The information entropy of quantum mechanical states

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Collaboration:

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Reference:

A. Stotland, A.A. Pomeransky, E. Bachmat, D. Cohen, Europhysics Letters 67, 700 (2004)

Information theory point of view

Shannon:

$$\mathcal{S}[\rho|\mathcal{A}] = -\sum_r p_r \ln(p_r)$$

ρ - state of the system

$\mathcal{A}$ - measurement setup

What is the label r?

r labels the possible outputs of a measurement.

Definite output:

$\mathcal{S} = 0$

Output one of n possibilities:

$\mathcal{S} = \ln(n)$

Maximally mixed state:

$\mathcal{S} = \ln(N)$

N - dimension of Hilbert space

Quantal definition of absolute entropy

$$S_{\text{total}} = S[\mathcal{A}] + \sum_{\mathcal{A}} P(\mathcal{A}) S[\rho|A]$$

Average over all possible basis sets:

$$S[\rho] \;=\; \overline{S[\rho|\mathcal{A}]} \;=\; S_0(N) + F(p_1, p_2, ...)$$

Minimum uncertainty entropy:

$$S_0(N) \;=\; \sum_{k=2}^{N} \frac{1}{k} \;\approx\; \ln(N) - (1-\gamma) + \frac{1}{2N}$$

Excess statistical entropy:

$$F(p_1, p_2, ...) = -\sum_r \left[\prod_{r'(\neq r)} \frac{p_r}{p_r - p_{r'}} \right] \; p_r \ln(p_r)$$

It is a measure for lack of purity.

Should be compared with:

$$S_{\text{von Neumann}} = -\sum_r p_r \ln p_r$$

Derivation - part one

$f(s) = -s \ln(s)$

$$
\begin{aligned}
S &= \overline{\sum_a f\left(\sum_r p_r |\langle r|a\rangle|^2\right)}^{A} \\
&= \overline{\sum_s f\left(\sum_r p_r |\langle r|U|s\rangle|^2\right)}^{U} \\
&= \overline{N f\left(\sum_r p_r |\langle r|\Psi\rangle|^2\right)}^{\Psi} \\
&= \overline{N f\left(\sum_r p_r (x_r^2 + y_r^2)\right)}^{\text{sphere}} \\
&= N \int_0^\infty f(s)\ P(s) ds
\end{aligned}
$$

$$s = \sum_r p_r |\Psi_r|^2 = \sum_{r=1}^{N} p_r (x_r^2 + y_r^2)$$

We have to find $P(s)$, and do the integral...

Derivation - part 2

$$P(s) = \left\langle \delta(s - \sum_r p_r(x_r^2 + y_r^2)) \right\rangle_{\text{sphere}}$$

$$\begin{aligned}
&= (N-1)! \int_0^\infty ds_1..ds_N \;\delta(1-\sum_r s_r)\delta(s-\sum_r p_r s_r) \\
&= (N-1)! \int_0^\infty .. \int \frac{d\omega d\nu}{(2\pi)^2} \mathrm{e}^{(1-\sum_r s_r)(i\nu+0)+i(s-\sum_r p_r s_r)\omega} \\
&= (N-1)! \int \frac{d\omega d\nu}{(2\pi)^2} \mathrm{e}^{i\nu+i\omega s} \prod_r \frac{1}{i\omega p_r + i\nu + 0} \\
&= \int \frac{d\omega}{2\pi} \frac{(N-1)!}{(i\omega)^{N-1}} \sum_r \mathrm{e}^{i\omega(s-p_r)} \prod_{r'(\neq r)} \frac{1}{p_{r'} - p_r} \\
&= (N-1) \sum_{(p_r>s)} \left[\prod_{r'(\neq r)} \frac{1}{p_r - p_{r'}} \right] (p_r - s)^{N-2}
\end{aligned}$$

$$\int_0^p (p-s)^{N-2} s \ln(s) ds = \frac{p^N}{N(N-1)} \left[\ln(p) - \sum_{k=2}^{n} \frac{1}{k} \right]$$

Main results

Pure state:

$$S_0(N) \;=\; \sum_{k=2}^{N} \frac{1}{k} \;\approx\; \ln(N) - (1-\gamma) + \frac{1}{2N}$$

$\rightsquigarrow$ $$S_{\text{F}}[\rho] \;<\; 1-\gamma$$

Mixed state:

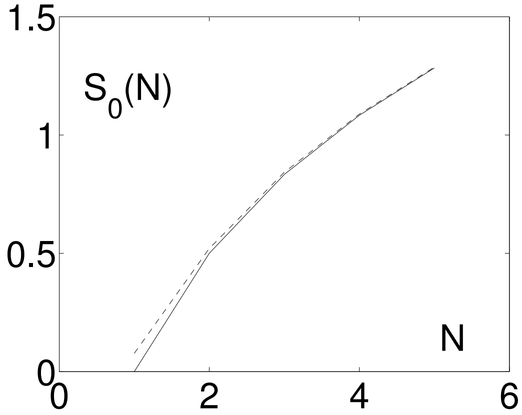
$$S_{\text{F}}[\rho] = -\sum_r \left[\prod_{r'(\neq r)} \frac{p_r}{p_r - p_{r'}} \right] \; p_r \ln(p_r)$$

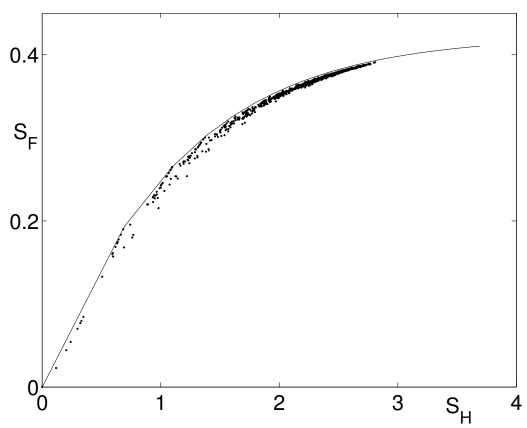
Mixture of two states:

$$S_{\text{F}}[\rho] = -\frac{1}{p_1 - p_2}\left(p_1^2 \ln(p_1) - p_2^2 \ln(p_2)\right)$$

