Lecture # 4, Quantum physics 3

Main points of # 3

- Finished discussion of harmonic oscillator
- Discussed Ehrenfest theorem
- Discussed Lagrange & Hamiltonian formulation of classical mechanics
- Derived the following representation of evolution operator in QM:

$$\langle x_f | U(t_f, t_i) | x_i \rangle = \lim_{N \to \infty} \int \mathcal{D}p \mathcal{D}x \, e^{i/\hbar S_{cl}}$$

$$\mathcal{D}p \mathcal{D}x = \frac{dp_N}{2\pi\hbar} \cdots \frac{dp_{N-1} dx_{N-1}}{2\pi\hbar} \cdots \frac{dp_1 dx_1}{2\pi\hbar}$$

$$S_{cl} = \left[p_N \left(\frac{x_N - x_{N-1}}{\Delta t} \right) + \ldots p_1 \frac{x_1 - x_0}{\Delta t} \right] \Delta t$$

$$- \left[H(p_N, x_{N-1}) + \ldots + H(p_1, x_0) \right] \Delta t \simeq$$

$$\simeq \int_{t_i}^{t_f} (p\dot{x} - H) dt$$

- Integrated over momenta in „continuum" representation,

$$\langle x_f | U | x_i \rangle = \int \mathcal{D}p \mathcal{D}x \ \exp\left[\frac{i}{\hbar}\int_{t_i}^{t_f}\left(p\dot{x} - \frac{p^2}{2m} - V(x)\right)dt\right] =$$

$$\bar{N} \int \mathcal{D}x \ \exp \frac{i}{\hbar} S_{cl}$$

where $\bar{N}$ is some constant we did not compute, and

$$S = \int_{t_i}^{t_f}\left(\frac{\dot{x}^2}{2m} - V(x)\right)dt$$ is the

classical action

Plan:

- Computation of $\bar{N}$
- Computation of path integral for free particle
- Physical interpretation
- Principle of minimal action from path integral

Integral over momentum, precisely:

$$\int \frac{dp_N}{(2\pi\hbar)} \exp\left[\left\{-\frac{p_N^2}{2m} + \frac{p_N(x_N - x_{N-1})}{\Delta t}\right\} \cdot \frac{i}{\hbar} \Delta t\right]$$

F-la for Gaussian integrals:

$$\int_{-\infty}^{+\infty} e^{-ax^2+bx} dx = \sqrt{\frac{\pi}{a}}\, e^{\frac{b^2}{4a}} \text{ , if } \operatorname{Re} a > 0$$

In our case a and b are pure imaginary, $a = i|a|$, $b = i|b|$.

Analytic continuation:

$$\int_{-\infty}^{+\infty} e^{-i|a|x^2+bx} dx \to \int_{-\infty}^{+\infty} e^{-i|a|x^2+bx-\varepsilon|x|} dx,$$

ε is small positive number, $\varepsilon \to 0$

$$= \sqrt{\frac{\pi}{i|a|}} \exp\left(\frac{b^2}{4a}\right)$$

For our case: $a = + \frac{1}{2m} \cdot \frac{i}{\hbar} \Delta t$

$$b = (x_N - x_{N-1}) \cdot \frac{i}{\hbar}$$

$$* = \frac{1}{(2\pi\hbar)} \cdot \sqrt{\frac{\pi}{+\frac{1}{2m}\frac{i}{\hbar}\Delta t}} \exp\left[-\frac{(x_N - x_{N-1})^2 \frac{1}{\hbar^2}}{2 \cdot \cancel{2} \cdot \left(+\frac{1}{\cancel{2}m}\frac{i}{\hbar}\Delta t\right)}\right]$$

$$= \frac{1}{(2\pi\hbar)} \left(\frac{2\pi m \hbar}{i \Delta t}\right)^{1/2} \exp\left[+ \frac{m(x_N - x_{N-1})^2}{2 \cdot \Delta t} \frac{i}{\hbar}\right]$$

