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Chapter 6

Equations of Motion, Classical limit &

§6-2 WKB (Wentzel - Kramers - Brillouin) approximation

Heisenberg picture v.s. Schrödinger picture

$$|\psi(t)\rangle = \hat{U}(t,t_0)\,|\psi(t_0)\rangle$$

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \left(i\hbar \frac{d\hat{U}(t,t_0)}{dt}\right)|\psi(t_0)\rangle$$

$$= \hat{H}\,|\psi(t)\rangle$$

$$= \hat{H}\,\hat{U}(t,t_0)\,|\psi(t_0)\rangle$$

$$\therefore\ i\hbar \frac{d\hat{U}(t,t_0)}{dt} = H\,\hat{U}(t,t_0) \qquad -i\hbar\frac{d\hat{U}^+}{dt} = \hat{U}^+ H$$

If H is independent of t, $\hat{U} = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}$

$$\therefore\ |\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}\,|\psi(0)\rangle$$

Consider an operator $\hat{A}$ (no explicit t dependence, e.g. $\hat{A}=\hat{x}$, or $\hat{p}$, ...)

$$\langle \hat{A}\rangle_t \equiv \langle\psi(t)|\,\hat{A}\,|\psi(t)\rangle \Leftarrow \text{Schrödinger picture} \begin{cases}\psi(t)\\ A \text{ indept. of } t.\end{cases}$$

Heisenberg:

$$\langle \hat{A}\rangle_t = \langle\psi(t)\,|\hat{A}|\,\psi(t)\rangle.$$

$$= \langle\psi(0)|\,e^{\frac{i}{\hbar}\hat{H}t}\,\hat{A}\,e^{-\frac{i\hat{H}t}{\hbar}}\,|\psi(0)\rangle$$

Can define $A(t) = e^{\frac{i}{\hbar}\hat{H}t}\,\hat{A}\,e^{-i\frac{\hat{H}}{\hbar}t}$ $\Rightarrow$ time-dependent

use $|\psi(0)\rangle \Leftarrow$ indept. of t.

11/5, 10/16/96 revision

In Schrödinger picture

$|\psi(t)\rangle$ carries the time-dependence

One needs the equation of motion for $|\psi(t)\rangle$, which is the Schrödinger eq.

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle$$

In the Heisenberg picture

more general

$$A_H(t) = U^\dagger(t,0)\, A\, U(t,0)$$

$$A_H(t) \equiv e^{\frac{i}{\hbar}Ht} \underset{\underset{A_S}{\Uparrow}}{A}\, e^{-\frac{i}{\hbar}Ht}$$ carries the time dependence.

One needs the equation of motion for $\hat{A}_H(t)$

$$\frac{dA_H(t)}{dt} = e^{\frac{i}{\hbar}Ht}\left[\frac{i}{\hbar}HA_S - \frac{i}{\hbar}A_S H\right] e^{-\frac{i}{\hbar}Ht}$$

$$+\ e^{\frac{i}{\hbar}Ht}\frac{\partial A_S}{\partial t}e^{-\frac{i}{\hbar}Ht}$$

$$= \frac{i}{\hbar}[H, A_H(t)] + \frac{\partial A_H}{\partial t}.$$

Remarks (i) $[f(A)]_H = f(A_H)$

e.g. $f(A) = A^2$

$$e^{\frac{i}{\hbar}Ht} f(A)\, e^{-\frac{i}{\hbar}Ht} = e^{\frac{i}{\hbar}Ht} A\, e^{-\frac{i}{\hbar}Ht} e^{\frac{i}{\hbar}Ht} A\, e^{-\frac{i}{\hbar}Ht}$$

$$= A_H^2$$

(ii) $H_H = H_S \equiv H$

(iii) $\frac{d}{dt}A_H(t)$ and $\frac{\partial A_H}{\partial t}$ are different, while

~~$\frac{dA_S}{dt} = \frac{\partial A_S}{\partial t}$:~~

example. $A_S = X_S^2 \cos\omega t$, in Schrödinger picture
X_S is independent of t

$$\therefore \frac{dA_S}{dt} = -\omega X_S^2 \sin\omega t = \frac{\partial A_S}{\partial t}.$$

But in Heisenberg picture, $A_H = X_H^2 \cos\omega t$

$$\frac{dA_H}{dt} = \frac{dX_H}{dt} X_H \cos\omega t + X_H \frac{dX_H}{dt} \cos\omega t - \omega \sin\omega t\, X_H^2$$

$$= \left\{ \frac{i}{\hbar}[H, X_H] X_H + \frac{i}{\hbar} X_H [H, X_H] \right\} \cos\omega t - \omega \sin\omega t\, X_H^2$$

$$= \frac{i}{\hbar}[H, A_H] \cancel{\cos\omega t} \underbrace{- \omega \sin\omega t\, X_H^2}$$

$$\frac{\partial A_H}{\partial t} = -\omega \sin\omega t\, X_H^2$$

* <u>Ehrenfest theorem</u>

$$\frac{d}{dt}\langle A \rangle = \frac{i}{\hbar}\langle [H, A] \rangle + \langle \frac{\partial A}{\partial t} \rangle$$

This is independent of which picture we use.

Consequence & examples :

(i) $[H, A] = 0$. A independent of time.

$$\frac{d\langle A \rangle}{dt} = 0 \qquad \langle A \rangle = \text{constant (time-indept)}$$

$\therefore$ initially, if $|\psi\rangle$ is an eigenket of A,
$\langle A \rangle = a$, (a = eigenvalue), $|\psi(t)\rangle$ will always
be the eigenket of A!

