Lecture # 3, Quantum physics 3

Main points of Lecture # 2

- Found coherent states $|\alpha\rangle$:

$$a|\alpha\rangle = \alpha|\alpha\rangle,$$

$$|\alpha\rangle = D(\alpha)\cdot|0\rangle; \quad D(\alpha) = \exp(\alpha a^{+} - \overset{*}{\alpha} a) -$$

unitary operator

- Found that $|\alpha\rangle$ - states minimise uncertainty relation,

$$\delta p \cdot \delta x = \frac{\hbar}{2}$$

- Found wave-function of $\alpha$-state in $x$ - representation and demonstrated that the probability distribution is a Gaussian packet which does not change its form and moves according to classical equations of motion

Plan:

- Ehrenfest theorem
- Path integral

The lessons from these considerations:

- the average values of observables follow classical evolution. We got this in two examples, but in fact this is true in general: Ehrenfest theorem.

For a generic 1d system:

$$H = \frac{p^2}{2m} + V(x) ;$$

in Heisenberg representation:

$$-\frac{\hbar}{i}\dot{\hat{x}} = [\hat{x}, \hat{H}] = \frac{i\hbar \hat{p}}{m} \Rightarrow \dot{\hat{x}} = \frac{\hat{p}}{m}$$

$$-\frac{\hbar}{i}\dot{\hat{p}} = [\hat{p}, \hat{H}] = -i\hbar \frac{\partial V}{\partial x} \Rightarrow$$

$$\dot{\hat{p}} = -\frac{\partial V}{\partial x} = F(x)$$

For any state we get

$$\left.\begin{aligned} \langle \dot{x} \rangle &= \frac{1}{m} \langle p(t) \rangle \\ \langle \dot{p} \rangle &= \langle F(x) \rangle \end{aligned}\right\} \text{ almost classical equations.}$$

Difference: $\langle F(x) \rangle \neq F(\langle x \rangle)$ for non-linear systems.

There are specific "semiclassical" states: Gaussian wave packet for a free particle and coherent states for harmonic oscillator which behave like classical states within some limitation. So, classical physics is indeed a limiting case of quantum mechanics for particular situations.

Now, we will construct a systematic approach to quantum mechanics which will make the connection more obvious. It is based on Feynman path integral representation of Quantum mechanics.

# Quantum mechanics and path integrals

path integral ≡ functional integral

Plan

- Reminder of classical analytical mechanics
- Path - integral representation of the quantum evolution operator
- Schrödiger equation from path integral
- Physics interpretation
- Classical principle of minimal action from QM

Detailed study of path integral:
lectures by Alessandro Vichi,
Quantum physics 4, next semester

# Reminder of classical mechanics

## (i) Lagrangian formalism

State of the system: $x, \dot{x}$

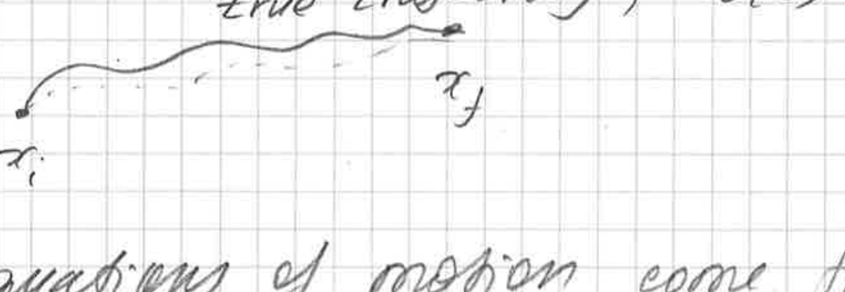
$x$ - generalized coordinate

$\dot{x}$ - generalized velocity

Main function, describing dynamics - Lagrangian $\mathcal{L}$, $\mathcal{L} = \mathcal{L}(x, \dot{x})$

Action principle: the system moves from point $x(t_i) = x_i$ to the point $x(t_f) = x_f$ is such a way that the action is minimal,

$$S \equiv \int_{t_i}^{t_f} \mathcal{L}(x, \dot{x})\, dt .$$




Equations of motion come from variation of the action. Action is a functional of trajectory, $S = S[x(t)]$

$x(t) = x_0(t) + \delta x(t)$; $\delta x(t) = 0$ for

$t = t_i$ and $t = t_f$.