Uniform mixture of n states:

$$S_{\text{F}}[\rho] \;=\; \ln(n) - \sum_{k=2}^{n} \frac{1}{k}$$





Inequalities

Entropy of a subsystem:

$$S[\sigma] < S[\rho]$$

System composed of two independent subsystems:

$$S[\rho|\mathcal{A}\otimes\mathcal{B}] = S[\sigma_{\rm A}|\mathcal{A}] + S[\sigma_{\rm B}|\mathcal{B}]$$

Hence

$$S[\rho] \geq S[\sigma_{\rm A}] + S[\sigma_{\rm B}]$$

A particular case is:

$$S_0(NM) > S_0(N) + S_0(M)$$

On the other hand (generalization):

$$S_{\rm F}[\rho] \leq S_{\rm F}[\sigma_{\rm A}] + S_{\rm F}[\sigma_{\rm B}]$$

As in the case with Von-Neumann:

$$S_{\rm H}[\rho] \leq S_{\rm H}[\sigma_{\rm A}] + S_{\rm H}[\sigma_{\rm B}]$$

Summary

We have found explicit expressions
for the minimum uncertainty entropy $S_0(N)$,
and for the excess statistical entropy $F(p_1, p_2, ...)$.

$F(p_1, p_2, ...)$ can be used as a measure for lack of purity of quantum mechanical states, and it is strongly correlated with the Von-Neumann entropy $S_{\mathrm{H}}[\rho]$.

$F(p_1, p_2, ...)$ is bounded from above by $(1 - \gamma)$.

The total information entropy $S[\rho]$, unlike the Von-Neumann entropy, has properties that do make sense from information theory point of view.

Time evolution under non-perturbative circumstances

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Collaborations:

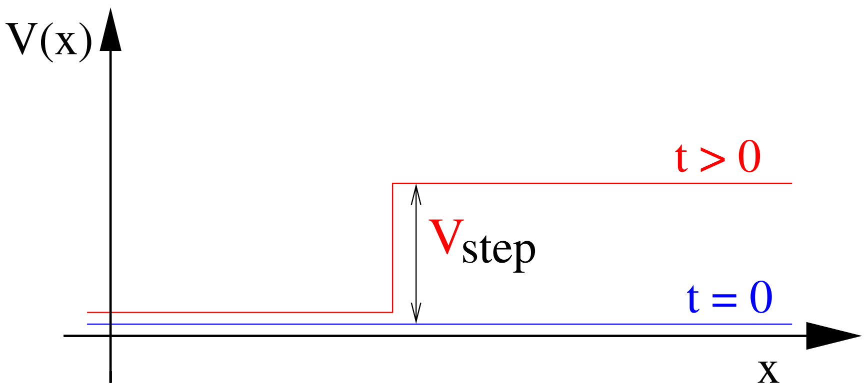
Doron Cohen (BGU)

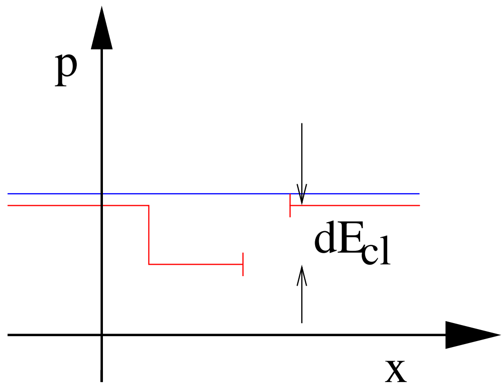
Discussions:

