Lecture # 6, Quantum physics 3

- Discussed and constructed WKB wave function,

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

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

- Discussed applicability of WKB approximation,

$$\left|\frac{d\lambda}{dx}\right| \ll 1, \quad \text{where} \quad \lambda = \frac{\hbar}{p} -$$

De Broglie wavelength

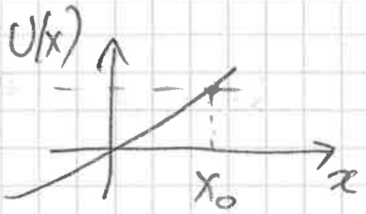
- Discussed classicaly allowed and forbidden regions

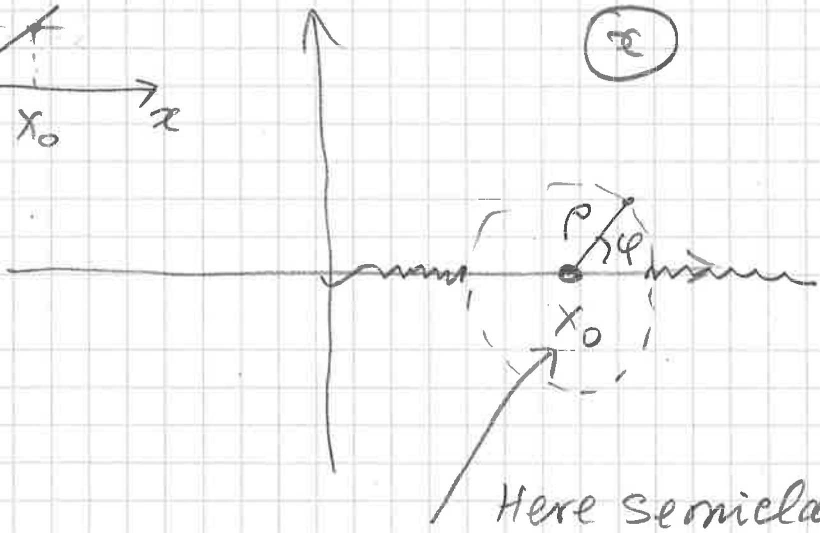
Plan

- matching conditions at the turning points
- Applicability of the result for matching conditions
- Bohr- Sommerfeld quantisation condition

Matching conditions for turning points

Way # 2. Consider ψ as a function of complex x and connect the region $x < x_0$ and $x > x_0$ in complex plane everywhere in the region where semiclassical solution is valid:





Here semiclassical solution is not valid

For real x, and for $x > x_0$ we take:

$$\psi = \frac{C}{2\sqrt{|p|}} \exp\left(-\frac{1}{\hbar}\int_{x_0}^{x} |p|\, dx'\right), \ C\text{-real}$$

For real x, $x < x_0$ we have:

$$(*) \quad \psi = \frac{C_1}{\sqrt{p}} \exp\left[-\frac{i}{\hbar}\int_{x}^{x_0} p\, dx\right] + \frac{C_2}{\sqrt{p}} \exp\left[+\frac{i}{\hbar}\int_{x}^{x_0} p\, dx\right]$$

ψ must be real everywhere (equation is real).

Near the turning point $U(x) = E + F(x-x_0) \Rightarrow$

$$p(x) = \sqrt{2m(E-U)} \approx \sqrt{-2mF(x-x_0)} \Rightarrow$$

on real axis,

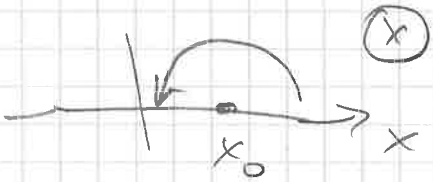
$$\psi = \frac{c}{2\sqrt{(2mF)^{1/2}}} \frac{1}{(x-x_0)^{1/4}} \exp\left[-\frac{1}{\hbar}\int_{x_0}^{x}\sqrt{2mF(x-x_0)}\,dx\right]$$

$$= \frac{c}{2\sqrt{(2mF)^{1/2}}} \frac{1}{(x-x_0)^{1/4}} \exp\left[-\frac{2}{3\hbar}\sqrt{2mF_0}\,(x-x_0)^{3/2}\right]$$

for complex x, $(x-x_0) = \rho e^{i\varphi}$,

$$(x-x_0)^{1/4} = \rho^{1/2} e^{i\varphi/4}; \quad (x-x_0)^{3/2} = \rho^{3/2} e^{3i\varphi/2}$$