(ii) $H = \frac{p^2}{2m} + U(x)$

$$\frac{d\langle x\rangle}{dt} = \frac{i}{\hbar}\langle [H, x]\rangle$$

$$= \frac{i}{\hbar}\langle [\frac{p^2}{2m}, x]\rangle$$

$$\underset{\uparrow}{=} \langle \frac{p}{m}\rangle \Leftrightarrow \text{classical } m\frac{dx}{dt} = p$$

$[p^2, x] = -2i\hbar p$

more generally $\underset{x = i\hbar \frac{\partial}{\partial p}}{=} \langle \frac{\partial H(x,p)}{\partial p}\rangle \Leftrightarrow \text{classical } \dot{x} = \frac{\partial H}{\partial p}$

$$\frac{d\langle p\rangle}{dt} = \frac{i}{\hbar}\langle [V(x), p]\rangle$$

$$= -\langle \frac{dV(x)}{dx}\rangle \left[= -\langle \frac{\partial H}{\partial x}\rangle \text{ more generally} \right]$$

When $\langle \frac{d\,U(x)}{dx}\rangle \simeq \frac{d\,V(\langle x\rangle)}{d\langle x\rangle}$ - - - - ①

$$\Rightarrow \frac{d\langle p\rangle}{dt} = -\frac{dV(\langle x\rangle)}{d\langle x\rangle} \Leftrightarrow \text{classical } \frac{dp}{dt} = -\frac{dU}{dx}$$

example: suppose $U(x) = 0$ (free particle)

$\frac{d\langle p\rangle}{dt} = 0$. $\langle p\rangle$ = constant fixed

but $\langle p^2\rangle$ is not as shown in Exercises.

($\Delta p(t)$ is a function of t.)

But when is ① valid? i.e. when do we recover classical results (classical limit is valid).

To answer this question, we ~~must~~ realise that we are essentially asking when

$\langle f(x)\rangle \cong f(\langle x\rangle)$?

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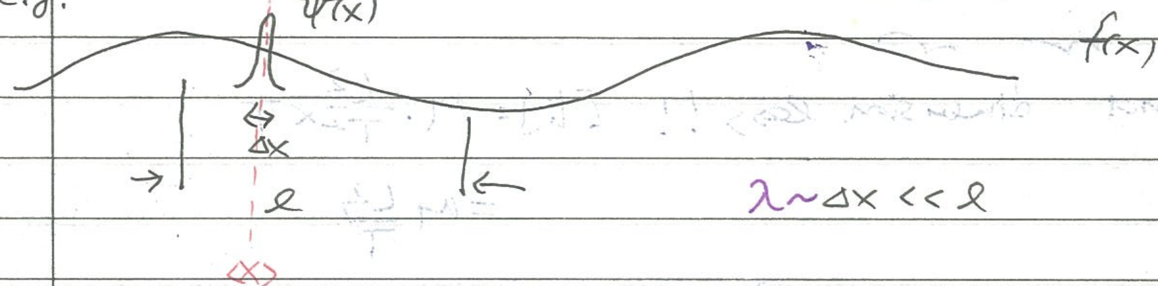
Since $\langle f(x) \rangle = \int_{-\infty}^{\infty} dx \, |\psi(x)|^2 f(x)$, it is obvious that this is true when Δx of $\psi(x) \ll$ the spatial variation length of $f(x)$.

e.g.



$\lambda \sim \Delta x \ll l$

$$\langle f(x) \rangle \sim f(\langle x \rangle)$$ The above is for mean value only!

How can a macroscopic particle be described by Classical Mechanics?

first: We have to prepare an initial state resembling the state of classical Mech.

i.e. well defined x & p.

But this is impossible in Q.M. The best one can do is to prepare a state with

$\langle x \rangle = x_0$, $\langle p \rangle = p_0$ and $\underbrace{\Delta x = \Delta \ \& \ \Delta p \simeq \frac{\hbar}{\Delta}}$ as small as possible.

$$\psi \sim \left(\frac{1}{\pi \Delta^2}\right)^{\frac{1}{4}} e^{\frac{i p_0 x}{\hbar}} e^{-\frac{(x-x_0)^2}{2\Delta^2}}$$

$\hbar \sim 1 \times 10^{-27}$ dyne-sec

Δ in cm Δp in g cm/sec dimension not right?

以c.g.s為單位之數字!

try to make $\Delta + \frac{\hbar}{\Delta}$ min $\therefore \Delta \propto \sqrt{\hbar}$

mass = 1g

$\therefore \Delta \simeq 10^{-13}$ cm (1F) $\Delta p \simeq 10^{-14}$ g cm/sec $\Delta v \sim 10^{-14} \frac{cm}{sec}$

far below experimental detectable range!

$\sim 10^{\ldots}$

✓ $\Delta(t) = \Delta\sqrt{1+\frac{\hbar^2 t^2}{m^2\Delta^2}} \sim 1\,mm$. $t \sim 3\times10^6$ year !