Vladimir Goland

Problems and their classical treatment

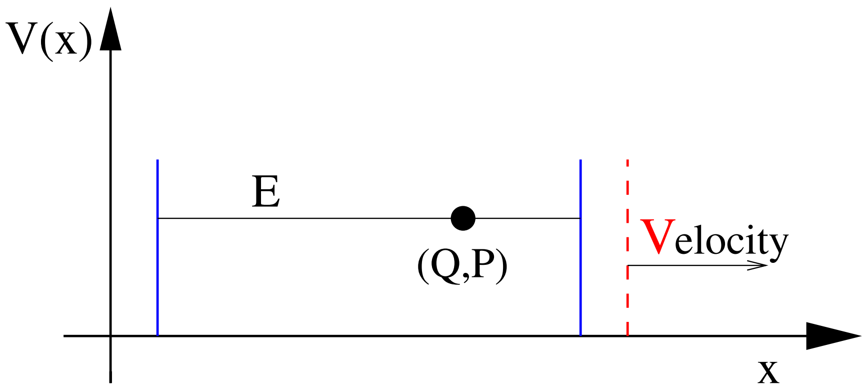
- Step potential

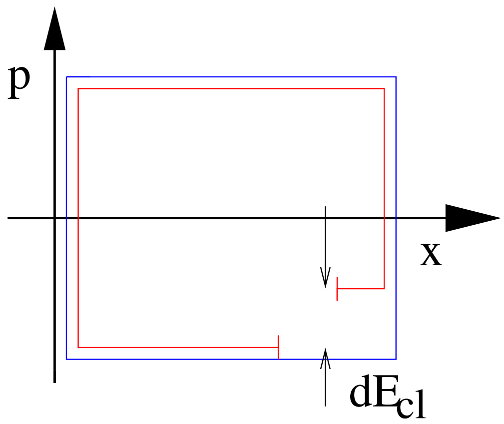




$$\delta E_{\text{cl}} = V_{\text{step}}$$

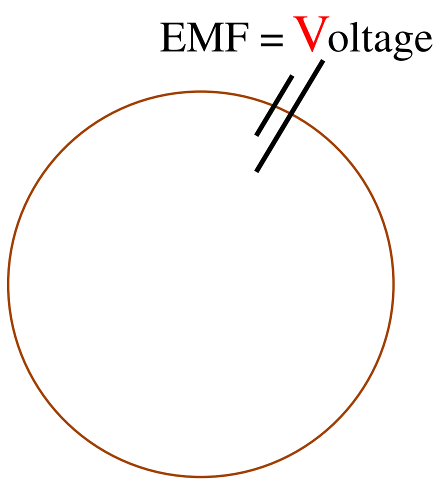
- Moving wall

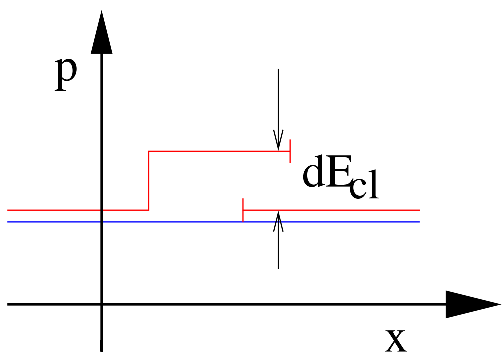




$$\delta E_{\text{cl}} = 2MvV$$

- Ring

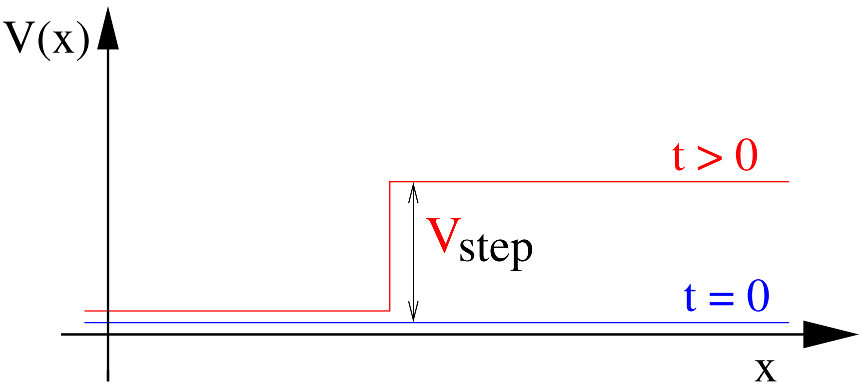


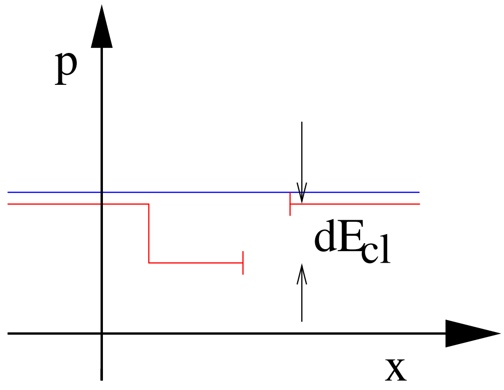


$$\delta E_{\text{cl}} = eV$$

$\delta \mathbf{E}_{\text{cl}} \gg \mathbf{\Delta}$ - semiclassical case

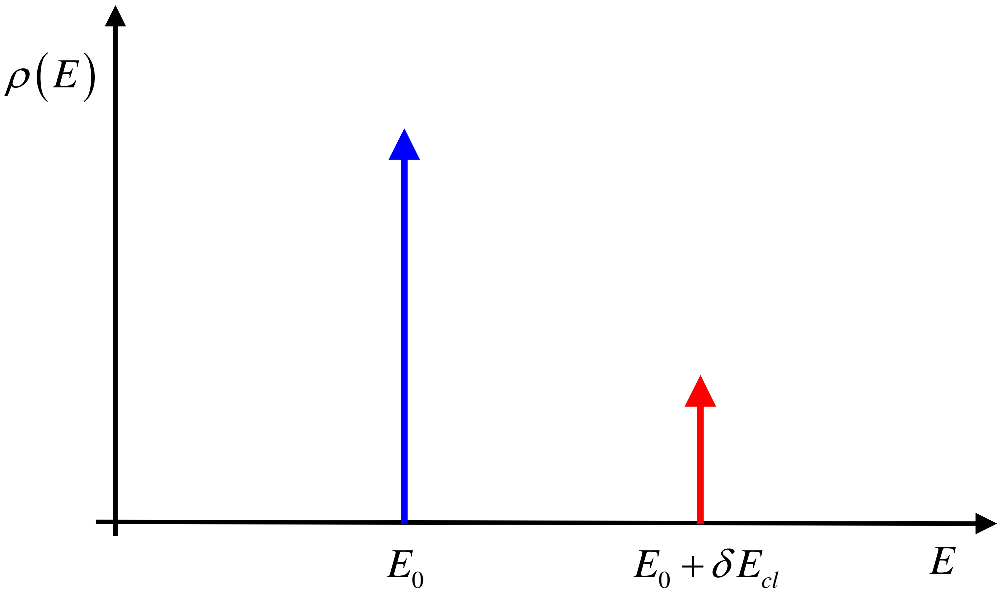
Step potential



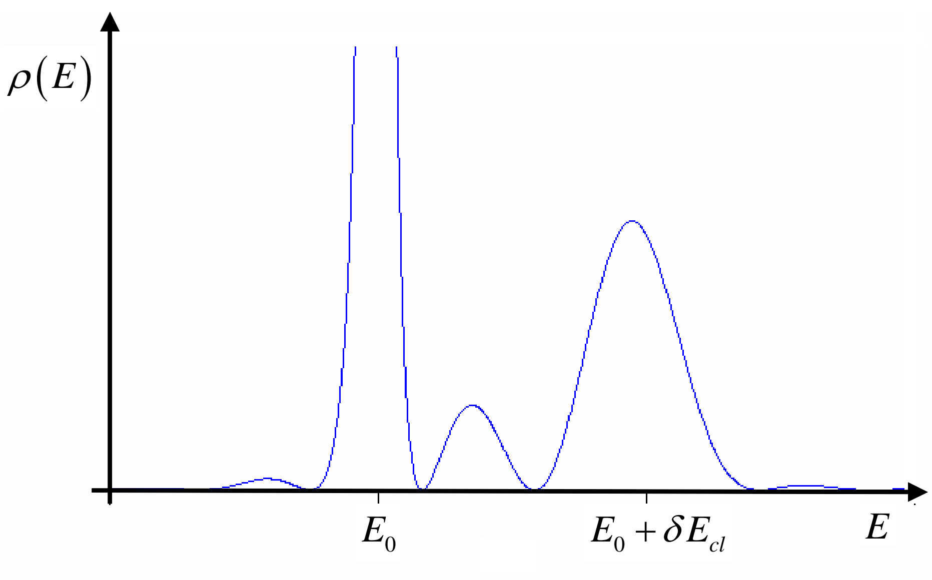


$$\delta E_{\mathrm{cl}} = V_{\mathrm{step}}$$

- Classical energy distribution



- QM energy distribution



Quantum Classical Correspondence

Energy distribution moments:

$$\delta E^r = \int p_t(E) E^r dE$$

$r = 1$ - expectation value

$r = 2$ - variance

Bohr QCC:

- Gaussian wavepacket
- smooth potentials

$\Rightarrow$ the same moments

But not always the wavepackets are gaussian...

LRT: the long time behavior is determined by the short time behavior.

