BHH - dimer system

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Upgraded version of "Lecture Notes in Quantum Mechanics" [quant-ph/060518] Sect.[38], with added appendix on Wigner function, to be integrated in a long paper.

[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. The dimension of the Hilbert space is $\mathcal{N} = N + 1$. Later we assume $N \gg 1$ so $\mathcal{N} \sim N$. For simplicity we might further assume N to be even, and define $j = N/2$, so as to have $\mathcal{N} = 2j+1$. The Hamiltonian is

$$\mathcal{H} \;=\; \sum_{i=1,2} \left[\mathcal{E}_i \hat{n}_i + \frac{U}{2}\hat{n}_i(\hat{n}_i - 1)\right] - \frac{K}{2}(\hat{a}_2^\dagger \hat{a}_1 + \hat{a}_1^\dagger \hat{a}_2) \tag{1}$$

where we denote by K the hopping, by U the interaction, and by $\mathcal{E} = \mathcal{E}_2 - \mathcal{E}_1$ the bias. Since $n_1 + n_2 = N$ is constant of motion, the Hamiltonian for a given N is formally equivalent to the Hamiltonian of a spin j particle. Defining

$$J_z \;\equiv\; \frac{1}{2}(\hat{n}_1 - \hat{n}_2) \;\equiv\; \hat{n} \tag{2}$$

$$J_+ \;\equiv\; \hat{a}_1^\dagger \hat{a}_2 \tag{3}$$

we can re-write the Hamiltonian as

$$\mathcal{H} \;=\; U\hat{J}_z^2 - \mathcal{E}\hat{J}_z - K\hat{J}_x + \text{const} \tag{4}$$

In the absence of interaction this is like having a spin in magnetic field with precession frequency $\Omega = (K, 0, \mathcal{E})$. In order to analyze the dynamics for finite U it is more convenient to re-write this Hamiltonian with canonically conjugate variables. Formally we are dealing with two coupled oscillators. So for each we can define action-angle variables in the following way (no approximations involved):

$$\hat{a}_i \;=\; \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix} \;=\; \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \sqrt{1} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{3} \end{pmatrix} \;\equiv\; \mathrm{e}^{i\boldsymbol{\varphi}}\sqrt{\hat{n}_i} \;=\; \sqrt{\hat{n}_i{+}1}\;\mathrm{e}^{i\boldsymbol{\varphi}} \tag{5}$$

One should be aware that the *ladder* operator $\mathrm{e}^{i\boldsymbol{\varphi}}$ is in fact non-unitary because it annihilates the ground state. We shall denote its adjoint operator as $\mathrm{e}^{-i\boldsymbol{\varphi}}$, so we have $\hat{a}_i^\dagger = \sqrt{\hat{n}_i}\mathrm{e}^{-i\boldsymbol{\varphi}_i}$. Now it is possible to re-write the Hamiltonian using the variable $\hat{n} \equiv \hat{n}_1$ and the associated ladder operator $\mathrm{e}^{\boldsymbol{\varphi}} \equiv \mathrm{e}^{\boldsymbol{\varphi}_1}\mathrm{e}^{-\boldsymbol{\varphi}_2}$ as follows: corrected

$$\mathcal{H} \;=\; Un^2 \;-\; \mathcal{E}n \;-\; \frac{K}{2}\left[\sqrt{[(N/2) - \hat{n}][(N/2) + \hat{n} + 1]}\;\mathrm{e}^{i\boldsymbol{\varphi}} + \text{h.c.}\right] \tag{6}$$

So far no approximation are involved. But now we want to allow an approximation which is valid for the dynamics as long as $|n|$ is not close to its extreme value $N/2$. Consequently we can ignore the small corrections that are associated with the proper ordering of the operators and write

$$\mathcal{H} \;\approx\; U\hat{n}^2 \;-\; \mathcal{E}\hat{n} \;-\; K\sqrt{(N/2)^2 - \hat{n}^2}\;\cos(\boldsymbol{\varphi}) \tag{7}$$