What happens with this function if we change φ from 0 to π?



$$\psi \to \frac{c}{2\sqrt{(2mF)^{1/2}}} \frac{1}{\rho^{1/4}} e^{-i\pi/4} \exp\left[-\frac{2}{3\hbar}\sqrt{2mF_0}\,\rho^{3/2}(-i)\right]$$

$$= \frac{c}{2\sqrt{(2mF)^{1/2}}} \frac{1}{(x_0-x)^{1/4}} \exp\left[+\frac{i}{\hbar}\int_{x}^{x_0} p\,dx - i\frac{\pi}{4}\right]$$

This is a second term in expression for $x < x_0 \Rightarrow$

$$C_2 = \frac{c}{2} e^{-i\pi/4}$$

If we consider going from $\varphi = 0$ to $\varphi = -\pi$ (lower plane), we get

$$\psi \to \frac{c}{2\sqrt{(2mF)^{1/2}}} \frac{1}{(\xi)^{1/4}} e^{+i\pi/4} \exp\left[-\frac{i}{\hbar}\int_x^{x_0} p\,dx\right],$$

which is exactly the first term $\Rightarrow$

$$C_1 = \frac{c}{2} e^{i\pi/4}$$

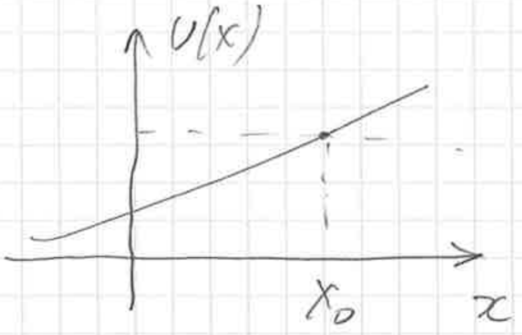
So, wave function in classically alowed region is

$$\frac{c}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int_x^{x_0} p\,dx - \frac{\pi}{4}\right)$$

Why we got different answers in different directions?

Important remark

- Semiclassical wave function in the classically forbidden region:



$U(x) > E$: classically forbidden region,

$$\psi = \frac{C_1}{\sqrt{|p|}} \exp\left[\frac{1}{\hbar}\int_{x_0}^{x} |p| dx'\right] + \frac{C_2}{\sqrt{|p|}} \exp\left[-\frac{1}{\hbar}\int_{x_0}^{x} |p| dx'\right]$$

$$p^2 = 2m\left(E - U(x)\right)$$

Important: if $C_1 \neq 0$, there is no sense to keep the part of the wave-function proportional to C_2, as it is exponentially smaller in the classically forbidden region.

However, if $C_1 \equiv 0$, the exponentially small function represents a valid solution.

Behaviour of ψ in different regions of complex plane, $\psi = \ldots \exp\left(-\frac{2}{3\hbar}\sqrt{2mF_0}\,(x-x_0)^{3/2}\right)$

$$\exp\left(\frac{3i\varphi}{2}\right) = \cos\frac{3\varphi}{2} + i\sin\frac{3\varphi}{2}, \quad x - x_0 = \rho e^{i\varphi}$$

$$\psi = \exp\left(-\frac{2}{3\hbar}\sqrt{2mF_0}\,\rho\left(\cos\frac{3\varphi}{2} + i\sin\frac{3\varphi}{2}\right)\right)$$

$$\cos\frac{3\varphi}{2} > 0 \quad \text{for} \quad -\frac{\pi}{2} < \frac{3\varphi}{2} < \frac{\pi}{2} \Rightarrow$$