Second moment $\Rightarrow$ Central limit theorem

- $r = 2$ - robust QCC
- $r > 2$ - fragile QCC

We tried to find a "sick" problem. The worst problem for Bohr: Step potential

Is there a QCC in this problem???

Step - analytical results

- Detailed QCC ($r > 2$) is destroyed.
- Restricted QCC ($r = 2$) is preserved.

Classical moments:

$$\langle (p - p_0)^r \rangle \; = \; u^r \times |A|^2 v_{\mathrm{E}} t$$

$u = -U_0 / v_{\mathrm{E}}$ is the momentum change

QM analytical solution:

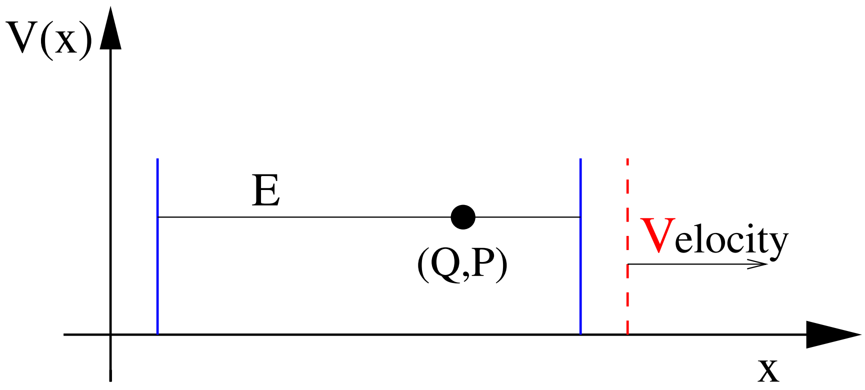
$$|\langle p_2 | \mathcal{U} | p_1 \rangle|^2 = 4u^2 \frac{\sin^2 \frac{(p_2 - p_1 - u) v_{\mathrm{E}} t}{2}}{(p_2 - p_1)^2 (p_2 - p_1 - u)^2}$$

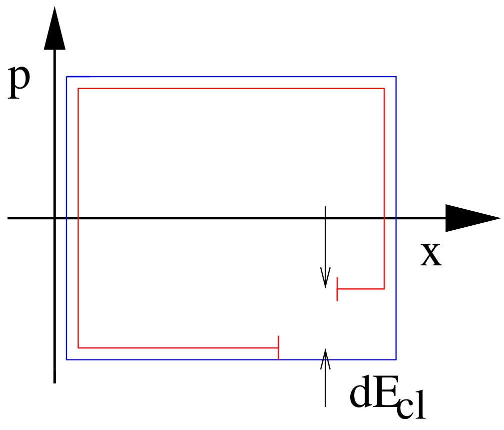
QM moments:

- $r = 1$
  $\langle p_2 - p_1 \rangle \; = 2\pi u \times v_{\mathrm{E}} t - 2\pi \sin(u v_{\mathrm{E}} t)$
- $r = 2$
  $\langle (p_2 - p_1)^2 \rangle \; = 2\pi u^2 \times v_{\mathrm{E}} t$
- $r > 2$
  $\langle (p_2 - p_1)^r \rangle = \infty$

The second moment is identical to the classical one, and the first moment has a modulation part in addition.

Moving Wall



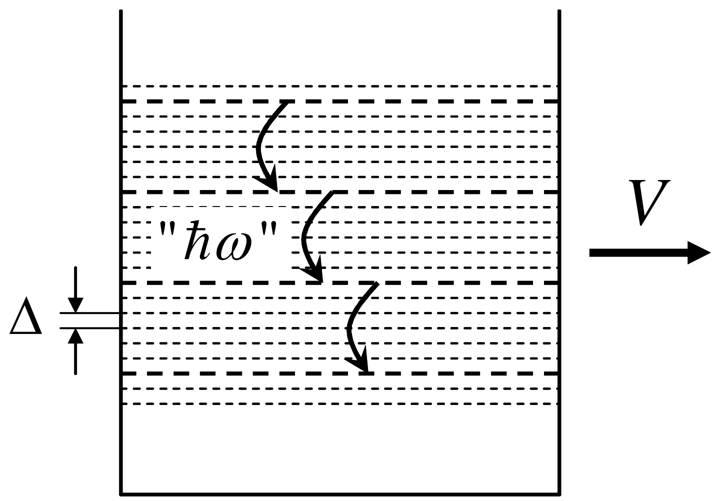


$\delta E_{\rm cl} = 2MvV$

- QM picture

$\delta E_{\rm cl} \ll \Delta \iff V \ll \frac{\hbar}{ML} \iff$ adiabatic behavior

Otherwise, the behavior is different:



AC driving $\implies$ FGR: $\hbar\omega = E_n - E_m$

In our problem there is no AC driving!

Is there a self-generated ω?:

$"\hbar\omega" = dE_{\rm col} = 2MvV$

YES!

Moving Wall

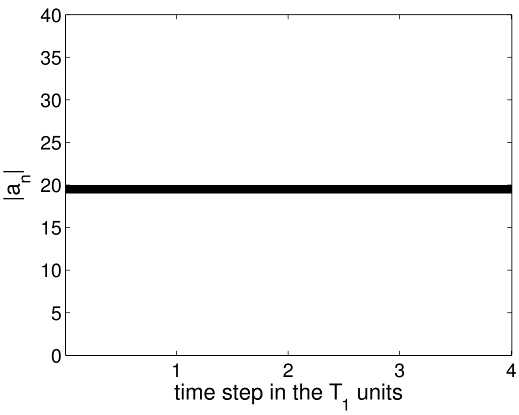
Numerical Solution

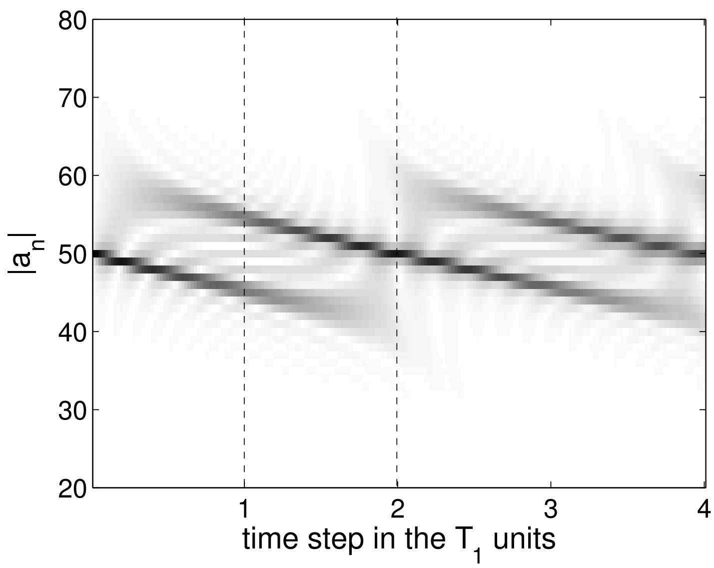
$$\frac{da_n}{dt} = -\frac{i}{\hbar}E_n a_n - \frac{V}{L}\sum_{m(\neq n)} \frac{2nm}{n^2 - m^2}\, a_m$$