Finally,

$$\langle x_f | U | x_i \rangle = \lim_{N \to \infty} \underbrace{\left[\frac{1}{2\pi\hbar}\left(\frac{2\pi m \hbar}{i \Delta t}\right)^{1/2}\right]^N}_{\left(\frac{m}{2\pi i \hbar \Delta t}\right)^{N/2}} \cdot$$

$$\cdot \int dx_{N-1} \ldots dx_1 \cdot$$

$$\cdot \exp\left[\frac{i}{\hbar}\left\{\frac{m(x_N - x_{N-1})^2}{2(\Delta t)^2} + \ldots \frac{m(x_1 - x_0)^2}{2(\Delta t)^2} - \right.\right.$$

$$\left.\left. - V(x_{N-1}) - \ldots - V(x_0)\right\} \cdot \Delta t\right]$$

This gives the value of $\overline{N}$

Computation of path-integrals.

Simplest example: free particle,

$$L = \frac{m\dot{x}^2}{2}$$

$$\langle x_f | U(t_f, t_i) | x_i \rangle = \bar{N} \int \Pi dx \exp\left[+ \frac{i}{\hbar} \int_{t_i}^{t_f} \frac{m\dot{x}^2}{2} \right] =$$

$$= \lim_{\varepsilon \to 0} \left[\frac{m}{2\pi i \hbar \Delta t} \right]^{\frac{1}{2} \cdot N} \cdot \int dx_1 \ldots dx_{N-1} \cdot$$

$$\cdot \exp\left[\frac{i}{\hbar} \sum_{i=1}^{N} \frac{(x_i - x_{i-1})^2 \cdot m}{2 \Delta t} \right],$$

with $x_N = x_f$; $x_0 = x_i$

Let us take for simplicity even N

"odd" integrations

$x_4 \quad x_3 \quad x_2 \quad x_1 \quad x_0$

even integration

Compute integration over x_1: $(x_2 - x_1)^2 + (x_1 - x_0)^2 =$

$$x_2^2 - 2x_2 x_1 + x_1^2 + x_1^2 - 2x_1 x_0 + x_0^2 \to$$

$$\to x_2^2 + x_0^2 + 2\left(x_1^2 - x_1(x_0 + x_2)\right)$$

$$\int dx_1 \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{1/2} \exp\left[\frac{im}{2\Delta t\hbar}\left(2x_1^2 - 2x_1(x_0+x_2) + x_0^2 + x_2^2\right)\right.$$

$$= \int dx_1 \left[\frac{m}{2\pi i\hbar\cdot\Delta t}\right]^{1/2} \cdot \exp\left[\frac{im}{2\hbar\Delta t}\left[(\delta x_1)^2\cdot 2\right.\right.$$

$$\left.\left. + 2\left(\frac{x_0+x_2}{2}\right)^2 - 2\frac{(x_0+x_2)^2}{2} + (x_0^2+x_2^2)\right]\right]$$

For Gaussian integral:

$$\frac{\partial}{\partial x_1}\left(x_1^2 - x_1(x_0+x_2)\right) = 2x_1 - (x_0+x_2) \Rightarrow$$

Change of variables $x_1 = \frac{x_0+x_2}{2} + \delta x_1$

$$\frac{\partial^2}{\partial x_1^2}(\qquad) = 2$$

$$= \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{1/2} \cdot \exp\left[\frac{im}{2\hbar\Delta t}\left(x_0^2+x_2^2 - \frac{1}{2}x_0^2 - \frac{1}{2}x_2^2 - x_0x_2\right)\right]$$

$$\cdot \left(\frac{2\pi\hbar\Delta t}{-im\cdot 2}\right)^{1/2} =$$

$$= \frac{1}{\sqrt{2}} \cdot \exp\left[\frac{im}{2\hbar\cdot 2\Delta t}(x_0-x_2)^2\right]$$

So, after integration over odd points, we get the integration over even points, with replacement everywhere of Δt to $2\Delta t$, due to prefactor $\frac{1}{\sqrt{2}}$

and due to $\Delta t \to 2\Delta t$ in the exponential.

