Classical Mechanics

Given a potential $U(x)$, the Hamiltonian is:

$$H = \frac{p^2}{2m} + U(x) = E \leftarrow \text{constant of motion}$$

You form the eqn of motion:

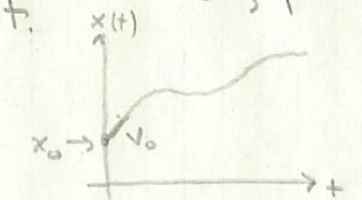
$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m} \qquad \dot{p} = -\frac{\partial H}{\partial x} = -\frac{dU}{dx}$$

$$\searrow \quad \swarrow$$

$$\frac{dp}{dt} = -\frac{dU}{dx} = F \Rightarrow m\ddot{x} = F$$

Solve subject to initial conditions $x(0) = x_0$, $\dot{x}(0) = v_0$.

The solution is $x(t)$, position of the particle at time t.



Quantum Mechanics

Start from the Hamiltonian again:

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

this time, we view H, p & x as <u>operators</u>

$$x \longrightarrow x, \quad p \longrightarrow \frac{\hbar}{i}\frac{\partial}{\partial x} \quad E \longrightarrow i\hbar\frac{\partial}{\partial t} \qquad (0)$$

w/ some built-in properties:

$[x,p] \equiv xp - px$ act on test-function

$$[x,p]f(x) = x\frac{\hbar}{i}\frac{df}{dx} - \frac{\hbar}{i}\frac{d}{dx}(xf)$$

$$= x\frac{\hbar}{i}\frac{df}{dx} - x\frac{\hbar}{i}\frac{df}{dx} - \frac{\hbar}{i}f$$

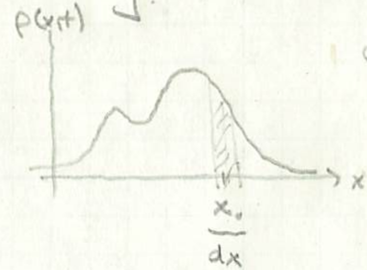
$$= i\hbar f(x) \Rightarrow [x,p] = i\hbar$$

Using the rules in (0) and allowing the operators to act on a function $\psi(x,t)$:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + U(x)\psi = i\hbar\frac{\partial\psi}{\partial t} \quad \text{Schrödinger's eqn.}$$

solve for $\psi(x,t)$ given initial $\psi(x,0) = \psi_0$ & b.c., typically $\psi(x,t) \xrightarrow[|x|\to\infty]{} 0$

$P(x,t) \equiv |\psi(x,t)|^2$ is prob. of finding the particle in the vicinity of x at time t



$$dP(x_0,t) = |\psi(x_0,t)|^2 dx$$

w/

$$P(a,b) = \int dP = \int_a^b |\psi(x,t)|^2 dx$$

then $P(-\infty,\infty) = ?$ (normalization condition) we can use the probability density to construct averages:

$$\langle x\rangle = \int_{-\infty}^{+\infty} x\rho(x)dx = \int_{-\infty}^{+\infty} \psi^* x \psi dx$$

$$\langle x^2\rangle = \int_{-\infty}^{+\infty} \psi^* x^2 \psi dx$$

& variances: $\sigma_x^2 \equiv \langle (x-\langle x\rangle)^2\rangle$

$$= \langle x^2 - 2x\langle x\rangle + \langle x\rangle^2\rangle$$

$$= \langle x^2\rangle - 2\langle x\rangle^2 + \langle x\rangle^2$$

$$= \langle x^2\rangle - \langle x\rangle^2$$

sim. for p: $\langle p\rangle = \int_{-\infty}^{+\infty} \psi^* \frac{\hbar}{i}\frac{\partial}{\partial x}\psi dx.$

etc. In general, for an operator A:

$$\langle A\rangle = \int_{-\infty}^{+\infty} \psi^* A \psi dx$$

& $\sigma_A^2 \equiv \langle A^2\rangle - \langle A\rangle^2$

<u>Example</u> - <u>free particle</u>

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = i\hbar\frac{\partial\psi}{\partial t}$$ use mult. S.O.V.