Density plots of $a_n(t)$:

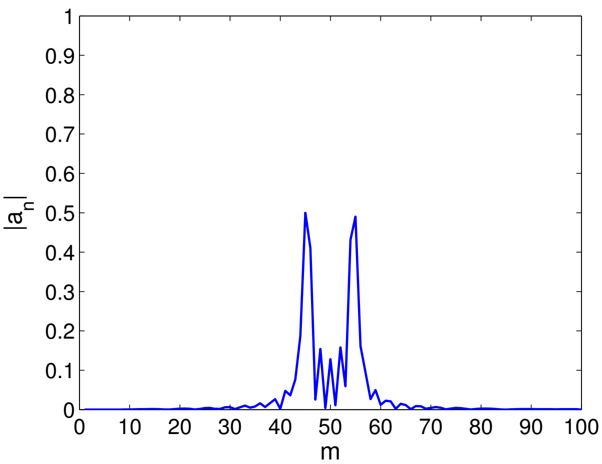
Semiclassical:

Adiabatic:

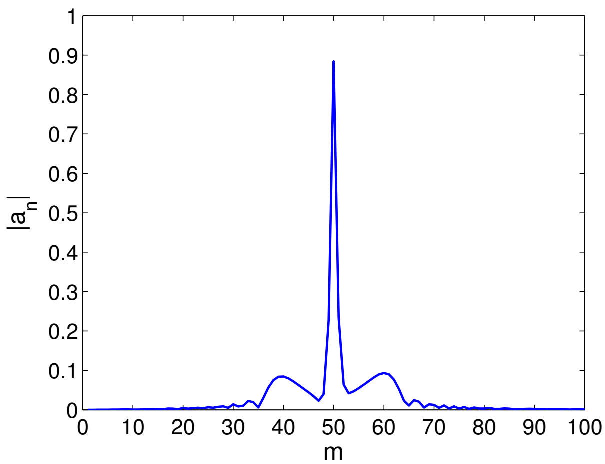




a_n VS. m for T_1 time



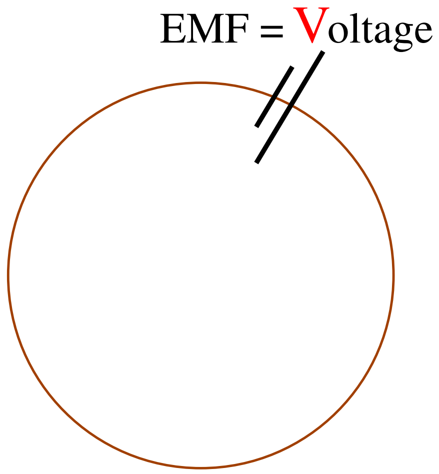
a_n VS. m for $2T_1$ time

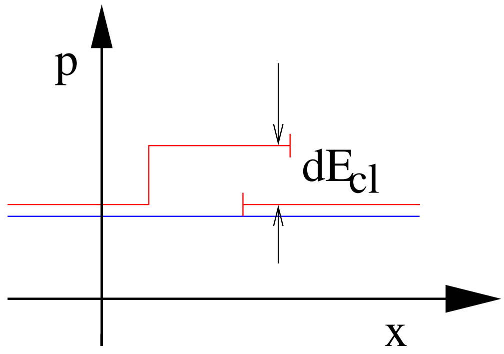


The plots are not so simple!

Ring

Description





$\delta E_{\text{cl}} = eV$

$A = \Phi\delta(x - x_0)$ - the vector potential.

$\mathcal{E} = -\frac{1}{c}\dot{\Phi}\delta(x - x_0)$ - the electric field.

Note: Gauge Invariance

$$A' = A - \nabla\Lambda \qquad U' = U + \frac{1}{c}\frac{\partial\Lambda}{\partial t}$$

The problem was solved in the following ways:

- Analytical solution (for linear energies)
- Numerical solution (for linear energies)
- Numerical solution (for quadratic energies)

Ring

Numerics/Solution

Hamiltonian:

$$H = \frac{1}{2M}\left(p - \frac{e}{c}A(t)\right)^2$$

Periodic boundary conditions:

$$\Psi(x) = \Psi(x+L)$$

Schrodinger equation:

$$\frac{da_n}{dt} = -\frac{\imath}{\hbar}a_n E_n - \alpha \sum_{m(\neq n)} \frac{1}{n-m} a_m, \quad \alpha = \frac{\dot{\Phi}}{\Phi_0}$$

$$E_n = \frac{1}{2M}\left(\frac{2\pi\hbar}{L}\right)^2\left(n - \frac{\Phi(t)}{\Phi_0}\right)^2$$

Analytical solution for $E_n = \Phi_c^2 - 2\Phi_c n$:

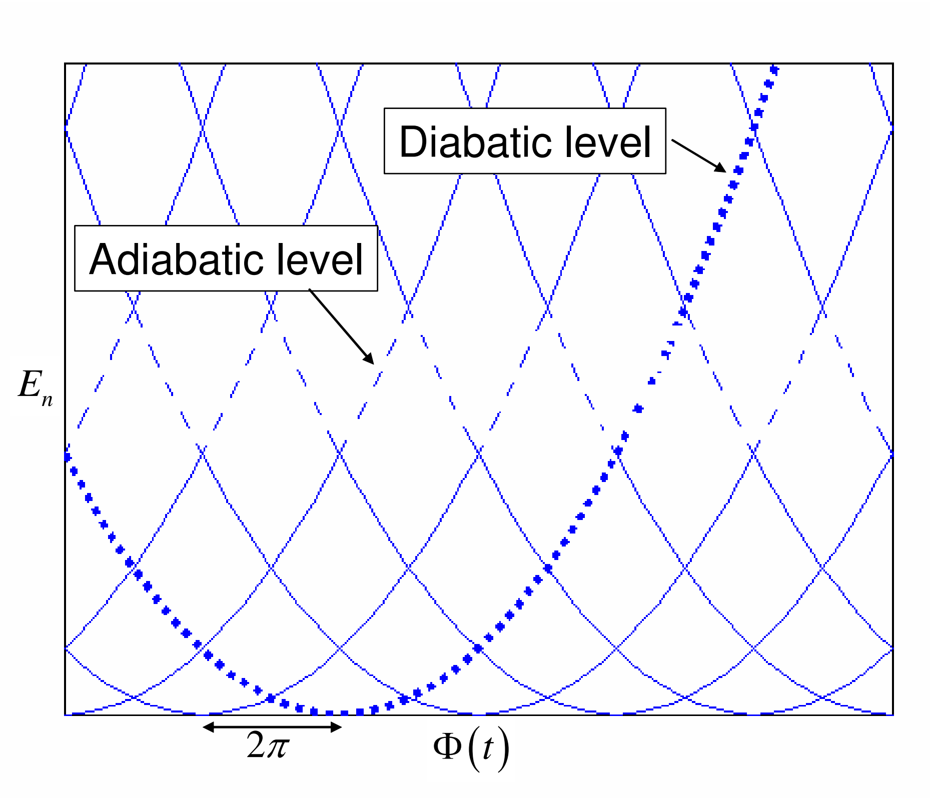
$$|a_n(t)|^2 = \left(\frac{\alpha}{\Phi_c}\right)^2 \frac{\sin^2\left(\Phi_c t\left(n - n_0 + \alpha(t - \frac{\pi}{\Phi_c})\right)\right)}{(n - n_0 + \alpha t)^2 (n - n_0 + \alpha(t - \frac{\pi}{\Phi_c}))^2}$$

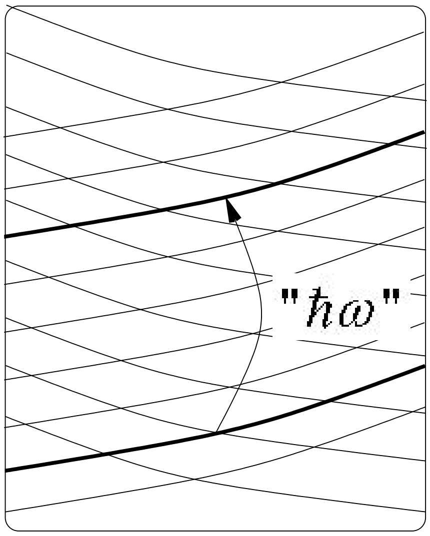
MOVIE

Ring

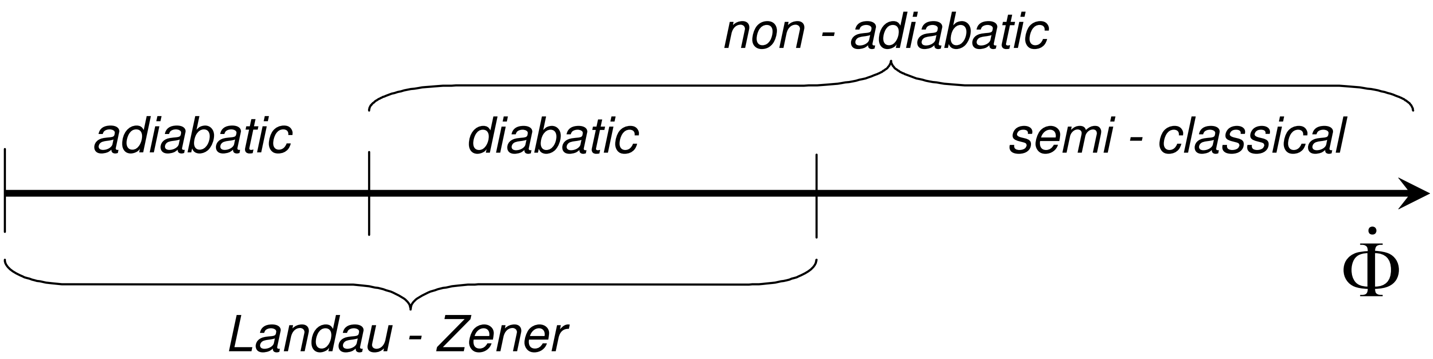
QM picture

Energy levels: $E_n = \frac{1}{2M}\left(\frac{2\pi\hbar}{L}\right)^2\left(n - \frac{\Phi}{\Phi_0}\right)^2$





Different regimes:



Is there a self-generated ω?

"$\hbar\omega$" $= eV$

YES!

Ring

Analysis

Hamiltonian:

$$H = \frac{1}{2M}\left(p - \frac{e}{c}A(t)\right)^2$$

Periodic boundary conditions:

$$\Psi(x) = \Psi(x+L)$$

The Schrodinger equation:

$$\frac{da_n}{dt} = -\frac{\imath}{\hbar}a_n E_n - \frac{\dot{\Phi}}{\Phi_0}\sum_{m(\neq n)}\frac{1}{n-m}a_m$$

where

$$E_n = \frac{1}{2M}\left(\frac{2\pi\hbar}{L}\right)^2\left(n - \frac{\Phi(t)}{\Phi_0}\right)^2$$

Note: Moving Wall

$$\frac{da_n}{dt} = -\frac{i}{\hbar}E_n a_n - \frac{V}{L}\sum_{m(\neq n)}\frac{2nm}{n^2-m^2}\,a_m$$

$$E_n = \frac{\hbar^2\pi^2}{2ML^2}n^2$$

Ring

Derivation of the "ring" equation

Strategy:

- $A = \tilde{A} + \nabla\Lambda$ does not change the fields.
- Find a potential which can be solved easily and then find the gauge function Λ.
  $\Longrightarrow \quad \tilde{A} = \frac{\Phi}{L}$

$$\Lambda(x) = \begin{cases} -\frac{\Phi}{L}x & , \; 0 < x < \frac{L}{2} \\ -\frac{\Phi}{L}x + \Phi & , \; \frac{L}{2} < x < L \end{cases}$$