Now, we repeat the procedure, and get for exponential

$$\exp\left[\frac{im}{2\hbar(t_f - t_i)}(x_f - x_i)^2\right],$$

and for the pre-factor

$$\left[\frac{m}{2\pi i\hbar(t_f - t_i)}\right]^{1/2},$$ making the result

$$\langle x_f | U(t_f, t_i) | x_i \rangle =$$

$$\left[\frac{m}{2\pi i\hbar(t_f - t_i)}\right]^{1/2} \exp\left[\frac{im}{2\hbar(t_f - t_i)}(x_f - x_i)^2\right]$$

In fact, it is very easy to get an exponential factor in the saddle-point approximation:

action: $\int_{t_i}^{t_f} \frac{m(\dot{x})^2}{2} dt$

Classical trajectory:

$$\ddot{x} = 0 \Rightarrow \dot{x} = \text{const} \Rightarrow x = at + b.$$

initial condition:

$$x_i = a t_i + b$$

final point:

$$x_f = a t_f + b$$

$$\Rightarrow x_f - x_i = a(t_f - t_i); \quad a = \frac{x_f - x_i}{t_f - t_i} \Rightarrow$$

$$x = \frac{x_f - x_i}{t_f - t_i} \cdot t + b \Rightarrow$$

$$\dot{x} = \left(\frac{x_f - x_i}{t_f - t_i}\right) \Rightarrow$$

$$S_{cl} = \frac{1}{2} m \left(\frac{x_f - x_i}{t_f - t_i}\right)^2 \cdot (t_f - t_i)$$

So, in saddle-point approximation

$$\langle x_f | U(t_f, t_i) | x_i \rangle =$$

$$\exp\left[\frac{i}{\hbar} \frac{m}{2} \frac{(x_f - x_i)^2}{(t_f - t_i)}\right] \cdot \underbrace{\bar{N} \int \mathcal{D}x \left[\frac{i}{\hbar} \int_{t_i}^{t_f} m \frac{(\delta \dot{x})^2}{2} dt\right]}_{\text{„prefactor"}},$$

where the boundary conditions for δx are : $\delta x\big|_{t_i} = \delta x\big|_{t_f} = 0$

The accurate computation we done before, fixes the prefactor.

Double check: „old" quantum mechanics:

$$\langle x_f | \exp\left[-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}(t_f - t_i)\right] | x_i \rangle =$$

$$= \int \langle x_f | \exp\left[-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}(t_f - t_i)\right] | p \rangle \langle p | x_i \rangle \, dp$$

$$= \int \exp\left[-\frac{i}{\hbar}\frac{p^2}{2m}(t_f - t_i)\right] \langle x_f | p \rangle \langle p | x_i \rangle \, dp$$

$$= \int \exp\left[-\frac{i}{\hbar}\frac{p^2}{2m}(t_f - t_i) + i\frac{p(x_f - x_i)}{\hbar}\right] \frac{dp}{2\pi\hbar} = *$$

again change of variables :

$$-\frac{i}{\hbar}\frac{p}{m}(t_f - t_i) + \frac{i}{\hbar}(x_f - x_i) = 0;$$

$$p = \frac{m(x_f - x_i)}{(t_f - t_i)}$$

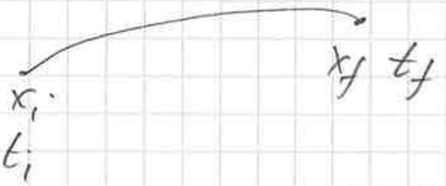
$$* = \underbrace{\exp\left[\frac{i}{\hbar} m \frac{(x_f - x_i)^2}{(t_f - t_i)}\right]}_{e^{iS_{cl}/\hbar}} \cdot \int_{-\infty}^{+\infty} e^{-\frac{i}{\hbar}\frac{p^2}{2m}(t_f - t_i)} \cdot \frac{dp}{2\pi\hbar} =$$

$$= \exp\left(\frac{i}{\hbar} S_{cl}\right) \cdot \frac{1}{2\pi\hbar} \cdot \sqrt{\frac{2\pi}{+\frac{i}{\hbar}\,\frac{t_f - t_i}{m}}} =$$

$$= \exp\left(\frac{i}{\hbar} S_{cl}\right) \cdot \left[\frac{m}{2\pi i \hbar (t_f - t_i)}\right]^{1/2} \qquad \underline{QED}$$

