§ Connection of the classical and Quantum mechanics.

Erenfest theorem renders:

$$\frac{d\hat{A}}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{A}]$$ which gives:

$$(1) \begin{cases} \dfrac{d\hat{x}}{dt} = \dfrac{\hat{p}}{m} \\ \dfrac{d\hat{p}}{dt} = -\dfrac{\partial u}{\partial x} \end{cases}$$ an analogue of the Hamiltons equations from classical mechanics.

let's discuss what / when (1) → to classical case

$$(2) \begin{cases} \dot{x} = \dfrac{p}{m} \\ \dot{p} = -\dfrac{\partial u}{\partial x} \end{cases}$$

it is rather clear that as the 1^{st} step in (1) we shall go to $\langle \cdot\cdot \rangle$

let $\langle \cdots \rangle$ (1)

$$(3) \begin{cases} \dfrac{d}{dt}\langle x \rangle = \dfrac{\langle \hat{p} \rangle}{m} \\ \dfrac{d}{dt}\langle \hat{p} \rangle = -\left\langle \dfrac{\partial u}{\partial x} \right\rangle \end{cases}$$

if in the r.h.s. of (3.2) we would have

$\frac{\partial u(\langle x \rangle)}{\partial \langle x \rangle}$ instead of $\left\langle \frac{\partial u(x)}{\partial x} \right\rangle$, we would have

the usual classical equations of motion.

lets discuss conditions when such a equality may hold:

lets write $x = \langle x \rangle + \Delta x$

$$(4) \quad U(x) = U(\langle x \rangle + \Delta x) = U(\langle x \rangle) + U'(\langle x \rangle)\Delta x + \frac{1}{2!}U''(\langle x \rangle)\Delta x^2 + \frac{1}{3!}U'''(\langle x \rangle)(\Delta x)^3 + \dots$$

Sub (4) into equation for momentum and use $\langle \Delta x \rangle = 0$ and $\frac{\partial}{\partial x} = \frac{\partial}{\partial \Delta x}$

$$\frac{d\langle p \rangle}{dt} = -U'(\langle x \rangle) - \frac{U'''(\langle x \rangle)}{2}\langle (\Delta x)^2 \rangle + \dots$$

if we keep in the r.h.s. of the above equation only the 1st term we have the classical Newton's equation: So the rest of the terms are the quantum corrections, which are small under condition

$$\boxed{\frac{1}{2}\left|U'''(\langle x \rangle)\right| \langle (\Delta x)^2 \rangle \ll \left|U'(\langle x \rangle)\right|}$$

This is the condition of transition from the quantum to classical description, known as the quasiclassical condition.

it is true for slow changing $U(x)$, and

$\langle (\Delta x)^2 \rangle$ is small.

The second condition will always be broken for long times, when $\langle (\Delta x)^2 \rangle$ grows (spreading ~~of~~ dispersion of the wavepacket).

The remeady is to have large p. Indeed from

$$\langle (\Delta \hat{x})^2 \rangle \cdot \langle (\Delta \hat{p})^2 \rangle \geq \frac{\hbar^2}{4} \rightarrow$$

that $\langle (\Delta \hat{p})^2 \rangle$ must be large as well as the moment itself must be large

Otherwise $\frac{p^2}{2m}$ would be small compared to quatum mechanical contribution to the kinetic energy $\frac{\langle (\Delta \hat{p})^2 \rangle}{2m}$.

At the classical turning points:

$p = \sqrt{2m(E - U(x))} = 0$ this breaks down.
"quasiclassic condition"

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§ - The wavefunction in the quasiclassical approximation.

Wentzel - Kramers - Brillouin approximation.

Mathematically this amount to find approximate solution to the S.E. when $\hbar \to 0$

Let a particle of mass m be subject to potential $U(x)$, stationary wave function is presented as

$$\psi(x) = e^{\frac{i}{\hbar}\sigma(x)}$$ sub. into S.E. $\Rightarrow$

$$-\frac{\hbar^2}{2m}\psi'' + U\psi = E\psi \quad \Rightarrow$$

$$\frac{\sigma'^2}{2m} + \frac{\hbar}{2mi}\sigma'' = E - U$$

$$\sigma' = \frac{d\sigma}{dx}$$
$$\sigma'' = \frac{d^2\sigma}{dx^2}$$

Zeroth order $(\hbar = 0)$ solution coincides with tehe Hamilton - Jacobi equation for the classical abbreviated ~~shortened~~ action $\sigma = \cancel{\int L \cdot dt} \int p\, dx$

