^\dagger\right] = \delta_{r,s}(1 - 2\hat{a}_r^\dagger \hat{a}_r) \tag{51.36}$$

is manifestly not invariant under a change of one-particle basis. The only hope is to have in *any* basis

$$\left[\hat{a}_r, \hat{a}_s^\dagger\right]_+ = \delta_{r,s} \tag{51.37}$$

which means that a_r and a_s for $r \neq s$ should anti-commute rather than commute. Can we define the operators a_r in such a way? It turns out that there is such a possibility:

$$\hat{a}_r^\dagger\,|n_1, n_2, \ldots, n_r, \ldots\rangle = (-1)^{\sum_{s(>r)} n_s}\sqrt{1+n_r}\,|n_1, n_2, \ldots, n_r+1, \ldots\rangle \tag{51.38}$$

For example, it is easily verified that we have:

$$a_2^\dagger a_1^\dagger |0,0,0,\ldots\rangle = -a_1^\dagger a_2^\dagger |0,0,0,\ldots\rangle = |1,1,0,\ldots\rangle \tag{51.39}$$

With the above convention if we create particles in the "natural order" then the sign comes out plus, while for any "violation" of the natural order we get a minus factor.

══════ [51.5] Algebraic characterization of field operators

In this section we establish a mathematical observations that we have used in previous sections, namely, that the *occupation rules* are dictated by the algebra. The algebra is required to be invariant under change of the "orbital" basis, and hence we ensure the same occupation rules is *any* basis. The algebra that we are discussing is defined as follows:

$$[\hat{a}_r, \hat{a}_s]_{\mp} = 0 \tag{51.40}$$
$$[\hat{a}_r, \hat{a}_s^\dagger]_{\mp} = \delta_{r,s} \tag{51.41}$$

where $\mp$ refers to Bosons and Fermions respectively. This algebra is manifestly invariant for change of orbital basis. What we want to clarify is that the respective occupations rules are implied, namely, $n = 0, 1, 2, \cdots$ for Bosons, and $n = 0, 1$ for Fermions.

Given operators n and a, we say that a is a lowering operator provided

$$\hat{n}\left(\hat{a}\,|n\rangle\right) = (n-1)\left(\hat{a}\,|n\rangle\right) \qquad \text{for any } n \tag{51.42}$$

which is equivalent to

$$\hat{n}\hat{a} = \hat{a}(\hat{n} - 1) \tag{51.43}$$

A raising operator is similarly characterized by $\hat{n}\hat{a}^\dagger = \hat{a}^\dagger(\hat{n} + 1)$.

It is possible to make a more interesting statement. Given that

$$[a, a^\dagger] = aa^\dagger - a^\dagger a = 1 \tag{51.44}$$

we deduce that a and $a^\dagger$ are lowering and raising operators with respect to $\hat{n} = a^\dagger a$. The proof follows directly from the implied identity $\hat{n}\hat{a}^\dagger = \hat{a}^\dagger(\hat{n} \pm 1)$, as discussed in the previous paragraph. Furthermore, we get

$$||a|n\rangle|| = \langle n|a^\dagger a|n\rangle = n \tag{51.45}$$
$$||a^\dagger|n\rangle|| = \langle n|aa^\dagger|n\rangle = 1 + n \tag{51.46}$$

Since the norm is a non-negative value it follows that $n = 0$ and hence also all the positive integer values $n = 1, 2, \ldots$ form its spectrum. Thus in such case a and $a^\dagger$ describe a system of Bosons.

Similar deduction applies to the Fermionic algebra. Here we start with the anti-commutation relations:

$$[a, a]_+ = 2aa = 0 \tag{51.47}$$
$$[a, a^\dagger]_+ = aa^\dagger + a^\dagger a = 1 \tag{51.48}$$

Again we define $\hat{n} = a^\dagger a$ and observe that a and $a^\dagger$ are characterized by $\hat{n}\hat{a} = \hat{a}(1 - \hat{n})$ and $\hat{n}\hat{a}^\dagger = \hat{a}^\dagger(1 - \hat{n})$. Hence we deduce that both a and $a^\dagger$ simply make transposition of two n states $|\epsilon\rangle$ and $|1-\epsilon\rangle$. Furthermore

$$||a|n\rangle|| = \langle n|a^\dagger a|n\rangle = n \tag{51.49}$$
$$||a^\dagger|n\rangle|| = \langle n|aa^\dagger|n\rangle = 1 - n \tag{51.50}$$

Since the norm is a non-negative value it follows that $0 \leq \epsilon \leq 1$. Thus we deduce that the representation of a is

$$\hat{a} = \begin{pmatrix} 0 & \sqrt{\epsilon} \\ \sqrt{1-\epsilon} & 0 \end{pmatrix} \tag{51.51}$$

One can check whether the desired anti-commutations are satisfied. Then one observes that is order to satisfy the trivial requirement $aa = 0$, the only possibilities are either $\epsilon = 0$ or $\epsilon = 1$, aka particle-hole duality.

═══════ [51.6] Bogoliubov transformations

Consider a vector z_μ of coordinates. The coordinates are either $z = (\boldsymbol{q}, \boldsymbol{p})$, or $z = (\boldsymbol{a}, \bar{\boldsymbol{a}})$, where $\boldsymbol{a} = (\boldsymbol{q} + i\boldsymbol{p})/\sqrt{2}$. They have the algebra

$$[z_\mu, z_\nu] \;=\; \boldsymbol{J}_{\mu,\nu} \;=\; \text{metric} \tag{51.52}$$

where $[\cdots]$ stands for either Poisson brackets (for oscillators), or commutator (for bosons), or anti-commutators (for fermions), depending on the context. Note that we can always use "bosons" language in order to discuss "oscillators". The symplectic metric is

$$\boldsymbol{J} \;=\; \begin{pmatrix} \boldsymbol{0} & \boldsymbol{1} \\ \mp\boldsymbol{1} & \boldsymbol{0} \end{pmatrix} \tag{51.53}$$

where the $\mp$ sign refers to bososn and fermions respectively. Note that $\boldsymbol{J}^2 = \mp\boldsymbol{1}$.

A symplectic transformation (in the manybody context aka Bogoliubov transformation) is required to preserve the metric. Writing the transformation as $\tilde{z} = \boldsymbol{S}z$, the requirement is $\boldsymbol{S}\boldsymbol{J}\boldsymbol{S}^t = \boldsymbol{J}$. The simplest example is a Bogoliubov transformation for a single site system:

$$\boldsymbol{c}^\dagger \;=\; u\boldsymbol{a}^\dagger + v\boldsymbol{a} \tag{51.54}$$

The corresponding transformation matrix is

$$\boldsymbol{S} \;=\; \begin{pmatrix} u^* & v^* \\ v & u \end{pmatrix}, \qquad \boldsymbol{T} = \boldsymbol{S}^{-1} = \boldsymbol{J}\boldsymbol{S}^t\boldsymbol{J}^{-1} = \begin{pmatrix} u & -v^* \\ -v & u^* \end{pmatrix}, \tag{51.55}$$

We use here a sign convention that prevails in the treatment of the GP equation (see lecture regarding site system with bosons). The symplectic condition implies $|u|^2 - |v|^2 = 1$, and $\boldsymbol{T}$ is the inverse transformation. In $z = (\boldsymbol{q}, \boldsymbol{p})$ coordinates $\boldsymbol{S}$ is real with determinant that equals to unity. In other words, for one degree of freedom, the symplectic group coincides with the group of area preserving linear transformation (Sp(2) = SL(2)). It is illuminating to write the transformation explicitly. For simplicity assume that u and v are real. We write them as $u = \cosh(\theta)$ and $v = \sinh(\theta)$. Then we get

$$\tilde{\boldsymbol{q}} \;=\; (u+v)\boldsymbol{q} \;=\; e^\theta\boldsymbol{q} \;=\; U(\theta)^\dagger\boldsymbol{q}U(\theta) \tag{51.56}$$
$$\tilde{\boldsymbol{p}} \;=\; (u-v)\boldsymbol{p} \;=\; e^{-\theta}\boldsymbol{p} \;=\; U(\theta)^\dagger\boldsymbol{p}U(\theta) \tag{51.57}$$

where $U(\theta) = \exp(-i\theta\boldsymbol{G})$. This transformation is called "squeeze", and its generator is

$$\boldsymbol{G} \;=\; \frac{1}{2}\left(\boldsymbol{q}\boldsymbol{p} + \boldsymbol{p}\boldsymbol{q}\right) \;=\; -\frac{i}{2}\left(\boldsymbol{a}\boldsymbol{a} - \boldsymbol{a}^\dagger\boldsymbol{a}^\dagger\right) \tag{51.58}$$

Note that the new vacuum-state is defined by the equation $\boldsymbol{c}|\Psi\rangle = 0$, and can be obtained by an inverse squeeze operation, namely, $|\tilde{0}\rangle = \exp(i\theta\boldsymbol{G})|0\rangle$. In general u and v can be complex. Then get an SL(2) transformation of the $(\boldsymbol{q}, \boldsymbol{p})$ coordinates. In particular, the transformation $\boldsymbol{c} = e^{i\varphi}\boldsymbol{a}$ is a φ rotation, that is generated by $\boldsymbol{G} = -\boldsymbol{a}^\dagger\boldsymbol{a}$. In the general case any real matrix that has unit determinant of SL(2) can be decomposed (SVD/KAK) into a sequence of rotation, squeeze, and a second rotation.

Writing $\boldsymbol{c}^\dagger = u\boldsymbol{a}^\dagger + v\boldsymbol{a}$, we can ask what is the analogous transformation for fermions. We realize that the condition $[\boldsymbol{c}, \boldsymbol{c}]_\mp = 0$ is trivial for bosons, but not for fermions. In the latter case we get the condition $uv = 0$, which leads to

triviality (particle hole duality). For fermions a non-trivial Bogoliubov transformation requires system that has more than one site. A common Bogoliubov transformation that involves two sites is

$$\boldsymbol{c}_1^\dagger = u\boldsymbol{a}_1^\dagger + v\boldsymbol{a}_2 \tag{51.59}$$

$$\boldsymbol{c}_2^\dagger = u\boldsymbol{a}_2^\dagger \pm v\boldsymbol{a}_1 \tag{51.60}$$

with $|u|^2 \mp |v|^2 = 1$ for bosons and fermions respectively. For real u and v the Bosonic transformation corresponds to a simple coordinate transformation $\tilde{\boldsymbol{q}}_1 = u\boldsymbol{q}_1 + v\boldsymbol{q}_2$ and $\tilde{\boldsymbol{q}}_2 = u\boldsymbol{q}_2 + v\boldsymbol{q}_1$, which implies a $\pm\theta$ squeeze of the $q_\pm = q_1 \pm q_2$ coordinates, hence $\boldsymbol{G} = (\boldsymbol{q}_1\boldsymbol{p}_2 + \boldsymbol{p}_1\boldsymbol{q}_2) = -i(\boldsymbol{a}_1\boldsymbol{a}_2 - \boldsymbol{a}_1^\dagger\boldsymbol{a}_2^\dagger)$.

===== [51.7] Quadratic Hamiltonians

In the classical context, equations of motion are derived from an Hamiltonian. If $z = (\boldsymbol{q}, \boldsymbol{p})$ the prescription is $\dot{z}_\mu = \boldsymbol{J}_{\mu,\nu}\partial_\nu\mathcal{H}$. With $z = (\boldsymbol{a}, \bar{\boldsymbol{a}})$ coordinates, the prescription is

$$\dot{z}_\mu = -i\sum_\nu \boldsymbol{J}_{\mu,\nu}\partial_\nu\mathcal{H} \tag{51.61}$$

Consider an Hamiltonian that has a quadratic form

$$\mathcal{H} = \frac{1}{2}\sum_{\mu,\nu} \boldsymbol{H}_{\mu,\nu}z_\mu z_\nu = \frac{1}{2}z^t\boldsymbol{H}z \tag{51.62}$$

where $\boldsymbol{H}^t = \boldsymbol{H}$ is the Hessian matrix. The equations of motion and their solution are

$$\dot{z} = -i[\boldsymbol{J}\boldsymbol{H}]z \tag{51.63}$$

$$z(t) = \exp[-it\boldsymbol{J}\boldsymbol{H}]z(0) \tag{51.64}$$

The same equation with matrix that satisfies $\boldsymbol{H}^t = -\boldsymbol{H}$ can be derived for fermions. The difference between bosons and fermions in this context is the implication of the symplectic condition: to have $\boldsymbol{S}\boldsymbol{J}\boldsymbol{S}^t = \boldsymbol{J}$ for an infinitesimal transformation that is generated by $\boldsymbol{J}\boldsymbol{H}$, is equivalent to $\boldsymbol{H}^t = \pm\boldsymbol{H}$, for bosons and fermions respectively. As an example we consider a two site system with bosons:

$$\mathcal{H} = \varepsilon_1\boldsymbol{a}_1^\dagger\boldsymbol{a}_1 + \varepsilon_2\boldsymbol{a}_2^\dagger\boldsymbol{a}_2 + K(\boldsymbol{a}_2^\dagger\boldsymbol{a}_1 + \boldsymbol{a}_1^\dagger\boldsymbol{a}_2) + \Delta(\boldsymbol{a}_2^\dagger\boldsymbol{a}_1^\dagger + \boldsymbol{a}_1\boldsymbol{a}_2) + \text{const} \tag{51.65}$$

$$\boldsymbol{H} = \begin{pmatrix} 0 & \Delta & \varepsilon_1 & K \\ \Delta & 0 & K & \varepsilon_2 \\ \varepsilon_1 & K & 0 & \Delta \\ K & \varepsilon_2 & \Delta & 0 \end{pmatrix}, \qquad \boldsymbol{J}\boldsymbol{H} = \begin{pmatrix} \varepsilon_1 & K & 0 & \Delta \\ K & \varepsilon_2 & \Delta & 0 \\ 0 & -\Delta & -\varepsilon_1 & -K \\ -\Delta & 0 & -K & -\varepsilon_2 \end{pmatrix} \tag{51.66}$$

We can look for a symplectic transformation $\boldsymbol{T}$ to new coordinates, such that the Hamiltonian becomes a sum over independent modes. We call such procedure *decoupling*. In $z = (\boldsymbol{a}, \bar{\boldsymbol{a}})$ coordinates it means that $\boldsymbol{J}\tilde{\boldsymbol{H}}$ should be diagonal. This is the matrix that generates the symplectic evolution, aka the Bogoliubov deGennes Hamiltonian. After the decoupling transformation, the equations of motion for the $\boldsymbol{a}$ coordinates are decoupled. We explain below that *decoupling* (in the sense of matrix congruence) can be achieved via *diagonalization* (in the sense of matrix similarity). We note that in the above example the 4x4 matrix decomposes into two 2x2 blocks if $K = 0$. Namely,

$$[\boldsymbol{J}\boldsymbol{H}]^{(1)} = \begin{pmatrix} \varepsilon_1 & \pm\Delta \\ -\Delta & -\varepsilon_2 \end{pmatrix}, \qquad [\boldsymbol{J}\boldsymbol{H}]^{(2)} = \begin{pmatrix} \varepsilon_2 & \Delta \\ \mp\Delta & -\varepsilon_1 \end{pmatrix}, \tag{51.67}$$

where the $\pm$ is for bosons and fermions respectively. After diagonalization we get four frequencies $(\omega_1, -\omega_2; \omega_2, -\omega_1)$, which implies $\mathcal{H} = \sum \omega_q \boldsymbol{c}_q^\dagger \boldsymbol{c}_q$, with $q = 1, 2$. If $\Delta = 0$ we get $\omega_q = \varepsilon_q$. If $\varepsilon_2 = \varepsilon_1 = \varepsilon$ the two frequencies become identical, and for non-zero Δ we get $\omega_q = \sqrt{\varepsilon^2 \mp \Delta^2}$ for bosons and fermions respectively.

Diagonalization procedure.– Diagonalization (in the sense of similarity transformation) means that we find a matrix $\boldsymbol{T}$ such that $\boldsymbol{T}^{-1}[\boldsymbol{JH}]\boldsymbol{T}$ is diagonal. The columns of $\boldsymbol{T}$ are the eigenvectors. A key observation is that $\boldsymbol{T}$, with proper normalization of its columns, is symplectic. This is analogous to the statement that diagonalization of a normal matrix can be achieved by a unitary transformation. Proof of this lemma is provided in the next paragraph. It follows that a properly normalized $\boldsymbol{T}$ satisfies $\boldsymbol{TJT}^t = \boldsymbol{J}$, and therefore the inverse matrix is $\boldsymbol{T}^{-1} = \boldsymbol{JT}^t\boldsymbol{J}^{-1}$. Accordingly we deduce that $\boldsymbol{J}[\boldsymbol{T}^t\boldsymbol{HT}]$ is diagonal, which is what we wanted to achieve (decoupling).

Diagonalization lemma.– Given an operator A we can find a new basis such that it becomes diagonal, namely, $T^{-1}AT = \Lambda$. The choice of T is not unique: we have freedom to normalize and gauge each column. Below we generalize the statement that a unitary matrix can be diagonalized by a unitary transformation. Namely, we claim that a symplectic matrix can be diagonalized by a symplectic transformation. The same applies to generators of symplectic evolution. Let us assume that A preserves the metric J in the quadratic form $z^t J z$. This means $A^t J A = G$. Then it follows that $A^{-1} = J^{-1}A^t J$. And therefore, from $\det[\lambda - A^{-1}] = \det[\lambda - A]$ it follows that the eigenvalues come in pairs $\{\lambda, \lambda^{-1}\}$. Note that if A is real then also the conjugate values belong to the spectrum. Given two eigenvectors "1" and "2" that belong to different blocks ($\lambda_1\lambda_2 \neq 1$) we deduce that "$1 \perp 2$" relative to the metric J. Construct transformation matrix T that consists of all the eigenvectors of A, it follows that $T^t J T$ is block diagonal, and has non-zero entries in one-to-one correspondence with J. Using the normalization freedom for the columns of T, we can have all the non-zero entries of $T^t J T$ equal to ± 1, so we can make it such that $T^t J T = J$. The above lemma can be generalized for any metric G. A preliminary step would be to adopt a standard basis in which G is diagonal with entries ± 1 in accordance with Sylvester's law of inertia.

Majorana operators.– Consider system with fermions we define a symplectic transformation to hermitian coordinates. This is done in analogy with the bosonic case. Namely

$$\text{Bosonic case:} \qquad a \;\equiv\; \frac{1}{\sqrt{2}}(q + ip) \tag{51.68}$$

$$\text{Fermionic case:} \qquad a \;\equiv\; \frac{1}{2}\left(\sigma_x + i\sigma_y\right) \tag{51.69}$$

Here we consider a one-site (one-degree-of-freedom) system, but the generalization to many-site system is straightforward. The algebra of the Majorana operators can be characterized in a very compact way

$$[\sigma_\mu, \sigma_\nu]_+ \;\;=\;\; 2\delta_{\mu,\nu} \tag{51.70}$$

We can go in reverse: given the σ algebra we define an a algebra, construct n operators, and hence construct an associated Fock space. Note the following relations:

$$\text{Bosonic case:} \qquad \hat{n} \;=\; a^\dagger a \;=\; \frac{1}{2}\left(x^2 + p^2\right) \tag{51.71}$$

$$\text{Fermionic case:} \qquad \hat{n} \;=\; a^\dagger a \;=\; \frac{1}{2}\left(1 + i\sigma_x\sigma_y\right) \tag{51.72}$$

With the Majorana operators the hamiltonian is written as

$$\mathcal{H} \;\;=\;\; \frac{i}{4}\sum_{\mu,\nu} \boldsymbol{H}_{\mu,\nu}\sigma_\mu\sigma_\nu \tag{51.73}$$

where $\boldsymbol{H}_{\mu,\nu}$ is a real anti-symmetric matrix. Note that $i\boldsymbol{H}$ is hermitian with eigenvalues that come in pairs $\pm\epsilon_k$. Symplectic transformations that preserve the hermiticity of the σ operators are represented by an orthogonal matrices. The "diagonal" form of the Hamiltonian is $\sum \epsilon_k b_k^\dagger b_k$.