In the $|n| \ll (N/2)$ region of phase space this resembles the so-called Josephson Hamiltonian, which is essentially the Hamiltonian of a pendulum

$$\mathcal{H}_{\text{Josephson}} \;=\; E_C(\hat{n}-n_\varepsilon)^2 \;-\; E_J\cos(\boldsymbol{\varphi}) \tag{8}$$

with $E_c = U$ and $E_J = KN/2$, while n_ε is linearly related to $\mathcal{E}$. The Josephson Hamiltonian is an over-simplification because it does not capture correctly the global topology of phase space. In order to shed better light on the actual Hamiltonian it is convenient to define in addition to the $\boldsymbol{\varphi}$ operator also a $\boldsymbol{\theta}$ operator such that $J_z \equiv (N/2)\cos(\boldsymbol{\theta})$ while $J_x \approx (N/2)\sin(\boldsymbol{\theta})\cos(\boldsymbol{\varphi})$. It is important to realize that $\boldsymbol{\varphi}$ and $\boldsymbol{\theta}$ do not commute. We get:

$$\mathcal{H} \;\approx\; \frac{NK}{2}\left[\frac{1}{2}u(\cos\boldsymbol{\theta})^2 - \varepsilon\cos\boldsymbol{\theta} - \sin\boldsymbol{\theta}\cos\boldsymbol{\varphi}\right] \tag{9}$$

where the scaled parameters are

$$u \equiv \frac{NU}{K}, \qquad\qquad \varepsilon \equiv \frac{\mathcal{E}}{K} \tag{10}$$

We can describe phase space using the canonical coordinates $(\boldsymbol{\varphi}, n)$, so the total area of phase space is $2\pi N$ and Planck cell is $2\pi\hbar$ with $\hbar = 1$. Optionally we can use spherical coordinates $(\boldsymbol{\varphi}, \boldsymbol{\theta})$, so the total area of phase space is 4π and Planck cell $4\pi/N$. Note that an area element in phase space can be written as $d\boldsymbol{\varphi} d\cos\boldsymbol{\theta}$.

Within the framework of the semiclassical picture a quantum state is described as a distribution in phase space, and the eigenstates are associated with strips that are stretched along contour lines $H(\boldsymbol{\varphi}, \boldsymbol{\theta}) = E$ 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 a family of states $|\boldsymbol{\theta}, \boldsymbol{\varphi}\rangle$ that are called coherent states. If U is large, $\mathcal{E} = 0$, and K is very small, then the eigenstates are the symmetric and the antisymmetric superpositions of the $|\pm n\rangle$ states. In particular we have "cat states" of the type:

$$|\text{CatState}\rangle \;=\; |n_1{=}N, n_2{=}0\rangle \;+\; \mathrm{e}^{i\text{phase}}|n_1{=}0, n_2{=}N\rangle \tag{11}$$

If a coherent state evolves, then the non-linearity (for non zero U) will stretch it. Sometimes the evolved state might resemble a cat state. We can characterize the one-body coherence of a state by defining the one-body reduced probability matrix as

$$\rho^{(1)}_{ji} \;=\; \frac{1}{N}\langle \hat{a}^\dagger_i \hat{a}_j\rangle \;=\; \frac{1}{2}(\mathbf{1} + \langle S\rangle\cdot\boldsymbol{\sigma}) \tag{12}$$

where $S_i = (2/N)J_i$ and the so called polarization vector is $\langle S\rangle = (\langle S_x\rangle, \langle S_y\rangle, \langle S_z\rangle)$. Note that

$$\text{AverageOccupation} \;=\; (N/2)\,[1 + \langle S_z\rangle] \tag{13}$$

$$\text{OneBodyPurity} \;=\; (1/2)\left[1 + \langle S_x\rangle^2 + \langle S_y\rangle^2 + \langle S_z\rangle^2\right] \tag{14}$$

$$\text{FringeVisibility} \;=\; \left[\langle S_x\rangle^2 + \langle S_y\rangle^2\right]^{1/2} \tag{15}$$

The coherent states have maximum OneBodyPurity. This purity can be diminished due to non-linear effects or due to interaction with environmental degrees of freedom. [hidden text]

[2] Digression: an M site system with N Bosons

A double well system with Bosons has formally the same Hilbert space as that of spin $N/2$ particle. The generalization of this statement is straightforward. The following model systems have formally the same Hilbert space:

- The "N particle" states of a Bosonic system with M sites.
- The "N quanta" states of M Harmonic oscillators.
- The states of a dim(N) "spin" of the $SU(M)$ group.