$2\pi - \frac{\pi}{2} < \frac{2\varphi}{3} < 2\pi + \frac{\pi}{2}$

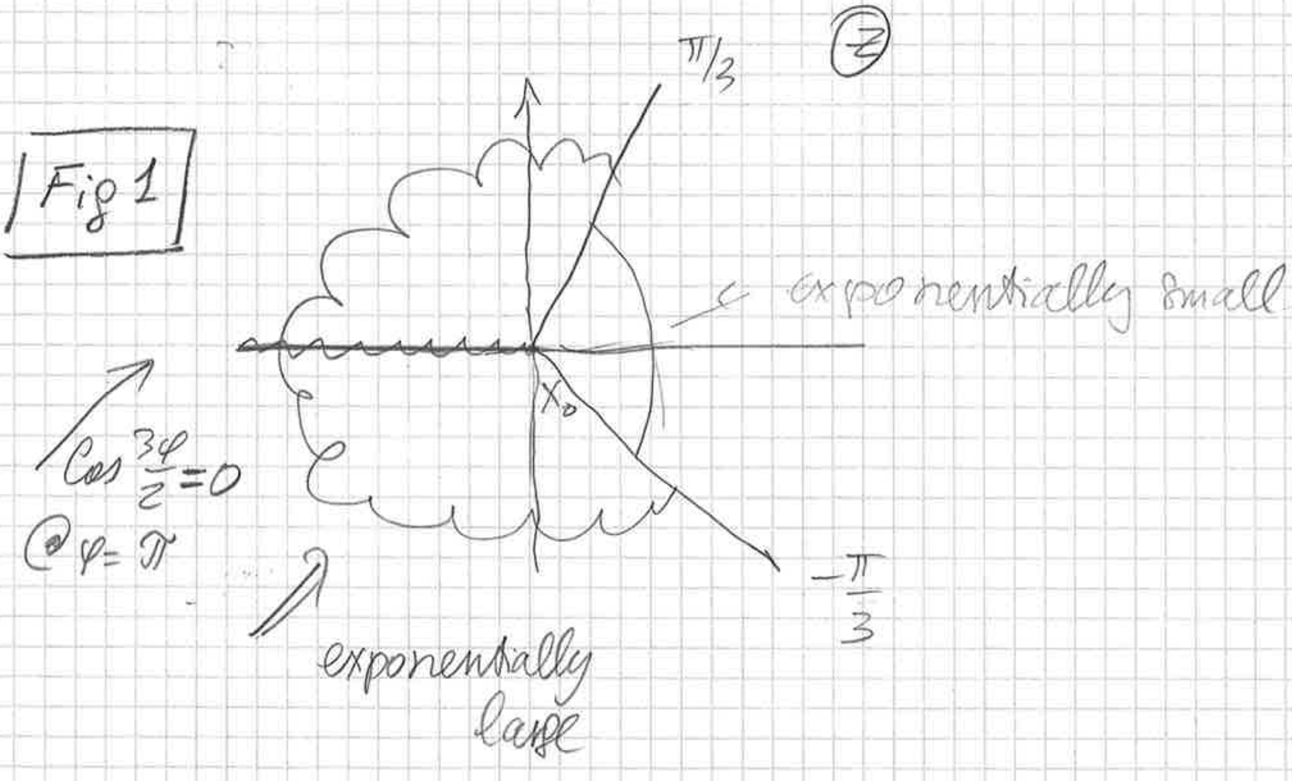
$\varphi <$

$$-\frac{\pi}{3} < \varphi < \frac{\pi}{3}$$

$$\cos\frac{3\varphi}{2} < 0: \quad \frac{\pi}{2} < \frac{3\varphi}{2} < \frac{3\pi}{2} \Rightarrow \frac{\pi}{3} < \varphi < \pi$$

$$-\frac{3\pi}{2} < \frac{3\varphi}{2} < -\frac{\pi}{2} \Rightarrow -\pi < \varphi < -\frac{\pi}{3}$$

Fig 1



Behaviour of

$$\psi = \frac{C}{\sqrt{p}} \exp\left[-\frac{i}{\hbar}\int_x^{x_0} p\,dx\right]$$ in different

regions of the complex plane:

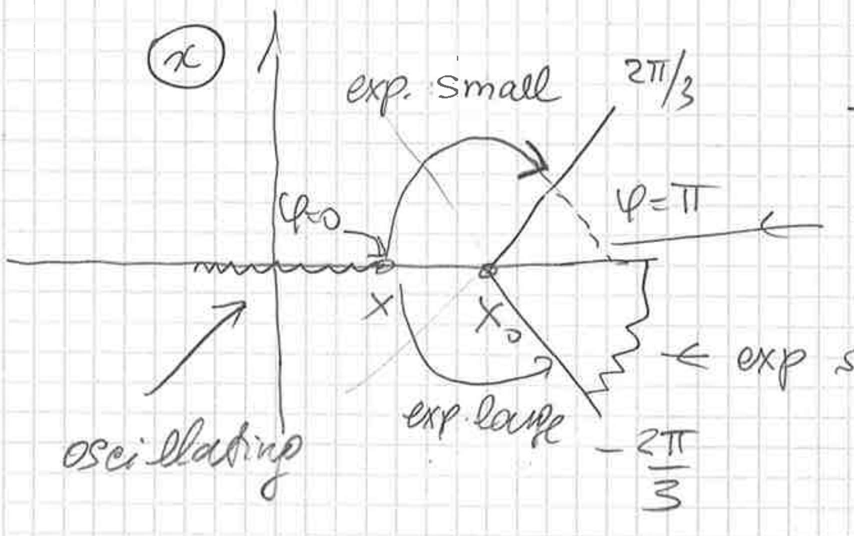
$$\exp\left[-\frac{i}{\hbar}\cdot\frac{2}{3}\sqrt{2mF_0}\,(x_0-x)^{3/2}\right] = \exp\left[-\frac{2i}{3\hbar}\sqrt{2mF_0}\,\rho\cdot e^{\frac{3i\varphi}{2}}\right]$$

