QM I

Phys 657

Lecture # 24

The classical limit

CM	QM
no uncertainty $\xleftarrow{\hbar \to 0}$	uncertainty
$\frac{dA}{dt} = [A, H]_{classical}$	$\frac{dA_H}{dt} = \frac{1}{i\hbar}[A_H, H]$ (QM) commutator
classical Hamiltonian, Poisson brackets	Heisenberg equation of motion
$\frac{\partial H}{\partial q}\frac{\partial A}{\partial p} - \frac{\partial A}{\partial q}\frac{\partial H}{\partial p}$	
generalized coordinate & momentum	

So, if there is a classical analog of QM operator, then the transition from CM to QM is

$$[\,,\,]_{classical} \longleftrightarrow \frac{[\,,\,]_{QM}}{i\hbar}$$

Dirac's rule

Examples of no classical analog? $\Rightarrow$ spin!

QM: $\frac{dS_H}{dt} = \frac{1}{i\hbar}[S_H, H]$, but no classical analog!

CM	QM
Harmonic oscillator:	
minimal energy $E=0$	minimal energy $E_0 = \frac{\hbar\omega}{2}$
$\Leftarrow \hbar \to 0$	
continuous	discrete
energy	spectrum

Consider the wave function

$$\Psi(\vec{x},t) = \underbrace{\sqrt{\rho(\vec{x},t)}}_{\Uparrow} e^{\frac{i}{\hbar}S(\vec{x},t)} \qquad (25.1)$$

probability density

$$\rho(\vec{x},t) = |\Psi(\vec{x},t)|^2$$

physical meaning?
$\Downarrow$
Recall Lecture #26
$\Downarrow$
probability flux

Substitute (25.1) into this $\Rightarrow$ $\vec{j}(\vec{x},t) = \frac{\hbar}{m} \mathrm{Im}(\Psi^* \vec{\nabla}\Psi)$

$$\vec{j}(\vec{x},t) = \frac{\hbar}{m} \mathrm{Im}\left[\sqrt{\rho}\, e^{-\frac{i}{\hbar}S} \cdot \left(e^{\frac{i}{\hbar}S} \vec{\nabla}(\sqrt{\rho}) + \frac{i}{\hbar}\sqrt{\rho}\, e^{\frac{i}{\hbar}S} \cdot \vec{\nabla}S\right)\right] = \frac{\hbar}{m} \mathrm{Im}\left[\sqrt{\rho}\,\vec{\nabla}(\sqrt{\rho}) + \frac{i}{\hbar}\underbrace{(\sqrt{\rho})^2}_{=\rho} \vec{\nabla}S\right] =$$

$$= \frac{\cancel{\hbar}}{m} \frac{\rho}{\cancel{\hbar}} \vec{\nabla}S = \frac{\rho}{m} \vec{\nabla}S$$

spatial variation of the phase of the wave function is dir related to the probability flux

If $\Psi(\vec{x},t) \sim e^{i\frac{\vec{p}\cdot\vec{x}}{\hbar}}\, e^{-\frac{i}{\hbar}Et}$ $\Rightarrow$ what is $\vec{\nabla} S$?

$\uparrow$ plane wave

$$\mathrm{Im}\left[\Psi^* \vec{\nabla}\Psi\right] \sim \left[\frac{i}{\hbar}\vec{p}\right] = \frac{\vec{p}}{\hbar}$$

$$\boxed{\vec{\nabla} S = \vec{p}} \Leftarrow \vec{j}(x,t) \sim \frac{\hbar}{m}\cdot\frac{\vec{p}}{\hbar} = \frac{1}{m}\vec{\nabla} S$$

$\uparrow$ $\rho = 1$ for simplicity

What if we substitude (25.1) into the Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \left(-\frac{\hbar^2}{2m}(\vec{\nabla})^2 + V\right)\Psi \Rightarrow \; ?$$

$$i\hbar\left[\frac{\partial\sqrt{\rho}}{\partial t} + \frac{i}{\hbar}\sqrt{\rho}\frac{\partial S}{\partial t}\right]e^{\frac{i}{\hbar}S} \overset{?}{=} -\frac{\hbar^2}{2m}\Delta\left(\sqrt{\rho}e^{\frac{i}{\hbar}S}\right) + V\sqrt{\rho}e^{\frac{i}{\hbar}S}$$

$$\Delta\left(\sqrt{\rho}e^{\frac{i}{\hbar}S}\right) = \Delta(\sqrt{\rho})\cdot e^{\frac{i}{\hbar}S} + \left(\frac{i}{\hbar}\sqrt{\rho}\,\Delta S + \frac{2i}{\hbar}(\vec{\nabla}\sqrt{\rho})(\vec{\nabla}S) - \frac{1}{\hbar^2}\sqrt{\rho}\,|\vec{\nabla}S|^2\right)e^{\frac{i}{\hbar}S} \Rightarrow$$