11/5 ~~due to $\hbar$ is very small~~

i.e., the experimental determined H is an averaged version of true $\hat{H}$. The averaged lengthscale $\gg \Delta x, \Delta p$

In other words, in the classical scale, the ψ has well-defined x & p at x_0 & p_0.

$$\therefore \left\langle \frac{\partial H(x,p)}{\partial p} \right\rangle \simeq \frac{\partial H(x_0,p_0)}{\partial p_0}$$

$$\left\langle \frac{\partial H(x,p)}{\partial x} \right\rangle \simeq \frac{\partial H(x_0,p_0)}{\partial x_0}.$$

$$\therefore \frac{d\langle x\rangle}{dt} = \left\langle \frac{\partial H(x,p)}{\partial p} \right\rangle$$

reduces to $\dot{x}_0 \simeq \frac{\partial H(x_0,p_0)}{\partial p_0}$

while $\frac{d\langle p\rangle}{dt} = -\left\langle \frac{\partial H(x,p)}{\partial x} \right\rangle$

reduces to $\dot{p}_0 \simeq -\frac{\partial H(x_0,p_0)}{\partial x_0}$.

the equality holds when $\hbar \to 0$. This statement is generally true as we'll show it when discussing path integral method.

WKB approximation (semi-classical approximation) $\boxed{\S\,16.2}$

$\boxed{\text{idea}}$:

If $V = \text{const}$. we have $\psi(x) = \psi(0)\, e^{\pm\frac{ipx}{\hbar}}$

$$p = \sqrt{2m(E-V)} \qquad E > 0$$

note $e^{+i\omega t} \Rightarrow +\ \leftarrow\ ,\ -\ \rightarrow \qquad (\omega = \frac{E}{\hbar})$

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

Now, suppose $V(x)$ varies slowly, then

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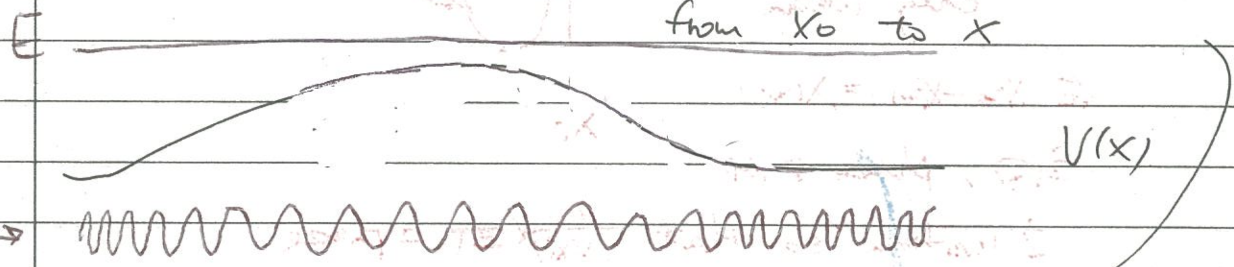
we expect $\lambda \to \lambda(x) = \frac{2\pi\hbar}{p(x)} = \frac{2\pi\hbar}{\sqrt{2m(E-V(x))}}$

$= |\psi(x_0)|\, e^{i\alpha(x_0) + i\,\text{accumulated phase from } x_0 \to x}$

$$\psi(x) = \psi(x_0)\exp\Big[\underbrace{\frac{\pm i}{\hbar}\int_{x_0}^{x} p(x')\,dx'}_{\shortparallel}\Big]$$

accumulated phase shift from x_0 to x



Amplitude fixed

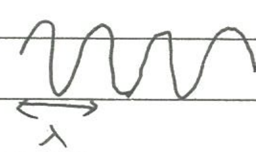
$$\frac{1}{\hbar}\,p(x')dx' = \frac{2\pi\,dx}{\lambda(x)}$$

Heuristic arguement for validity

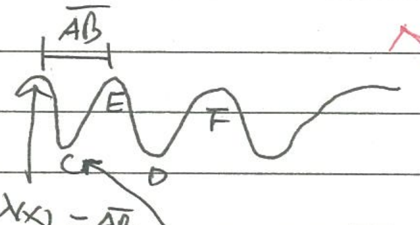
For $\lambda(x)$ to be well-defined, the change of λ over a period $(\lambda) \equiv \delta\lambda$ should be $\ll \lambda$

i.e. $\left|\frac{\delta\lambda}{\lambda}\right| \ll 1 \quad \because\ \delta\lambda = \frac{d\lambda}{dx}\cdot\lambda$

$\Rightarrow \left|\frac{d\lambda}{dx}\right| \ll 1$



$\overline{AB} \simeq \overline{CD}$



$\lambda(x_E) = \overline{EF}$

$\lambda(x) = \overline{AB}$ $\quad \lambda(x) = \overline{CD}$

$\frac{2\pi\,dx}{\lambda(x)}$ then describe the phase shift due to dx

$$\lambda(x) \ll \left|\frac{E-V(x)}{\frac{dV}{dx}}\right|$$

characteristic length of $V(x)$

Theorize the idea:

(see over)

$$\left[\frac{d^2}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\right]\psi(x)$$

$\Rightarrow \left[\frac{d^2}{dx^2} + \frac{p(x)^2}{\hbar^2}\right]\psi(x) = 0$, we now write $\psi(x) = e^{\frac{i\phi(x)}{\hbar}}$

$\phi(x)$ needs not to be real!

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$\Phi(x)$ satisfies   i.e. $i\hbar\Phi''(x) - \Phi'^2 + p^2 = 0$

$$-\left(\frac{\Phi'(x)}{\hbar}\right)^2 + \frac{i\Phi''}{\hbar} + \frac{p^2(x)}{\hbar^2} = 0 \quad \text{--- ①}$$

$\because$ $\lambda(x) = \dfrac{2\pi\hbar}{p(x)} \to 0$ as $\hbar \to 0$,

$\therefore$ at $\hbar \to 0$, $\lambda(x)$ is small compared to any finite variations of $U(x)$!!