Consider a tight-binding Hamiltonian for a ring with paring interaction [Kitaev]. Depending on the model parameters the b-s are associated either with sites or with bonds. In the latter case, if we disconnect the ring, we get a an $\epsilon_0 \sim 0$ Majorana mode. So we have two anti-commuting operators σ_L and σ_R that form a single degree of freedom $b_0 = (1/2)[\sigma_L + i\sigma_R]$, which provide a degeneracy with respect to a quantum number n_0.

══════ [51.8] One Body Additive Operators

Let us assume that we have an additive quantity V which is not the same for different one-particle states. One example is the (total) kinetic energy, another example is the (total) potential energy. It is natural to define the many body operator that corresponds to such a property in the basis where the one-body operator is diagonal. In the case of potential energy it is the position basis:

$$\boldsymbol{V} = \sum_\alpha V_{\alpha,\alpha} \hat{n}_\alpha = \sum_\alpha \hat{a}_\alpha^\dagger V_{\alpha,\alpha} \hat{a}_\alpha \tag{51.74}$$

This counts the amount of particles in each α and multiplies the result with the value of V at this site. If we go to a different one-particle basis then we should use the transformation

$$\hat{a}_\alpha = \sum_k T_{k,\alpha}^* \hat{a}_k \tag{51.75}$$

$$\hat{a}_\alpha^\dagger = \sum_{k'} T_{k',\alpha} \hat{a}_{k'}^\dagger$$

leading to

$$\boldsymbol{V} = \sum_{k,k'} \hat{a}_{k'}^\dagger V_{k',k} \hat{a}_k \tag{51.76}$$

Given the above result we can calculate the matrix elements from a transition between two different occupations:

$$|\langle n_1 - 1, n_2 + 1 | \boldsymbol{V} | n_1, n_2 \rangle|^2 = (n_2 + 1)\, n_1\, |V_{2,1}|^2 \tag{51.77}$$

What we get is quite amazing: in the case of Bosons we get an amplification of the transition if the second level is already occupied. In the case of Fermions we get "blocking" if the second level is already occupied. Obviously this goes beyond classical reasoning. The latter would give merely n_1 as a prefactor.

══════ [51.9] Two Body "Additive" Operators

It is straightforward to make a generalization to the case of two body "additive" operators. Such operators may represent the two-body interaction between the particles. For example we can take the Coulomb interaction, which is diagonal in the position basis. Thus we have

$$\boldsymbol{U} = \frac{1}{2} \sum_{\alpha \neq \beta} U_{\alpha\beta,\alpha\beta} \hat{n}_\alpha \hat{n}_\beta + \frac{1}{2} \sum_\alpha U_{\alpha\alpha,\alpha\alpha}\, \hat{n}_\alpha (\hat{n}_\alpha - 1) \tag{51.78}$$

Using the relation

$$\hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger \hat{a}_\beta \hat{a}_\alpha = \begin{cases} \hat{n}_\alpha \hat{n}_\beta & \text{for } \alpha \neq \beta \\ \hat{n}_\alpha(\hat{n}_\alpha - 1) & \text{for } \alpha = \beta \end{cases} \tag{51.79}$$

We get the simple expression

$$\boldsymbol{U} = \frac{1}{2} \sum_{\alpha,\beta} \hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger\, U_{\alpha\beta,\alpha\beta}\, \hat{a}_\beta \hat{a}_\alpha \tag{51.80}$$

and for a general one-particle basis

$$\boldsymbol{U} = \frac{1}{2} \sum_{k'l',kl} \hat{a}_{k'}^{\dagger} \hat{a}_{l'}^{\dagger} \; U_{k'l',kl} \; \hat{a}_l \hat{a}_k \tag{51.81}$$

We call such operator "additive" (with quotations) because in fact they are not really additive (see below). It is useful to notice that if we multiply two one-body operators, say $\boldsymbol{C} = \boldsymbol{AB}$ we get in general a non-additive two-body operator. But if we consider the commutator $\boldsymbol{C} = [\boldsymbol{A}, \boldsymbol{B}]$, we realize that it is equivalent to a one-body additive operator that corresponds to $C = [A, B]$. This observation is very important for the theory of linear response (Kubo formula).

═══════ [51.10] Matrix elements with N particle states

One-body operator are *additive*. This is reflected in the calculation of the expectation value of a state that has n_k particles in the k-th orbital, namely,

$$\langle \boldsymbol{V} \rangle \;\; = \;\; \sum_k n_k \, \langle V \rangle_k \tag{51.82}$$

Let us consider specifically an N particle state of a Fermionic system, which is characterized by a definite occupation of k orbitals:

$$|N\rangle = \hat{a}_N^{\dagger} \ldots \hat{a}_2^{\dagger} \hat{a}_1^{\dagger} |0\rangle \tag{51.83}$$

For the expectation value of a one body operator we get

$$\langle N | \boldsymbol{V} | N \rangle = \sum_{k \in N} \langle k | V | k \rangle \tag{51.84}$$

because only the terms with $k = k'$ do not vanish. If we have two N particle states with definite occupations, then the matrix element of V would be in general zero unless they differ by a single electronic transition, say from an orbital k_0 to another orbital k_0'. In the latter case we get the result V_{k_0', k_0} as if the other electrons are not involved.

For the two body operator we get for the expectation value a more interesting result that goes beyond the naive expectation. The only non-vanishing terms in the sandwich calculation are those with either $k' = k$ and $l' = l$ or with $k' = l$ and $l' = k$. All the other possibilities give zero. Consequently

$$\langle N | \boldsymbol{U} | N \rangle = \frac{1}{2} \sum_{k,l \in N} \underset{direct}{\langle kl | U | kl \rangle} - \underset{exchange}{\langle lk | U | kl \rangle} \tag{51.85}$$

A common application of this formula is in the context of multi-electron atoms and molecules, where U is the Coulomb interaction. The direct term has an obvious electrostatic interpretation, while the exchange term reflects the implications of the Fermi statistics. In such application the exchange term is non-vanishing whenever two orbitals have a non-zero spatial overlap. Electrons that occupy well separated orbitals have only a direct electrostatic interaction.

══════ [51.11] Introduction to the Kondo problem

One can wonder whether the Fermi energy, due to the Pauli exclusion principle, is like a lower cutoff that "regularize" the scattering cross section of of electrons in a metal. We explain below that this is not the case unless the scattering involves a spin flip. The latter is known as the Kondo effect. The scattering is described by

$$V = \sum_{k',k} a_{k'}^{\dagger} V_{k',k} a_k \tag{51.86}$$

hence:

$$T^{[2]} = \left\langle k_2 \left| V \frac{1}{E - \mathcal{H} + i0} V \right| k_1 \right\rangle = \sum_{k_b',k_b} \sum_{k_a',k_a} \left\langle k_2 \left| a_{k_b'}^{\dagger} V_{k_b',k_b} a_{k_b} \frac{1}{E - \mathcal{H} + i0} a_{k_a'}^{\dagger} V_{k_a',k_a} a_{k_a} \right| k_1 \right\rangle \tag{51.87}$$

where both the initial and the final states are zero temperature Fermi sea with one additional electron above the Fermi energy. The initial and final states have the same energy:
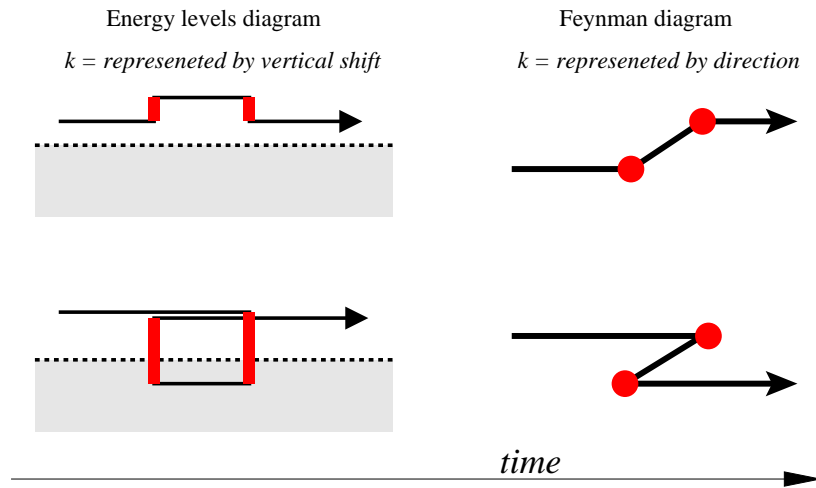
$$E = E_0 + \epsilon_{k_1} = E_0 + \epsilon_{k_2} \tag{51.88}$$

where E_0 is the total energy of the zero temperature Fermi sea. The key observation is that all the intermediate states are with definite occupation. Therefore we can pull out the resolvent:

$$T^{[2]} = \sum_{k_b',k_b,k_a',k_a} \frac{V_{k_b',k_b} V_{k_a',k_a}}{E - E_{k_a,k_a'}} \left\langle k_2 \left| a_{k_b'}^{\dagger} a_{k_b} a_{k_a'}^{\dagger} a_{k_a} \right| k_1 \right\rangle \tag{51.89}$$

where

$$E_{k_a,k_a'} = E_0 + \epsilon_{k_1} - \epsilon_{k_a} + \epsilon_{k_a'} \tag{51.90}$$

Energy levels diagram

k = represeneted by vertical shift

Feynman diagram

k = represeneted by direction

time

As in the calculation of "exchange" we have two non-zero contribution to the sum. These are illustrated in the figure above: Either (k_b', k_b, k_a', k_a) equals (k_2, k', k', k_1) with k' above the Fermi energy, or (k', k_1, k_2, k') with k' below the Fermi energy. Accordingly $E - E_{k_a,k_a'}$ equals either $(\epsilon_{k_1} - \epsilon_{k'})$ or $-(\epsilon_{k_1} - \epsilon_{k'})$. Hence we get

$$T^{[2]} = \sum_{k'} \left[\frac{V_{k_2,k'} V_{k',k_1}}{+(\epsilon_{k_1} - \epsilon_{k'}) + i0} \left\langle k_2 \left| a_{k_2}^{\dagger} a_{k'} a_{k'}^{\dagger} a_{k_1} \right| k_1 \right\rangle + \frac{V_{k',k_1} V_{k_2,k'}}{-(\epsilon_{k_1} - \epsilon_{k'}) + i0} \left\langle k_2 \left| a_{k'}^{\dagger} a_{k_1} a_{k_2}^{\dagger} a_{k'} \right| k_1 \right\rangle \right] \tag{51.91}$$

Next we use

$$\left\langle k_2 \left| a_{k_2}^\dagger a_{k'}^\dagger a_{k'} a_{k_1} \right| k_1 \right\rangle = \left\langle k_2 \left| a_{k_2}^\dagger (1 - n_{k'}) a_{k_1} \right| k_1 \right\rangle = +1 \times \left\langle k_2 \left| a_{k_2}^\dagger a_{k_1} \right| k_1 \right\rangle \tag{51.92}$$

which holds if k' is above the Fermi energy (otherwise it is zero). And

$$\left\langle k_2 \left| a_{k'}^\dagger a_{k_1} a_{k_2}^\dagger a_{k'} \right| k_1 \right\rangle = \left\langle k_2 \left| a_{k_1} (n_{k'}) a_{k_2}^\dagger \right| k_1 \right\rangle = -1 \times \left\langle k_2 \left| a_{k_2}^\dagger a_{k_1} \right| k_1 \right\rangle \tag{51.93}$$

which holds if k' is below the Fermi energy (otherwise it is zero). Note that without loss of generality we can assume gauge such that $\langle k_2 | a_{k_2}^\dagger a_{k_1} | k_1 \rangle = 1$. Coming back to the transition matrix we get a result which is not divergent at the Fermi energy:

$$T^{[2]} = \sum_{k' \in \text{above}} \frac{V_{k_2,k'} V_{k',k_1}}{\epsilon_{k_1} - \epsilon_{k'} + i0} + \sum_{k' \in \text{below}} \frac{V_{k_2,k'} V_{k',k_1}}{\epsilon_{k_1} - \epsilon_{k'} - i0} \tag{51.94}$$

If we are above the Fermi energy, then it is as if the Fermi energy does not exist at all. But if the scattering involves a spin flip, as in the Kondo problem, the divergence for ϵ close to the Fermi energy is not avoided. Say that we want to calculate the scattering amplitude

$$\langle k_2 \uparrow, \Downarrow | T | k_1, \uparrow, \Downarrow \rangle \tag{51.95}$$

where the double arrow stands for the spin of a magnetic impurity. It is clear that the only sequences that contribute are those that take place *above* the Fermi energy. The other set of sequences, that involve the creation of an electron-hole pair do not exist: Since we assume that the magnetic impurity is initially "down", it is not possible to generate a pair such that the electron spin is "up".

======= [51.12] Green functions for many body systems

The Green function in the one particle formalism is defined via the resolvent as the Fourier transform of the propagator. In the many body formalism the role of the propagator is taken by the time ordered correlation of field operators. In both cases the properly defined Green function can be used in order to analyze scattering problems in essentially the same manner. It is simplest to illustrate this observation using the example of the previous section. The Green function in the many body context is defined as

$$G_{k_2,k_1}(\epsilon) \quad = \quad -i\text{FT}\left[\left\langle \Psi \middle| \mathcal{T} a_{k_2}(t_2) a_{k_1}^\dagger(t_1) \middle| \Psi \right\rangle \right] \tag{51.96}$$

If Ψ is the vacuum state this coincides with the one particle definition of the Green function:

$$G_{k_2,k_1}(\epsilon) \quad = \quad -i\text{FT}\left[\Theta(t_2 - t_1) \langle k_2 | U(t_2 - t_1) | k_1 \rangle \right] \tag{51.97}$$

But if Ψ is (say) a non-empty zero temperature Fermi sea then also for $t_2 < t_1$ we get a non-zero contribution due to the possibility to annihilate an electron in an occupied orbital. Thus we get

$$G_{k_2,k_1}(\epsilon) = \sum_{\epsilon_k > \epsilon_F} \frac{\delta_{k_1,k} \delta_{k_2,k}}{\epsilon - \epsilon_k + i0} + \sum_{\epsilon_k < \epsilon_F} \frac{\delta_{k_1,k} \delta_{k_2,k}}{\epsilon - \epsilon_k - i0} \tag{51.98}$$

One should observe that the many-body definition is designed so as to reproduce the correct T matrix as found in the previous section. The definition above allows us to adopt an optional point of view of the scattering process: *a one particle point of view instead of a many body point of view!* In the many body point of view an electron-hole pair can be created, and later the hole is likely to be annihilated with the injected electron. In the one particle point of view the injected electron can be "reflected" to move backwards in time and then is likely to be scattered back to the forward time direction. The idea here is to regard antiparticles as particles that travel backwards in time. This idea is best familiar in the context of the Dirac equation.

[52] Wigner function and Wigner-Weyl formalism

════════ [52.1] The classical description of a state

Classical states are described by a probability function. Given a random variable $\hat{x}$, we define $\rho(x) = \text{Prob}(\hat{x} = x)$ as the probability of the event $\hat{x} = x$, where the possible values of x are called the spectrum of the random variable $\hat{x}$. For a random variable continuous spectrum we define the probability density function via $\rho(x)dx = \text{Prob}(x < \hat{x} < x + dx)$. The expectation value of a random variable $\hat{A} = A(\hat{x})$ is defined as

$$\langle \hat{A} \rangle = \sum \rho(x)\ A(x) \tag{52.1}$$

and for a continuous variable as. For simplicity we use, from now on, a notation as if the random variables have a discrete spectrum, with the understanding that in the case of a continuous spectrum we should replace the $\sum$ by an integral with the appropriate *measure* (e.g. dx or $dp/(2\pi\hbar)$). Unless essential for the presentation we set $\hbar = 1$.

Let us consider two random variables $\hat{x}, \hat{p}$. One can ask what is the joint probability distribution for these two variables. This is a valid question only in classical mechanics. In quantum mechanics one usually cannot ask this question since not all variables can be measured in the same measurement. In order to find the joint probability function of these two variables in quantum mechanics one needs to build a more sophisticated method. The solution is to regard the expectation value as the fundamental outcome and to define the probability function as an expectation value. In the case of one variable such as $\hat{x}$ or $\hat{p}$, we define probability functions as

$$\rho(X) \equiv \langle\ \delta(\hat{x} - X)\ \rangle$$
$$\rho(P) \equiv \langle\ 2\pi\delta(\hat{p} - P)\ \rangle \tag{52.2}$$

Now we can also define the joint probability function as

$$\rho(X, P) = \langle 2\pi\delta(\hat{p} - P)\ \delta(\hat{x} - X)\ \rangle \tag{52.3}$$

This probability function is normalized so that

$$\int \rho(X, P)\frac{dXdP}{2\pi} = \left\langle \int \delta(\hat{p} - P)dP \int \delta(\hat{x} - X)dX \right\rangle = 1 \tag{52.4}$$

In the next section we shall define essentially the same object in the framework of quantum mechanics.

════════ [52.2] Wigner function

Wigner function is a real normalized function which is defined as

$$\rho_{\text{W}}(X, P) = \left\langle\ \left[\ 2\pi\delta(\hat{p} - P)\ \delta(\hat{x} - X)\ \right]_{\text{sym}}\ \right\rangle \tag{52.5}$$

In what follows we define what we mean by symmetrization ("sym"), and we relate $\rho_{\text{W}}(X, P)$ to the conventional probability matrix $\rho(x', x'')$. We recall that the latter is defined as

$$\rho(x', x'') = \left\langle P^{x'x''} \right\rangle = \left\langle\ |x''\rangle\langle x'|\ \right\rangle \tag{52.6}$$

The "Wigner function formula" that we are going to prove is

$$\rho_{\text{W}}(X, P) = \int \rho\left(X + \frac{1}{2}r, X - \frac{1}{2}r\right) e^{-iPr} dr \tag{52.7}$$

Thus to go from the probability matrix to the Wigner function is merely a Fourier transform, and can be loosely regarded as a change from "position representation" to "phase space representation".

Moreover we can use the same transformation to switch the representation of an observable $\hat{A}$ from $A(x', x'')$ to $A(X, P)$. Then we shall prove the "Wigner-Weyl formula"

$$\mathsf{trace}(A\rho) = \int A(X, P)\rho_\mathrm{W}(X, P)\frac{dXdP}{2\pi} \tag{52.8}$$

This formula implies that expectation values of an observable can be calculated using a semi-classical calculation. This extension of the Wigner function formalism is known as the Wigner-Weyl formalism.