We shall explain and formulate mathematically the above statements, and later we shall use the formal analogy with "spin" in order to shed light on the dynamics of N Bosons in $M = 2$ site system.

To regard Bosonic site as an Harmonic "mode" is just a matter of language: We can regard the "creation" operator $a_i^\dagger$ as a "raising" operator, and we can regard the "occupation" of the ith site $\hat{n}_i = a_i^\dagger a_i$ as the number of quanta stored in ith mode. The one particle states of an M site system form an M dimensional Hilbert space. The set of unitary transformations within this space is the $SU(M)$ group. Let us call these transformation generalized "rotations". If we have N particles in M sites then the dimensionality of Hilbert space is $\dim(N) = (N{+}1)!/[(M{-}1)!N{-}M{+}2)!]$. For example for $M = 2$ system we have $\dim(N) = N{+}1$ 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 $SU(M)$ group. By definition these "rotations" can be expressed as a linear combination of the $SU(M)$ generators J_μ, and they all commute with $\hat{N}$. We shall see that the many body 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". Still we assume that $\mathcal{H}$ commutes with $\hat{N}$, so we can work within $\dim(N)$ subspace.

There is a common *mean field approximation* which is used in order to analyze the dynamics of many Bosons system. In the semiclassical framework the dynamics in phase space is generated by the Hamilton equations of motion for the action-variables $\dot{n}_i$ and $\dot{\boldsymbol{\varphi}}_i$. These are the "polar coordinates" that describe each of the oscillators. Optionally one can define a "macroscopic wavefunction"

$$\psi_i \;\equiv\; \sqrt{n_i}\, \mathrm{e}^{i\boldsymbol{\varphi}} \qquad \text{representing a single point in phase space} \tag{16}$$

The equation for $\dot{\Psi}_i$ is known as the discrete version of the non-linear Schrodinger (DNLS) equation:

$$i\frac{d\psi_i}{dt} \;=\; \Big(\epsilon_i + U|\psi_i|^2\Big)\Psi_i - \frac{K}{2}\left(\psi_{i+1} + \psi_{i-1}\right) \tag{17}$$

In the continuum limit this equations is known as the Gross-Pitaevskii equation:

$$i\frac{d\psi(x)}{dt} \;=\; \Big[V(x) + g_s|\psi(x)|^2 - \frac{1}{2\mathsf{m}}\nabla^2\Big]\psi(x) \tag{18}$$

The potential $V(x)$ corresponds to the ϵ_i of the DNLS equation, and the mass m is associated with the hopping amplitude K using the standard prescription. 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 $g_s = 4\pi a_s/\mathsf{m}$.

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 goes beyond the conventional mean field approximation. The latter 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") and accordingly it is characterized by $\overline{n}_i = \langle n_i\rangle$ and $\overline{\boldsymbol{\varphi}}_i = \langle\boldsymbol{\varphi}_i\rangle$ or equivalently by the mean field

$$\overline{\psi}_i = \langle\psi_i\rangle \qquad \text{representing the center of a wavepaket} \tag{19}$$

To the extend that the mean field assumption can be trusted the equation of motion for $\overline{\psi}_i$ is the DNLS. Indeed if $U = 0$ there is no non-linear spreading and the mean field description becomes exact. Otherwise it is a crude approximation.