One thus expects $\hbar$ is the parameter to expand,

$\therefore$ We expand (treat $\hbar$ as small variable even though $\hbar$ is a const.)

$$\Phi(x) = \Phi_0(x) + \hbar\Phi_1(x) + \hbar^2\Phi_2(x) + \ldots$$

↳ as long as $O(\hbar^n) = 0$, ⇐ 反過來 ① 也 ② is satisfied!

Substitute ② into ①,

$O(\hbar^0) \Rightarrow \quad \Phi_0'^2 + p^2(x) = 0 \qquad \Phi_0'(x) = \pm p(x)$

$$\therefore \Phi_0 = \pm \int^x p(x')\,dx'$$

$$\therefore \quad \Psi(x) = A \exp\left[\pm\frac{i}{\hbar}\int^x p(x')\,dx'\right]$$

$$= \Psi(x_0) \exp\left[\frac{\pm i}{\hbar}\int_{x_0}^x p(x')\,dx'\right]$$

反之不真:

① = 0

= ( ) + $\hbar$( ) + . + $\hbar^2$ . .

doesn't imply

( )

( )

⋮

=0 !

Which recovers the previous result.

$O(\hbar) \qquad i\hbar\Phi_0'' - 2\hbar\Phi_0'\Phi_1' = 0$

$$\therefore i\Phi_0'' = 2\Phi_0'\Phi_1'$$

$$\frac{(\Phi_0')'}{\Phi_0'} = -2i\Phi_1' \Rightarrow \ln\Phi_0' = -2i\Phi_1 + C$$

$$\Phi_1 = i\ln(\Phi_0')^{\frac{1}{2}} + \frac{C}{2i} = C' + i\ln p^{\frac{1}{2}}$$

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$$\therefore \psi(x) = e^{i\frac{\phi(x)}{\hbar}} \cong e^{i\frac{\phi_0(x)}{\hbar} + i\phi_1(x)}$$

$$= A\, e^{-\ln(p(x))^{\frac{1}{2}}} \exp\left[\pm\frac{i}{\hbar}\int^x p(x')dx'\right]$$

$$= \frac{A}{\sqrt{p(x)}} \exp\left[\frac{\pm i}{\hbar}\int^x p(x')\, dx'\right]$$

$$\psi(x_0) = \frac{A}{\sqrt{p(x_0)}} \exp\left[\frac{\pm i}{\hbar}\int^{x_0} p(x')dx'\right]$$

$$\underbrace{\psi(x) = \psi(x_0)\sqrt{\frac{p(x_0)}{p(x)}} \exp\left[\frac{\pm i}{\hbar}\int_{x_0}^{x} p(x')\, dx'\right]}$$

<u>WKB Approximation</u>! $\Uparrow$ p(x) can be imaginary!

<u>argument for $\frac{1}{\sqrt{p(x)}}$</u>:

classically,

Probability at $x \sim \frac{1}{v(x)} \sim \frac{1}{p(x)}$

$$\therefore \psi(x) \sim \frac{1}{\sqrt{p(x)}}!$$

<u>Validity of WKB approximation</u>

before setting $=0$!

$$i\hbar\phi'' - \phi'^2 + p^2 = \underbrace{(p^2 - \phi_0'^2) + i\hbar(\phi_0'' - 2\phi_0'\phi_1')}_{} + \cdots = 0$$

expansion is valid if

$$(p^2 - \phi_0'^2) \gg \hbar(\phi_0'' - 2\phi_0'\phi_1')$$

take $\phi_0'^2$ as a measure of $p^2 - \phi_0'^2$

ϕ_0'' as " of $\phi_0'' - 2\phi_0'\phi_1'$

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or from eq. ①

$|\hbar\phi''| << \phi'^2$

Obviously, WKB is not valid near turning point ($\frac{1}{\sqrt{p(x)}} = \infty$!)

$\therefore \quad \phi_0'^2 >> |\hbar\phi_0''|$

i.e. $\left| \frac{\hbar \frac{d\phi_0'}{dx}}{\phi_0'^2} \right| << 1$

$\left| \hbar \frac{d \frac{1}{\phi_0'}}{dx} \right| << 1$

$\left| \hbar \frac{d \frac{1}{p(x)}}{dx} \right| << 1 \Rightarrow \frac{1}{2\pi} \left|\frac{d\lambda}{dx}\right| << 1$

$$\frac{\hbar}{\sqrt{2m(E-U(x))}} << \frac{2(E-U(x))}{\left|\frac{dU(x)}{dx}\right|}$$

$$\frac{\hbar}{\sqrt{2m(E-U(x))}} = \frac{\lambda(x)}{2\pi}$$

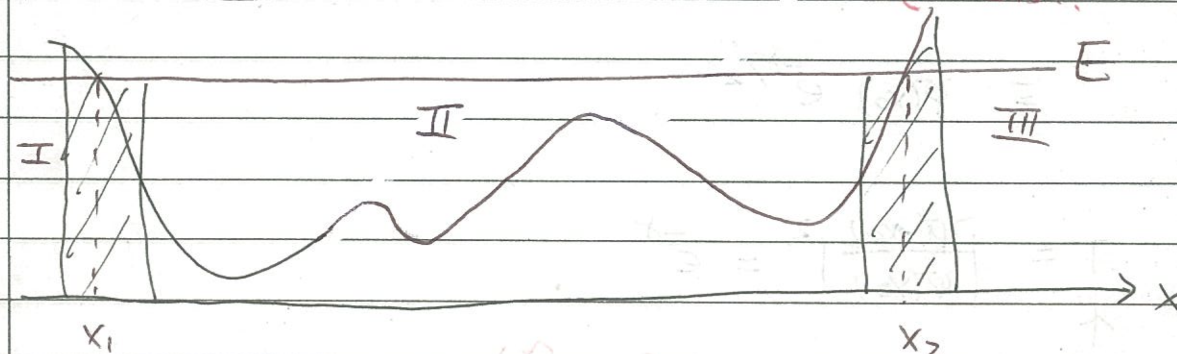
Characteristic variation length of $U(x)$

agree with the heuristic arguement.

for bound state $\boxed{n>>1}$ guarantees this!!