$$i\hbar\left[\frac{\partial\sqrt{\rho}}{\partial t} + \frac{i}{\hbar}\sqrt{\rho}\frac{\partial S}{\partial t}\right] = \frac{-\hbar^2}{2m}\left[\Delta(\sqrt{\rho}) + \frac{i}{\hbar}\sqrt{\rho}\,\Delta S + \frac{2i}{\hbar}\cdot(\vec{\nabla}\sqrt{\rho})\cdot\vec{\nabla}S - \frac{1}{\hbar^2}\sqrt{\rho}\,|\vec{\nabla}S|^2\right] + V\sqrt{\rho}\;; \qquad (25.2)$$

$$i\hbar\frac{\partial\sqrt{\rho}}{\partial t} - \sqrt{\rho}\frac{\partial S}{\partial t} = -\frac{\hbar^2}{2m}\Delta(\sqrt{\rho}) - \frac{i\hbar}{2m}\sqrt{\rho}\,\Delta S - \frac{i\hbar}{m}(\vec{\nabla}\sqrt{\rho})\vec{\nabla}S + \frac{\sqrt{\rho}}{2m}|\vec{\nabla}S|^2$$

If we set $\hbar \to 0$ in (25.2) $\Rightarrow$

$$+\sqrt{\rho}\frac{\partial S}{\partial t} + \frac{\sqrt{\rho}}{2m}|\vec{\nabla} S|^2 + V\sqrt{\rho} = 0 \Rightarrow$$

$$\boxed{\frac{1}{2m}|\vec{\nabla} S(\vec{x},t)|^2 + V(\vec{x}) + \frac{\partial S(\vec{x},t)}{\partial t} = 0} \quad (25.3)$$

Hamilton–Jacobi equation in classical mechanics!!

$S(\vec{x},t) \to$ Hamilton's principal function

So,

CM	QM
$S(\vec{x},t)$	$\hbar \cdot \frac{S}{\hbar}$

$\frac{S}{\hbar}$ ← phase of the wave function

If $H \neq H(t) \Rightarrow S(\vec{x},t) = W(\vec{x}) - Et \quad (25.4)$

$W(\vec{x})$ ↑ Hamilton's characteristic function

$$\Psi(\vec{x},t) = \underbrace{\sqrt{\rho}\, e^{\frac{i}{\hbar}W(\vec{x})}\, e^{-\frac{i}{\hbar}Et}}_{\text{stationary state}}$$

Let's substitute (25.4) into (25.3) $\Rightarrow$

$$\frac{1}{2m}|\vec{\nabla} W(\vec{x})|^2 + V(\vec{x}) = E \Rightarrow |\vec{\nabla} W|^2 = 2m(E - V(\vec{x}))$$

$$\vec{\nabla} W = \pm\sqrt{2m(E - V(\vec{x}))}\,; \quad W = \pm\int_0^{x} dx'\, \sqrt{2m(E - V(x'))}$$

in 1D $\Rightarrow$

0 ↑ or where $V(x)$ is ~~def...~~ defined

Semiclassical (WKB) approximation

Consider 1D case $\Rightarrow$ $S(x,t) = \pm \int^x \sqrt{2m(E-V(x'))}\,dx' - Et$;

Recall conservation of probability:

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0 \quad ; \quad j = \frac{\rho}{m}\frac{\partial S}{\partial x} \Rightarrow$$

Consider a stationary state $\Rightarrow$ $\frac{\partial \rho}{\partial t} = 0 \Rightarrow$

$$\frac{\partial}{\partial x}\left[\rho \frac{\partial S}{\partial x}\right] = 0 \Rightarrow \rho \underbrace{\left[\frac{dW}{dx}\right]}_{=\pm\sqrt{2m(E-V(x))}} = \text{const} \Rightarrow$$

integrate over x

$$\sqrt{\rho} \sim \frac{\text{constant}}{\big(\underbrace{E - V(x)}\big)^{1/4}} \sim \frac{1}{\sqrt{v_{\text{classical}}}}$$

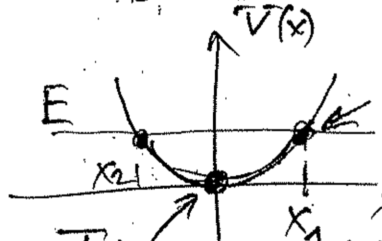
$\sqrt{\rho} \Updownarrow \psi$

kinetic energy $\sim v^2_{\text{classical}}$

Classically: the probability for finding a particle at a given point is inversely proportional to its velocity