- Verify that $\oint \tilde{A} \cdot dl = \oint A \cdot dl$.
- Find the new wave functions for our original potential by: $\Psi = \tilde{\Psi} \exp\left(\frac{\imath e}{\hbar c}\Lambda\right)$

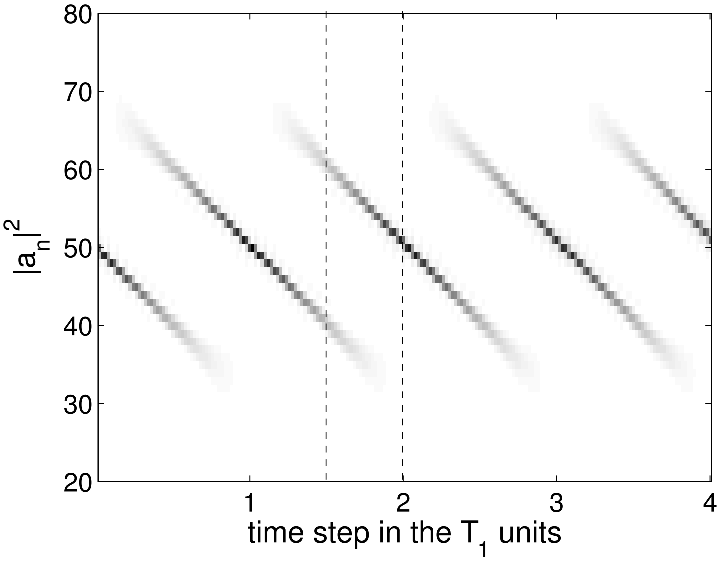
Use the standard procedure and obtain:

$$\frac{da_n}{dt} = -\frac{\imath}{\hbar} a_n E_n - \sum_{m(\neq n)} a_m \left\langle \psi_m \middle| \frac{d}{dt} \middle| \psi_n \right\rangle$$

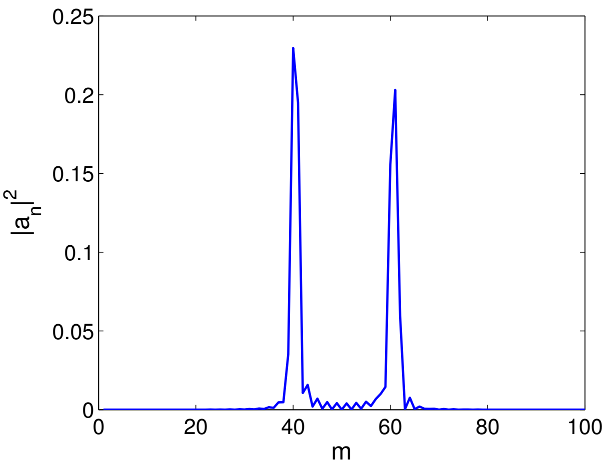
Ring

Numerical Solution - Evolution Matrix

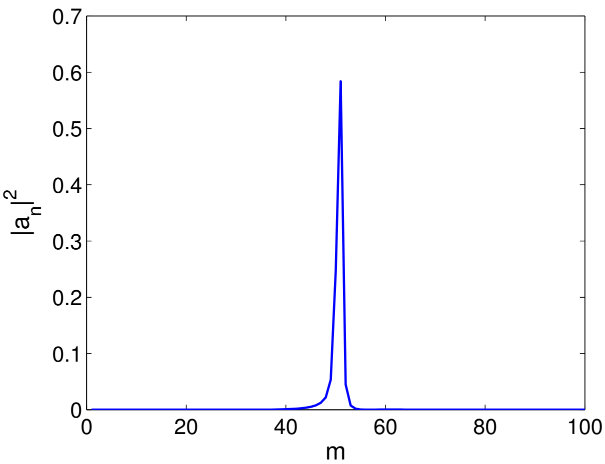
The density plot of $a_n(t)$



The plot of a_n VS. m for $1.5T_1$ time



The plot of a_n VS. m for $2T_1$ time



The Hamiltonian depends on time explicitly.

$\Rightarrow$ The evolution operator $U = e^{-\frac{i}{\hbar}Ht}$ is meaningless.

BUT: If $\Phi(t) \gg \dot{\Phi}t$ we may approximate $\Phi(t) = \text{const}$.

Ring

Fourier Method

The equation:

$$\frac{da_n}{dt} = -\frac{\imath}{\hbar} E_n a_n + \alpha \sum_{m(\neq n)} \frac{1}{n-m} a_m$$

$$E_n = \frac{1}{2M}\left(\frac{2\pi\hbar}{L}\right)^2 \left(n - \frac{\Phi(t)}{\Phi_0}\right)^2 , \qquad \Phi(t) = \Phi_{\text{const}} + \dot{\Phi} t$$

If $\Phi(t) \gg \dot{\Phi} t$ we may approximate $\Phi(t) = \text{const}$.

$$A_k = \sum_{n=-\infty}^{\infty} a_n \mathrm{e}^{-\imath k n}$$

$$a_n = \frac{1}{2\pi} \int_0^{2\pi} A_k \mathrm{e}^{\imath k n}$$

Bloch electorns in a lattice $\Rightarrow$ k basis.

$\sum_{m(\neq n)} \frac{1}{n-m} a_m$ is a convolution for m!!!

Omitting prefactors: $E_n = n^2 - 2\Phi_c n + \Phi_c^2$

- $E_n = 0,\ E_n = \Phi_c^2 - 2\Phi_c n$ - Analytical
- $E_n = \Phi_c^2 - 2\Phi_c n,\ E_n = (n - \Phi_c)^2$ - Numerical

Ring

Preliminary calculation

$$\frac{da_n}{dt} = \alpha \sum_{m(\neq n)} \frac{1}{n-m} a_m \; , \quad (E_n = 0)$$

Initial conditions: $a_n(t) = \delta_{n,n_0}$.