⇒ Tunneling Amplitude see over

Bound states



x_1, x_2 = turning points

WKB region

I $\quad \psi(x) \sim \frac{A}{\left(\sqrt{2m(V(x)-E)}\right)^{\frac{1}{2}}} \exp\left[\frac{1}{\hbar}\int^x \sqrt{2m(V(x')-E)}\, dx'\right]$

III $\quad \psi(x) \sim \frac{A}{\left(\sqrt{2m(V(x)-E)}\right)^{\frac{1}{2}}} \exp\left[\frac{-1}{\hbar}\int^x \sqrt{2m(V(x')-E)}\, dx'\right]$

II: $\quad \psi(x) = \frac{A}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int^x p(x')\,dx' + B\right]$

$\boxed{A, B = \text{Real}}$

$\boxed{1/1}$ region : $E \simeq V(x)$, $\lambda(x) = \dfrac{h}{\sqrt{2m(E-V(x))}} \to \infty$

thus , $\lambda(x) \ll \dfrac{2(E-V(x))}{\left|\frac{dV(x)}{dx}\right|}$ is not valid!

$\therefore$ WKB is not valid !

Need to solve Schrödinger equation directly :
(no free lunch !)

but $\because V(x) \simeq V(x_i) + V'(x_i)(x-x_i)$ $\quad i=1,2$

$= E + V'(x_i)(x-x_i)$

$\Rightarrow$ We can solve for linear potential .

Results :

near x_1^+ : $\beta = -\frac{\pi}{4}$

$$\psi_{II}(x) = \frac{A}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_{x_1}^{x} p(x')dx' - \frac{\pi}{4}\right]$$

near x_2^- , $\beta = \frac{\pi}{4}$

$$\psi_{II}(x) = \frac{A'}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_{x_2}^{x} p(x')dx' + \frac{\pi}{4}\right]$$

To be self consistent , $\psi_{II}(x)$ single value see over

$|A| = |A'|$

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

$n =$ odd , $A' = -A$

$n =$ even , $A' = A$

Theorem: regarding $x \to z$ if $V(z)$ is entire

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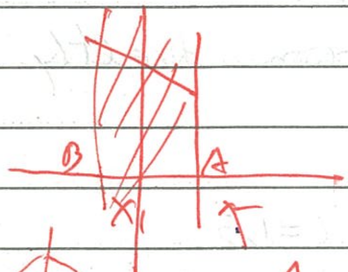
$\psi(z)$ has to be an entire function

Quick way to understand $\pm\frac{\pi}{4}$

Imagine that we can analytically continue

$x \to$ complex plane so that we can avoid $(x_1, 0)$



$$\frac{A}{\sqrt{2m(E-V(x))}}\left[e^{\frac{i}{\hbar}\int^x \sqrt{2m(E-V(x'))}\,dx' + iB} + e^{-\frac{i}{\hbar}\int^x \cdots + iB}\right]$$

$$\frac{1}{\sqrt{2m(V(x)-E)}}\, e^{\frac{1}{\hbar}\int^x \sqrt{2m(V(x')-E)}\,dx'}$$

dominant one (see Gottfried's book page 219-221)

When we go from x_A to x_B

$$\sqrt{2m(E-V(x))} \to \sqrt{2m(V(x)-E)}\; i$$

$$\frac{1}{(\sqrt{2m(E-V(x))})^{1/2}} \to \frac{1}{(\sqrt{2m(V(x)-E)})^{1/2}}\, i^{-\frac{1}{2}}$$

$$e^{-\frac{\pi}{4}i}$$

$\frac{\pi}{4} \pm \phi$ required coeff $= 0$

$$e^{\frac{1}{\hbar}\int^x \cdots - iB}$$

$\therefore B + \frac{\pi}{4} = 0$

also imply

$$\mathrm{I} = \frac{2A}{\sqrt{p(x)}}\, e^{\frac{i}{\hbar}\int^x p(x')\,dx'}$$

$$\mathrm{II} = \frac{2A}{\sqrt{p(x)}}\cos\left(\frac{1}{\hbar}\int^x p(x')\,dx' - \frac{\pi}{4}\right) \qquad \therefore B = -\frac{\pi}{4}$$

$$\mathrm{III} = \frac{A}{\sqrt{p(x)}}\, e^{-\frac{1}{\hbar}\int^x p(x')\,dx'}$$

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meaning $p = \frac{2\pi\hbar}{\lambda} \Rightarrow \frac{2\pi(x_2 - x_1)}{\lambda} = (n+\frac{1}{2})\pi$

$2L = (n+\frac{1}{2})\lambda_n \Rightarrow$ see over

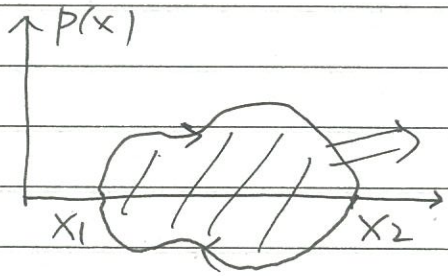
$$\Rightarrow \int_{x_1}^{x_2} p(x')\,dx' = \hbar(n+1/2)\pi$$

$$\text{i.e. } \int_{x_1}^{x_2} p(x')\,dx' + \int_{x_2}^{x_1} p(x')(-dx') = 2\hbar(n+1/2)\pi$$

$$\therefore \oint p(x)\,dx = (n+1/2)h$$

, $n\uparrow$, $P\uparrow$, $\lambda\downarrow$.