===== [52.3] Mathematical derivations

Fourier transform reminder:

$$
\begin{aligned}
F(k) &= \int f(x)\mathrm{e}^{-ikx}dx \\
f(x) &= \int \frac{dk}{2\pi}F(k)\mathrm{e}^{ikx}
\end{aligned}
\tag{52.9}
$$

The inner product is invariant under change of representation

$$\int f^*(x)g(x)dx = \int \frac{dk}{2\pi}F^*(k)G(k) \tag{52.10}$$

For the matrix representation of an operator A we use the notation

$$A(x', x'') = \langle x'|A|x''\rangle \tag{52.11}$$

It is convenient to replace the row and column indexes by diagonal and off-diagonal coordinates:

$$
\begin{aligned}
X &= \frac{1}{2}(x' + x'') = \text{the diagonal coordinate} \\
r &= x' - x'' = \text{the off diagonal coordinate}
\end{aligned}
\tag{52.12}
$$

such that $x' = X + (r/2)$ and $x'' = X - (r/2)$, and to use the alternate notation

$$A(X, r) = \left\langle X + \frac{1}{2}r \middle| A \middle| X - \frac{1}{2}r \right\rangle \tag{52.13}$$

Using this notation, the transformation to phase space representations can be written as

$$A(X, P) = \int A(X, r)\mathrm{e}^{-iPr}dr \tag{52.14}$$

Consequently the inner product of two matrices can be written as a phase space integral

$$\mathsf{trace}(A^\dagger B) = \int A^*(x', x'')B(x', x'')dx'dx'' = \int A^*(X, r)B(X, r)dXdr = \int A^*(X, P)B(X, P)\frac{dXdP}{2\pi} \tag{52.15}$$

This we call the "Wigner-Weyl formula". Note that if A is hermitian then $A(X, -r) = A^*(X, +r)$, and consequently $A(X, P)$ is a real function.

For the derivation of the "Wigner function formula" we have to explain how the operators $\delta(\hat{p} - P)\delta(\hat{x} - X)$ are symmetrized, and that that they form a complete set of observables that are linearly related to the standard set $|x'\rangle\langle x''|$. First we recall that a projector can be written as a delta function. This is quite transparent in discrete notation, namely $|n_0\rangle\langle n_0| = \delta_{\hat{n}, n_0}$. The left hand side is a projector whose only non-zero matrix element is $n = m = n_0$. The right hand side is a function of $f(\hat{n})$ such that $f(n) = 1$ for $n = n_0$ and zero otherwise. Therefore the right hand side is also diagonal in n with the same representation. In continuum notation

$$|X\rangle\langle X| \;\; = \;\; \delta(\hat{x} - X) \;\; = \;\; \int \frac{dp}{2\pi} \mathrm{e}^{ip(\hat{x} - X)} \tag{52.16}$$

With the same spirit we *define* the symmetrized operator

$$\left[\, 2\pi\delta(\hat{p} - P)\,\delta(\hat{x} - X)\,\right]_{\mathrm{sym}} \;\; \equiv \;\; \int \frac{drdp}{2\pi}\, \mathrm{e}^{ir(\hat{p} - P) + ip(\hat{x} - X)} \;\; = \;\; \int dr \mathrm{e}^{-irP} \int \frac{dp}{2\pi} \mathrm{e}^{ir\hat{p} + ip(\hat{x} - X)} \tag{52.17}$$

The inner integral can be carried out:

$$\int \frac{dp}{2\pi} \mathrm{e}^{ir\hat{p} + ip(\hat{x} - X)} \;\; = \;\; \int \frac{dp}{2\pi} \mathrm{e}^{i(r/2)\hat{p}} \mathrm{e}^{ip(\hat{x} - X)} \mathrm{e}^{i(r/2)\hat{p}} \;\; = \;\; \mathrm{e}^{i(r/2)\hat{p}} \delta(\hat{x} - X) \mathrm{e}^{i(r/2)\hat{p}} \tag{52.18}$$

where we used the identity $\mathrm{e}^{\hat{A} + \hat{B}} = \mathrm{e}^{\hat{A}} \mathrm{e}^{\hat{B}} \mathrm{e}^{\frac{1}{2}[\hat{A}, \hat{B}]}$, and the commutation $[\hat{x}, \hat{p}] = i$, in order to split the exponents, as in the equality $\mathrm{e}^{\hat{x} + \hat{p}} = \mathrm{e}^{\hat{p}/2} \mathrm{e}^{\hat{x}} \mathrm{e}^{\hat{p}/2}$. Replacing the $\delta(\hat{x} - X)$ by $|X\rangle\langle X|$, and operating on the ket and on the bra with the displacement operators $\mathrm{e}^{\pm i(r/2)\hat{p}}$ we find that

$$\left[\, 2\pi\delta(\hat{p} - P)\,\delta(\hat{x} - X)\,\right]_{\mathrm{sym}} \;\; = \;\; \int dr \mathrm{e}^{-irP}\, \Big|X - (r/2)\Big\rangle\Big\langle X + (r/2)\Big| \tag{52.19}$$

Taking the trace of both sides with ρ we deduce that $\rho_{\mathrm{W}}(X, P)$ is related to $\rho(X, r)$ via a Fourier transform in the r variable.

═══════ [52.4] Applications of the Wigner Weyl formalism

In analogy with the definition of the Wigner function $\rho_{\mathrm{W}}(X, P)$ which is associated with $\hat{\rho}$ we can define a Wigner-Weyl representation $A_{\mathrm{WW}}(X, P)$ of any hermitian operator $\hat{A}$. The phase space function $A_{\mathrm{WW}}(X, P)$ is obtained from the standard representation $A(x', x'')$ using the same "Wigner function formula" recipe. Let us consider the simplest examples. First consider how the recipe works for the operator $\hat{x}$:

$$\langle\, x'|\hat{x}|x''\rangle \;\; = \;\; x'\delta(x' - x'') \;\; = \;\; X\delta(r) \;\; \overset{\mathrm{WW}}{\longmapsto} \;\; X \tag{52.20}$$

Similarly $\hat{p} \overset{WW}{\to} P$. Further examples are:

$$f(\hat{x}) \quad \overset{\mathrm{WW}}{\longmapsto} \quad f(X) \tag{52.21}$$

$$g(\hat{p}) \quad \overset{\mathrm{WW}}{\longmapsto} \quad g(P) \tag{52.22}$$

$$\hat{x}\hat{p} \quad \overset{\mathrm{WW}}{\longmapsto} \quad XP + \frac{1}{2}i \tag{52.23}$$

$$\hat{p}\hat{x} \quad \overset{\mathrm{WW}}{\longmapsto} \quad XP - \frac{1}{2}i \tag{52.24}$$

$$\frac{1}{2}(\hat{x}\hat{p} + \hat{p}\hat{x}) \quad \overset{\mathrm{WW}}{\longmapsto} \quad XP \tag{52.25}$$

In general for appropriate ordering we get that $f(\hat{x}, \hat{p})$ is represented by $f(X, P)$. But in practical applications $f(\hat{x}, \hat{p})$ will not have the desired ordering, and therefore this recipe should be considered as a leading term in a semiclassical $\hbar$ expansion.

There are two major applications of the Wigner Weyl formula. The first one is the calculation of the partition function.

$$\mathcal{Z}(\beta) = \sum_r e^{-\beta E_r} = \sum_r \langle r|e^{-\beta H}|r\rangle = \mathsf{trace}(e^{-\beta H}) = \int \frac{dXdP}{2\pi}(e^{-\beta H(X,P)}) + \mathcal{O}(\hbar) \tag{52.26}$$

The second one is the calculation of the number of eigenstates up to a given energy E

$$\begin{aligned}\mathcal{N}(E) &= \sum_{E_r \leq E} 1 = \sum_r \Theta(E - E_r) = \mathsf{trace}[\Theta(E - \hat{H})] \\ &\approx \int \frac{dXdP}{2\pi}\Theta(E - H(X,P)) = \int_{H(X,P)\leq E} \frac{dXdP}{2\pi}\end{aligned} \tag{52.27}$$

Below we discuss some further applications that shed light on the dynamics of wavepackets, interference, and on the nature of quantum mechanical states. We note that the time evolution of Wigner function is similar but not identical to the evolution of a classical distribution unless the Hamiltonian is a quadratic function of $\hat{x}$ and $\hat{p}$.

═══ [52.5] Wigner function for a Gaussian wavepacket

A Gaussian wavepacket in the position representation is written as

$$\Psi(x) = \frac{1}{\sqrt{\sqrt{2\pi}\sigma}}e^{-\frac{(x-x_0)^2}{4\sigma^2}}e^{ip_0 x} \tag{52.28}$$

The probability density matrix is

$$\begin{aligned}\rho(X,r) &= \Psi\left(X+\frac{1}{2}r\right)\Psi^*\left(X-\frac{1}{2}r\right) \\ &= \frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{((X-x_0)+\frac{1}{2}r)^2}{4\sigma^2}-\frac{((X-x_0)-\frac{1}{2}r)^2}{4\sigma^2}+ip_0 r} = \frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(X-x_0)^2}{2\sigma^2}-\frac{r^2}{8\sigma^2}+ip_0 r}\end{aligned} \tag{52.29}$$

Transforming to the Wigner representation

$$\rho_{\mathrm{W}}(X,P) = \int \frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(X-x_0)^2}{2\sigma^2}-\frac{r^2}{8\sigma^2}-i(P-p_0)r}dr = \frac{1}{\sigma_x\sigma_p}e^{-\frac{(X-x_0)^2}{2\sigma_x^2}-\frac{(P-p_0)^2}{2\sigma_p^2}} \tag{52.30}$$

where $\sigma_x = \sigma$ and $\sigma_p = \frac{1}{2\sigma}$. It follows that $\sigma_x\sigma_p = 1/2$. Let us no go backwards. Assume that have a Gaussian in phase space, which is characterized by some σ_x and σ_p. Does it represent a legitimate quantum mechanical state? The normalization condition $\mathsf{trace}(\rho) = 1$ is automatically satisfied. We also easily find that

$$\mathsf{trace}(\rho^2) = \int \frac{1}{\sigma_x^2\sigma_p^2}e^{-\frac{(X-x_0)^2}{\sigma_x^2}-\frac{(P-p_0)^2}{\sigma_p^2}}\frac{dXdP}{2\pi} = \frac{1}{2\sigma_x\sigma_p} \tag{52.31}$$

We know that $\mathsf{trace}(\rho^2) = 1$ implies pure state. If $\mathsf{trace}(\rho^2) < 1$ it follows that we have a mixed state, whereas $\mathsf{trace}(\rho^2) > 1$ is not physical. It is important to remember that not any $\rho(X,P)$ corresponds to a legitimate quantum mechanical state. There are classical states that do not have quantum mechanical analog (e.g. point like preparation). Also the reverse is true: not any quantum state has a classical analogue. The latter is implied by the possibility to have negative regions in phase space. These is discussed in the next example.

══════ [52.6] The Winger function of a bounded particle

Wigner function may have some modulation on a fine scale due to an interference effect. The simplest and most illuminating example is the Wigner function of the nth eigenstate of a particle in a one dimensional box ($0 < x < L$). The eigen-wavefunction that correspond to wavenumber $k = (\pi/L) \times$ integer can be written as the sum of a right moving and a left moving wave $\psi(x) = (1/\sqrt{2})(\psi_1(x) + \psi_2(x))$ within $0 < x < L$, and $\psi(x) = 0$ otherwise. The corresponding Wigner function is zero outside of the box. Inside the box it can be written as

$$\rho_{\rm W}(X,P) = \frac{1}{2}\rho_1(X,P) + \frac{1}{2}\rho_2(X,P) + \rho_{12}(X,P) \tag{52.32}$$

where ρ_{12} is the interference component. The semiclassical components are concentrated at $P = \pm k$, while the interference component is concentrated at $P = 0$. The calculation of $\rho_1(X,P)$ in the interval $0 < x < L/2$ is determined solely by the presence of the hard wall at $x = 0$. The relevant component of the wavefunction is

$$\psi_1(x) = \frac{1}{\sqrt{L}}\Theta(x)e^{ikx} \tag{52.33}$$

and hence

$$\rho_1(X,P) = \int_{-\infty}^{\infty} \psi_1(X+(r/2))\psi_1^*(X-(r/2))e^{-iPr}dr = \frac{1}{L}\int_{-\infty}^{\infty} \Theta(X+(r/2))\Theta(X-(r/2))e^{-i(P-k)r}dr$$

$$= \frac{1}{L}\int_{-2X}^{2X} e^{-i(P-k)r}dr = \frac{4X}{L}\operatorname{sinc}(2X(P-k)) \tag{52.34}$$

This shows that as we approach the sharp feature the non-classical nature of Wigner function is enhanced, and the classical (delta) approximation becomes worse. The other components of Wigner function are similarly calculated, and for the interference component we get

$$\rho_{12}(X,P) = -\cos(2kX) \times \frac{4X}{L}\operatorname{sinc}(2XP) \tag{52.35}$$

It is easily verified that integration of $\rho_{\rm W}(X,P)$ over P gives $\rho(x) = (1/L)[1 - \cos(2kX)] = (2/L)(\sin(kX))^2$.

In many other cases the energy surface in phase space is "soft" (no hard walls) and then one can derive a uniform semiclassical approximation [Berry, Balazs]:

$$\rho_{\rm W}(X,P) = \frac{2\pi}{\Delta_{sc}(X,P)}\operatorname{Ai}\left(\frac{\mathcal{H}(X,P) - E}{\Delta_{sc}(X,P)}\right) \tag{52.36}$$

where for $\mathcal{H} = p^2/(2{\sf m}) + V(x)$

$$\Delta_{sc} = \frac{1}{2}\left[\hbar^2\left(\frac{1}{\sf m}|\nabla V(X)|^2 + \frac{1}{{\sf m}^2}(P\cdot\nabla)^2 V(X)\right)\right]^{1/3} \tag{52.37}$$

What can we get out of this expression? We see that $\rho_{\rm W}(X,P)$ decays exponentially as we go outside of the energy surface. Inside the energy surface we have oscillations due to interference.

The interference regions of the Wigner function might be very significant. A nice example is given by Zurek. Let us assume that we have a superposition of $N \gg 1$ non-overlapping Gaussian. we can write the Wigner function as $\rho = (1/N)\sum\rho_j + \rho_{\rm intrfr}$. We have $\operatorname{trace}(\rho) = 1$ and also $\operatorname{trace}(\rho^2) = 1$. This implies that $\operatorname{trace}(\rho_{\rm intrfr}) = 0$, while $\operatorname{trace}(\rho_{\rm intrfr}^2) \sim 1$. The latter conclusion stems from the observation that the classical contribution is $N \times (1/N)^2 \ll 1$. Thus the interference regions of the Wigner function dominate the calculation.

===== [52.7] The Winger picture of a two slit experiment

The textbook example of a two slit experiment will be analyzed below. The standard geometry is described in the upper panel of the following figure. The propagation of the wavepacket is in the y direction. The wavepacket is scattered by the slits in the x direction. The distance between the slits is d. The interference pattern is resolved on the screen. In the lower panel the phase-space picture of the dynamics is displayed. Wigner function of the emerging wavepacket is projected onto the (x, p_x) plane.
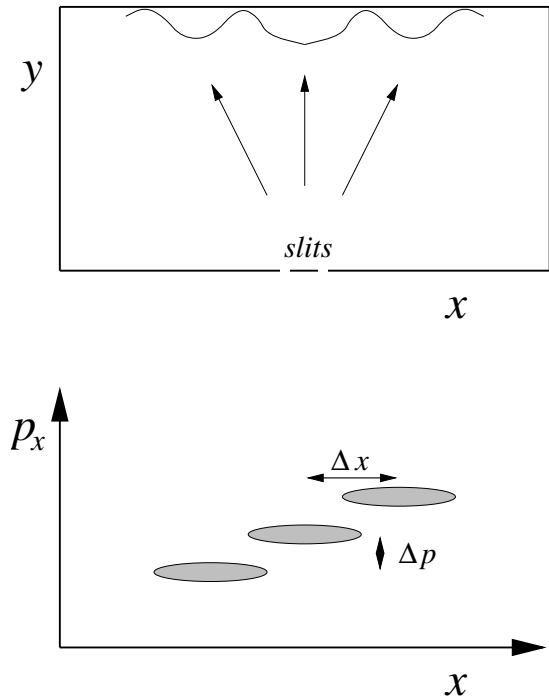
The wavepacket that emerges from the two slits is assumed to be a superposition

$$\Psi(x) \approx \frac{1}{\sqrt{2}}(\varphi_1(x) + \varphi_2(x)) \tag{52.38}$$

The approximation is related to the normalization which assumes that the slits are well separated. Hence we can regard $\varphi_1(x) = \varphi_0(x + (d/2))$ and $\varphi_2(x) = \varphi_0(x - (d/2))$ as Gaussian wavepackets with a vanishingly small overlap. The probability matrix of the superposition is

$$\rho(x', x'') = \Psi(x')\Psi^*(x'') = (\varphi_1(x') + \varphi_2(x'))(\varphi_1^*(x'') + \varphi_2^*(x'')) = \frac{1}{2}\rho_1 + \frac{1}{2}\rho_2 + \rho_{\text{interference}} \tag{52.39}$$

All the integrals that are encountered in the calculation are of the Wigner function are of the type

$$\int \varphi_0\left((X - X_0) + \frac{1}{2}(r - r_0)\right) \varphi_0\left((X - X_0) - \frac{1}{2}(r - r_0)\right) e^{-iPr} dr \equiv \rho_0(X - X_0, P) e^{-iPr_0} \tag{52.40}$$

where $X_0 = \pm d/2$ and $r_0 = 0$ for the classical part of the Wigner function, while $X_0 = 0$ and $r_0 = \pm d/2$ for the interference part. Hence we get the result

$$\rho_W(X, P) = \frac{1}{2}\rho_0\left(X + \frac{d}{2}, P\right) + \frac{1}{2}\rho_0\left(X - \frac{d}{2}, P\right) + \cos(Pd)\,\rho_0(X, P) \tag{52.41}$$

Note that the momentum distribution can be obtained by integrating over X

$$\rho(P) \ = \ (1 + \cos(Pd))\rho_0(P) \ = \ 2\cos^2(\frac{Pd}{2})\rho_0(P) \tag{52.42}$$

In order to analyze the dynamics it is suggestive to write $\rho(X, P)$ schematically as a sum of partial-wavepackets, each characterized by a different transverse momentum:

$$\rho_{\mathrm{W}}(X, P) \ = \ \sum_{n=-\infty}^{\infty} \rho_n(X, P) \tag{52.43}$$

By definition the partial-wavepacket ρ_n equals ρ for $|P - n \times (2\pi\hbar/d)| < \pi\hbar/d$ and equals zero otherwise. Each partial wavepacket represents the possibility that the particle, being scattered by the slits, had acquired a transverse momentum which is an integer multiple of

$$\Delta p \ = \ \frac{2\pi\hbar}{d} \tag{52.44}$$

The corresponding angular separation is

$$\Delta\theta \ = \ \frac{\Delta p}{P} \ = \ \frac{\lambda_B}{d} \tag{52.45}$$

as expected. The associated spatial separation if we have a distance y from the slits to the screen is $\Delta x = \Delta\theta y$. It is important to distinguish between the "preparation" zone $y < d$, and the far-field (Franhaufer) zone $y \gg d^2/\lambda_B$. In the latter zone we have $\Delta x \gg d$ or equivalently $\Delta x \Delta p \gg 2\pi\hbar$.