$$x_0 - x = \rho\exp(-i\varphi)$$

$0<\varphi<\pi$: upper half plane

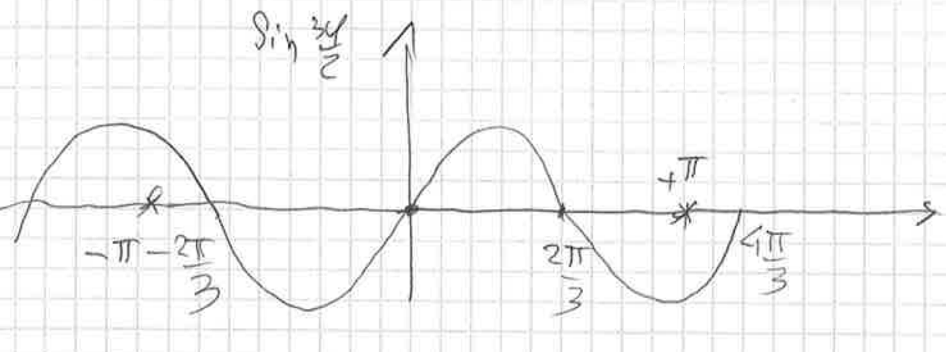
$-\pi<\varphi<0$ lower half plane

Fig 2



$$-ie^{\frac{3i\varphi}{2}} = -i\cos\frac{3\varphi}{2} + \sin\frac{3\varphi}{2}$$

$$\sin\frac{3\varphi}{2} = 0 \Rightarrow \varphi = 0;\ \frac{2\pi}{3},\ -\frac{2\pi}{3}$$



Behaviour of function with C_2: opposite.

Comparison of Fig 1 and Fig 2 shows that the function $\sim C_1$ to the left of the turning point is the same as the one $\sim C$ to the right of the turning point in the lower part of the complex plane.

In the upper part of the complex plane function $\sim C_2$ is the same as the one $\sim C$.

If both (exponentially large and small) parts are present, we can only rely on exponentially large part. This explains why we got different answers in different analytical continuations.

Summary:

$$\psi(x) = \begin{cases} \dfrac{C}{2\sqrt{|p|}} \exp\left[-\dfrac{1}{\hbar}\displaystyle\int_{x_0}^{x} |p|\,dx'\right], & x > x_0 \\ \dfrac{C}{\sqrt{p}} \cos\left(\dfrac{1}{\hbar}\displaystyle\int_{x}^{x_0} |p|\,dx' - \dfrac{\pi}{4}\right), & x < x_0 \end{cases}$$

$V(x) > E$ for $x > x_0$

Applicability of the result for matching condition.

We used expansion of the potential near the turning point:

$$U(x) = E + \frac{\partial U}{\partial x}\Big|_{x_0}(x-x_0) + \frac{1}{2}\frac{\partial^2 U}{\partial X^2}(x-x_0)^2 + \dots$$

and only kept the second term, so it is needed that

$$\frac{1}{2}U''_{(x_0)}(x-x_0) << U'(x_0), \text{ so that}$$

$$(x-x_0) << \frac{2U'}{U''}$$

At the same time, semiclassical approximation is valid at

$$\left|\frac{d}{dx}\frac{\hbar}{p}\right| << 1.$$

in the vicinity of the turning point

$$p = \sqrt{2mU'\cdot(x-x_0)}, \text{ and}$$

$$\left|\hbar\frac{d}{dx}\frac{1}{p}\right| = \left|\frac{\hbar}{\sqrt{2mU'}}\cdot\frac{1}{2}\frac{1}{(x-x_0)^{3/2}}\right|,$$

and this must be $<< 1$.