$\therefore$ $\lambda <$ characteristic length of U is satisfied!



Area is quantized:

# of states belonging to the phase space volume $\Delta x \Delta p = \frac{\Delta x \Delta p}{2\pi\hbar}$ $(2\pi\hbar = h)$

~ Old quantum theory by Sommerfeld & W. Wilson

$(n+1/2 \to n)$, 1915 (resulting from $\pm\frac{\pi}{4}$!)

$\because$ $P = \sqrt{2m(E-U(x))} \Rightarrow E$ is quantized : E_n!

<u>Example</u> : Simple harmonic oscillator (Ex 16.2, 4)

$$E = \frac{p^2}{2m} + \frac{1}{2}kx^2 \qquad \frac{k}{m} = \omega^2$$

$$P = \sqrt{2m(E - \frac{1}{2}kx^2)} \qquad x_1 = -\left(\frac{2E}{k}\right)^{\frac{1}{2}}$$

$$x_2 = \sqrt{\frac{2E}{k}}$$

$$\int_{x_1}^{x_2} p(x)\,dx = \sqrt{2mE}\int_{x_1}^{x_2}\sqrt{1-\frac{k}{2E}x^2}\,dx$$

$$= 2\sqrt{\frac{m}{k}}\,E\int_{-1}^{1}\sqrt{1-y^2}\,dy = \frac{2E}{\omega}\int_{-1}^{1}\sqrt{1-y^2}\,dy$$

$$= \frac{\pi E}{\omega} = \pi\hbar(n+1/2), \quad \therefore E_n = \hbar\omega(n+1/2)$$ exact!!

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Validity of WKB approximation:

Recall that $i\hbar\phi'' - \phi'^2 + p^2 = 0$

$\therefore \phi'^2 - i\hbar\phi'' = p^2$

RHS is independent of ϕ. For LHS, we do the expansion:

$$\phi'^2 - i\hbar\phi'' = \phi_0'^2 - i\hbar(\phi_0'' - 2\phi_0'\phi_1') + \cdots$$

the expansion is valid if

$$|\hbar\phi_0''| \ll |\phi_0'^2| \quad \cdots ①$$

& $\hbar|2\phi_0'\phi_1'| \ll |\phi_0'^2|$ $\Rightarrow \hbar\phi_1' \ll |\phi_0'| = p(x)$

$\Rightarrow \hbar \frac{1}{\sqrt{p}} \frac{d\sqrt{p}}{dx} < p$

$\Rightarrow \frac{\hbar}{p}\frac{dp}{dx} < p$

$\Rightarrow \hbar \frac{d}{dx}\left(\frac{1}{p(x)}\right) < 1$

Now ① implies $|\hbar\phi_0''| \ll |\phi_0'|^2$

i.e. $\left|\hbar \frac{d\frac{1}{\phi_0'}}{dx}\right| \ll 1$

With the solution, $\phi_0' = \pm p(x)$, same !

we get $\left|\hbar \frac{d}{dx}\left(\frac{1}{p(x)}\right)\right| \ll 1$

$$\therefore \frac{1}{2\pi}\left|\frac{d\lambda}{dx}\right| \ll 1$$

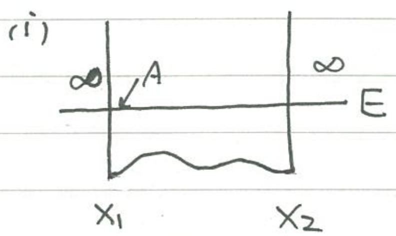
Remark: the quantization rule $\int_{x_1}^{x_2} p(x')\,dx' = \hbar\pi(n+\frac{1}{2})$

only applies to smooth potential such that

$\frac{1}{2\pi}\frac{d\lambda}{dx} << 1$ where $\frac{\lambda(x)}{2\pi} = \frac{\hbar}{\sqrt{2m(E-V(x))}}$

It doesn't apply to violent potentials such as:

(i)



or (ii)

However, near the point with ∞ potential (e.g. point A)

$\lambda(x) = \frac{h}{\sqrt{2\pi(E-V(x))}}$ = finite, there is actually no

intersection of E & $V(x)$! ∴ WKB approximation

is valid down to the ∞ points !

∴ For (i) $\psi(x) = \frac{A}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_{x_1}^{x} p(x')\,dx' + B\right]$

$\psi(x_1) = \psi(x_2) = 0$. $B = \frac{1}{2}\pi$, $\int_{x_1}^{x_2} p(x')\,dx = \hbar n\pi$, $n = 1, 2, 3, \ldots$

* if $V=0$ $x_1 < x < x_2$. $\sqrt{2mE}(x_2 - x_1) = n\pi\hbar \Rightarrow E = \frac{n^2\pi^2\hbar^2}{2m(x_2-x_1)^2}$

(ii) $\psi(x) = \frac{A}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_{x_2}^{x} p(x')\,dx' + \frac{\pi}{4}\right]$