WKB

[3] Phase space and semiclassics

We can describe phase space using the canonical coordinates $(\boldsymbol{\varphi}, n)$, so the total area of phase space is $2\pi\mathcal{N}$ and Planck cell is $2\pi\hbar$ with $\hbar = 1$. Optionally we can use normalized coordinates $(\boldsymbol{\varphi}, \cos\boldsymbol{\theta})$, such that an area element in phase space is $d\boldsymbol{\varphi} d\cos\boldsymbol{\theta}$, and the total area of phase space is 4π. It is convenient to define a scaled Planck constant

$$h \quad = \quad \text{Planck cell area in steradians} \quad = \quad \frac{4\pi}{\mathcal{N}} \quad , \qquad\qquad [\mathcal{N} = N{+}1 = 2j{+}1] \tag{20}$$

Within the framework of the semiclassical picture a quantum state is described as a distribution in phase space, and the eigenstates are associated with *strips* of area h that are stretched along contour lines $H(\boldsymbol{\varphi}, \boldsymbol{\theta}) = E$ of the Hamiltonian. The associated WKB quantization condition is

$$A(E_n) \quad = \quad \left(\frac{1}{2} + n\right) h \tag{21}$$

where $A(E)$ is defined as the phase space area enclosed by an E contour in *steradians*:

$$A(E) \quad \equiv \quad \int\!\!\int \Theta(E - \mathcal{H}(\boldsymbol{\varphi}, \boldsymbol{\theta}))\; d\boldsymbol{\varphi} d\cos\boldsymbol{\theta} \tag{22}$$

while the area of phase space in Plank units is $A(E)/h$. The frequency of oscillations at energy E is

$$\omega(E) \quad \equiv \quad \frac{dE}{dn} \quad = \quad \left[\frac{1}{h} A'(E)\right]^{-1} \tag{23}$$

If we have non-linear oscillators then the eigenenergies are not equally spaced, and within some small interval around $n \sim n_0$ one can make the approximation

$$\omega(E_n) \quad \approx \quad (1 + \alpha(n - n_0))\;\omega_0 \tag{24}$$

$$E_n \quad \approx \quad E_0 + \left((n - n_0) + \frac{1}{2}\alpha(n - n_0)^2\right)\omega_0 \tag{25}$$

It is straightforward to find that the nonlinearity parameter at energy E is given by

$$\alpha(E) \quad \equiv \quad \frac{1}{\omega}\frac{d\omega}{dn} \quad = \quad \omega(E)^2 \left[\frac{1}{h} A''(E)\right] \tag{26}$$

[4] Frequencies

For $u = 0$ there is only one frequency, which is the Rabi frequency

$$\omega_K \quad = \quad K \tag{27}$$

For $u < 1$ the frequencies around the two stable fixed points are slightly modified:

$$\omega_\pm \quad = \quad \omega(E_\pm) \quad = \quad \sqrt{(K \pm NU)K} \tag{28}$$

For $u \gg 1$ we have the Josephson oscillation frequency near the minimum point:

$$\omega_J \;=\; \omega(E_-) \;\approx\; \sqrt{NUK} \;=\; \sqrt{u}\,\omega_K \tag{29}$$

while at the top of the islands:

$$\omega_+ \;=\; \omega(E_+) \;\approx\; NU \;=\; u\,\omega_K \tag{30}$$

From now on our interest in this $u \gg 1$ regime. The approximations for the phase space area in the 3 energy regions are corrected:

$$\frac{1}{h}A(E) \;=\; \left(\frac{E-E_-}{\omega_J}\right) \qquad \text{[low energies]} \tag{31}$$

$$\frac{1}{h}A(E) \;=\; \frac{1}{h}A(E_{\text{x}}) + \left(\frac{E-E_{\text{x}}}{\omega_J}\right)\log\left|\frac{NK}{E-E_x}\right| \qquad \text{[separatrix]} \tag{32}$$

$$\frac{1}{h}A(E) \;=\; \frac{4\pi}{h} - \left(\frac{E_+-E}{U}\right)^{1/2} \qquad \text{[high energies, disregarding pairing]} \tag{33}$$

It follows that in the vicinity of the separatrix

$$\omega(E) \;\approx\; \left[\log\left|\frac{NK}{E-E_x}\right|\right]^{-1}\omega_J \tag{34}$$

[5] WKB quantization

Away form the separatrix the WKB quantization recipe implies that the local level spacing at energy E is $\omega(E)$ given by Eq.(**??**). In particular the law energy levels have spacing ω_J, while the high energy levels are doubly-degenerate with spacing ω_+.