For $(x-x_0) \simeq \frac{2U'}{U''}$ semiclassical approximation must work:

$$\frac{\hbar}{\sqrt{2mU'}} \cdot \frac{1}{2}\left(\frac{U''}{2U'}\right)^{3/2} \ll 1,$$

leading to condition (factor ~2 are taken away)

$$(U')^2 \gg \frac{\hbar}{\sqrt{m}} (U'')^{3/2} \qquad (*)$$

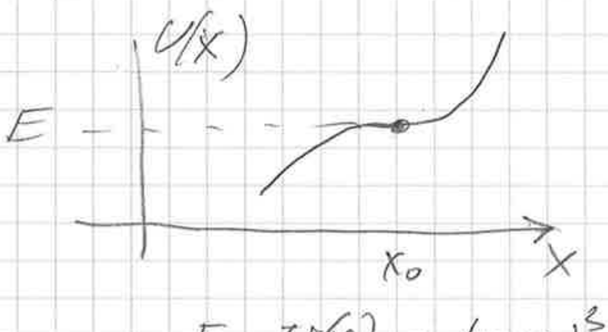
Check of dimension:

$[GeV]^4$ & $[GeV^3]^{3/2}\, GeV^{-1/2} = [GeV]^4$

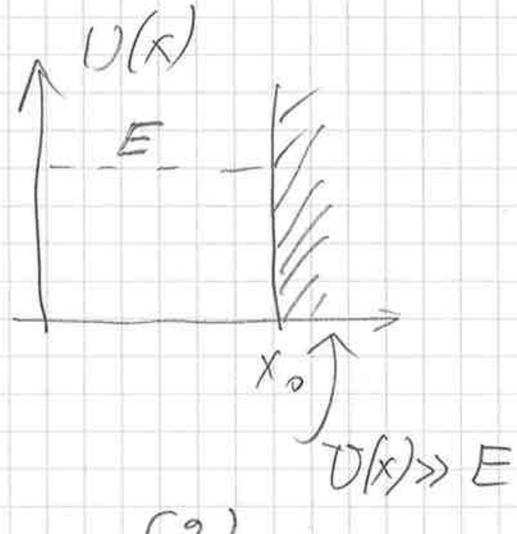
ok!

If this condition is not satisfied, then the analysis must be redone.

Examples:



(1)



(2)

For example, for the case (2), fig 2 in the page 4, $U(x) \gg E$ right after x_0, whereas to the left of x_0 the semiclassical description is valid, since $E \gg U(x)$. So, the boundary condition for the wave-function in the classically allowed region is $\psi(x_0) = 0$, leading to

$$\psi \sim \cos\left(\frac{1}{\hbar}\int_x^{x_0} |p|\,dx - \frac{\pi}{2}\right) \sim$$

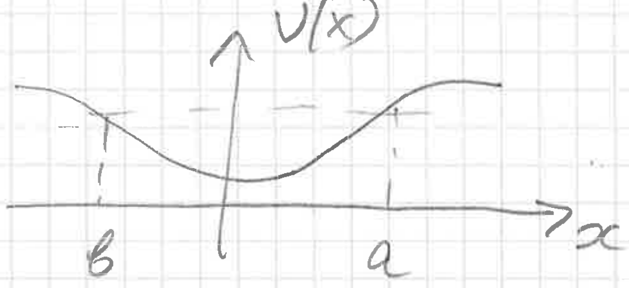
$$\sin\left(\frac{1}{\hbar}\int_x^{x_0} |p|\,dx\right).$$

In general, the semiclassical wave function in the allowed region has a generic form $\sim$

$$\cos\left(\frac{1}{\hbar}\int_x^{x_0} |p|\,dx - \varphi\right),$$ where φ is a phase determined by the structure of the turning point.