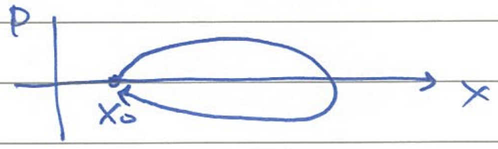
$\psi(x_1) = 0$ ∴ $\frac{1}{\hbar}\int_{x_2}^{x_1} p(x')\,dx' + \frac{\pi}{4} = -\frac{2n-1}{2}\pi$, $n = 1, 2, \ldots$

∴ $\int_{x_1}^{x_2} p(x')\,dx' = \hbar(n - \frac{1}{4})\pi$, $n = 1, 2, 3, \ldots$

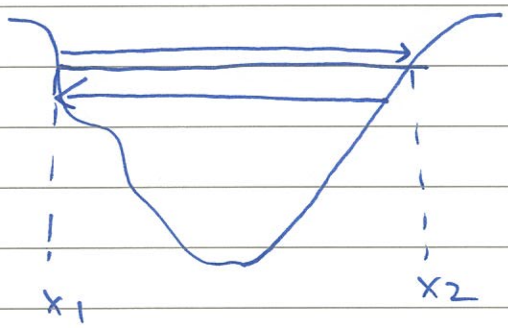
Meaning of $\oint p(x)\,dx = (n+\frac{1}{2})h$

wavefunction is single-valued.

$\therefore$ Starting from x_0

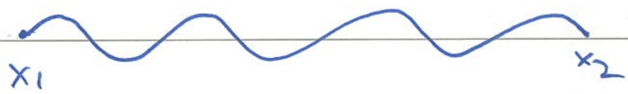


the accumulated phase $\oint = 2\pi \times n$!



Now, 由 $x_1 \to x_2$ 之 accumulated phase

$= \frac{1}{\hbar}\int_{x_1}^{x_2} p(x')\,dx'$ ($= k(x_2 - x_1)$ if $p = \text{const}$)



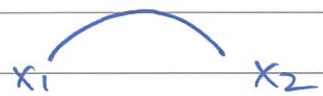
同理, $x_2 \to x_1$ 之 accumulated phase (>0)

$$= \frac{1}{\hbar}\int_{x_1}^{x_2} p(x')\,dx' \text{ too!}$$

$$= \frac{1}{\hbar}\int_{x_2}^{x_1} (-p(x'))\,dx \quad (p(x') \text{ is reversed})$$

(Note that $\neq \frac{1}{\hbar}\int_{x_2}^{x_1} p(x')\,dx'$. For example :

(i)

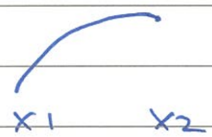


$x_1 \to x_2$: $\frac{\lambda}{2} = \pi$

$x_2 \to x_1$ (在 x_2 為 0) : 但是 $\frac{\lambda}{2} = \pi$

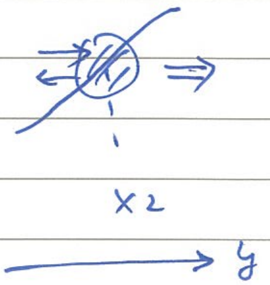
$\therefore$ total phase accumulated $= 2\pi$

(ii)



$x_1 \to x_2$: $\frac{\lambda}{4} = \pi/2$
$x_2 \to x_1$: $\frac{\lambda}{4} = \pi/2$
total $= \pi$ not allowed !)

turning phase :



$$e^{\frac{i}{\hbar}\int_{x_2}^{x} p(x')\,dx' + \frac{\pi}{4}i} + e^{-\frac{i}{\hbar}\int_{x_2}^{x} p(x')\,dx' - \frac{\pi}{4}i}$$

$$= e^{+iky + \frac{\pi}{4}i} + e^{-\frac{i}{\hbar}ky - \pi/4\, i}$$

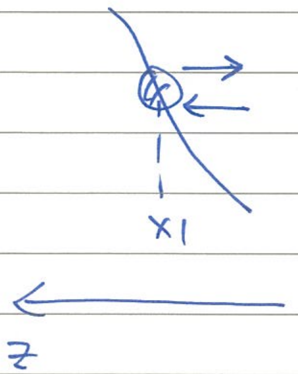
$\uparrow$ 向右入射 ~~outgoing~~　　$\uparrow$ incoming 向左

$y = \cancel{x_2 - x}\ x - x_2$　　~~(essentially $k \to -k$)~~

$\therefore$ turning phase $= \frac{\pi}{4} - (-\frac{\pi}{4}) = \pi/2$

入射　反射

another view: $\frac{1}{\sqrt{p(x)}} \rightarrow +\frac{1}{\sqrt{-p(x)}} = \frac{1}{\sqrt{p(x)}} e^{-i\pi/2}$



$$e^{\frac{i}{\hbar}\int_{x_1}^{x} p(x')\,dx' - \frac{\pi}{4}i} + e^{-\frac{i}{\hbar}\int_{x_1}^{x} p(x')\,dx' + \frac{\pi}{4}i}$$

$$= e^{+ikz - \pi/4\, i} + e^{-ikz + \pi/4\, i}$$

向右　向左

$z = x_1 - x$ ~~(or see $k \to -k$)~~ 入射

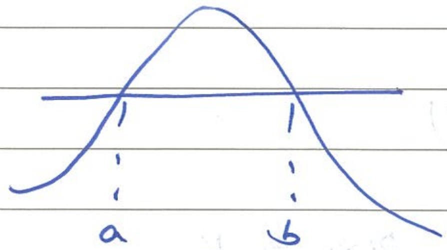
turning phase $= \frac{\pi}{4} - (-\frac{\pi}{4}) = \pi/2$