Fourier transforms:

$$\begin{aligned} A_k(t) &= \sum_{n=-\infty}^{\infty} a_n \mathrm{e}^{-\imath kn} \\ E_k &= \alpha \sum_{n=-\infty}^{\infty} \frac{\mathrm{e}^{-\imath kn}}{n}, \quad n \neq 0 \end{aligned}$$

Therefore:

$$\begin{aligned} \frac{d}{dt} A_k(t) &= E_k A_k(t) \\ A_k(t=0) &= \mathrm{e}^{-\imath k n_0} \end{aligned}$$

Solving the equation and performing the inverse transform one can obtain:

$$a_n(t) = \frac{\sin \pi \alpha t}{\pi(\alpha t + n - n_0)}$$

Ring

Analytical Solution

$$\frac{da_n}{dt} = -\imath E_n a_n + \alpha \sum_{m(\neq n)} \frac{1}{n-m} a_m$$

$$a_n = \tilde{a}_n \mathrm{e}^{-\imath E_n t}$$

$$\Rightarrow \frac{d\tilde{a_n}}{dt} = \alpha \sum_{m(\neq n)} \frac{\mathrm{e}^{\imath(E_n - E_m)t}}{n-m} \tilde{a}_m$$

The RHS is a convolution for $E_n - E_m \sim n - m$.

So approximate: $E_n = \Phi_c^2 - 2\Phi_c n$.

This equation can be solved analytically using the Fourier method (but the solution is a little bit tricky...)

$$|a_n(t)|^2 = \left(\frac{\alpha}{\Phi_c}\right)^2 \frac{\sin^2\left(\Phi_c t \left(n - n_0 + \alpha(t - \frac{\pi}{\Phi_c})\right)\right)}{(n - n_0 + \alpha t)^2 (n - n_0 + \alpha(t - \frac{\pi}{\Phi_c}))^2}$$

Ring

Analytical Solution - Discussion

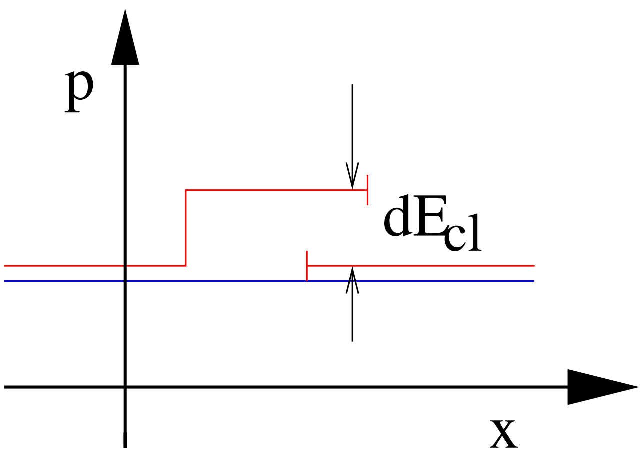
The solution:

$$|a_n(t)|^2 = \left(\frac{\alpha}{\Phi_c}\right)^2 \frac{\sin^2\left(\Phi_c t\left(n - n_0 + \alpha(t - \frac{\pi}{\Phi_c})\right)\right)}{(n - n_0 + \alpha t)^2 (n - n_0 + \alpha(t - \frac{\pi}{\Phi_c}))^2}$$

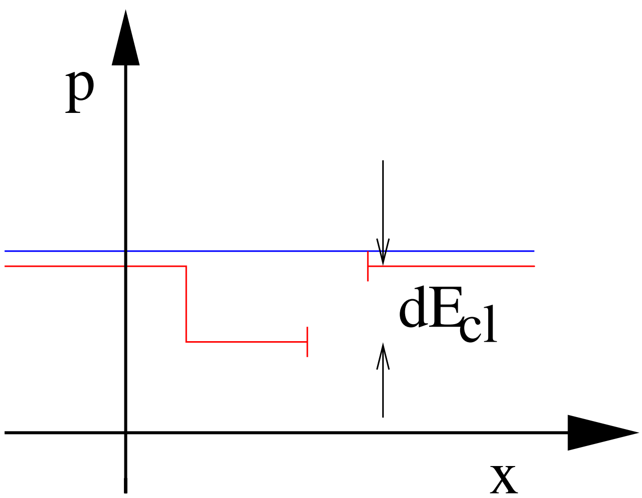
Compare to the "step potential":

$$|\langle p_2|\mathcal{U}|p_1\rangle|^2 = 4u^2 \frac{\sin^2 \frac{(p_2 - p_1 - u)v_{\mathrm{E}} t}{2}}{(p_2 - p_1)^2 (p_2 - p_1 - u)^2}$$

- The behavior is very similar!



"Ring"



"Step"

Ring

Numerical Solution

Write **the** equation

$$\frac{da_n}{dt} = -\imath E_n a_n + \alpha \sum_{m(\neq n)} \frac{1}{n-m} a_m = P_1 a_n + P_2 a_n$$

We saw that for $a_n(0) = \delta_{n,n_0}$ the solution for $E_n = 0$ is:

$$a_n(t) = \frac{\sin \pi\alpha t}{\pi(\alpha t + n - n_0)}$$

For the case of $a_n(0) = b_n$ the solution for $E_n = 0$ is:

$$a_n(t) = \frac{\sin \pi\alpha t}{\pi} \sum_m \frac{b_n}{\alpha t + n - m}$$

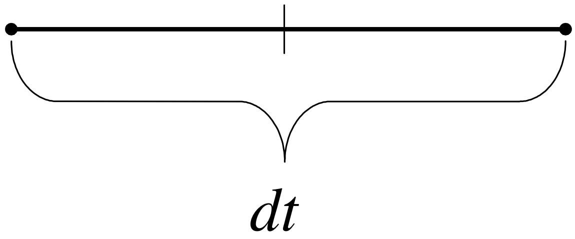
It is a convolution!!!

The equation $\frac{da_n}{dt} = P_1 a_n$ is solved analytically.

Ring

Numerical Solution - Cont.

"Split" algorithm



1. P_1 with the step $\Delta t = 0.5dt$
2. P_2 with the step $\Delta t = 0.5dt$ and the initial conditions which are the results of the previous step.
   Calculated using the FFT algorithm.
3. P_1 with the step $\Delta t = 0.5dt$ and the initial conditions which are the results of the previous step.

Advantages of this algorithm:

- has no limitations for E_n - it may depend on time **explicitly**
- much faster than the "evolution matrix method"
- uses less memory

Summary

1. The theory of response requires a theory for an energy spreading.

   $\delta E^r = ?\ , \qquad r = 1, 2, ...$

2. Beyond the Bohr correspondence:
   distinction between the restricted and detailed QCC.

3. Detailed QCC is fragile.

   Examples:

   - step
   - moving wall
   - ring

4. We shed new light on the energy spreading process in the case of a EMF-driven ring.

5. The semi-classical limit is not perturbative.

6. In order to derive the "LRT" one cannot use perturbation theory - even not to the infinite order.