Newtonian Mechanics:

Given initial conditions $(x(0), v_x(0))$,

Find $x(t)$

Use Newton's Law

$$m\frac{d^2x}{dt^2} = F$$

If F is conservative

$$\oint \vec{F}\cdot d\vec{\ell} = 0, \quad \vec{\nabla}\times\vec{F} = 0$$

Then $\vec{F} = -\vec{\nabla}U$

$$m\frac{d^2\vec{r}}{dt^2} = -\vec{\nabla}U$$

$$m\frac{d^2x}{dt^2} = -\frac{\partial U}{\partial x}$$

$$m\frac{d^2y}{dt^2} = -\frac{\partial U}{\partial y}$$

$$\cdots$$

In QM, we are interested not in $\vec{r}(t)$

but $\Psi(\vec{r}, t)$

Where Ψ is the wave-function

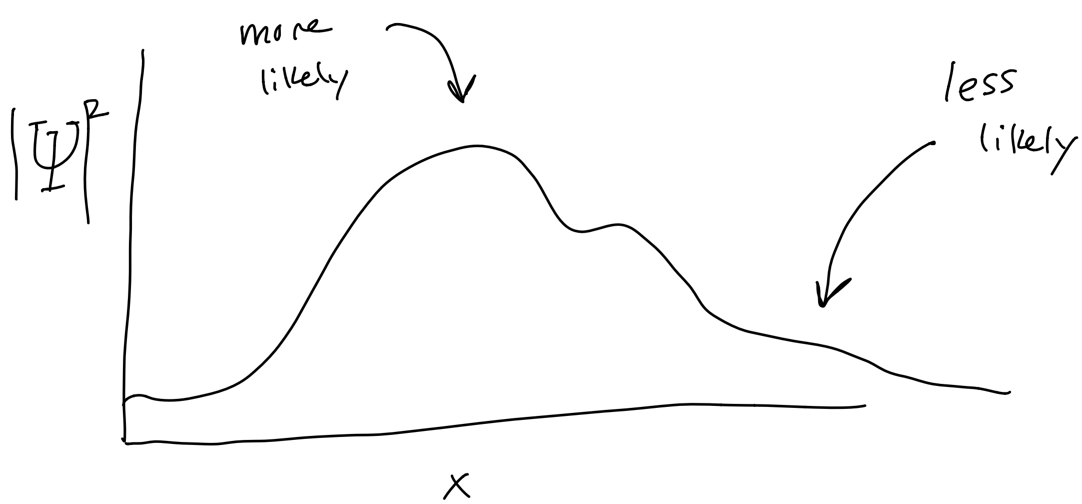
if $\Psi = \Psi(x, t)$

then

$$\int_a^b |\Psi(x,t)|^2 dx = \text{Probability of finding particle between } a \,\&\, b, \text{ at time } t$$

Particles don't have a precise position/velocity etc

instead: probability distribution



Properties of the wave function:

- Complex

$$|\psi|^2 = \psi^* \psi$$

z^* is complex conjugate

$$z = x + iy$$
$$z^* = x - iy$$

$$*: \; i \longrightarrow -i$$

- $$\int_{-\infty}^{\infty} |\psi|^2 = 1$$

Probability

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

- Solution determined by Schrödinger equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi$$

$V \longleftrightarrow \mathcal{U}$

V = Potential Energy

IN 1D:

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

$\hbar$: Reduced Planck constant

$$= \frac{h}{2\pi} = 1.054 \ldots \times 10^{-34} \text{ Js}$$

Most of a QM class is learning techniques to solve!