入射　反射

$\therefore\ \frac{\pi}{2} \times 2 + \frac{1}{\hbar}\oint p(x')\,dx' = 2\pi n$

$$\oint p(x')\,dx' = (n + \tfrac{1}{2})h \qquad (n - 1/2 \Rightarrow n + 1/2)$$

Application to tunneling



I II III

$$\text{III} \quad \psi(x) = \frac{\overset{\text{transmission}}{t}}{\sqrt{|p(x)|}}\, e^{\frac{i}{\hbar}\int_b^x |p(x')|dx' - \frac{\pi}{4}}$$

$$\text{II}: \quad \psi(x) = \frac{t}{\sqrt{|p(x)|}}\, e^{\frac{1}{\hbar}\int_x^b |p(x')|dx'}$$

$$= \underbrace{\frac{t}{\sqrt{|p(x)|}}\, e^{\frac{1}{\hbar}\int_a^b |p(x')|dx'}}\, e^{-\frac{1}{\hbar}\int_a^x |p(x')|dx'}$$

$$\downarrow$$

$$\text{I}: \quad \psi(x) = 2\frac{t}{\sqrt{|p(x)|}}\, e^{\frac{1}{\hbar}\int_a^b |p(x')|dx'} \cos\left(\frac{1}{\hbar}\int_a^x p(x')dx' + \frac{\pi}{4}\right)$$

counting from turning point.

~~incident flux~~ $\cancel{= \frac{|t|^2}{|p(x)|} e^{\frac{2}{\hbar}\int_a^b |p(x')|dx'}}$

Now, assuming $x \ll a$, $U \sim 0 \Rightarrow p(x) \to k = \sqrt{\frac{2mE}{\hbar^2}}$

$x \gg b$, $U \sim 0 \Rightarrow p(x) \to k = \sqrt{\frac{2mE}{\hbar^2}}$

$\therefore \frac{1}{\sqrt{|p(x)|}}$ is the same, and can be dropped

$\rightarrow$ or assuming $\frac{U_{+\infty}}{U_{-\infty}} \to 1$. $\therefore p(x\to\infty) = p(x\to-\infty)$

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Date

$$\cos\left(\frac{1}{\hbar}\int_a^x p(x')dx' + \frac{\pi}{4}\right)$$

$$\to \quad e^{\frac{i}{\hbar}\int_a^x p(x')dx + \frac{\pi}{6}i} \quad (\text{incident})$$

flux, $\quad \nabla\psi \Rightarrow \quad \nabla\int_a^x p(x')dx' = p(x) \to K$

$\Rightarrow \therefore$ incident flux $= |t|^2 e^{2/\hbar \int_a^b p(x')dx'} \cdot \left(\frac{1}{\sqrt{K}}\right)^2 \times K$ ①

transimissin

flux $= |t|^2 \left(\frac{1}{\sqrt{K}}\right)^2 K$ 구ㅡ! ②

$$\therefore T = \frac{②}{①} = e^{\frac{-2}{\hbar}\int_a^b p(x')dx'}$$

DCT Dream Come True

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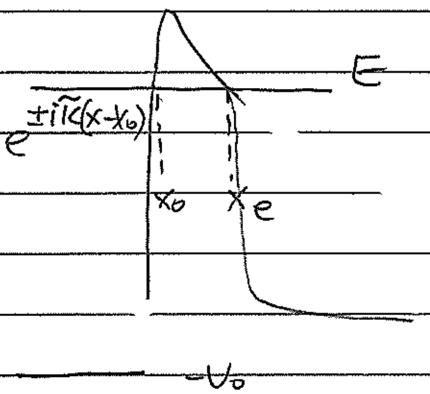
Tunneling Amplitude

$\psi \simeq \psi(x_0)\, e^{\pm i\tilde{\kappa}(x-x_0)}$



$\psi \simeq \psi(x_e)\, e^{ik(x-x_e)}$

$k = \frac{1}{\hbar}\sqrt{E \cdot 2m}$

$\tilde{\kappa} = \frac{1}{\hbar}\sqrt{2m(V_0+E)}$

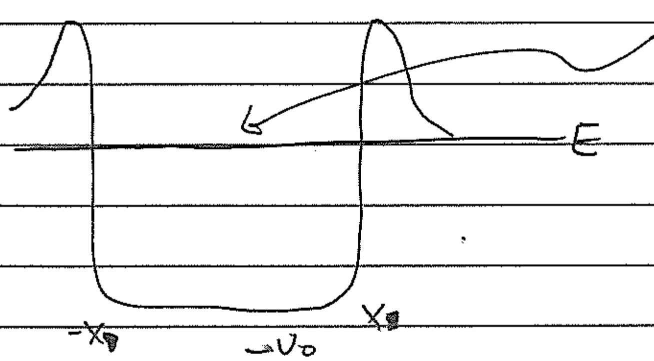
$$\psi(x_e) = \psi(x_0)\exp\left[\frac{-1}{\hbar}\int_{x_0}^{x_e} \sqrt{2m[V(x)-E]}\, dx\right]$$

$$\equiv \psi(x_0)\, e^{-\gamma/2}$$

$$\therefore\ T = \left|\frac{\psi(x_e)}{\psi(x_0)}\right|^2 = e^{-\gamma}$$

tunneling propability (if $k = \tilde{\kappa}$)

$v = \frac{\hbar \tilde{\kappa}}{m}$



frequency of collision with the barrier

$= \frac{v}{2x_1}$

$\therefore\ R$ (escaping rate) $= \frac{v}{2x_1} e^{-\gamma}$

$\tau \equiv$ life time $= \frac{1}{R}$

Angel