Lagrangian

where also $\sigma' = p$ is the particle moment.

the full action (for $E = const$) is given by

$$S(x,t) = \int_{t_0}^{t} L\, dt = -E \cdot t + \sigma(x).$$

assuming σ is an analytic function of $\hbar$

we write:

$$\sigma = \sigma_0 + \frac{\hbar}{i}\sigma_1 + \left(\frac{\hbar}{i}\right)^2 \sigma_2 + \dots$$

$\sigma_0 \to$ classical action, and $\sigma_1, \sigma_2, \dots$ quatum corrections.

Comment. eq. on $\sigma(x)$ establishes a connection between quantum description ~~and~~ in terms of probability amplitude and the classical one in terms of the action functional.

$$\begin{cases} \hbar^0: & \dfrac{\sigma_0'^2}{2m} = E - U \quad (1) \\ \hbar^1: & \sigma_0' \sigma_1' + \dfrac{\sigma_0''}{2} = 0, \quad (2) \\ & \dots\dots \end{cases}$$

$$(1) \to \quad \sigma_0' = \pm\sqrt{2m[E - U(x)]}$$

let's us introduce classical moment

$p(x) = \sqrt{2m(E - U(x))}$. in the classically allowed region $p(x) \in \mathbb{R}$, and

$$\sigma_0' = \pm p \quad \to \quad \sigma_0 = \pm \int p\,dx + \text{Const}$$

$$(2) \to \quad 2p\sigma_1' + p' = 0$$

$$\sigma_1' = -\frac{p'}{2p} \qquad \int \dots \qquad \to$$

$$\sigma_1 = -\frac{1}{2}\ln p + \text{const}$$

up to ~~seco~~ $O(\frac{\hbar}{i})$ we have

$$\psi(x) \approx e^{\frac{i}{\hbar}(\sigma_0 + \frac{\hbar}{i}\sigma_1)} \cancel{= c\, e^{\pm\frac{i}{\hbar}(\sigma_0 + \frac{\hbar}{i}\sigma_1)}}$$

$$= c\, e^{\pm\frac{i}{\hbar}\int p\,dx - \frac{1}{2}\ln p} = \frac{c}{\sqrt{p}}\, e^{\pm\frac{i}{\hbar}\int p\,dx}$$

a general solution we take as a linear superposition:

$$\psi(x) \approx \frac{c_1}{\sqrt{p}}\, e^{\frac{i}{\hbar}\int p\,dx} + \frac{c_2}{\sqrt{p}}\, e^{-\frac{i}{\hbar}\int p\,dx}$$

c_1 and c_2 normalisation constants,

$|\psi(x)|^2 \sim \frac{1}{p}$, which may be interpreted as the time for particle to spend in the vicinity of x is inverse proportional to p.

- if $E < U(x) \rightarrow p = i|p| = i\sqrt{2m\,[U(x) - E]}$

and

$$\psi(x) = \frac{c_1'}{\sqrt{|p|}} \cdot e^{-\frac{1}{\hbar}\int |p|\,dx} + \underbrace{\frac{c_2'}{\sqrt{|p|}}\, e^{\frac{1}{\hbar}\int |p|\,dx}}_{\text{diverging to exclude.}}$$

Let's reexamine the validity of the approximation; which may be written as

$$\left| \frac{\overbrace{\hbar\,\sigma''}^{\text{quantum correction}}}{\underbrace{\sigma'^2}_{\text{classical term}}} \right| \ll 1$$

or $\left|\frac{d}{dx}\frac{\hbar}{\sigma'}\right| \ll 1$

as $\sigma' \sim p \rightarrow \left|\frac{d}{dy}\frac{\hbar}{p}\right| \ll 1$ (1)

relation between p and de Broglie wave length:

$$p = \frac{2\pi\hbar}{\lambda}$$

$$(1) \Rightarrow \left|\frac{1}{2\pi}\frac{d\lambda}{d\cancel{x}}\right| \ll 1.$$

$\Rightarrow$ quasiclasiccal approximation is applicable whe

λ depends weakly upon x.