Normalisation of the classical wave-function:

Between turning points b and a



we have:

$$\psi = \frac{C}{\sqrt{|p|}} \cos\left(\frac{1}{\hbar}\int_b^x |p|\,dx - \varphi\right),$$

and exponentially small for $x > a$ and $x < b$

$$\int |\psi|^2 dx \approx \int_b^a \frac{C^2}{p} \cos^2\left(\frac{1}{\hbar}\int_b^x |p|\,dx - \varphi\right) \approx$$

$$\approx \frac{1}{2} C^2 \int_b^a \frac{dx}{|p|} = \frac{1}{2} C^2 \int_b \frac{dx\,dt}{m\,dx} =$$

$$= \frac{1}{2} C^2 \frac{1}{m} \cdot \frac{T}{2} = 1 \Rightarrow C = 2\sqrt{\frac{m}{T}}$$

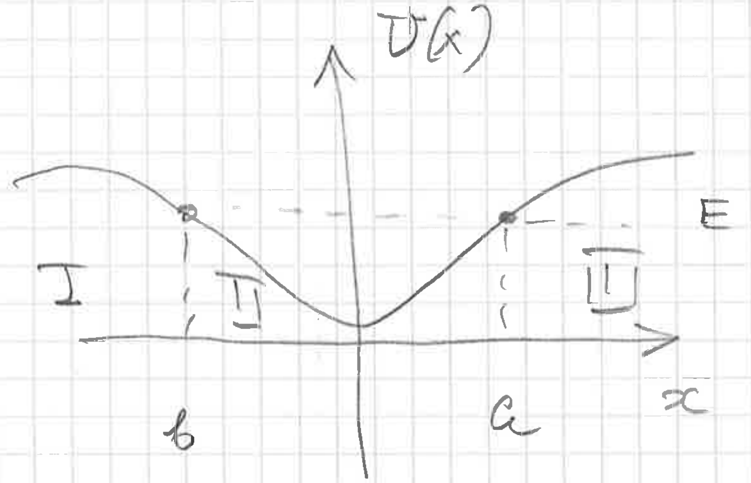
T: classical period of oscillations

$$\psi = 2\sqrt{\frac{m}{pT}} \cos(\ldots) = \sqrt{\frac{2\omega}{\pi v}} \cos(\ldots)$$

where $\omega = \frac{2\pi}{T}$, and v is the velocity.

Bohr - Sommerfeld quantisation condition

Let us use the semiclassical wave function for potential of the form:



wave - function for $x > a$:

$$\text{III} \quad \frac{c}{2|p|} \exp\left[-\frac{1}{\hbar}\int_a^x |p|\,dx'\right]$$

wave - function for $x < a$;

$$\text{II} \quad \frac{c}{\sqrt{p}} \cos\left[\frac{1}{\hbar}\int_x^a p(x')\,dx' - \frac{\pi}{4}\right]$$

wave - function for $x < b$

$$\left.\begin{array}{l} \text{I} \quad \dfrac{\tilde{c}}{2\sqrt{|p|}} \exp\left[-\displaystyle\int_x^b |p|\,dx'\right] \\[2ex] \text{II} \quad \dfrac{c}{\sqrt{p}} \cos\left[\dfrac{1}{\hbar}\displaystyle\int_b^x p(x) - \dfrac{\pi}{4}\right] \end{array}\right\} \text{will be derived at exersise}$$

Functions in the region $\underline{II}$ must be identical $\Rightarrow$ $\cos A = \pm \cos B$;

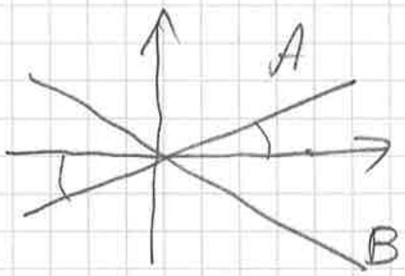
$$A = B + 2\pi n \qquad A = \pi - B + 2\pi n$$

$$A = -B + 2\pi n \qquad A = \pi + B + 2\pi n$$

$$\Downarrow$$

$$A + B = \pi n \text{ , or}$$

$$A - B = \pi n$$



two possibilities:

$$\frac{1}{\hbar}\int_x^a p\,dx - \frac{\pi}{4} + \frac{1}{\hbar}\int_b^x p\,dx - \frac{\pi}{4} = \pi n$$

or $$\frac{1}{\hbar}\int_x^a p\,dx - \frac{\pi}{4} - \frac{1}{\hbar}\int_b^x p\,dx + \frac{\pi}{4} = \pi n$$

1st condition:

$$\frac{1}{\hbar}\int_b^a p\,dx = \pi\left(n + \frac{1}{2}\right) \qquad (*)$$

2nd condition: cannot be satisfied for all x

The ef (*) in page 14 can be rewritten as

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

integral over one period of classical motion.

This is exactly Bohr-Sommerfeld quantisation condition. Remark: ef (*) in page 10 must be satisfied.