$S[x(t)] - S[x_0(t)] =$

$$\int_{t_i}^{t_f} dt \left\{ \mathcal{L}(x_0 + \delta x, \dot{x}_0 + \delta \dot{x}) - \mathcal{L}(x_0, x_0) \right\} =$$

$$= \int_{t_i}^{t_f} dt \left\{ \frac{\partial \mathcal{L}}{\partial x} \delta x + \frac{\partial \mathcal{L}}{\partial \dot{x}} \delta \dot{x} \right\} dt =$$

(integrate by parts the second term)

$$= \int_{t_i}^{t_f} dt \, \delta q \left\{ \frac{\partial \mathcal{L}}{\partial x} - \frac{d}{dt}\left( \frac{\partial \mathcal{L}}{\partial \dot{x}} \right) \right\} = 0 \Rightarrow$$

Lagrange equations for true trajectory $x_0(t)$

$$\frac{\partial \mathcal{L}}{\partial x} - \frac{d}{dt}\left( \frac{\partial \mathcal{L}}{\partial \dot{x}} \right) = 0$$

Note: in integration by parts the boundary terms dissappear since $\delta x(t) = 0$ @ $t_i$ & $t_f$.

(ii) Hamiltonian formalism:

Define generalized momentum as

(*) $p = \frac{\partial \mathcal{L}}{\partial \dot{x}}$ and Hamiltonian as

$H = p\dot{x} - \mathcal{L}$, where $\dot{x}$ is expressed via $p$ from eq. (*). $H$ is a function of $p$ and $x$. Equations of motion are:

$$\dot{p} = -\frac{\partial H}{\partial x} \; ; \quad \dot{x} = \frac{\partial H}{\partial p} \; , \text{ or,}$$

for any variable,

$$\frac{\partial f}{\partial t} = \{f, H\} \, ,$$ where $\{\, , \}$ are the Poisson brackets,

$$\{f, H\} = \frac{\partial f}{\partial p}\frac{\partial H}{\partial x} - \frac{\partial f}{\partial x}\frac{\partial H}{\partial p}$$

Action via Hamiltonian:

$$S = \int_{t_i}^{t_f} [p\dot{x} - H] dt$$

# Path-integral representation of the evolution operator in quantum mechanics.

Schrödinger equation

$-\frac{\hbar}{i}\frac{\partial\psi}{\partial t} = H\psi$ has the solution

$$\psi(t_f) = e^{-\frac{i}{\hbar}H(t_f - t_i)}\psi_i \equiv U(t_f, t_i)\psi_i$$

(We assume that $H$ is time-independent.

Let us find the matrix element

$\langle x_f | U(t_f, t_i) | x_i \rangle$, which determines completely the evolution of the quantum system. We consider Hamiltonians of the type $\hat{H} = \frac{p^2}{2m} + V(x)$.

Reminder: in $x$-representation

$$|x_i\rangle = \delta(x - x_i)\ ;\ |x_f\rangle = \delta(x - x_f);$$

$$|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left[\frac{ipx}{\hbar}\right]$$

what can be written as

$$\langle x|x_i\rangle = \delta(x-x_i)\,; \quad \langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left[\frac{ipx}{\hbar}\right]$$

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left[-\frac{ipx}{\hbar}\right]$$

For Hamiltonian, we have:

$$\langle p|\hat{H}|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{-\frac{ipx}{\hbar}}\, \underbrace{H(p,x)}_{\text{classical Hamiltonian}}$$

Let us consider first the case when $t_f - t_i$ is very small. Then

$$U(t_f, t_i) \approx 1 - \frac{iH}{\hbar}(t_f - t_i), \quad \text{so that}$$

$$\langle p|U(t_f,t_i)|x\rangle \approx \frac{1}{\sqrt{2\pi\hbar}}\left(1 - \frac{iH(p,x)}{\hbar}(t_f - t_i)\right)\cdot$$

$$e^{-\frac{ipx}{\hbar}} \approx \frac{1}{\sqrt{2\pi\hbar}}\exp\left[-\frac{ipx}{\hbar} - \frac{iH(p,x)}{\hbar}(t_f - t_i)\right]$$

Then,

$$\langle x_f|U(t_f,t_i)|x_i\rangle = \int_{-\infty}^{+\infty}\langle x_f|p\rangle\langle p|U(t_f,t_i)|x_i\rangle\, dp$$

$$\approx \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dp\, \exp\left[\frac{ip(x_f - x_i)}{\hbar} - \frac{iH(p,x)(t_f - t_i)}{\hbar}\right]$$