===== [52.8] Thermal states

A stationary state $\partial\rho/\partial t$ has to satisfy $[\mathcal{H}, \rho] = 0$. This means that ρ is diagonal in the energy representation. It can be further argued that in typical circumstances the thermalized mixture is of the canonical type. Namely

$$\hat{\rho} = \sum |r\rangle p_r \langle r| = \frac{1}{\mathcal{Z}} \sum |r\rangle \mathrm{e}^{-\beta E_r} \langle r| = \frac{1}{\mathcal{Z}} \mathrm{e}^{-\beta \hat{H}} \tag{52.46}$$

Let us consider some typical examples. The first example is spin $1/2$ in a magnetic field. In this case the energies are $E_\uparrow = \epsilon/2$ and $E_\downarrow = \epsilon/2$. Therefore ρ takes the following form:

$$\rho = \frac{1}{2\cosh(\frac{1}{2}\beta\epsilon)} \begin{pmatrix} \mathrm{e}^{\beta\frac{\epsilon}{2}} & 0 \\ 0 & \mathrm{e}^{-\beta\frac{\epsilon}{2}} \end{pmatrix} \tag{52.47}$$

Optionally one can represent the state of the spin by the polarization vector

$$\vec{M} \ = \ \left(0, 0, \tanh(\frac{1}{2}\beta\epsilon)\right) \tag{52.48}$$

The next example is a free particle. The Hamiltonian is $H = \hat{p}^2/2\mathsf{m}$. The partition function is

$$\mathcal{Z} \ = \ \int \frac{dk}{(2\pi)/L} \mathrm{e}^{-\beta\frac{k^2}{2m}} \ = \ \int \frac{dXdP}{2\pi} \mathrm{e}^{-\beta\frac{P^2}{2m}} \ = \ L\left(\frac{m}{2\pi\beta}\right)^{\frac{1}{2}} \tag{52.49}$$

The probability matrix ρ is diagonal in the p representation, and its Wigner function representation is identical with the classical expression. The standard $\hat{x}$ representation can be calculated either directly or via inverse Fourier transform of the Wigner function:

$$\rho(x', x'') = \left(\frac{1}{L} \right) e^{-\frac{m}{2\beta}[x' - x'']^2} \tag{52.50}$$

Optionally it can be regarded as a special case of the harmonic oscillator case. In the case of an harmonic oscillator the calculation is less trivial because the Hamiltonian is not diagonal neither in the x nor in the p representation. The eigenstates of the Hamiltonian are $H|n\rangle = E_n|n\rangle$ with $E_n = \left(\frac{1}{2} + n \right) \omega$. The probability matrix $\rho_{nn'}$ is

$$\rho_{nn'} = \frac{1}{\mathcal{Z}} \delta_{nn'} e^{-\beta\omega\left(\frac{1}{2} + n \right)} \tag{52.51}$$

where the partition function is

$$\mathcal{Z} = \sum_{n=0}^{\infty} e^{-\beta E_n} = \left(2\sinh\left(\frac{1}{2}\beta\omega \right) \right)^{-1} \tag{52.52}$$

In the $\hat{x}$ representation

$$\rho(x', x'') = \sum_n \langle x'|n\rangle p_n \langle n|x''\rangle = \sum_n p_n \varphi^n(x') \varphi^n(x'') \tag{52.53}$$

The last sum can be evaluated by using properties of Hermite polynomials, but this is very complicated. A much simpler strategy is to use of the Feynman path integral method. The calculation is done as for the propagator $\langle x'|\exp(-i\mathcal{H}t)|x''\rangle$ with the time t replaced by $-i\beta$. The result is

$$\rho(x', x'') \propto e^{-\frac{m\omega}{2\sinh(\beta\omega)}\left[\cosh(\beta\omega)\left((x''^2 + x'^2) - 2x'x'' \right) \right]} \tag{52.54}$$

which leads to the Wigner function

$$\rho_{\mathrm{W}}(X, P) \propto e^{-\beta\left(\frac{\tanh\left(\frac{1}{2}\beta\omega \right)}{\frac{1}{2}\beta\omega} \right)\left[\frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2 \right]} \tag{52.55}$$

It is easily verified that in the zero temperature limit we get a minimal wavepacket that represent the pure ground state of the oscillator, while in high temperatures we get the classical result which represents a mixed thermal state.

[53] Quantum states, operations and measurements

═════ [53.1] The reduced probability matrix

In this section we consider the possibility of having a system that has interacted with its surrounding. So we have "system $\otimes$ environment" or "system $\otimes$ measurement device" or simply a system which is a part of a larger thing which we can call "universe". The question that we would like to ask is as follows: Assuming that we know what is the sate of the "universe", what is the way to calculate the state of the "system"?

The mathematical formulation of the problem is as follows. The pure states of the "system" span N_{sys} dimensional Hilbert space, while the states of the "environment" span N_{env} dimensional Hilbert space. So the state of the "universe" is described by $N \times N$ probability matrix $\rho_{i\alpha,j\beta}$, where $N = N_{\text{sys}}N_{\text{env}}$. This means that if we have operator A which is represented by the matrix $A_{i\alpha,j\beta}$, then it expectation value is

$$\langle A \rangle \;\; = \;\; \text{trace}(A\rho) \;\; = \;\; \sum_{i,j,\alpha,\beta} A_{i\alpha,j\beta}\, \rho_{j\beta,i\alpha} \tag{53.1}$$

The probability matrix of the "system" is defined in the usual way. Namely, the matrix element $\rho_{j,i}^{\text{sys}}$ is defined as the expectation value of $P^{ji} = |i\rangle\langle j| \otimes \mathbf{1}$. Hence

$$\rho_{j,i}^{\text{sys}} = \langle P^{ji} \rangle = \text{trace}(P^{ji}\rho) = \sum_{k,\alpha,l,\beta} P_{k\alpha,l\beta}^{ji}\rho_{l\beta,k\alpha} = \sum_{k,\alpha,l,\beta} \delta_{k,i}\delta_{l,j}\delta_{\alpha,\beta}\; \rho_{l\beta,k\alpha} = \sum_{\alpha} \rho_{j\alpha,i\alpha} \tag{53.2}$$

The common terminology is to say that ρ^{sys} is the *reduced* probability matrix, which is obtained by *tracing out* the environmental degrees of freedom. Just to show mathematical consistency we note that for a general system operator of the type $A = A^{\text{sys}} \otimes \mathbf{1}^{\text{env}}$ we get as expected

$$\langle A \rangle \;\; = \;\; \text{trace}(A\rho) \;\; = \;\; \sum_{i,\alpha,j,\beta} A_{i\alpha,j\beta}\rho_{j\beta,i\alpha} \;\; = \;\; \sum_{i,j} A_{i,j}^{\text{sys}} \rho_{j,i}^{\text{sys}} \;\; = \;\; \text{trace}(A^{\text{sys}}\rho^{\text{sys}}) \tag{53.3}$$

═════ [53.2] Entangled superposition

Of particular interest is the case where the universe is in a pure state Ψ. Choosing for the system $\otimes$ environemnt an arbitrary basis $|i\alpha\rangle = |i\rangle \otimes |\alpha\rangle$, we can expand the wavefunction as

$$|\Psi\rangle \;\; = \;\; \sum_{i,\alpha} \Psi_{i\alpha}|i\alpha\rangle \tag{53.4}$$

By summing over α we can write

$$|\Psi\rangle \;\; = \;\; \sum_{i} \sqrt{p_i}|i\rangle \otimes |\chi^{(i)}\rangle \tag{53.5}$$

where $|\chi^{(i)}\rangle \propto \sum_{\alpha} \Psi_{i\alpha}|\alpha\rangle$ is called the "relative state" of the environment with respect to the ith state of the system, while p_i is the associated normalization factor. Note that the definition of the relative state implies that $\Psi_{i\alpha} = \sqrt{p_j}\chi_{\alpha}^{(i)}$. Using these notations it follows that the reduced probability matrix of the system is

$$\rho_{j,i}^{\text{sys}} \;\; = \;\; \sum_{\alpha} \Psi_{j\alpha}\Psi_{i\alpha}^* \;\; = \;\; \sqrt{p_i p_j}\, \langle \chi^{(i)}|\chi^{(j)}\rangle \tag{53.6}$$

The prototype example for a system-environment entangled state is described by the superposition

$$|\Psi\rangle \;\; = \;\; \sqrt{p_1}\,|1\rangle \otimes |\chi^{(1)}\rangle + \sqrt{p_2}\,|2\rangle \otimes |\chi^{(2)}\rangle \tag{53.7}$$

where $|1\rangle$ and $|2\rangle$ are orthonormal states of the system. The singlet state of two spin $1/2$ particles is possibly the simplest example for an entangled superposition of this type. Later on we shall see that such entangled superposition may come out as a result of an interaction between the system and the environment. Namely, depending on the state of the system the environment, or the measurement apparatus, ends up in a different state χ. Accordingly we do not assume that $\chi^{(1)}$ and $\chi^{(2)}$ are orthogonal, though we normalize each of them and pull out the normalization factors as p_1 and p_2. The reduced probability matrix of the system is

$$\rho_{j,i}^{\text{sys}} \;\; = \;\; \begin{pmatrix} p_1 & \lambda^* \sqrt{p_1 p_2} \\ \lambda \sqrt{p_1 p_2} & p_2 \end{pmatrix} \tag{53.8}$$

where $\lambda = \langle\chi^{(1)}|\chi^{(2)}\rangle$. At the same time the environment is in a mixture of non-orthogonal states:

$$\rho^{\text{env}} \;\; = \;\; p_1\,|\chi^{(1)}\rangle\langle\chi^{(1)}| + p_2\,|\chi^{(2)}\rangle\langle\chi^{(2)}| \tag{53.9}$$

The purity of the state of the system in the above example is determined by $|\lambda|$, and can be characterized by $\text{trace}(\rho^2) = 1 - 2p_1 p_2(1-|\lambda|^2)$. The value $\text{trace}(\rho^2) = 1$ indicates a pure state, while $\text{trace}(\rho^2) = 1/N$ with $N = 2$ characterizes a 50%-50% mixture. Optionally the purity can be characterized by the Von Neumann entropy as discussed in a later section: This gives $S[\rho] = 0$ for a pure state and $S[\rho] = \log(N)$ with $N = 2$ for a 50%-50% mixture.

===== [53.3] Schmidt decomposition

If the "universe" is in a pure state we cannot write its ρ as a *mixture* of product states, but we can write its Ψ as an entangled superposition of product states.

$$|\Psi\rangle \;\; = \;\; \sum_i \sqrt{p_i}|i\rangle \otimes |B_i\rangle \tag{53.10}$$

where the $|B_i\rangle$ is the "relative state" of subsystem B with respect to the ith state of subsystem A, while p_i is the associated normalization factor. The states $|B_i\rangle$ are in general not orthogonal. The natural question that arise is whether we can find a decomposition such that the $|B_i\rangle$ are orthonormal. The answer is positive: Such decomposition exists and it is unique. It is called Schmidt decomposition, and it is based on singular value decomposition (SVD). Let us regard $\Psi_{i\alpha} = W_{i,\alpha}$ as an $N_A \times N_B$ matrix. From linear algebra it is known that any matrix can be written in a unique way as a product:

$$W_{(N_A \times N_B)} = U^A_{(N_A \times N_A)} D_{(N_A \times N_B)} U^B_{(N_B \times N_B)} \tag{53.11}$$

where U^A and U^B are the so called left and right unitary matrices, while D is a diagonal matrix with so called (positive) singular values. Thus we can re-write the above matrix multiplication as

$$\Psi_{i\alpha} \;\; = \;\; \sum_r U^A_{i,r}\,\sqrt{p_r}\,U^B_{r,\alpha} \;\; \equiv \;\; \sum_r \sqrt{p_r}\,u^{A_r}_i\,u^{B_r}_\alpha \tag{53.12}$$

Substitution of this expression leads to the result

$$|\Psi\rangle \;\; = \;\; \sum_{i,\alpha} \Psi_{i\alpha}|i\alpha\rangle \;\; = \;\; \sum_r \sqrt{p_r}|A_r\rangle \otimes |B_r\rangle \tag{53.13}$$

where $|A_r\rangle$ and $|B_r\rangle$ are implied by the unitary transformations. We note that the normalization of Ψ implies $\sum p_r = 1$. Furthermore the probability matrix is $\rho_{i\alpha,j\beta}^{A+B} = W_{i,\alpha}W_{j,\beta}^*$, and therefore the calculation of the reduced probability matrix can be written as:

$$
\begin{aligned}
\rho^A &= \quad WW^\dagger \quad = (U^A)D^2(U^A)^\dagger \\
\rho^B &= (W^T)(W^T)^\dagger \ = [(U^B)^\dagger D^2(U^B)]^*
\end{aligned}
\tag{53.14}
$$

This means that the matrices ρ^A and ρ^B have the same non-zero eigenvalues $\{p_r\}$, or in other words it means that the degree of purity of the two subsystems is the same.

═════ [53.4] The violation of the Bell inequality

We can characterize the entangled state using a correlation function as in the EPR thought experiment. The correlation function $C(\theta) = \langle\hat{C}\rangle$ is the expectation value of a so-called "witness operator". If we perform the EPR experiment with two spin 1/2 particles (see the Fundamentals II section), then the witness operator is $\hat{C} = \sigma_z \otimes \sigma_\theta$, and the correlation function comes out $C(\theta) = -\cos(\theta)$, which violates Bell inequality.

Let us see how the result for $C(\theta)$ is derived. For pedagogical purpose we present 3 versions of the derivation. One possibility is to perform a straightforward calculation using explicit *standard-basis* representation:

$$
|\Psi\rangle \mapsto \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}, \qquad \hat{C} = \sigma_z \otimes \sigma_\theta \mapsto \begin{pmatrix} \sigma_\theta & 0 \\ 0 & -\sigma_\theta \end{pmatrix}, \qquad \langle\hat{C}\rangle = \frac{1}{2}\Big(\langle\sigma_\theta\rangle_\downarrow - \langle\sigma_\theta\rangle_\uparrow\Big),
\tag{53.15}
$$

leading to the desired result. The second possibility is to use the "appropriate" basis for the C measurement:

$$
\mathrm{MeasurementBasis} \ = \ \Big\{ |z\theta\rangle, \ \ |z\bar{\theta}\rangle, \ \ |\bar{z}\theta\rangle, \ \ |\bar{z}\bar{\theta}\rangle \Big\}
\tag{53.16}
$$

where $\bar{z}$ and $\bar{\theta}$ label polarization in the $-z$ and $-\theta$ directions respectively. The singlet state in this basis is

$$
|\psi\rangle \ = \ \frac{1}{\sqrt{2}}\left(|\theta\bar{\theta}\rangle - |\bar{\theta}\theta\rangle\right) \ = \ \frac{1}{\sqrt{2}}\cos\left(\frac{\theta}{2}\right)\left(|z\bar{\theta}\rangle - |\bar{z}\theta\rangle\right) + \frac{1}{\sqrt{2}}\sin\left(\frac{\theta}{2}\right)\left(|z\theta\rangle + |\bar{z}\bar{\theta}\rangle\right)
\tag{53.17}
$$

Therefore the probabilities to get $C=1$ and $C=-1$ are $|\sin(\theta/2)|^2$ and $|\cos(\theta/2)|^2$ respectively, leading to the desired result for the average value $\langle\hat{C}\rangle$.

Still there is a third version of this derivation, which is more physically illuminating. The idea is to relate correlation functions to *conditional* calculation of expectation values. Let $A = |a_0\rangle\langle a_0|$ be a projector on state a_0 of the first subsystem, and let B some observable which is associated with the second subsystem. We can write the state of the whole system as an entangled superposition

$$
\Psi \ = \ \sum_a \sqrt{p_a} \, |a\rangle \otimes |\chi^{(a)}\rangle
\tag{53.18}
$$

Then it is clear that $\langle A \otimes B\rangle = p_{a_0}\langle\chi^{(a_0)}|B|\chi^{(a_0)}\rangle$. More generally if $A = \sum_a |a\rangle a\langle a|$ is any operator then

$$
\langle A \otimes B\rangle \ = \ \sum_a p_a \, a \, \langle\chi^{(a)}|B|\chi^{(a)}\rangle
\tag{53.19}
$$

Using this formula with $A = \sigma_z = |\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|$, and $B = \sigma_\theta$ we have $p_\uparrow = p_\downarrow = 1/2$, and we get the same result for $\langle\hat{C}\rangle$ as in the previous derivation.

===== [53.5] Quantum entanglement

Let us consider a system consisting of two sub-systems, "A" and "B", with no correlation between them. Then, the state of the system can be factorized:

$$\rho^{A+B} = \rho^A \rho^B \tag{53.20}$$

But in reality the state of the two sub-systems can be correlated. In classical statistical mechanics ρ^A and ρ^B are probability functions, while ρ^{A+B} is the joint probability function. In the classical state we can always write

$$\rho^{A+B}(x,y) = \sum_{x',y'} \rho^{A+B}(x',y') \, \delta_{x,x'} \, \delta_{y,y'} \equiv \sum_r p_r \, \rho^{A_r}(x) \, \rho^{B_r}(y) \tag{53.21}$$

where x and y label classical definite states of subsystems A and B respectively, and $r = (x', y')$ is an index that distinguish pure classical states of $A \otimes B$. The probabilities $p_r = \rho^{A+B}(x', y')$ satisfy $\sum p_r = 1$. The distribution ρ^{A_r} represents a pure classical state of subsystem A, and ρ^{B_r} represents a pure classical state of subsystem B. Thus any classical state of $A \otimes B$ can be expressed as a *mixture* of product states.

By definition a quantum state is *not entangled* if it is a product state or a mixture of product states. Using explicit matrix representation it means that it is possible to write

$$\rho_{i\alpha,j\beta}^{A+B} = \sum_r p_r \, \rho_{i,j}^{(A_r)} \, \rho_{\alpha,\beta}^{(B_r)} \tag{53.22}$$

It follows that an entangled state, unlike a non-entangled state, cannot have a classical interpretation. This means that it cannot be described by a classical joint probability function. The latter phrasing highlights the relation between entanglement and the failure of the hidden-variable-hypothesis of the EPR experiment.

The question how to detect an entangled state is still open. Clearly the violation of the Bell inequality indicates entanglement. Adopting the GHZ-Mermin perspective (see "Optional tests of realism" section) this idea is presented as follows: Assume you have two sub-systems (A, B). You want to characterize statistically the outcome of possible measurements using a *joint* probability function $f(a_1, a_2, a_3, ...; b_1, b_2, b_3, ...)$. You measure the correlations $C_{ij} = \langle a_i b_j \rangle$. Each C imposes a restriction on the hypothetical fs that could describe the state. If the state is non-classical (*entangled*) the logical conjunction of all these restrictions gives NULL.

===== [53.6] Purity and the von-Neumann entropy

The purity of a state can be characterized by the von-Neumann entropy:

$$S[\rho] = -\text{trace}(\rho \log \rho) = -\sum_r p_r \log p_r \tag{53.23}$$

In the case of a pure state we have $S[\rho] = 0$, while in the case of a uniform mixture of N states we have $S[\rho] = \log(N)$. From the above it should be clear that while the "universe" might have zero entropy, it is likely that a subsystem would have a non-zero entropy. For example if the universe is a zero entropy singlet, then the state of each spin is unpolarized with $\log(2)$ entropy.

