Lecture # 5, Quantum physics 3

Main points of # 4.

- found that

$$\langle x_f | U(t_f, t_i) | x_i \rangle = \bar{N} \int \mathcal{D}x \, \exp\left[\frac{i}{\hbar} S_{cl}\right] \quad (*)$$

$$S_{cl} = \int_{t_i}^{t_f} dt \left(\frac{mv^2}{2} - V(x)\right) \text{- classical action}$$

- Discussed physical interpretation
- discussed saddle point method and found that formally, when $\hbar \to 0$, saddle point of $(*)$ coincides with classical trajectory $\frac{\delta S_{cl}}{\delta x} = 0$

- Mathematical aspects of the saddle-point method are discussed in Addendum to lecture # 4 and in exercises to Lecture # 3

Plan

- Semiclassical (WKB) approximation

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Semiclassical Approximation

Other name: WKB approximation

W = Wentzel

K = Kramers

B = Brillouin

intuition: if $\hbar = 0$, then we should get classical physics: $[\hat{p}, \hat{x}] = -i\hbar$ and if $\hbar = 0$, then $[\hat{p}, \hat{x}] = 0 \Rightarrow p$ & x are not operators, just c-numbers, as we expect them to be in classical physics. So, we should try to find a limit of QM when $\hbar \to 0$

Remark: $\hbar$ is a dimenfull quantity, with dimension of erg·s (or joule·s), so it does not make sense to say that $\hbar \to 0$. It is some dimensionless ratio, to be specified later, which must go to zero.

Let us start from time-independent problem: determination of energy levels of quantum-mechanical system in 1 dim:

$$H\psi = E\psi; \quad -\frac{\hbar^2}{2m}\psi'' + U(x)\psi(x) = E\psi(x)$$

Formal limit $\hbar = 0$ leads to nonsense.

Idea: use some clever representation for ψ, which will make formal expansion with respect to $\hbar$ possible.

$$\psi = e^{\frac{i}{\hbar}S} \quad \Rightarrow \quad \psi' = \frac{i}{\hbar}S' e^{\frac{i}{\hbar}S}$$

$$\psi'' = \frac{i}{\hbar}S'' e^{\frac{i}{\hbar}S} - \frac{1}{\hbar^2}(S')^2 e^{\frac{i}{\hbar}S}$$

Equation for S:

$$\left\{-\frac{\hbar^2}{2m}\left[\frac{i}{\hbar}S'' - \frac{1}{\hbar^2}(S')^2\right] + U(x)\right\} = E$$

or, $-\frac{i\hbar}{2m}S'' + \frac{1}{2m}(S')^2 = E - U$

Price to pay: linear eq for ψ is transformed into non-linear equation for S, but expansion with respect to $\hbar$ now becomes possible:

$$S = S_0 + \frac{\hbar}{i} S_1 + \left(\frac{\hbar}{i}\right)^2 S_2 + \ldots$$

$$S' = S_0' + \frac{\hbar}{i} S_1' + \left(\frac{\hbar}{i}\right)^2 S_2'$$

$$(S')^2 = (S_0')^2 + \frac{\hbar}{i} 2 S_0' S_1' + \left(\frac{\hbar}{i}\right)^2 \left(2 S_0' S_2' + (S_1')^2\right)$$

$$+ \ldots$$

$$S'' = S_0'' + \frac{\hbar}{i} S_1'' + \left(\frac{\hbar}{i}\right)^2 S_2''$$

0 order in $\hbar$:

$$\frac{1}{2m} (S_0')^2 = E - U \ ;$$

$$S_0 = \pm \int \sqrt{2m(E-U)}\, dx$$

For a classical system we would have: $\dfrac{p^2}{2m} + U(x) = E$, i.e

$$p = \sqrt{2m(E-U)}$$

So, we can write

$$S_0 = \pm \int p(x)\, dx$$

1st order in $\hbar$:

$$-\frac{i\hbar}{2m} S_0'' + \frac{1}{2m} \cdot \frac{\hbar}{i} 2 S_0' S_1' = 0$$

or, $$S_0'' + 2 S_0' S_1' = 0 \Rightarrow$$

$$S_1' = -\frac{S_0''}{2S_0'} \Rightarrow S_1 = -\frac{1}{2} \log(S_0') =$$

$$= -\frac{1}{2} \log(p(x)) + \text{Const} = \log \frac{1}{\sqrt{p}} + \text{Const}$$

2nd order in $\hbar$ can be also considered, but is left for exersise.