let $\psi(x,t) = X(x)T(t)$, then:

$$-\frac{\hbar^2}{2m}\frac{X''}{X} = i\hbar\frac{\dot{T}}{T} \Rightarrow -\frac{\hbar^2}{2m}\frac{X''}{X} = E = i\hbar\frac{\dot{T}}{T}$$

name based on units: J·s·1/s = J ✓

$$X(x) = Ae^{i\sqrt{\frac{2mE}{\hbar^2}}x} + Be^{-i\sqrt{\frac{2mE}{\hbar^2}}x}$$

$$T(t) = e^{-iEt/\hbar}$$

for a classical free particle, $E = p^2/2m$

so

$$\psi(x,t) = e^{-iEt/\hbar}\left[Ae^{ipx/\hbar} + Be^{-ipx/\hbar}\right]$$

left & right travelling oscillations. (which is which?)

Take $\psi(x,t) = Ae^{-iEt/\hbar}e^{ipx/\hbar}$, what is $\psi^*\psi = ?$

$|\psi|^2 = |A|^2$ — particle could be <u>anywhere</u> w/ equal probability, not normalizable.

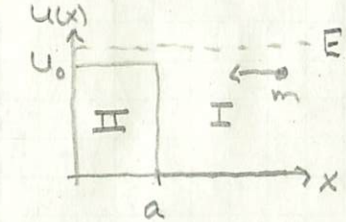
act on ψ w/ the momentum operator $\hat{p}$:

$$\hat{p}\psi = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi = \frac{\hbar}{i}\cdot\frac{i}{\hbar}p\psi = p\psi$$

ψ is an eigenfunction of the $\hat{p}$ operator, w/ e-value p.

position is uncertain, momentum is not.

Comparison of CM + QM



$E_1 = \frac{p^2}{2m} + U(x)$

so

$\frac{p^2}{2m} = E_1 - U(x)$

particle goes faster when $E_1 - U(x)$ is bigger,

$$p = \pm\sqrt{2m(E_1 - U(x))}$$

in region I, $p_I = -\sqrt{2mE_1}$

in region II, $p_{II} = -\sqrt{2m(E_1 - U_0)}$

Quantum version – focus on t-indep. piece:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi(x) = E_1\psi(x)$$

in region I: $\psi(x) = Ae^{-ipx/\hbar}$ w/ $p = -\sqrt{2mE_1}$

oscillatory ψ w/ wavelength λ:

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

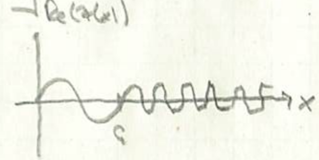
in region II,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U_0\psi = E_1\psi \Rightarrow \psi'' = -\frac{2m}{\hbar^2}(E_1 - U_0)\psi$$

$$\psi = Be^{-i\sqrt{\frac{2m}{\hbar^2}(E_1-U_0)}\,x} = Be^{-i\frac{x}{\hbar}\sqrt{p^2-2mU_0}}$$

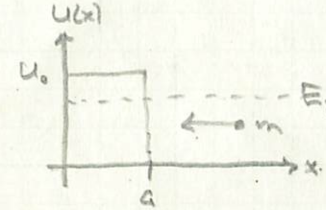
oscillation w/ wavelength $\lambda_{II} = \frac{2\pi\hbar}{\sqrt{p^2-2mU_0}} > \lambda_I$

$\psi(x)$ is continuous + deriv. continuous everywhere (for finite pot'l.), so



(sketch)

What happens if $E_2 < U_0$:



CM: $x<a$: $p = -\sqrt{2m\underbrace{(E_2 - U_0)}_{<0}}$ imaginary.

? What happens physically ?

QM: for $x<a$, $-\frac{\hbar^2}{2m}\psi'' + U_0\psi = E_2\psi$

gives $\psi'' = -\frac{2m}{\hbar^2}\underbrace{(E_2 - U_0)}_{<0}\psi$

this time ψ has growing + decaying exponential behavior, + the particle will be found in the $x<a$ region w/ non-zero probability.