We would like to emphasize that the von-Neumann entropy $S[\rho]$ should not be confused with the Boltzmann entropy $S[\rho|A]$. The definition of the latter requires to introduce a partitioning A of phase space into cells. In the quantum case this "partitioning" is realized by introducing a complete set of projectors (a basis). The p_r in the case of the Boltzmann entropy are probabilities in a given basis and not eigenvalues. In the case of an isolated system out of equilibrium the Von Neumann entropy is a constant of the motion, while the appropriately defined Boltzmann entropy increases with time. In the case of a canonical thermal equilibrium the Von Neumann entropy $S[\rho]$ turns out to be equal to the thermodynamic entropy $\mathcal{S}$. The latter is defined via the equation $dQ = Td\mathcal{S}$, where $T = 1/\beta$ is an integration factor which is called the absolute temperature.

If the von-Neumann entropy were defined for a classical distributions $\rho = \{p_r\}$, it would have all the classical "information theory" properties of the Shanon entropy. In particular if we have two subsystems A and B one would expect

$$S[\rho^{\mathrm{A}}],\ S[\rho^{\mathrm{B}}] \quad \leq \quad S[\rho^{\mathrm{AB}}] \quad \leq \quad S[\rho^{\mathrm{A}}] + S[\rho^{\mathrm{B}}] \tag{53.24}$$

Defining $N = \exp(S)$, the inequality $N_{\mathrm{AB}} < N_{\mathrm{A}} N_{\mathrm{B}}$ has a simple graphical interpertation.

The above ineqiality is satisfied also in the quantum case provided the subsystems are not entangled. We can use this mathematical observation in order to argue that the zero entropy singlet state is an entangled state: It cannot be written as a product of pure states, neither it cannot be a mixture of product states.

The case where ρ^{A+B} is a zero entropy pure state deserves further attention. As in the special case of a singlet, we can argue that if the state cannot be written as a product, then it must be an entangled state. Moreover for the Schmidt decomposition procedure it follows that the entropies of the subsystems satisfy $S[\rho^{\mathrm{A}}] = S[\rho^{\mathrm{B}}]$. This looks counter intuitive at first sight because subsystem A might be a tiny device which is coupled to a huge environment B. We emphasize that the assumption here is that the "universe" $A \otimes B$ is prepared in a zero order pure state. Some further thinking leads to the conjecture that the entropy of the subsystems in such circumstance is proportional to the area of surface that divides the two regions in space. Some researchers speculate that this observation is of relevance to the discussion of black holes entropy.

===== [53.7] Quantum operations

The quantum evolution of an isolated system is described by a unitary operator, hence $\tilde{\rho} = U\rho U^{\dagger}$. We would like to consider a more general case. The system is prepared in some well-controlled initial state ρ, while the environment is assumed to be in some mixture state $\sigma = \sum_{\alpha} |\alpha\rangle p_{\alpha} \langle \alpha|$. The state of the universe is $R = \rho \otimes \sigma$. The evolution of the universe is represented by $U(n\alpha|n'\alpha')$. Hence the evolution of the reduced probability matrix can be written as a linear operation, so called "quantum operation", namely

$$\tilde{\rho}_{n,m} \;=\; \sum_{n',m'} \mathcal{K}(n,m|n',m')\, \rho_{n',m'}, \qquad \mathcal{K}(n,m|n',m') \equiv \sum_{\alpha\alpha'} p_{\alpha'} U(n,\alpha|n'\alpha') U(m,\alpha|m',\alpha')^{*} \tag{53.25}$$

With slight change of notations this can be re-written in a way that is called "Kraus representation"

$$\tilde{\rho} \;=\; \sum_{r} [K^{r}]\, \rho\, [K^{r}]^{\dagger}, \qquad \sum_{r} [K^{r}]^{\dagger}\, [K^{r}] \;=\; \mathbf{1} \tag{53.26}$$

where the sum rule reflects trace preservation (conservation of probability). Below we are using the following terminology: The quantum operation is induced by a linear $\mathcal{K}$-map, that is represented by a $\mathcal{K}$-kernel $\mathcal{K}(n,m|n',m')$, with an associated $\mathcal{K}$-matrix $\mathcal{K}_{nn',mm'} \equiv \mathcal{K}(n,m|n',m')$. Note the order of indices.

Not any matrix ρ can be regarded as representing a quantum state. Disregarding normalization $\mathsf{trace}(\rho) = 1$ one requires that $\mathsf{trace}(\rho P) > 0$ for any projector, or equivalently $\langle \psi|\rho|\psi\rangle > 0$ for any ψ. This is called "positivity". Upon diagonalization the eigenvalues p_r have to be non-negative. It follows that one can define a matrix V such that $\rho_{n,m} = \sum_{r} V_{n,r} V_{m,r}^{*}$, or in abstract notations $\rho = VV^{\dagger}$.

It can be easily verify that the linear kernel $\mathcal{K}$ preserves the positivity of ρ. This positivity is essential for the probabilistic interpretation of ρ. In fact $\mathcal{K}$ is "completely positive". This means that if we consider any "positive" matrix R that describes the universe, possibly an entangled state, the result of the operation $\mathcal{K} \otimes \mathbf{1}$ would be "positive" too. Explicitly it means that for any R we get a positive matrix $\tilde{R}_{n\alpha,m\beta} = \sum_{n'm'} \mathcal{K}_{nn',mm'} R_{n'\alpha,m'\beta}$.

It is now possible to turn things around, and claim that any trace-preserving completely-positive linear mapping of Hermitian matrices has a "Kraus representation". Given $\mathcal{K}$, it follows from the Hermiticity requirement that $\mathcal{K}_{nn',mm'}$ is Hermitian matrix. Therefore it has real eigenvalues λ_r, with transformation matrix $T(nn'|r)$ such that

$$\mathcal{K}(n,m|n',m') \;\equiv\; \mathcal{K}_{nn',mm'} \;=\; \sum_{r} T(nn'|r)\, \lambda_r\, T(r|mm') \;=\; \sum_{r} \lambda_r [K^{r}_{nn'}][K^{r}_{mm'}]^{*} \tag{53.27}$$

where $\mathsf{trace}([K^r]^\dagger[K^s]]) = \delta_{r,s}$, due to the orthonormality of the transformation matrix. From the "complete positivity" it follows that all the λ_r are positive (see proof below) hence we can absorb $\lambda_r^{1/2}$ into the definition of the K^r, and get the Kraus representation. We note that in this derivation the Kraus representation comes out orthogonal. One can switch to an optional Kraus representation using a linear transformation $\tilde{K}^r = \sum_s u_{rs} K^s$ were u_{rs} is any unitary matrix. After such transformation the $\tilde{K}^r$ are no longer orthogonal.

The statement that complete positivity implies $\lambda_r > 0$, is paraphrasing of Choi's theorem. The theorem states that if the $\mathcal{K}$-map is completely positive then the $\mathcal{K}$-matrix is positive, hence we get the Kraus representation as described above. The proof is misleadingly simple: write the condition of complete positivity for the spacial case $R = |\Psi\rangle\langle\Psi|$, with the entangled state $|\Psi\rangle = \sum_n |n, \alpha_n\rangle$, where the relative states α_n are orthogonal. Then it follows that $\tilde{R}_{n\alpha,m\beta} = \mathcal{K}_{n\alpha,m\beta}$ has to be positive.

Extension of the above reasoning is used in order to derive a master equation that describes the evolution of ρ. The key non-trivial assumption is that the environment can be regarded as effectively factorized from the system at any moment. Then we get the Lindblad equation:

$$\frac{d\rho}{dt} = -i[\mathcal{H}_0, \rho] + \sum_r [W^r]\rho[W^r]^\dagger - \frac{1}{2}[\Gamma\rho + \rho\Gamma], \qquad \Gamma = \sum_r [W^r]^\dagger[W^r] \qquad (53.28)$$

where the Lindblad operators W^r parallel the Kraus operators K^r, and Γ is implied by conservation of probability. The Lindblad equation is the most general form of a Markovian master equation for the probability matrix. We emphasize that in general the Markovian assumption does not hold, hence Lindblad is not as satisfactory as the Kraus description.

===== [53.8] Measurements, the notion of collapse

In elementary textbooks the quantum measurement process is described as inducing "collapse" of the wavefunction. Assume that the system is prepared in state $\rho_{\text{initial}} = |\psi\rangle\langle\psi|$ and that one measures $\hat{P} = |\varphi\rangle\langle\varphi|$. If the result of the measurement is $\hat{P} = 1$ then it is said that the system has collapsed into the state $\rho_{\text{final}} = |\varphi\rangle\langle\varphi|$. The probability for this "collapse" is given by the projection formula $\text{Prob}(\varphi|\psi) = |\langle\varphi|\psi\rangle|^2$.

If one regard $\rho(x, x')$ or $\psi(x)$ as representing *physical reality*, rather than a probability matrix or a probability amplitude, then one immediately gets into puzzles. Recalling the EPR experiment this world imply that once the state of one spin is measured at Earth, then immediately the state of the other spin (at the Moon) would change from unpolarized to polarized. This would suggest that some spooky type of "interaction" over distance has occurred.

In fact we shall see that the quantum theory of measurement does not involve any assumption of spooky "collapse" mechanism. Once we recall that the notion of quantum state has a statistical interpretation the mystery fades away. In fact we explain (see below) that *there is "collapse" also in classical physics*! To avoid potential miss-understanding it should be clear that I do not claim that the classical "collapse" which is described below is an explanation of the the quantum collapse. The explanation of quantum collapse using a quantum measurement (probabilistic) point of view will be presented in a later section. The only claim of this section is that in probability theory a correlation is frequently mistaken to be a causal relation: "smokers are less likely to have Alzheimer" not because cigarettes help to their health, but simply because their life span is smaller. Similarly quantum collapse is frequently mistaken to be a spooky interaction between well separated systems.

Consider the thought experiment which is known as the "Monty Hall Paradox". There is a car behind one of three doors. The car is like a classical "particle", and each door is like a "site". The initial classical state is such that the car has equal probability to be behind any of the three doors. You are asked to make a guess. Let us say that you peak door #1. Now the organizer opens door #2 and you see that there is no car behind it. This is like a measurement. Now the organizer allows you to change your mind. The naive reasoning is that now the car has equal probability to be behind either of the two remaining doors. So you may claim that it does not matter. But it turns out that this simple answer is very very wrong! The car is no longer in a state of equal probabilities: Now the probability to find it behind door #3 has increased. A standard calculation reveals that the probability to find it behind door #3 is twice large compared with the probability to find it behind door #2. So we have here an example for a classical collapse.

If the reader is not familiar with this well known "paradox", the following may help to understand why we have this collapse (I thank my colleague Eitan Bachmat for providing this explanation). Imagine that there are billion doors.

You peak door #1. The organizer opens all the other doors except door #234123. So now you know that the car is either behind door #1 or behind door #234123. You want the car. What are you going to do? It is quite obvious that the car is almost definitely behind door #234123. It is also clear the that the collapse of the car into site #234123 does not imply any physical change in the position of the car.

===== [53.9] Quantum measurements

What do we mean by quantum measurement? In order to clarify this notion let us consider a system that is prepared in a superposition of states a. Additionally we have a detector that is prepared independently in a state $q=0$. In the present context the detector is called "von-Neumann pointer". The initial state of the system and the detector is

$$|\Psi\rangle \quad = \quad \left[\sum_a \psi_a |a\rangle\right] \otimes |q=0\rangle \tag{53.29}$$

As a result of an interaction we assume that the pointer is displaced. Its displacement is proportional to a. Accordingly the detector correlates with the system as follows:

$$\hat{U}_{\text{measurement}} \Psi \quad = \quad \sum \psi_a |a\rangle \otimes |q=a\rangle \tag{53.30}$$

We call such type of unitary evolution an *ideal projective measurement*. If the system is in a definite a state, then it is not affected by the detector. Rather, we gain information on the state of the system. One can think of q as representing a memory device in which the information is stored. This memory device can be of course the brain of a human observer. From the point of view of the observer, the result at the end of the measurement process is to have a definite a. This is interpreted as a "collapse" of the state of the system. Some people wrongly think that "collapse" is something that goes beyond unitary evolution. But in fact this term just makes over-dramatization of the above unitary process.

The concept of measurement in quantum mechanics involves psychological difficulties which are best illustrated by considering the "Schroedinger cat" experiment. This thought experiment involves a radioactive nucleus, a cat, and a human being. The half life time of the nucleus is an hour. If the radioactive nucleus decays it triggers a poison which kills the cat. The radioactive nucleus and the cat are inside an isolated box. At some stage the human observer may open the box to see what happens with the cat... Let us translate the story into a mathematical language. A time $t=0$ the state of the universe (nucleus⊗cat⊗observer) is

$$\Psi \quad = \quad |\uparrow = \text{radioactive}\rangle \otimes |q=1=\text{alive}\rangle \otimes |Q=0=\text{ignorant}\rangle \tag{53.31}$$

where q is the state of the cat, and Q is the state of the memory bit inside the human observer. If we wait a very long time the nucleus would definitely decay, and as a result we will have a definitely dead cat:

$$U_{\text{waiting}} \Psi \quad = \quad |\downarrow = \text{decayed}\rangle \otimes |q=-1=\text{dead}\rangle \otimes |Q=0=\text{ignorant}\rangle \tag{53.32}$$

If the observer opens the box he/she would see a dead cat:

$$U_{\text{seeing}} U_{\text{waiting}} \Psi \quad = \quad |\downarrow = \text{decayed}\rangle \otimes |q=-1=\text{dead}\rangle \otimes |Q=-1=\text{shocked}\rangle \tag{53.33}$$

But if we wait only one hour then

$$U_{\text{waiting}} \Psi \quad = \quad \frac{1}{\sqrt{2}}\Big[|\uparrow\rangle \otimes |q=+1\rangle + |\downarrow\rangle \otimes |q=-1\rangle\Big] \otimes |Q=0=\text{ignorant}\rangle \tag{53.34}$$

which means that from the point of view of the observer the system (nucleus+cat) is in a superposition. The cat at this stage is neither definitely alive nor definitely dead. But now the observer open the box and we have:

$$U_{\text{seeing}} U_{\text{waiting}} \Psi \quad = \quad \frac{1}{\sqrt{2}}\Big[|\uparrow\rangle \otimes |q=+1\rangle \otimes |Q=+1\rangle + |\downarrow\rangle \otimes |q=-1\rangle \otimes |Q=-1\rangle\Big] \tag{53.35}$$

We see that now, from the point of view of the observer, the cat is in a definite(!) state. This is regarded by the observer as "collapse" of the superposition. We have of course two possibilities: one possibility is that the observer sees a definitely dead cat, while the other possibility is that the observer sees a definitely alive cat. The two possibilities "exist" in parallel, which leads to the "many worlds" interpretation. Equivalently one may say that only one of the two possible scenarios is realized from the point of view of the observer, which leads to the "relative state" concept of Everett. Whatever terminology we use, "collapse" or "many worlds" or "relative state", the bottom line is that we have here merely a unitary evolution.

====== [53.10] Measurements and the macroscopic reality

The main message of the Schroedinger's cat thought experiment is as follows: if one believes that a microscopic object (atom) can be prepared in a superposition state, then also a macroscopic system (atom+cat) can be prepared in a superposition state. Accordingly the quantum mechanical reasoning should be applicable also in the macroscopic reality.

In fact there are more sophisticated schemes that allow to perform so called "quantum teleportation" of state from object to object. However, one can prove easily the "no cloning" theorem: a quantum state cannot be copied to other objects. Such duplication would violate unitarity. The proof goes as follows: Assume that there were a transformation U that maps (say) a two spin state $|\theta\rangle \otimes |0\rangle$ to $|\theta\rangle \otimes |\theta\rangle$. The inner product $\langle\theta'|\theta\rangle$ would be mapped to $\langle\theta'|\theta\rangle^2$. This would not preserve norm, hence a unitary cloning transformation is impossible.

Many textbooks emphasize that in order to say that we have a measurement, the outcome should be macroscopic. As far as the thought experiment of the previous section is concerned this could be achieved easily: we simply allow the system to interact with one pointer, then with a second pointer, then with a third pointer, etc. We emphasize again that during an *ideal* measurement the pointer is not affecting the system, but only correlates with it. In other words: the measured observable $\hat{A}$ is a constant of the motion.

A more interesting example for a measurement with a macroscopic outcome is as follows: Consider a ferromagnet that is prepared at temperature $T > T_c$. The ferromagnet is attached to the system and cooled down below T_c. The influence of the system polarization (spin up/down) on the detector is microscopically small. But because of the symmetry breaking, the ferromagnet (huge number of coupled spins) will become magnetized in the respective (up/down) direction. One may say that this is a generic model for a *macroscopic pointer*.

====== [53.11] Measurements, formal treatment

In this section we describe mathematically how an ideal projective measurement affects the state of the system. First of all let us write how the U of a measurement process looks like. The formal expression is

$$\hat{U}_{\text{measurement}} \quad = \quad \sum_a \hat{P}^{(a)} \otimes \hat{D}^{(a)} \tag{53.36}$$

where $\hat{P}^{(a)} = |a\rangle\langle a|$ is the projection operator on the state $|a\rangle$, and $\hat{D}^{(a)}$ is a translation operator. Assuming that the measurement device is prepared in a state of ignorance $|q=0\rangle$, the effect of $\hat{D}^{(a)}$ is to get $|q=a\rangle$. Hence

$$\begin{aligned} \hat{U}\Psi \quad &= \quad \left[\sum_a \hat{P}^{(a)} \otimes \hat{D}^{(a)}\right] \left(\sum_{a'} \psi_{a'}|a'\rangle \otimes |q=0\rangle\right) \\ &= \quad \sum_a \psi_a|a\rangle \otimes \hat{D}^{(a)}|q=0\rangle \quad = \quad \sum_a \psi_a|a\rangle \otimes |q=a\rangle \end{aligned} \tag{53.37}$$

A more appropriate way to describe the state of the system is using the probability matrix. Let us describe the above measurement process using this language. After "reset" the state of the measurement apparatus is $\sigma^{(0)} = |q{=}0\rangle\langle q{=}0|$. The system is initially in an arbitrary state ρ. The measurement process correlates that state of the measurement

apparatus with the state of the system as follows:

$$\hat{U}\rho \otimes \sigma^{(0)}\hat{U}^{\dagger} \quad = \quad \sum_{a,b} \hat{P}^{(a)}\rho\hat{P}^{(b)} \otimes [\hat{D}^{(a)}]\sigma^{(0)}[\hat{D}^{(b)}]^{\dagger} \quad = \quad \sum_{a,b} \hat{P}^{(a)}\rho\hat{P}^{(b)} \otimes |q{=}a\rangle\langle q{=}b| \tag{53.38}$$

Tracing out the measurement apparatus we get

$$\rho^{\text{final}} \quad = \quad \sum_{a} \hat{P}^{(a)}\rho\hat{P}^{(a)} \quad \equiv \quad \sum_{a} p_a \rho^{(a)} \tag{53.39}$$

where p_a is the trace of the projected probability matrix $\hat{P}^{(a)}\rho\hat{P}^{(a)}$, while $\rho^{(a)}$ is its normalized version. We see that the effect of the measurement is to turn the superposition into a mixture of a states, unlike unitary evolution for which

$$\rho^{\text{final}} \quad = \quad U \, \rho \, U^{\dagger} \tag{53.40}$$

So indeed a measurement process looks like a non-unitary process: it turns a pure superposition into a mixture. A simple example is in order. Let us assume that the system is a spin $1/2$ particle. The spin is prepared in a pure polarization state $\rho = |\psi\rangle\langle\psi|$ which is represented by the matrix

$$\rho_{ab} \quad = \quad \psi_a \psi_b^* \quad = \quad \begin{pmatrix} |\psi_1|^2 & \psi_1 \psi_2^* \\ \psi_2 \psi_1^* & |\psi_2|^2 \end{pmatrix} \tag{53.41}$$

where 1 and 2 are (say) the "up" and "down" states. Using a Stern-Gerlach apparatus we can measure the polarization of the spin in the up/down direction. This means that the measurement apparatus projects the state of the spin using

$$P^{(1)} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \qquad \text{and} \qquad P^{(2)} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{53.42}$$

leading after the measurement to the state

$$\rho^{\text{final}} \quad = \quad P^{(1)}\rho P^{(1)} + P^{(2)}\rho P^{(2)} \quad = \quad \begin{pmatrix} |\psi_1|^2 & 0 \\ 0 & |\psi_2|^2 \end{pmatrix} \tag{53.43}$$

Thus the measurement process has eliminated the off-diagonal terms in ρ and hence turned a pure state into a mixture. It is important to remember that this non-unitary non-coherent evolution arise because we look only on the state of the system. On a universal scale the evolution is in fact unitary.