Let us combine now 0 order in $\hbar$ and 1st order in $\hbar$:

$$\psi = \frac{c_1}{\sqrt{p}} \exp\left[+\frac{i}{\hbar} \int p(x)\,dx\right] + \frac{c_2}{\sqrt{p}} \exp\left[-\frac{i}{\hbar} \int p(x)\,dx\right] -$$

semilassical wave function.

Applicability of expansion

Easy way - require that $O(\hbar)$ term in equation for S is much smaller than $O(1)$ terms:

$$-i\frac{\hbar}{2m}S'' + \frac{1}{2m}(S')^2 = E - U \Rightarrow$$

$$|\hbar S''| \ll |(S')^2| \quad \text{or}$$

$$\left|\hbar \frac{d}{dx}\left(\frac{1}{S'}\right)\right| \ll 1$$

in the first approximation $S' = p(x)$.

Reminder of QM I & II : De Broglie wave-length is

$$\lambda(x) = \frac{2\pi\hbar}{p}$$ [Coming from the

momentum wave-function,

$$\psi_p \sim e^{ipx/\hbar} = e^{2\pi i \frac{x}{\lambda}}$$

So $\left|\hbar \frac{d}{dx}\left(\frac{1}{S'}\right)\right| = \left|\frac{d}{dx}\frac{\hbar}{p}\right| = \frac{1}{2\pi}\frac{d}{dx}(\lambda) \ll 1.$

So, semiclassical approximation is only valid when De-Broglie wavelength λ of a particle is changing slowly over the distance $= \lambda$.

Important remark: the applicability of the semiclassical expansion can also be found from the form of the wave function. At the first side, it is

$$|S_0| \gg |\hbar S_1| \gg |\hbar^2 S_2| \text{ etc.}$$

However, in fact, this is not enough. Indeed, in zero approximation

$\psi_0 = e^{\frac{i}{\hbar} S_0}$, and $\hbar = 0$ is essentially singular point. In the first approximation

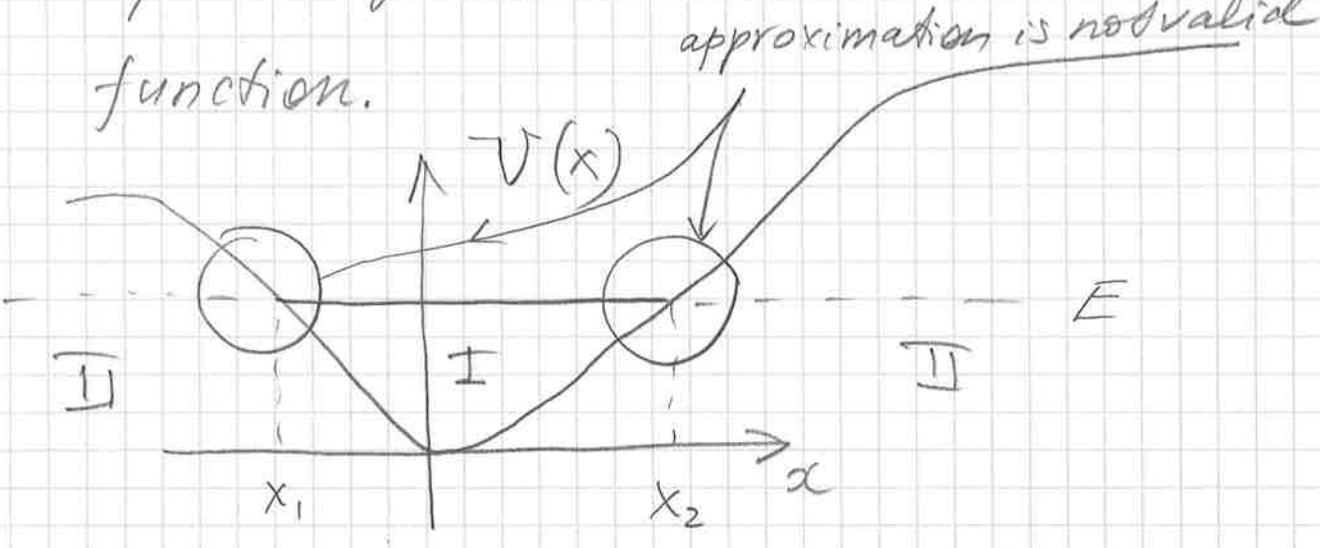
$\psi_1 = e^{\frac{i}{\hbar} S_0 + S_1}$, and even if $S_1 \ll \frac{S_0}{\hbar}$