$\Downarrow$

Example: harmonic oscillator



$T = E - V(x) \to 0$ at $x_{1\text{ or }2}$

$\Downarrow$

$v \to 0 \Rightarrow$ particle spends a lot of time there

T is maximal ($=E$) goes through fast

(6)

Now back to the wave function $\Rightarrow$

$$\underline{\Psi(x,t)} = \sqrt{\rho}\, e^{\frac{i}{\hbar}S} = \frac{\text{Const}}{(E-V(x))^{1/4}} e^{\frac{i}{\hbar}S} =$$

$$= \frac{\text{Const}}{(E-V(x))^{1/4}} \cdot e^{\frac{i}{\hbar}W(x)} e^{-\frac{i}{\hbar}Et} =$$

$$= \frac{\text{Const}}{(E-V(x))^{1/4}} \exp\left[\pm \frac{i}{\hbar}\int_0^x dx' \sqrt{2m(E-V(x'))} - \frac{i}{\hbar}Et\right] \quad (25.5)$$

assuming $E > V(x)$

Wentzel – Kramers – Brillouin (WKB) solution

<u>Note</u>: We obtained WKB solution in the "classical" limit ($\hbar \to 0$), i.e. $\hbar\left|\frac{d^2W}{dx^2}\right| \ll \left|\frac{dW}{dx}\right|^2$ or, substituting $W(x) = \pm\int^x dx' \sqrt{2m(E-V(x))} \Rightarrow$

$$\hbar \cdot \frac{\cancel{\sqrt{2m}}\left|\frac{dV}{dx}\right|}{\cancel{2}\sqrt{2m(E-V(x))}} \ll \cancel{2m}(E-V(x)) \Rightarrow$$

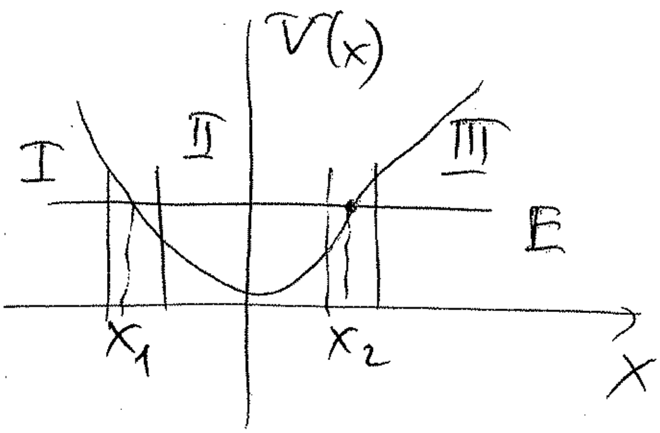
$$\underset{\text{de Broglie wavelength}}{\lambda\!\!\!^{-}_B} = \frac{\lambda_B}{2\pi} = \frac{1}{\underset{2\pi/\lambda}{K}} = \boxed{\frac{\hbar}{\underset{\hbar K}{\sqrt{2m(E-V(x))}}} \ll \frac{2(E-V(x))}{|dV/dx|}} \quad (25.6)$$

$\Rightarrow$ semi-classical picture works in the short-wavelength limit

What if $E < V(x) \Rightarrow$ then (25.5) 7

turns into

$$\Psi(x,t) = \frac{\text{constant}}{(V(x)-E)^{1/4}} \exp\left[\pm\frac{1}{\hbar}\int^{x} dx' \sqrt{2m(V(x')-E)} - \frac{i}{\hbar}Et\right] \quad (25.5')$$



<u>But</u> what if $E \simeq V(x)$ (around x_1, x_2)?

$\Downarrow$

(25.6) criterion for WKB validity breaks down.

in these regions $\Leftarrow$

we have to solve Schrödinger equation

<u>Good news</u>: $V(x_{1,2}) = E \Rightarrow$ around x_1, x_2 can approximate

$$V(x) \simeq \underbrace{E}_{V(x_{1,2})} + \left.\frac{dV}{dx}\right|_{x_{1,2}}(x-x_{1,2})$$

around $x_{1,2}$ $\Leftarrow$ constant!

$\Downarrow$

$$-\frac{\hbar^2}{2m}\Psi''(x) + \left.\frac{dV}{dx}\right|_{x_{1,2}}\cdot(x-x_{1,2})\Psi(x) = 0$$

same <u>kind</u> of equation for <u>any</u> $V(x)$!

Bessel equation $\Rightarrow$ solutions are Bessel functions!