===== [53.12] Weak measurement with post-selection

In the previous section we have assumed that the measurement operation takes zero time, and results in the translation of a pointer q. Such measurement is generated by an interaction term

$$\mathcal{H}_{\text{measurement}} \quad = \quad -\lambda g(t) \, \mathcal{A} \, \hat{x} \tag{53.44}$$

In this expression $\mathcal{A}$ is the system observable that we want to measure. It has a spectrum of values $\{a_i\}$. This observable is coupled to a von-Nuemann *pointer* whose canonical coordinates are $(\hat{x}, \hat{q})$. The coupling constant is λ, and its temporal variation is described by a short time normalized function $g(t)$. If $\mathcal{A} = a$ this interaction shifts the pointer $q \mapsto q + \lambda a$. Note that x unlike q is a constant of the motion. Note also that q is a dynamical variable, hence it has some uncertainty. For practical purpose it is useful to assume that the pointer has been prepared as minimal wave-packet that is initially centered at $x = q = 0$.

It is easily shown that for general preparation the average shift of the pointer is $\lambda\langle\mathcal{A}\rangle$. We would like to know how this result is modified if a *post-selection* is performed. Aharonov has suggested this scheme in order to treat the past and the future on equal footing. Namely: one assumes that the system is prepared in a state $|\Psi\rangle$, that is regarded as pre-selection; and keeps records of q only for events in which the final state of the system is post-selected as $|\Phi\rangle$. Below we shall prove that the average shift of the pointer is described by the complex number

$$\langle\mathcal{A}\rangle^{\text{weak}}_{\Phi,\Psi} \;\; = \;\; \frac{\langle\Phi|\mathcal{A}|\Psi\rangle}{\langle\Phi|\Psi\rangle} \tag{53.45}$$

It is important to realize that this "weak value" is not bounded: it can exceed the spectral range of the observable.

The evolution of the system with the pointer is described by

$$U_{\text{measurement}} \;\; = \;\; \mathrm{e}^{i\lambda\mathcal{A}\hat{x}} \;\; \approx \;\; 1 + i\lambda\mathcal{A}\hat{x} \tag{53.46}$$

where the latter approximation holds for what we regard here as "weak measurement". The x position of the von-Nuemann pointer is a constant of the motion. Consequently the representation of the evolution operator is

$$\langle\Phi, x|U|\Psi, x_0\rangle \;\; = \;\; U[x]_{\Phi,\Psi} \; \delta(x - x_0) \tag{53.47}$$

where $U[x]$ is a system operator that depends on the constant parameter x. If the system is prepared in state $P^\Psi = |\Psi\rangle\langle\Psi|$, and the pointer is prepared in state $\rho^{(0)}$, then after the interaction we get

$$\text{final state of the universe} \;\; = \;\; U\left[\, P^\Psi \, \rho^{(0)} \,\right] U^\dagger \tag{53.48}$$

The reduced state of the pointer after post selection is

$$\rho(x', x'') \;\; = \;\; \mathsf{trace}\left[\, P^\Phi P^{x',x''} \, UP^\Psi\rho^{(0)}U^\dagger \,\right] \;\; = \;\; \tilde{K}(x', x'') \; \rho^{(0)}(x', x'') \tag{53.49}$$

where $P^{x',x''} = |x''\rangle\langle x'|$. Note that this reduced state is not normalized: the trace is the probability to find the system in the post-selected state Φ. In the last equality we have introduced the notation

$$\tilde{K}(x', x'') \;\; = \;\; \langle\Phi|U[x']|\Psi\rangle \; \langle\Psi|U[x'']^\dagger|\Phi\rangle \tag{53.50}$$

Defining X and r as the average and the difference of x'' and x' respectively, we can write the evolution of the pointer in this representation as

$$\rho(r, X) \;\; = \;\; \tilde{K}(r, X) \; \rho^{(0)}(r, X), \qquad\qquad \tilde{K}(r, X) \;\; \equiv \;\; \left\langle\Psi\left|U\left[X - \frac{r}{2}\right]^\dagger\right|\Phi\right\rangle \left\langle\Phi\left|U\left[X + \frac{r}{2}\right]\right|\Psi\right\rangle \tag{53.51}$$

Optionally we can transform to the Wigner representation, and then the multiplication becomes a convolution:

$$\rho(q, X) \;\; = \;\; \int K(q - q'; X) \; \rho^{(0)}(q', X) \; dq', \qquad\qquad K(q - q'; X) \;\; \equiv \;\; \int \tilde{K}(r, X) \; \mathrm{e}^{-i(q - q')r} dr \tag{53.52}$$

If we summed over Φ we would get the standard result that apply to a measurement without post-selection, namely,

$$K(q - q'; X) \;\; = \;\; \sum_a |\langle a|\Psi\rangle|^2 \; \delta(q - q' - a) \;\; \sim \;\; \delta\!\left(q - q' - \lambda\langle\mathcal{A}\rangle\right) \tag{53.53}$$

The last rough equality applies since our interest is focused on the *average* pointer displacement. With the same spirit we would like to obtain a simple result in the case of post-selection. For this purpose we assume that the measurement is weak, leading to

$$\tilde{K}(r, X) \;\; = \;\; |\langle\Phi|\Psi\rangle|^2 + i\lambda\mathrm{Re}\left[\langle\Psi|\Phi\rangle\langle\Phi|\mathcal{A}|\Psi\rangle\right] r - \lambda\mathrm{Im}\left[\langle\Psi|\Phi\rangle\langle\Phi|\mathcal{A}|\Psi\rangle\right] X \tag{53.54}$$

Bringing the terms back up to the exponent, and transforming to the Wigner representation we get

$$K(q-q'; X) \;\; = \;\; |\langle\Phi|\Psi\rangle|^2 \; \mathrm{e}^{-\lambda\mathrm{Im}\langle\mathcal{A}\rangle^{\mathrm{weak}}X} \; \delta\left(q - q' - \lambda\mathrm{Re}\langle\mathcal{A}\rangle^{\mathrm{weak}}\right) \tag{53.55}$$

we see that the real and the imaginary parts if the "weak value" determine the shift of the pointer in phase space. Starting with a minimal Gaussian of width σ, its center is shifted as follows:

$$\text{q-shift} \;\; = \;\; \lambda \, \mathrm{Re}\left[\langle\mathcal{A}\rangle^{\mathrm{weak}}_{\Phi,\Psi}\right] \tag{53.56}$$

$$\text{x-shift} \;\; = \;\; \frac{\lambda}{2\sigma^2} \, \mathrm{Im}\left[\langle\mathcal{A}\rangle^{\mathrm{weak}}_{\Phi,\Psi}\right] \tag{53.57}$$

We emphasize again that the "weak value" manifest itself only if the coupling is small enough to allow linear approximation for the shift of the pointer. In contrast to that, without post-selection the average q-shift is $\lambda\langle\mathcal{A}\rangle$ irrespective of the value of λ.

════ [53.13] Weak continuous measurements

A more interesting variation on the theme of weak measurements arises due to the possibility to perform a continuous measurement. This issue has been originally discussed by Levitov in connection with theme of "full counting statistics" (FCS). Namely, let us assume that we have an interest in the current $\mathcal{I}$ that flows through a section of a wire. We formally define the counting operator as follows:

$$\mathcal{Q} \;\; = \;\; \int_{-\infty}^{\infty} \mathcal{I}(t) \, dt \tag{53.58}$$

The time window is defined by a rectangular function $g(t)$ that equals unity during the measurements. The interaction with the von-Nuemann *pointer* is

$$\mathcal{H}_{\mathrm{measurement}} \;\; = \;\; -\lambda g(t) \, \mathcal{I} \, \hat{x} \tag{53.59}$$

Naively we expect a shift $q \mapsto q + \lambda\langle\mathcal{Q}\rangle$, and more generally we might wonder what is the probability distribution of Q. It turns out that these questions are ill-defined. The complication arises here because $\mathcal{Q}$ is an integral over a time dependent operator that does not have to commute with itself in different times.

The only proper way to describe the statistics of Q is to figure out what is the outcome of the measurement as reflected in the final state of the von-Nuemann pointer. The analysis is the same as in the previous section, and the result can be written as

$$\rho(q, X) \;\; = \;\; \int K(q-q'; X) \, \rho^{(0)}(q', X) \, dq' \tag{53.60}$$

where

$$K(Q; x) \;\; = \;\; \frac{1}{2\pi} \int \left\langle \psi \middle| U[x - (r/2)]^{\dagger} U[x + (r/2)] \middle| \psi \right\rangle \mathrm{e}^{-iQr} dr \tag{53.61}$$

In the expression above it was convenient to absorb the coupling λ into the definition of $\mathcal{I}$. The derivation and the system operator $U[x]$ are presented below. The FCS kernel $K(Q; x)$ is commonly calculated for $x = 0$. It is a

quasi-probability distribution (it might have negative values). The kth quasi-moment of Q can be obtained by taking the kth derivative of the bra-ket expression in the integrand with respect to r, then setting $r = 0$.

We follow here the formulation of Nazarov. Note that his original derivation has been based on an over-complicated path integral approach. Here we present as much simpler version. The states of system can be expanded in some arbitrary basis $|n\rangle$, and accordingly for the system with the detector we can use the basis $|n, x\rangle$. The x position of the von-Nuemann pointer is a constant of the motion. Consequently the representation of the evolution operator is

$$U(n, x|n_0, x_0) \;=\; U[x]_{n, n_0} \; \delta(x - x_0) \tag{53.62}$$

where $U[x]$ is a system operator that depends on the constant parameter x. We formally write the explicit expression for $U[x]$ both in the Schrodinger picture and also in the interaction picture using time ordered exponentiation:

$$U[x] \;=\; \mathcal{T} \exp\left[-i \int_0^t (\mathcal{H} - x\mathcal{I})dt'\right] \;=\; U[0]\,\mathcal{T} \exp\left[ix \int_0^t \mathcal{I}(t')dt'\right] \tag{53.63}$$

The time evolution of the detector is described by its reduced probability matrix

$$\rho(x', x'') \;=\; \mathsf{trace}\left[P^{x', x''} \, U \rho^{\psi} \rho^{(0)} U^{\dagger} \right] \;=\; \tilde{K}(x', x'') \; \rho^{(0)}(x', x'') \tag{53.64}$$

where $\rho^{\psi} = |\psi\rangle\langle\psi|$ is the initial state of the system, and $\rho^{(0)}$ is the initial preparation of the detector, and

$$\tilde{K}(x', x'') \;=\; \sum_n \langle n|U[x']|\psi\rangle \, \langle\psi|U[x'']^{\dagger}|n\rangle \;=\; \langle\psi|U[x'']^{\dagger} \, U[x']|\psi\rangle \tag{53.65}$$

Transforming to the Wigner function representation as in the previous section we get the desired result.

======= [53.14] Interferometry

Interferometry refers to a family of techniques whose purpose is to deduce the "relative phase" in a superposition. The working hypothesis is that there is some preferred "standard" basis that allows measurements. In order to clarify this concept let us consider the simplest example, which is a "two slit" experiment. Here the relative phase of being in either of the two slits has the meaning of transverse momentum. Different momenta have different velocities. Hence the interferometry here is straightforward: one simply places a screen far away, such that transverse momentum transforms into transverse distance on the screen. This way one can use position measurement in order to deduce momentum. Essentially the same idea is used in "time of flight" measurments of Bose-Einstein condensates: The cloud is released and expands, meaning that its momentum distribution translates into position distribution. The latter can be captured by a camera. Another example for interferometry concerns the measurement of the relative phase of Bose condensed particles in a double well superposition. Here the trick is to induce a Rabi type "rotation" in phase space, ending up in a population imbalance that reflects the relative phase of the preparation.

[54] Theory of quantum computation

======= [54.1] Motivating Quantum Computation

Present day secure communication is based on the RSA two key encryption method. The RSA method is based on the following observation: Let N be the product of two unknown big prime numbers p and q. Say that we want to find are what are its prime factors. The simple minded way would be to try to divide N by 2, by 3, by 5, by 7, and so on. This requires a huge number ($\sim N$) of operations. It is assumed that N is so large such that in practice the simple minded approached is doomed. Nowadays we have the technology to build classical computers that can handle the factoring of numbers as large as $N \sim 2^{300}$ in a reasonable time. But there is no chance to factor larger numbers, say of the order $N \sim 2^{308}$. Such large numbers are used by Banks for the encryption of important transactions. In the following sections we shall see that factoring of a large number N would become possible once we have a quantum computer.

Computational complexity: A given a number N can be stored in an n-bit register. The size of the register should be $n \sim \log(N)$, rounded upwards such that $N \leq 2^n$. As explained above in order to factor a number which is stored in an n bit register by a classical computer we need an exponentially large number ($\sim N$) of operations. Obviously we can do some of the operations in parallel, but then we need an exponentially large hardware. Our mission is to find an efficient way to factor an n-bit number that do not require exponentially large resources. It turns out that a quantum computer can do the job with hardware/time resources that scale like power of n, rather than exponential in n. This is done by finding a number N_2 that has a common divisor with N. Then it is possible to use Euclid's algorithm in order to find this common divisor, which is either p or q.

Euclid's algorithm: There is no efficient algorithm to factor a large number $N \sim 2^n$. The classical computational complexity of this task is exponentially large in n. But if we have two numbers $N_1 = N$ and N_2 we can quite easily and efficiently find their greater common divisor $\text{GCD}(N_1, N_2)$ using Euclid's algorithm. Without loss of generality we assume that $N_1 > N_2$. The two numbers are said to be co-prime if $\text{GCD}(N_1, N_2) = 1$. Euclid's algorithm is based on the observation that we can divide N_1 by N_2 and take the reminder $N_3 = \text{mod}(N_1, N_2)$ which is smaller than N_2. Then we have $\text{GCD}(N_1, N_2) = \text{GCD}(N_2, N_3)$. We iterate this procedure generating a sequence $N_1 > N_2 > N_3 > N_4 > \cdots$ until the reminder is zero. The last non-trivial number in this sequence is the greater common divisor.

The RSA encryption method: The RSA method is based on the following mathematical observation. Given two prime numbers p and q define $N = pq$. Define also a and b such that $ab = 1 \mod [(p-1)(q-1)]$. Then we have the relations

$$B = A^a \quad \mod [N] \tag{54.1}$$
$$A = B^b \quad \mod [N] \tag{54.2}$$

This mathematical observation can be exploited as follows. Define

$$\text{public key} = (N, a) \tag{54.3}$$
$$\text{private key} = (N, b) \tag{54.4}$$

If anyone want to encrypt a message A, one can use for this purpose the public key. The coded message B cannot be decoded unless one knows the private key. This is based on the assumption that the prime factors p and q and hence b are not known.

======= [54.2] The factoring algorithm

According to Fermat's theorem, if N is prime, then $M^N = M \mod (N)$ for any number $M(< N)$. If the "seed" M is not divisible by N, this can be re-phrased as saying that the period of the function $f(x) = M^x \mod (N)$ is $r = N-1$. That means $f(x + r) = f(x)$. To be more precise the primitive period can be smaller than N (not any "seed" is "generator"). More generally if N is not prime, and the seed M has no common divisor with it, then the primitive period of $f(x)$ is called "the order".

The quantum computer is a black box that allows to find the period r of a function $f(x)$. How this is done will be discussed in the next section. Below we explain how this ability allows us to factor a given large number N.

(1) We have to store N inside an n-bit register.

(2) We pick a large number M, so called seed, which is smaller than N. We assume that M is co-prime to N. This assumption can be easily checked using Euclid'd algorithm. If by chance the chosen M is not co-prime to N then we are lucky and we can factor N without quantum computer. So we assume that we are not lucky, and M is co-prime to N.

(3) We build a processor that can calculate the function $f(x) = M^x \mod (N)$. This function has a period r which is smaller than N.

(4) Using a quantum computer we find one of the Fourier components of $f(x)$ and hence its period r. This means that $M^r = 1 \mod (N)$.

(5) If r is not even we have to run the quantum computer a second time with a different M. Likewise if $a^{r/2} = -1$. There is a mathematical theorem that guarantees that with probability of order one we should be able to find M with which we can continue to the next step.

(6) We define $Q = M^{r/2} \mod (N)$. We have $Q^2 = 1 \mod (N)$, and therefore $(Q-1)(Q+1) = 0 \mod (N)$. Consequently both $(Q-1)$ and $(Q+1)$ must have either p or q as common divisors with N.

(6) Using Euclid's algorithm we find the GCD of N and $\tilde{N} = (Q-1)$, hence getting either p or q.

The bottom line is that given N and M an an input, we would like to find the period r of the functions

$$f(x) = M^x \mod (N) \tag{54.5}$$

Why do we need a quantum computer to find the period? Recall that the period is expected to be of order N. Therefore the x register should be n_c bits, where n_c is larger or equal to n. Then we have to make order of 2^{n_c} operations for the purpose of evaluating $f(x)$ so as to find out its period. It is assumed that n is large enough such that this procedure is not practical. We can of course try to do parallel computation of $f(x)$. But for that we need hardware which is larger by factor of 2^n. It is assumed that to have such computational facility is equally not practical. We say that factoring a large number has an exponentially complexity.

The idea of quantum processing is that the calculation of $f(x)$ can be done "in parallel" without having to duplicate the hardware. The miracle happens due to the superposition principle. A single quantum register of size n_c can be prepared at $t = 0$ with all the possible input x values in superposition. The calculation of $f(x)$ is done in parallel on the prepared state. The period of $f(x)$ in found via a Fourier analysis. In order to get good resolution n_c should be larger than n so as to have $2^{n_c} \gg 2^n$. Neither the memory, nor the number of operation, are required to be exponentially large.

===== [54.3] The quantum computation architecture

We shall regard the computer as a machine that has registers for memory and gates for performing operations. The complexity of the computation is determined by the total number of memory bits which has to be used times the number of operations. In other words the complexity of the calculation is the product memory $\times$ time. As discussed in the previous section classical parallel computation do not reduce the complexity of a calculation. Both classical and quantum computers work according to the following scheme:

$$|\text{output}\rangle = U[\text{input}] |0\rangle \tag{54.6}$$

This means that initially we set all the bits or all the qubits in a zero state (a reset operation), and then we operate on the registers using gates, taking the input into account. It is assumed that there is a well define set of elementary gates. An elementary gate (such as "AND") operates on few bits (2 bits in the case of AND) at a time. The size of the hardware is determined by how many elementary gates are required in order to realize the whole calculation.