another form for the applicability criterium may be obtained using classical Force:

$$F = -\frac{\partial u}{\partial x} \;; \quad \left|\frac{d}{dx}\frac{\hbar}{p}\right| \ll 1 \Rightarrow \left|\frac{\hbar}{p^2}\frac{dp}{dx}\right| \ll 1$$

$$p = \sqrt{2m(E-u)} \qquad \frac{dp}{dx} = -\frac{1}{2}\cdot\frac{1\cdot(-2m)\,du/dx}{\sqrt{2m(E-u)}} =$$

$$= \frac{1}{2}\frac{\sqrt{2m}}{(E-u}$$

$$\left|\frac{\hbar}{p^2}\frac{1}{2\sqrt{2m(E-u)}}\cdot 2m\frac{du}{dx}\right| \ll 1$$

$$\Downarrow$$

$$\boxed{\frac{\hbar m}{p^3}|F| \ll 1}$$

Example: wave function in the vicinity of a classical turning point. $x = x_0 \Rightarrow U(x_0) = E$

no kinetic energy.

$$U(x) \cancel{\simeq} E + U'(x_0)(x - x_0) + O\left((x-x_0)^2\right)$$

S.E. in the momentum representation:

$$\left(\frac{p^2}{2m} + U'(x_0)\underbrace{i\hbar\frac{d}{dp}}_{\hat{x}}\right)c(p) - U'(x_0)x_0 C(p)$$

$U(x_0) = E$ these two term cancels and.

$$\frac{dc(p)}{dp} = i\left(\frac{p^2}{2m\hbar U'(x_0)} - \frac{x_0}{\hbar}\right)c(p)$$

integrating we find:

$$c(p) = \underbrace{C}_{\text{normalisatio const.}}\exp\left\{i\frac{p^3}{6m\hbar U'(x_0)} - \frac{i}{\hbar}px_0\right\}.$$

In the coordinate representation

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} e^{ipx/\hbar}\, c(p)\, dp =$$

$$= \frac{2C}{\sqrt{2\pi\hbar}}\int_0^{\infty}\cos\left[\frac{p^3}{6m\hbar U'(x_0)} + \frac{p}{\hbar}(x - x_0)\right]dp$$

Sin gives zero contribution as odd function

$$p \to q\left[6m\hbar U'(x_0)\right]^{1/3} \to$$

$$\psi(x) = A \int_0^\infty \cos\left(q^3 + qz\right) dq$$

$\hookrightarrow$ normalisation const.

$$z = \left(\frac{6mU'(x_0)}{\hbar^2}\right)^{1/3}(x - x_0)$$

and $\int_0^\infty \dots$ is the Airy function.

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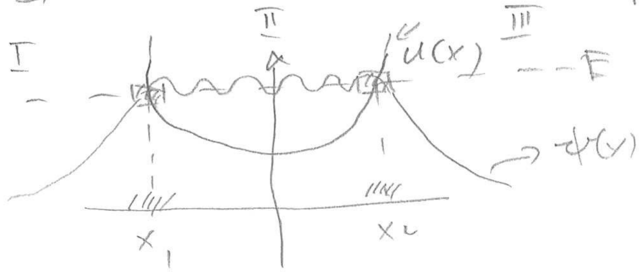
§ Bohr-Sommerfeld quantisation rule.



Using (continuity and smoothness) conditions across the turning point x_1, x_2

we may find the "old Q.M." quantisation

rules. B.-S.

For the regions I and II we use

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around point x_1: $\psi_I(x) = \frac{C_I}{2\sqrt{|p|}} e^{-\frac{1}{\hbar}\int_x^{x_1} |p|\, dx'}$

$$\psi_{II}^1(x) = \frac{C_{II}^1}{\sqrt{p}} e^{\frac{i}{\hbar}\int_x^{x_1} p\, dx'} + \frac{C_{II}^2}{\sqrt{p}} e^{\frac{-i}{\hbar}\int_x^{x_1} p\, dx'}$$

in the hatched area we use the "exact"

solution in terms of the Airy function,

this will give condition upon the

coefficients. $\Rightarrow \psi_{II}^1(x) = \frac{C_I}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int_x^{x_1} p\, dx' + \frac{\pi}{4}\right)$

around point x_2:

$$\psi_{II}^{2}(x) = \frac{D_{II}^{1}}{\sqrt{p}}\, e^{\frac{i}{\hbar}\int_{x_2}^{x} p\,dx'} + \frac{D_{II}^{2}}{\sqrt{p}}\, e^{-i/\hbar \int_{x_2}^{x} p\,dx'}$$

$$\psi_{III}(x) = \frac{D_{III}}{2\sqrt{|p|}} \cancel{\int_{x_2}^{x} e} \; e^{-\frac{1}{\hbar}\int_{x_2}^{x} |p|\,dx'}$$

and inside the hatched region we have exact solution in terms of the Airy function. Matchin all three brunches we find conditions on the coefficients and obtaine for

$$\psi_{II}^{2}(x) = \frac{D_{III}}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int_{x_2}^{x} p\,dx' + \pi/4\right)$$