S_1 can be large, and $\exp S_1$ even larger. In other words, we should use ψ accounting for S_0 and S_1. In the second order we have:

$$\psi_2 = e^{\frac{i}{\hbar} S_0 + S_1 + \frac{\hbar}{i} S_2} = \psi_1 e^{\frac{\hbar}{i} S_2}.$$

Requirement: $|\hbar S_2| \ll 1$ — in this case only $\psi_2 \approx \psi_1$. S_2 will be found at exercises session.

Properties of the semiclassical wave function.



I „Classically alowed" region:

If $x_1 < x < x_2$, then

$E > U(x)$, $p^2(x) = 2m(E-U) > 0$,

so p is real. Wave-function oscillates, and

$$|\Psi|^2 \sim \frac{1}{p}$$

Probability to find the particle is in agreement with classical physics:

time spent in interval Δx is inversely proportional to the velocity of the particle, i.e. momentum p.

For $x > x_2$ or $x < x_1$
we will get „classically forbidden regions": $p^2 = 2m(E-V) < 0$,
p is purely imaginary, and

$$\psi = \frac{c_1}{\sqrt{|p|}} \exp\left[-\frac{1}{\hbar}\int |p| dx\right] + \frac{c_2}{|\sqrt{p}|} \exp\left[+\frac{1}{\hbar}\int |p| x\right]$$

If we have exponentially small wave function, it would fit the intuition that the probability to find the particle in the forbidden region is small.

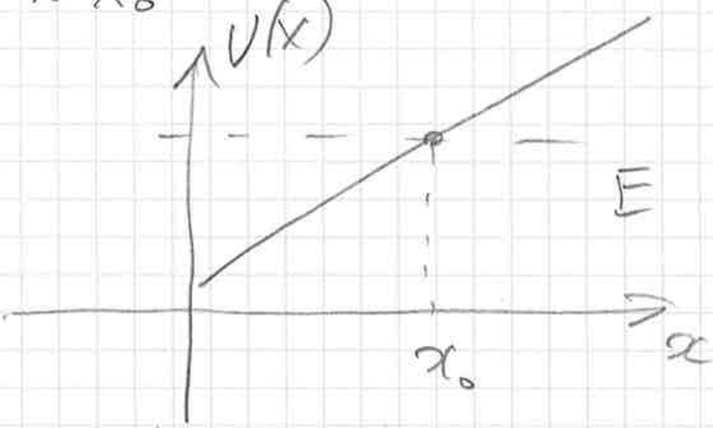
„Turning points" x_1 and x_2
(classical particle would turn at these points).
Here semiclassical approximation breaks down: $p(x) = 0$, and relation

$$\hbar \frac{d}{dx}\left(\frac{1}{p}\right) \ll 1 \text{ cannot be satisfied}$$

Next aim: to determine wave function globaly – go over turning points.

Several way to attack this problem

Way # 1 : if $x \approx x_0$



then close to this point

$$V(x) \approx E + \left.\frac{dV}{dx}\right|_{x_0} (x - x_0) \equiv E + F(x - x_0)$$

Exact equation can be replaced by approximate equation,

$$-\frac{\hbar^2}{2m}\psi'' + F(x - x_0)\psi = 0$$

This equation can be exactly solved

(i) by -yourself (Appendix of Landau-Lifshits, Scrucca lectures)

(ii) by matematisians, see, e.g.

NIST Handbook of Mathematical functions, http://dlmf.nist.gov

Solution: Airy functions

$$\psi = C_A Ai(\;) + C_B Bi(\;)$$