The quantum analog of the digital bits ("0" or "1") are the qubits, which can be regarded as spin 1/2 elements. These are "analog" entities because the "spin" can point in any direction (not just "up" or "down"). The set of states such that each spin is aligned either "up" or "down" is called the *computational basis*. Any other state of a register can be written a superposition:

$$|\Psi\rangle \;=\; \sum_{x_0, x_1, x_2, ...} \psi(x_0, x_1, x_2...) \, |x_0, x_1, x_2, ...\rangle \tag{54.7}$$

The architecture of the quantum computer which is requited in order to find the period r of the function $f(x)$ is illustrated in the figure below. We have two registers:

$$x \;=\; (x_0, x_1, x_2, ..., x_{n_c-1}) \tag{54.8}$$
$$y \;=\; (y_0, y_0, y_2, ..., y_{n-1}) \tag{54.9}$$

The registers x and y can hold binary numbers in the range $x < N_c$ and $y < \bar{N}$ respectively, where $N_c = 2^{n_c}$ and $\bar{N} = 2^n > N$. The y register is used by the CPU for processing $\mathrm{mod}(N)$ operations and therefore it requires a minimal number of n bits. The x register has n_c bits and it is used to store the inputs for the function $f(x)$. In order to find the period of $f(x)$ the size n_c of the latter register should be significantly larger compared with n. Note that that $n_c = n + 10$ implies that the x range becomes roughly $\times 1000$ larger than the expected period. Large n_c is required if we want to determine the period with large accuracy.
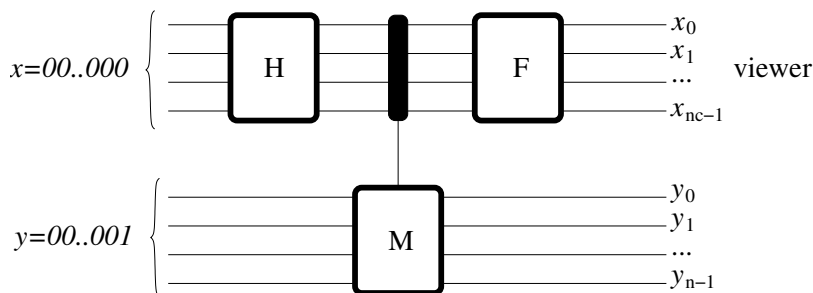
We are now ready to describe the quantum computation. In later sections we shall give more details, and in particular we shall see that the realization of the various unitary operations which are listed below does not require an exponentially large hardware. The preliminary stage is to make a "reset" of the registers, so as to have

$$|\Psi\rangle \;=\; |x; y\rangle = |0, 0, 0, ..., 0, 0; 1, 0, 0, ..., 0, 0\rangle \tag{54.10}$$

Note that it is convenient to start with $y = 1$ rather than $y = 0$. Then come a sequence of unitary operations

$$U \;=\; U_F U_M U_H \tag{54.11}$$

where

$$U_H \;=\; U_{\mathrm{Hadamard}} \otimes \mathbf{1} \tag{54.12}$$
$$U_M \;=\; \sum_x |x\rangle\langle x| \otimes U_M^{(x)} \tag{54.13}$$
$$U_F \;=\; U_{\mathrm{Fourier}} \otimes \mathbf{1} \tag{54.14}$$

The first stage is a unitary operation U_H that sets the x register in a democratic state. It can realized by operating on Ψ with the Hadamard gate. Disregarding normalization we get

$$|\Psi\rangle \;=\; \sum_x |x\rangle \otimes |y{=}1\rangle \tag{54.15}$$

The second stage is an x controlled operation U_M. This stage is formally like a quantum measurement: The x register is "measured" by the y register. The result is

$$|\Psi\rangle \;\; = \;\; \sum_x |x\rangle \otimes |y{=}f(x)\rangle \tag{54.16}$$

Now the y register is entangled with the x register. The fourth stage is to perform Fourier transform on the x register:

$$|\Psi\rangle \;\; = \;\; \sum_x \left[\sum_{x'} e^{i\frac{2\pi}{N_c}xx'}|x'\rangle \right] \otimes |f(x)\rangle \tag{54.17}$$

We replace the dummy integer index x' by $k = (2\pi/N_c)x'$ and re-write the result as

$$|\Psi\rangle \;\; = \;\; \sum_k |k\rangle \otimes \left[\sum_x e^{ikx}|f(x)\rangle \right] \;\; \equiv \;\; \sum_k p_k |k\rangle \otimes |\chi^{(k)}\rangle \tag{54.18}$$

The final stage is to measure the x register. The probability to get k as the result is

$$p_k \;\; = \;\; \left\| \sum_x e^{ikx}|f(x)\rangle \right\|^2 \tag{54.19}$$

The only non-zero probabilities are associated with $k = \text{integer} \times (2\pi/r)$. Thus we are likely to find one of these k values, from which we can deduce the period r. Ideally the error is associated with the finite length of the x register. By making the x register larger the visibility of the Fourier components becomes better.

══════ [54.4] Elementary qubit quantum gates

Classical operations can be constructed using single bit NOT gates, and two-bit AND gates. Similarly, quantum operations can be constructed using single qubit operations (rotations), and two-qubit CNOT gates. We review below the common gates that are used, e.g. in the IBM composer.

The single qubit gates can be regarded as spin rotations. It is useful to define the following notations for the observable that 'measures' the state of the qubit in the standard basis:

$$Q \;\; = \;\; \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \;\; = \;\; \frac{1}{2}(1 - Z) \;\; = \;\; |1\rangle\langle 1| \tag{54.20}$$

The notations X, Y, Z are used for the Pauli matrices. The notations RX, RY, RZ are used for rotations. A phase gate is defined as follows:

$$\mathrm{P}(\varphi) \;\; = \;\; e^{i\varphi Q} \;\; = \;\; e^{i(\varphi/2)}\mathsf{RZ}(\varphi) \;\; = \;\; |0\rangle\langle 0| + |1\rangle e^{i\varphi}\langle 1| \tag{54.21}$$

Note that

$$Z \;\; = \;\; \mathrm{P}(\pi) \;\; = \;\; i\mathrm{RZ}(\pi) \tag{54.22}$$

More interesting are two-qubit gates. The controlled-phase gate is

$$\mathrm{CP}(\varphi) \;\; = \;\; e^{i\varphi Q \otimes Q} \;\; = \;\; |0\rangle\langle 0| \otimes 1 + |1\rangle\langle 1| \otimes \mathrm{P}(\varphi) \tag{54.23}$$

This gate is symmetric: we can say that the first qubit controls the phase operation on the second qubit, or vice versa. In particular the controlled-Z gate is

$$\text{CZ} = \text{CP}(\pi) = e^{i\pi Q \otimes Q} = |0\rangle\langle 0| \otimes 1 + |1\rangle\langle 1| \otimes Z \tag{54.24}$$

Most useful is the controlled-X (CNOT) gate

$$\text{CX} = |0\rangle\langle 0| \otimes 1 + |1\rangle\langle 1| \otimes X = \begin{pmatrix} 1 & 0 & & 0 \\ 0 & 1 & & \\ & & 0 & 1 \\ 0 & & 1 & 0 \end{pmatrix} \tag{54.25}$$

Ising-type phase gates are defined as follows:

$$\text{RZZ}(\varphi) = e^{-i(\varphi/2)Z \otimes Z} \tag{54.26}$$

Similarly one can define RXX and RYY gates, etc.

For completeness we list some common notations:

$$T = P(\pi/4) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix} \tag{54.27}$$

$$S = T^2 = P(\pi/2) = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$$

$$Z = S^2 = P(\pi) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_z = i\text{RZ}(\pi)$$

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_x = ie^{-i\pi S_x} = i\text{RX}(\pi) = \text{NOT gate}$$

$$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \sigma_y = ie^{-i\pi S_y} = i\text{RY}(\pi)$$

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{1}{\sqrt{2}}(\sigma_x + \sigma_z) = ie^{-i\pi S_n} = \text{Hadamard gate}$$

$$R = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = \frac{1}{\sqrt{2}}(1 - i\sigma_y) = e^{-i(\pi/2)S_y} = \text{RY}(\pi/2) = 90\text{deg Rotation}$$

We have $R^4 = -1$ which is a 2π rotation in $SU(2)$. We have $X^2 = Y^2 = Z^2 = H^2 = 1$ which implies that these are π rotations in $U(2)$. We emphasize that though the operation of H on "up" or "down" states looks like $\pi/2$ rotation, it is in fact a π rotation around a 45° inclined axis:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \left(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}} \right) \cdot \vec{\sigma} = \vec{n} \cdot \vec{\sigma} \tag{54.28}$$

Global phase issue.– Mathematically we can define a U(1) operation on a qubit, namely, a multiplication by a phase. Let us use the notation $G(\varphi) = e^{i\varphi}$. Clearly, from a physical perspective this operation has no significance. Operations like X and $\text{RX}(\pi)$ are equivalent. If we have, say, a two-qubit register, then $[G(\varphi)|x_0\rangle] \otimes |x_1\rangle = e^{i\varphi}|x_0, x_1\rangle$. What about a controlled-G? For that we have the identity

$$\text{CG}(\varphi) = |0\rangle\langle 0| \otimes 1 + |1\rangle\langle 1| \otimes e^{i\varphi} = \text{P}(\varphi) \otimes 1 \tag{54.29}$$

Namely, CG is mathematically equivalent to an operation with a phase-gate on the control qubit. For that reason the G-gate is redundant.

[54.5] The CNOT quantum gate

It is popular to consider the controlled NOT (CNOT) gate as an elementary gate, with which we can construct more complicated gates. We shall use for it the notation CX. In the standard computational basis the control bit (x) of CX is not affected by its operation, while the controlled bit (y) undergoes NOT provided the x bit is turned-*on*. The gate is schematically illustrated in the following figure. We also provide in the figure another variation of CX that performs NOT provided the x bit is turned-*off*. Below we explain that CX can be constructed using CZ and R operations (right panel of the figure).
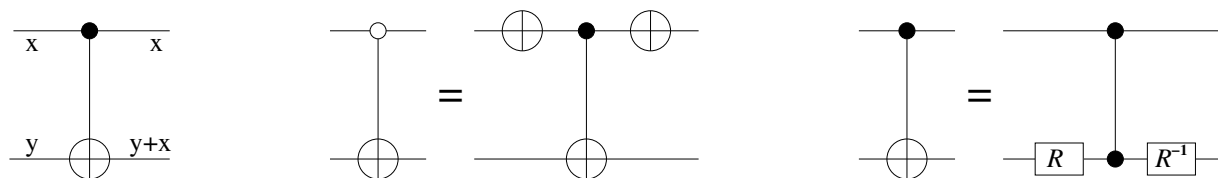

In order to realize a two qubit gate we need a coupling mechanism. If we regard the two qubits as spins, it is most natural to exploit the Ising spin-spin interaction ($\propto Z \otimes Z$) in order to realize an RZZ phase operation. But for pedagogical purpose it is more convenient to regard the qubits as dots that can be charges with $Q = 0, 1$ particles, such that the interaction is $\propto Q \otimes Q$. With such interaction we can construct a CZ operation. Then we can exploit the similarity transformation $R^{-1}ZR = X$ in order to get CX as follows:

$$\text{CX} \;=\; R^{-1}\,\text{CZ}\,R \;=\; |0\rangle\langle 0| \otimes 1 + |1\rangle\langle 1| \otimes X \tag{54.30}$$

where the rotations are performed on the controlled qubit (see figure). Here R is -90deg rotation around Y.

[54.6] CNOT-related operations

Having the ability to realize single-qubit operations, and the CNOT gate, we can construct all other possible gates and circuits. It is amusing to see how SWAP gate can be realized by combining 3 CNOT gates, as illustrated is the following diagram:
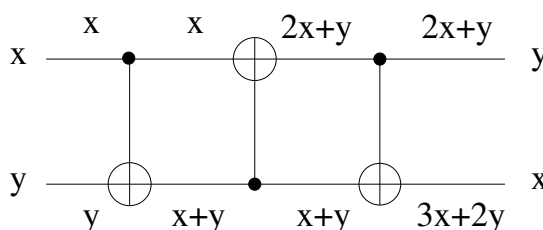

The controlled-not gate has misc generalizations. There are two aspects: (i) how to form controlled-rotations instead of control-not; (ii) how to have more then one control bit. The way to form a controlled RY or controlled RZ rotation is to write the rotation, call it W, as a sequence of two half-rotations, namely, $W = VV$. We use the notation $\bar{V} = V^\dagger = V^{-1}$ for the inverse rotation. We note that for either RY or RZ we have the identity $XVX = \bar{V}$. Then we can use the following circuit (see figure below for its illustration):

$$\text{CW} \;=\; (\text{CX}\,\bar{V}\,\text{CX})\,V \tag{54.31}$$

where V operates on the controlled qubit, and the CX performs on it a controlled-not. Note that if we want to get CRX, we can use the identity $\text{CRX} = \text{RZ}(-\pi/2)\,\text{CRY}\,\text{RZ}(\pi/2)$, where the RZ rotations operate on the controlled qubit. The way to have two control bits labelled as "1" and "2" is to write the desired rotation as $R = WW$, and then to use the following circuit (see figure below for its illustration):

$$\text{CCR} \;=\; \text{CW}^{2\mapsto 0}\;\text{CX}^{2\mapsto 1}\;\bar{\text{CW}}^{1\mapsto 0}\;\text{CX}^{2\mapsto 1}\;\text{CW}^{1\mapsto 0} \tag{54.32}$$

where the notation $C^{i \mapsto j}$ means that qubit i controls the operation on qubit j.
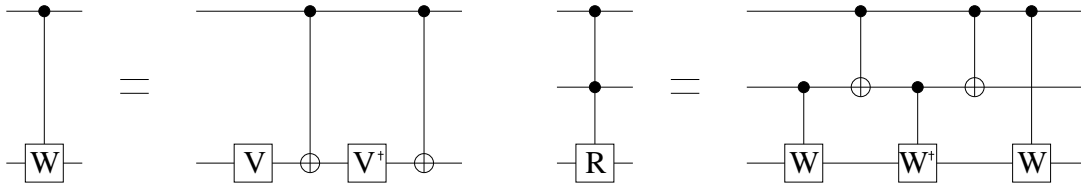
The CCX operation, where we have two qubit that control NOT operation, is known as Toffoli gate. The NOT operation is performed only if both control bits are turned on:
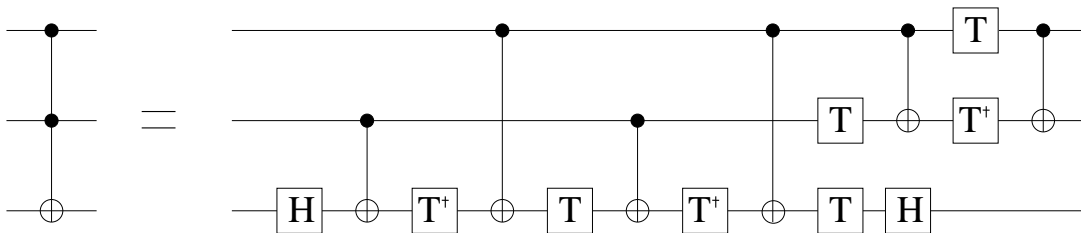
The realization of the Toffoli gate opens the way to the quantum realization of an AND operation. Namely, by setting $y = 0$ at the input, the output would be $y = x_1 \wedge x_2$. For generalization of the Toffoli gate to the case where the x register is of arbitrary size see p.184 of Nielsen and Chuang.

===== [54.7] Quantum Simulations

We have motivated quantum computation by considering the RSA decryption problem. We shall come back to that in the subsequent sections, providing details on the Hadamard transform, on the quantum Fourier transform, and on the required controlled computation of the $f(x)$ function.

But quantum computation can be used also for the purpose of quantum simulations. Clearly, if we have a large N-spin system, it is not feasible to perform a classical simulation with $2^N \times 2^N$ matrices, while it might be feasible to perform a simulation with an N qubit register. If we consider spin $1/2$ system, then each qubit can represent a spin. Evolution that is generated by, say, $S_x \otimes S_x$ interaction can be realized using RXX gates. The Hamiltonian might be a sum of several such terms, and therefore the use of the Trotter formula is required: each dt time step of the simulation is composed of a sequence of infinitesimal unitary operations that correspond to the terms in the Hamiltonian.

Slightly less natural is to perform simulation of a 2^N site system, where each site is labelled by an N digit binary number $\boldsymbol{x}$. The operation of a potential $V(\boldsymbol{x})$ can be simulated using controlled-phase operations. Note: if we apply a phase gate on a single qubit, say x_0, then all the sites that have $x_0 = 1$ are affected. If we want to change the phase of, say, $\boldsymbol{x} = \cdots 001$, we need a controlled operation that performs the phase operation only if all the other bits are 0. Similar treatment is required in order to induce hopping. Flipping one bit in $\boldsymbol{x}$, say x_0, means simultaneous transitions within any pair of sites whose $\boldsymbol{x}$ differ by digit x_0. If we want to induce transition between, say, only the first two sites ($\cdots 000$ and $\cdots 001$) we have to use a controlled operation on the x_0 bit, namely, it is "rotated" only if all the other bits equal 0. Accordingly, with controlled operation we can induce any transition between two sites whose $\boldsymbol{x}$ differs by a single binary digit. In order to induce transitions between sites whose $\boldsymbol{x}$ differ by more than one digit, we have to perform Gray-sequence of exchanges before the controlled operation, and after that reverse this sequence. For Hamiltonian of the type $H = T(\boldsymbol{p}) + V(\boldsymbol{x})$ we might use the identity $T(\boldsymbol{p}) = F^\dagger T(\boldsymbol{x}) F$, where F is the quantum Fourier transform operation (see below). Other trick can be used for e.g. simulating the effect of $T(\boldsymbol{p}) = \cos(\boldsymbol{p})$.

===== [54.8] The Hadamard Transform

In the following we discuss the Hadamard and the Fourier transforms. These are unitary operations that are defined on the multi-qubit x register. A given basis state $|x_0, x_1, x_3, ...\rangle$ can be regarded as the binary representation of an

integer number:

$$x = \sum_{r=0}^{n_c-1} x_r 2^r \tag{54.33}$$

We distinguish between the algebraic multiplication for which we use the notation xx', and the scalar product for which we use the notation $x \cdot x'$,

$$x \cdot x' = \sum_r x_r x'_r \tag{54.34}$$

$$xx' = \sum_{r,s} x_r x'_s 2^{r+s}$$

So far we have defined the single qubit Hadamard gate. If we have an multi-qubit register it is natural to define

$$U_{\text{Hadamard}} = H \otimes H \otimes H \otimes \cdots \tag{54.35}$$

The operation of a single-qubit Hadamard gate can be written as

$$|x_1\rangle \xrightarrow{H} \frac{1}{\sqrt{2}}\left(|0\rangle + (-1)^{x_1}|1\rangle\right) = \frac{1}{\sqrt{2}}\sum_{k_1=0,1}(-1)^{k_1 x_1}|k_1\rangle \tag{54.36}$$

If we have a multi-qubit register we simply have to perform (in parallel) an elementary Hadamard transform on each qubit:

$$|x_0, x_1, ..., x_r, ...\rangle \xrightarrow{H} \prod_r \frac{1}{\sqrt{2}}\left(|0\rangle + (-1)^{x_r}|1\rangle\right) = \frac{1}{\sqrt{2^{n_c}}}\prod_r\left[\sum_{k_r=0,1}(-1)^{k_r x_r}|k_r\rangle\right] \tag{54.37}$$

$$= \frac{1}{\sqrt{N_c}}\sum_{k_0,k_1,...}(-1)^{k_0 x_0 + k_1 x_1 + \cdots}|k_0, k_1, ..., k_r, ...\rangle = \frac{1}{\sqrt{N_c}}\sum_k (-1)^{k \cdot x}|k\rangle$$

The Hadmard transform is useful in order to prepare a "democratic" superposition state as follows:

$$|0, 0, ..., 0\rangle \xrightarrow{H} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes ... \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \mapsto \frac{1}{\sqrt{N_c}}\begin{pmatrix} 1 \\ 1 \\ . \\ . \\ . \\ 1 \end{pmatrix} \tag{54.38}$$

To operate with a unitary operator on this state is like making parallel computation on all the possible x basis states.