Demanding that

$$\psi_{II}^{1}(x) = \psi_{II}^{2}(x) \Rightarrow$$

$$\frac{C_I}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int_{x}^{x_1} p\,dx' + \frac{\pi}{4}\right) = \frac{D_{III}}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int_{x_2}^{x} p\,dx' + \pi/4\right)$$

$$\frac{C_I}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int_{x_1}^{x} p\,dx' - \pi/4\right) = \frac{D_{III}}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int_{x}^{x_2} p\,dx' - \pi/4\right)$$

for any $x \Rightarrow$ the sum of the argument must be multiple of π

$$\frac{1}{\hbar}\int_{x_1}^{x} p\,dx' - \frac{\pi}{4} + \frac{1}{\hbar}\int_{x}^{x_2} p\,dx' - \frac{\pi}{4} = n\pi$$

$n = 0, 1, 2, \ldots$ and

$$\boxed{C_I = (-1)^n D_{III}} \quad ?$$

$$\cos(f) + \cos(g) = 0 \qquad g = \pi - f$$

$$\cos(f) + \cos(\pi - f) = \cos f + \underbrace{\cos\pi}_{(-1)}\cdot\cos f - \underbrace{\sin\pi\,\sin f}_{0}$$

$$\cos(f) - \cos(g) = 0 \qquad g = 2\pi - f$$

$$\cos f - \cos 2\pi \cos f = 0$$

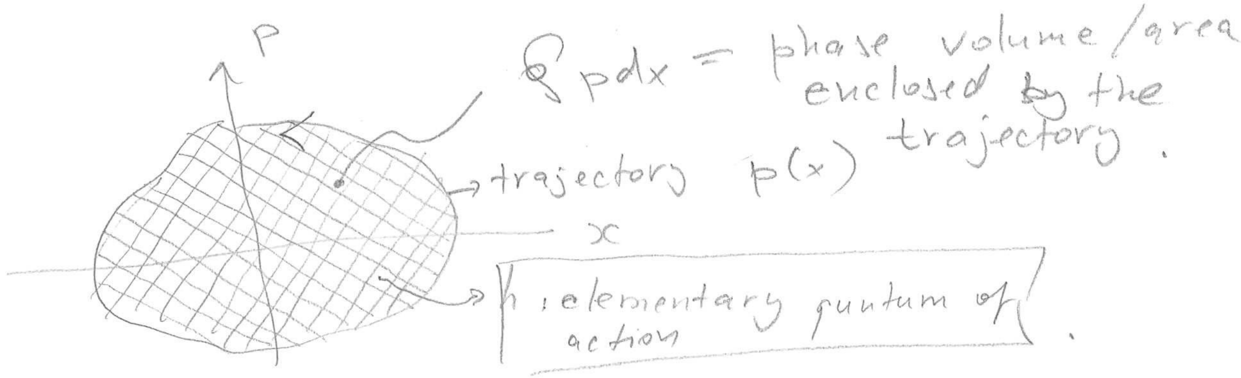
$$\Rightarrow \frac{1}{\hbar}\int_{x_1}^{x_2} p\,dx' = n\pi + \frac{\pi}{2} \quad \text{or}$$

$$\frac{2}{\hbar}\int_{x_1}^{x_2} p\,dx' = 2\pi\left(n + \frac{1}{2}\right)$$

The 1st integral with 2 is the integral over the full period of the classical motion:

$$\oint p\,dx' = 2\pi\hbar\left(n + \frac{1}{2}\right).$$

That is the Bohr-Sommerfeld quantisation rule of the old quantum mechanics.



B.S. quantisation rule state that

the area enclosed by the trajectory in the phase space is a multiple of

$$\boxed{h = 2\pi\hbar}$$

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