Physical interpretation:

The probability amplitude to go from point x_i at time t_i to point x_f at time t_f can be computed as follows:

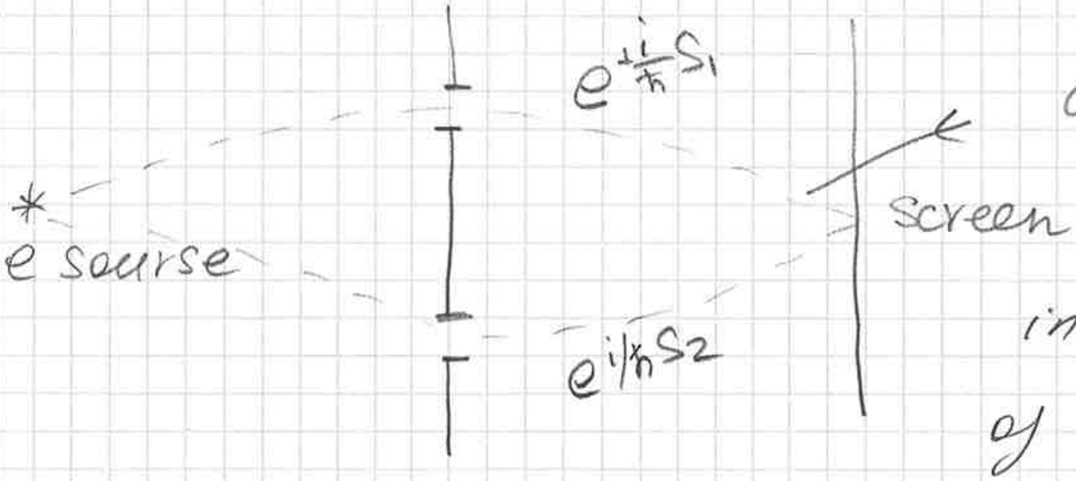


- take arbitrary trajectory connecting x_i and x_f, and compute classical action S corresponding this trajectory, the amplitude of probability is given by e^{iS}.

To get total amplitude, sum up all amplitudes corresponding to different trajectories,

$$A \sim \int \Pi dx \, e^{iS}$$

Electron and two holes:



complicated picture, interference of two possibilities.

Principle of minimal action.

Action S depends strongly on trajectory, and e^{iS} is in general a rapidly oscillating function. We can use this property to understand which trajectories are the most important ones. From mathematics: saddle point approximation:

$$\int_{-\infty}^{+\infty} dx\, f(x)\, e^{iA(x)} \approx \int_{-\infty}^{+\infty} dx\, f(x_0)\, e^{iA(x_0)} \cdot$$

$$\cdot \exp\left[i \tfrac{1}{2} A''(x_0)(x-x_0)^2\right] \approx f(x_0)\, e^{iA(x_0)} \cdot$$

$$(*) \qquad \cdot \sqrt{\frac{2\pi}{-iA''(x_0)}},$$

where $A'(x_0) = 0$, $A(x) \gg 1$ – i.e. we have a rapidly oscillating function.

[The validity of this f-la, coming from saddle point approximation, depends on analytic properties of function $A(x)$; square root in $(*)$ is defined in such a way that its real part is positive.]

For our path integral: the most-important trajectories are those for which

$\frac{\delta S}{\delta x(t)} = 0$ – exactly the principle of the minimal action! Under certain circumstances their contribution dominating the path integral, as all other contributions rapidly oscillate.

Applications of path integral:

statistical theory, QFT, theory of strong interactions.

Approximate methods:

numerics, N is finite; saddle point approximation.