We would like to have an expression for finite, not small $t_f - t_i$. Let us write

$$t_f - t_i = \Delta t \cdot N, \quad N \to \infty, \ \Delta t \to 0$$

(devide the time interval in many small steps)

$$U(t_f, t_i) = \left(\exp\left[-\frac{iH\Delta t}{\hbar}\right]\right)^N.$$


$$\exp\left[-\frac{iH\Delta t}{\hbar}\right]$$

$$\langle x_f | U(t_f, t_i) | x_i \rangle = \langle x_f | U(t_f, t_f - \Delta t) \cdot U(t_f - \Delta t, t_f - 2\Delta t) \ldots U(t_i + \Delta t, t_i) | x_i \rangle =$$

$$= \langle x_N | U_N \cdot U_{N-1} \ldots U_1 | x_0 \rangle =$$

$\boxed{\text{insertion of } |x\rangle\langle x| \text{ between}}$

$$= \int \langle x_N | U_N | x_{N-1} \rangle \langle x_{N-1} | U_{N-1} | x_{N-2} \rangle \ldots \langle x_1 | U_1 | x_0 \rangle \cdot dx_{N-1} \ldots dx_1$$

For every matrix element let us use the representation we found, introducing $p_1, \dots p_N$:

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

$$\exp\Big\{\frac{i}{\hbar}\Big[p_N(x_N - x_{N-1}) + p_{N-1}(x_{N-1} - x_{N-2}) + \dots\ p_1(x_1 - x_0)\Big]$$

$$- \frac{i}{\hbar}\Big[H(p_N, x_{N-1}) + \dots\ + H(p_1, x_0)\Big]\Delta t\Big\} \cdot$$

$$\cdot \frac{dp_N}{2\pi\hbar} \quad \frac{dp_{N-1}\, dx_{N-1}}{2\pi\hbar} \quad \dots \quad \frac{dp_1\, dx_1}{2\pi\hbar},$$

and the limit $N \to \infty$ should be taken.

Let us write (formally):

$$\frac{(x_N - x_{N-1})}{\Delta t} \cdot \Delta t = \dot{x}_N \Delta t,$$

$$\frac{x_{N-1} - x_{N-2}}{\Delta t} \cdot \Delta t = \dot{x}_{N-1} \Delta t,$$

Then,

$$\langle x_f | U(t_f, t_i) | x_i \rangle = \int \prod_t \frac{dp\, dx}{2\pi\hbar} \cdot \exp\Big(\frac{i}{\hbar}\int_{t_i}^{t_f} (p\dot{x} - H)\, dt\Big)$$

$$= \int \prod \frac{dp\, dx}{2\pi\hbar} \exp\Big(\frac{i}{\hbar}\int_{t_i}^{t_f} S_{cl}\, dt\Big)$$

This integral can be simplified, since integration over momenta is Gaussian:

$$\int \Pi \frac{dp\,dx}{2\pi\hbar} \exp\left[\frac{i}{\hbar}\int_{t_i}^{t_f}\left(p\dot{x}-\frac{p^2}{2m}-V(x)\right)dt\right]$$

According to the general rules for Gaussian integral computation, make a shift: $p \to p' + m\dot{x} \Rightarrow$

$$p\dot{x}-\frac{p^2}{2m} = -\frac{1}{2m}(p'+m\dot{x})^2 + (p'+m\dot{x})\cdot\dot{x} =$$

$$= -\frac{p'^2}{2m} + \frac{1}{2}m\dot{x}^2 \Rightarrow$$

$$\int \Pi \frac{dp\,dx}{2\pi\hbar} \exp\left[\frac{i}{\hbar}\int_{t_i}^{t_f}\left(-\frac{p'^2}{2m} - V(x) + \frac{1}{2}m\dot{x}^2\right)dt\right]$$

$$= \underbrace{\int \Pi \frac{dp'}{2\pi\hbar} \exp\left[-\frac{i}{\hbar}\int_{t_i}^{t_f}\frac{p'^2}{2m}\,dt\right]}\cdot$$

$$\cdot \int \Pi dx \exp\left[\frac{i}{\hbar}\int_{t_i}^{t_f}\left(\frac{\dot{x}^2}{2m} - V(x)\right)dt\right]$$

This is a factor which does not depend on

$x_i$ and $x_f$, we denote it $\bar{N}$.

Final result:

$$(**)\quad \langle x_f | U(t_f, t_i) | x_i \rangle = \bar{N} \int \prod dx \, \exp\left(\frac{i}{\hbar} S\right),$$

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

the classical action.