On the separatrix $\omega(E) = 0$. Consequently in the vicinity of the separatrix the level spacing becomes smaller but of course not zero. Rather we have to go back to the WKB quantization condition, and we find that the level spacing at the vicinity of the separatrix is *finite* and given by the expression

$$\omega_{\text{x}} \;=\; \left[\frac{1}{2}\log\left(\frac{N^2}{u}\right)\right]^{-1}\omega_J \tag{35}$$

In Fig. (**??**) we compare the WKB energies with exact eigenvalues and the analytical linear expressions with slopes ω_J for low energies, ω_x for near-separatrix energies, and ω_+ for high energies.

For later discussion we need also the nonlinearity in the separatrix region. Substitution of $A''(E) = 1/(\omega_0 E)$, and evaluating for $|E| \sim \omega_{\text{x}}$ we get:

$$\alpha(E_{\text{x}}) \;=\; \omega(E_{\text{x}})^2\left[\frac{1}{h}A''(E_{\text{x}})\right] \;\approx\; \frac{\omega_{\text{x}}}{\omega_J} \;\approx\; \left[\frac{1}{2}\log\left(\frac{N^2}{u}\right)\right]^{-1} \tag{36}$$

The importance of α is clarified later when we discuss the non-linear dynamics of wavepackets in phase space.

Wigner function

[6] The Wigner distribution on a sphere

The Hilbert space of a spin j entity has the dimension $\mathcal{N} = 2j{+}1$, and the associated space of operators has the dimensionality $\mathcal{N}^2$. The inner product of two operators is defined as trace$[A^\dagger B]$. The non-Hermitian multipole operators $\hat{T}^{lm}$ (see definition below) form a complete orthonormal set of operators. By orthogonal transformation we can define another complete orthonormal set of Hermitian operators $\hat{P}^{\theta\varphi}$ (see definition below). Respectively we can represent any operator A either by $A_{lm} = \text{trace}[(\hat{T}^{lm})^\dagger A]$ or by

$$A_{\text{W}}(\theta,\varphi) \quad = \quad \text{trace}[\hat{P}^{\theta\varphi}\rho] \tag{37}$$

Note that if the operator A is Hermitian, then its Wigner function $A_{\text{W}}(\theta,\varphi)$ is real. Accordingly the inner product of two operators becomes a simple phase space integral on the corresponding Wigner functions:

$$\text{tr}[\hat{\rho}\hat{A}] \quad = \quad \int \rho_{\text{W}}(\theta,\varphi)A_{\text{W}}(\theta,\varphi)d\Omega \tag{38}$$

We turn now to discuss the details. The defining expression for the multipole operators is

$$\hat{T}^{lm} = \sum_{m',m''} (-1)^{j-m'}\sqrt{2l+1}\begin{pmatrix} j & l & j \\ -m' & m & m'' \end{pmatrix} |m'\rangle\langle m''| \tag{39}$$

where we use the Wigner $3j$ symbols. The defining expression for the generalized phase space projectors is [**? ?**]

$$\hat{P}^{\theta\varphi} = \sum_{l=0}^{2j}\sum_{m=-l}^{l} Y^{lm}(\theta,\varphi)\hat{T}^{lm} \tag{40}$$

The Wigner representation of a projector or a pure state $\rho = |\Psi\rangle\langle\Psi|$ is

$$\rho_{\text{W}}(\theta,\varphi) = \sum_{l,m}\left[\sum_{m',m''}(-1)^{j-m'}\sqrt{2l+1}\begin{pmatrix} j & l & j \\ -m' & m & m'' \end{pmatrix}\Psi^*_{m'}\Psi_{m''}\right]Y^{lm}(\theta,\varphi) \tag{41}$$

The Wigner-Wyle representation of the identity operator is up to normalization the same as the Wigner function of a uniform mixed state

$$1_{\text{w}}(\theta,\varphi) \quad = \quad \sqrt{2j{+}1}\; Y^{0,0}(\theta,\varphi) \tag{42}$$

It follows that

$$\text{tr}[\hat{\rho}] = \sqrt{\frac{2j{+}1}{4\pi}}\int \rho_{\text{W}}(\theta,\varphi)d\Omega \tag{43}$$