===== [54.9] The quantum Fourier transform

The definitions of the Hadamard transform and the quantum Fourier transform are very similar in style:

$$U_{\text{Hadamard}}|x\rangle = \frac{1}{\sqrt{N_c}}\sum_k (-1)^{k \cdot x}|k\rangle \tag{54.39}$$

$$U_{\text{Fourier}}|x\rangle = \frac{1}{\sqrt{N_c}}\sum_k e^{-i\frac{2\pi}{N_c}kx}|k\rangle \tag{54.40}$$

Let us write the definition of the quantum Fourier transform using different style so as to see that it is indeed a Fourier transform operation in the conventional sense. First we notice that its matrix representation is

$$\langle x'|U_{\text{Fourier}}|x\rangle \quad = \quad \frac{1}{\sqrt{N_c}}\mathrm{e}^{-i\frac{2\pi}{N_c}x'x} \tag{54.41}$$

If we operate with it on the state $|\psi\rangle = \sum_x \psi_x|x\rangle$ we get $|\varphi\rangle = \sum_x \varphi_x|x\rangle$, where the column vector φ_x is obtained from ψ_x by a multiplication with the matrix that represents U_{Fourier}. Changing the name of the dummy index form x to k we get the relation

$$\varphi_k \quad = \quad \frac{1}{\sqrt{N_c}}\sum_{x=0}^{N_c-1}\mathrm{e}^{-i\frac{2\pi}{N_c}kx}\psi_x \tag{54.42}$$

This is indeed the conventional definition of

$$\begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ . \\ . \\ . \\ \psi_{N_c-1} \end{pmatrix} \xrightarrow{FT} \begin{pmatrix} \varphi_0 \\ \varphi_1 \\ \varphi_2 \\ . \\ . \\ . \\ \varphi_{N_c-1} \end{pmatrix} \tag{54.43}$$

The number of memory bits which are required to store these vectors in a classical register is of order $N \sim 2^n$. The number of operations which is involved in the calculation of a Fourier transform seems to be of order N^2. In fact there is an efficient "Fast Fourier Transform" (FFT) algorithm that reduces the number of required operations to $N\log N = n2^n$. But this is still an exponentially large number in n. In contrast to that a quantum computer can store these vectors in n qubit register. Furthermore, the "quantum" FT algorithm can perform the calculation with only $n^2\log n\log\log n$ operations. We shall not review here how the Quantum Fourier transform is realized. This can be found in the textbooks. As far as this presentation is concerned the Fourier transform can be regarded as a complicated variation of the Hadamard transform.

======= [54.10] Note on analog or optical computation

A few words are in order here regarding quantum computation versus classical analog computation. In an analog computer every analog "bit" can have a voltage within some range, so ideally each analog bit can store infinite amount of information. This is of course not the case in practice because the noise in the circuit defines some effective finite resolution. Consequently the performance is not better compared with a digital computers. In this context the analog resolution is a determining factor in the definition of the memory size. Closely related is optical computation. This can be regarded as a special type of analog computation. Optical Fourier Transform of a "mask" can be obtained on a "screen" that is placed in the focal plane of a lens. The FT is done in one shot. However, also here we have the same issue: Each pixel of the mask and each pixel of the screen is a hardware element. Therefore we still need an exponentially large hardware just to store the vectors. At best the complexity of FT with optical computer is of order 2^n.

======= [54.11] The U_M operation

The CNOT/Toffoli architecture can be generalized so as to realize any operation of the type $y = f(x_1, x_2, ...)$, as an x-controlled operation, where y is a single qubit. More generally we have

$$x \quad = \quad (x_0, x_1, x_2...x_{n_c-1}) \tag{54.44}$$
$$y \quad = \quad (y_0, y_1, y_2, ...y_{n-1}) \tag{54.45}$$

and we would like to realize a unitary controlled operation

$$U \;=\; \sum_x |x\rangle\langle x| \otimes U^{(x)} \;\equiv\; P^{(0)} \otimes U^{(0)} + P^{(1)} \otimes U^{(1)} + P^{(2)} \otimes U^{(2)} + \dots \tag{54.46}$$

This is formally like a measurement of the x register by the y register. Note that x is a constant of motion, and that U has a block diagonal form:

$$\langle x', y'|U|x, y\rangle \;=\; \delta_{x',x} U^{(x)}_{y',y} \;=\; \begin{pmatrix} U^{(0)} & & & \\ & U^{(1)} & & \\ & & U^{(2)} & \\ & & & \dots \end{pmatrix} \tag{54.47}$$

Of particular interest is the realization of a unitray operation that maps $y = 1$ to $y = f(x)$. Let us look on

$$U^{(x)}_M \big|y\big\rangle \;=\; \big|M^x y \mod (N)\big\rangle \tag{54.48}$$

If M is co-prime to N, then U is merely a permutation matrix, and therefore it is unitary. The way to realize this operation is implied by the formula

$$M^x \;=\; M^{\sum_s x_s 2^s} \;=\; \prod_s \left(M^{2^s}\right)^{x_s} \;=\; \prod_{s=0}^{n_c-1} M_s^{x_s} \tag{54.49}$$

which requires n_c stages of processing. The circuit is illustrated in the figure below. In the s stage we have to perform a controlled multiplication of y by $M_s \equiv M^{2^s} \mod (N)$.
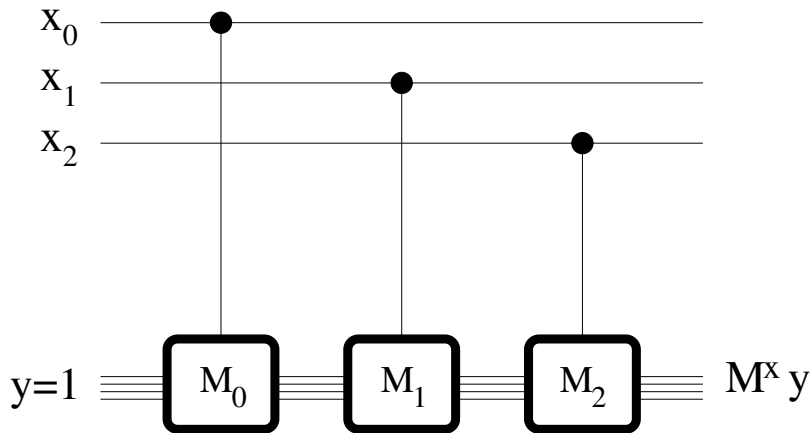
[55] The foundation of statistical mechanics

═════════ [55.1] The canonical formalism

Consider some system, for example particles that are confined in a box. The Hamiltonian is

$$\mathcal{H} \;=\; \mathcal{H}(\boldsymbol{r}, \boldsymbol{p}; X) \tag{55.1}$$

where X is some control parameter, for example the length of the box. The energy of the system is defined as

$$E \;\equiv\; \langle \mathcal{H} \rangle \;=\; \text{trace}(\mathcal{H}\rho) \;=\; \sum_r p_r E_r \tag{55.2}$$

where is the last equality we have assume that we are dealing with a stationary state. Similarly the expression for the generalized force y is

$$y \;\equiv\; \left\langle -\frac{\partial \mathcal{H}}{\partial X} \right\rangle \;=\; \sum_r p_r \left(-\frac{E_r}{dX} \right) \tag{55.3}$$

It is argued that the weak interaction with an environment that has a huge density of state ϱ_{env} leads after relaxation to a canonical state which is determined by the parameter $\beta = d \log(\varrho_{\text{env}}(E))/dE$ that characterizes the environment. The argument is based on the assumption that the universe (system+environment) is a closed system with some total energy E_{total}. After ergodization the system get into a stationary-like state. The probability p_r to find the system in state E_r is proportional to $\varrho_{\text{env}}(E_{\text{total}} - E_r) \approx \varrho_{\text{env}}(E_{\text{total}})e^{-\beta E_r}$. Accordingly

$$p_r = \frac{1}{Z} e^{-\beta E_r} \tag{55.4}$$

where the so-called partition function provides the normalization

$$Z(\beta; X) = \sum_r e^{-\beta E_r} \tag{55.5}$$

One observes that the energy can be obtained from

$$E \;=\; -\frac{\partial \ln Z}{\partial \beta} \tag{55.6}$$

while the generalized force is

$$y \;=\; \frac{1}{\beta} \frac{\partial \ln Z}{\partial X} \tag{55.7}$$

If we slightly change X and β and assume that the state of the system remains canonical then

$$dE \;=\; \sum_r dp_r E_r + \sum p_r dE_r \;\equiv\; TdS - ydX \tag{55.8}$$

where the absolute temperature is *defined* as the integration factor of the first term

$$T \;=\; \text{integration factor} \;=\; \frac{1}{\beta} \tag{55.9}$$

and the implied *definition* of the thermodynamic entropy is

$$S \;=\; -\sum p_r \ln p_r \tag{55.10}$$

Note that the thermodynamic entropy is an extensive quantity in the thermodynamic limit. At this state it is convenient to define the Helmholtz generating function

$$F(T, X) \;\equiv\; -\frac{1}{\beta} \ln Z(\beta; X) \tag{55.11}$$

which allows to write the state equation in an elegant way:

$$S \;=\; -\frac{\partial F}{\partial T} \tag{55.12}$$

$$y \;=\; -\frac{\partial F}{\partial X} \tag{55.13}$$

and

$$E \;=\; F + TS \tag{55.14}$$

══════ [55.2] Work

In the definition of work the system and the environment are regarded as one driven *closed* unit. On the basis of the "rate of change formula" we have the following exact expression:

$$\mathcal{W} \;=\; -\int \langle \mathcal{F} \rangle_t \, dX \tag{55.15}$$

where $\mathcal{F} = -d\mathcal{H}/dX$. Note that $\langle \mathcal{F} \rangle_t$ is calculated for the time dependent (evolving) state of the system. From linear response theory of driven closed systems we know that in leading order

$$\langle \mathcal{F} \rangle_t \;\approx\; \langle \mathcal{F} \rangle_X \;-\; \eta \dot{X} \tag{55.16}$$

The first terms is the conservative force, which is a function of X alone. The subscript implies that the expectation value is taken with respect to the instantaneous adiabatic state. The second term is the leading correction to the adiabatic approximation. It is the "friction" force which is proportional to the rate of the driving. The net conservative work is zero for a closed cycle while the "friction" leads to irreversible dissipation of energy with a rate $\eta \dot{X}^2$.

The above reasoning implies that for a quasi static process we can calculate the work as the sum of two contributions: $\mathcal{W} = -W + \mathcal{W}_{\text{irreversible}}$. The conservative work is defined as

$$W \;=\; \int_A^B y(X) dX \tag{55.17}$$

The rate of irreversible work is

$$\dot{\mathcal{W}}_{\text{irreversible}} \;=\; \eta \dot{X}^2 \tag{55.18}$$

where η is the "friction" coefficient, which can be calculated using linear response theory.

═════ [55.3] Heat

In order to understand which type of statements can be extracted form the canonical formalism we have to discuss carefully the physics of work and heat. We distinguish between the system and the environment and write the Hamiltonian in the form

$$\mathcal{H}_{\text{total}} = \mathcal{H}(\boldsymbol{r}, \boldsymbol{p}; X(t)) + \mathcal{H}_{\text{int}} + \mathcal{H}_{\text{env}} \tag{55.19}$$

It is implicit that the interaction term is extremely small so it can be ignored in the calculation of the total energy. We define

$$\mathcal{W} = \text{work} \ \equiv \ \left(\langle \mathcal{H}_{\text{total}} \rangle_B - \langle \mathcal{H}_{\text{total}} \rangle_A \right) \tag{55.20}$$

$$\mathcal{Q} = \text{heat} \ \equiv \ -\left(\langle \mathcal{H}_{\text{env}} \rangle_B - \langle \mathcal{H}_{\text{env}} \rangle_A \right) \tag{55.21}$$

$$E_{\text{final}} - E_{\text{initial}} \ \equiv \ \langle \mathcal{H} \rangle_B - \langle \mathcal{H} \rangle_A \ = \ \mathcal{Q} \ + \ \mathcal{W} \tag{55.22}$$

If for a general process we know the work $\mathcal{W}$ and the change in the energy of the system, then we can deduce what was the heat flow $\mathcal{Q}$. If we compare $dE = TdS - ydX$ with the expression $dE = đ\mathcal{Q} + đ\mathcal{W}$ we deduce that $TdS = đ\mathcal{Q} + đ\mathcal{W}_{\text{irreversible}}$. This implies that the change in the entropy of the system is $dS = (đ\mathcal{Q} + đ\mathcal{W}_{\text{irreversible}})/T$.

═════ [55.4] The second law of thermodynamics

The discussion of irreversible processes has been differed to *Lecture Notes in Statistical Mechanics and Mesoscopic*, arXiv:1107.0568

═════ [55.5] Fluctuations

The partition function and hence the thermodynamic equations of state give information only on the spectrum $\{E_n\}$ of the system. In the classical context this observation implies that a magnetic field has no influence on the equilibrium state of a system because the spectrum remains $E = \mathsf{m}v^2/2$ with $0 < |v| < \infty$. In order to probe the dynamics we have to look on the fluctuations $S(t) = \langle \mathcal{F}(t)\mathcal{F}(0) \rangle$, where $\mathcal{F}$ is some observable. The Fourier transform of $S(t)$ describes the power spectrum of the fluctuations:

$$\tilde{S}(\omega) \ = \ \int_{-\infty}^{\infty} S(t)\mathrm{e}^{i\omega\tau}d\tau \ = \ \sum_n p_n \sum_m |\mathcal{F}_{mn}|^2 \ 2\pi\delta\left(\omega - (E_m - E_n)\right) \tag{55.23}$$

This is the same object that appears in the Fermi-Golden-rule for the rate of transitions due to a perturbation term $V = -f(t)\mathcal{F}$. In the above formula $\omega > 0$ corresponds to absorption of energy (upward transitions), while $\omega < 0$ corresponds to emission (downward transitions). It is a straightforward algebra to show that for a canonical preparations with $p_n \propto \exp(-E_n/T)$ there is a detailed balance relation:

$$\tilde{S}(\omega) = \tilde{S}(-\omega) \ \exp\left(\frac{\hbar\omega}{T}\right) \tag{55.24}$$

This implies that if we couple to the system another test system (e.g. a two level "thermometer") it would be driven by the fluctuations into a canonical state with the same temperature.

The connection with Fermi-Golden-rule is better formalized within the framework of the so called fluctuation-dissipation relation. Assume that the system is driven by varying a parameter X, and define $\mathcal{F}$ as the associated generalized force. The Kubo formula (see *Dynamics and driven systems* lectures) relates the response kernel to $S(t)$. In particular the dissipation coefficient is:

$$\eta(\omega) \ = \ \frac{\tilde{S}(\omega) - \tilde{S}(-\omega)}{2\omega} \tag{55.25}$$

If the system is in a canonical state it follow that the zero frequency response is $\eta_0 = \tilde{S}(0)/(2T)$. If we further assume "Ohmic response", which means having constant $\eta(\omega) = \eta_0$ up to some cutoff frequency, then the above relation can be inverted:

$$\tilde{S}_{\text{ohmic}}(\omega) \;\; = \;\; \eta_0 \frac{2\omega}{1 - e^{-\omega/T}} \tag{55.26}$$

The best known application of this relation is known as the Nyquist theorem. If a ring is driven by an electro-motive force $-\dot{\Phi}$, then the rate of heating is $\dot{W} = G\dot{\Phi}^2$, which is know as Joule law. The generalized force which is associated with Φ is the current $\mathcal{I}$, and G is known as the conductance. Note that Joule law is equivalent to Ohm law $\langle \mathcal{I} \rangle = -G\dot{\Phi}$. It follows from the fluctuation-dissipation relation that the fluctuations of the current at equilibrium for $\omega \ll T$ are described by $\tilde{S}(\omega) = 2GT$. It should be clear that in non-equilibrium we might have extra fluctuations, which in this example are known as shot noise.

══════ [55.6] The modeling of the environment

It is common to model the environment as a huge collection of harmonic oscillators, and to say that the system is subject to the fluctuations of a field variable $\mathcal{F}$ which is a linear combination of the bath coordinates:

$$\mathcal{F} \;\; = \;\; \sum_{\alpha} c_\alpha Q_\alpha \;\; = \;\; \sum_{\alpha} c_\alpha \left(\frac{1}{2m_\alpha \omega_\alpha} \right)^{1/2} (a_\alpha + a_\alpha^\dagger) \tag{55.27}$$

For preparation of the bath in state $\boldsymbol{n} = \{n_\alpha\}$ we get

$$\tilde{S}(\omega) \;\; = \;\; \sum_{\alpha} \sum_{\pm} c_\alpha^2 \, |\langle n_\alpha \pm 1 | Q_\alpha | n_\alpha \rangle|^2 \; 2\pi\delta(\omega \mp \omega_\alpha) \tag{55.28}$$

Using

$$\langle n_\alpha + 1 | Q_\alpha | n_\alpha \rangle \;\; = \;\; \left(\frac{1}{2m_\alpha \omega_\alpha} \right)^{1/2} \sqrt{1 + n_\alpha} \tag{55.29}$$

$$\langle n_\alpha - 1 | Q_\alpha | n_\alpha \rangle \;\; = \;\; \left(\frac{1}{2m_\alpha \omega_\alpha} \right)^{1/2} \sqrt{n_\alpha} \tag{55.30}$$

we get

$$\tilde{S}(\omega) \;\; = \;\; \sum_{\alpha} \frac{1}{2m_\alpha \omega_\alpha} 2\pi c_\alpha^2 \Big[(1 + n_\alpha)\delta(\omega - \omega_\alpha) + n_\alpha \delta(\omega + \omega_\alpha) \Big] \tag{55.31}$$

For a canonical preparation of the bath we have $\langle n_\alpha \rangle = f(\omega_\alpha) \equiv 1/(e^{\omega/T} - 1)$. It follows that

$$\tilde{S}(\omega) \;\; = \;\; 2J(|\omega|) \times \begin{cases} (1 + f(\omega)) \\ f(-\omega) \end{cases} \;\; = \;\; 2J(\omega)\frac{1}{1 - e^{-\beta\omega}} \tag{55.32}$$

where we used $f(-\omega) = -(1 + f(\omega))$, and defined the spectral density of the bath as

$$J(\omega) \;\; = \;\; \frac{\pi}{2} \sum_{\alpha} \frac{c_\alpha^2}{m_\alpha \omega_\alpha} \delta(\omega - \omega_\alpha) \tag{55.33}$$

with anti-symmetric continuation. For an Ohmic bath $J(\omega) = \eta\omega$, with some cutoff frequency ω_c.