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

How to solve? (Assume $V = V(x)$, not t)

Separation of variables

Assume $\Psi(x,t) = \psi(x)\,\varphi(t)$

$$\frac{\partial \Psi}{\partial t} = \psi \frac{d\varphi}{dt}, \quad \frac{\partial^2 \Psi}{\partial x^2} = \varphi \frac{d^2\psi}{dx^2}$$

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

Becomes

$$i\hbar\psi \frac{d\varphi}{dt} = \frac{-\hbar^2}{2m}\varphi \frac{d^2\psi}{dx^2} + V\psi\varphi$$

Now $\div$ by $\psi \phi$

$$i\hbar \frac{1}{\phi}\frac{d\phi}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V$$

LHS $= f(t)$
RHS $= f(x)$

$f(t) = f(x)$

Both are <u>constant</u>

Call the constant E

$$i\hbar \frac{1}{\phi}\frac{d\phi}{dt} = E$$

$$\boxed{\frac{d\phi}{dt} = -\frac{i}{\hbar} E\phi} \qquad (1)$$

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V = E$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi} \qquad (2)$$

1 PDE $\longrightarrow$ 2 ODEs

(1)

$$\boxed{\frac{d\phi}{dt} = -\frac{i}{\hbar} E \phi}$$

$$\phi = C e^{-\frac{i}{\hbar} E t}$$

(2) Requires that we specify V

$$\boxed{-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi}$$

Time IND Schrödinger Eqn

specify V, solve ψ,

then

$$\Psi(x,t) = \psi(x) e^{-\frac{i}{\hbar} E t}$$

Claim:

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right) = H \quad \text{(hamiltonian)}$$

$$H = \frac{p^2}{2m} + V$$

$$\langle p \rangle = m\langle v \rangle = m\frac{d\langle x \rangle}{dt}$$

$$\langle x \rangle = \int \Psi^*(x)\Psi\, dx$$

$$\frac{d}{dt}\langle x \rangle = \int \frac{\partial}{\partial t}\left(\psi^*(x)\psi\right) dx$$

$$\frac{d}{dt}\langle x \rangle = \int x\left(\psi\frac{\partial \psi^*}{\partial t} + \psi^*\frac{\partial \psi}{\partial t}\right)$$

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \psi}{\partial x^2} + \frac{i}{\hbar}V\psi$$

$$\frac{\partial \psi^*}{\partial t} = \frac{-i\hbar}{2m}\frac{\partial^2 \psi^*}{\partial x^2} - \frac{i}{\hbar}V\psi^*$$

$$\psi \frac{\partial \psi^*}{\partial t} = \frac{-i\hbar}{2m} \psi \frac{\partial^2 \psi^*}{\partial x^2} - \frac{i}{\hbar} V \psi \psi^*$$

$$\psi^* \frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m} \psi^* \frac{\partial^2 \psi}{\partial x^2} + \frac{i}{\hbar} V \psi^* \psi$$

$$\psi \frac{\partial \psi^*}{\partial t} + \psi^* \frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m} \left(\psi^* \frac{\partial^2 \psi}{\partial x^2} - \psi \frac{\partial^2 \psi^*}{\partial x^2} \right)$$

$$= \frac{i\hbar}{2m} \frac{\partial}{\partial x} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right)$$

$$\boxed{\begin{aligned} \frac{\partial}{\partial x}\left(\psi^* \frac{\partial}{\partial x} \psi\right) &= \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} + \psi^* \frac{\partial^2 \psi}{\partial x} \\ &\quad - \frac{\partial \psi}{\partial x} \frac{\partial \psi^*}{\partial x} - \psi \frac{\partial^2 \psi^*}{\partial x} \end{aligned}}$$

$$\frac{d\langle x \rangle}{dt} = \frac{i\hbar}{2m} \int x \frac{\partial}{\partial x} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right) dx$$

$\int$ by parts

$$\frac{d\langle x \rangle}{dt} = \frac{-i\hbar}{2m} \int \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right) dx$$

$$\frac{d\langle x\rangle}{dt} = -\frac{i\hbar}{m}\int \Psi^* \frac{\partial}{\partial x}\Psi\, dx$$

$$\langle p\rangle = \int \Psi^* (p)\Psi\, dx = \int \Psi^* \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi\, dx$$

$\frac{\hbar}{i}\frac{\partial}{\partial x}$ is the momentum "operator" $\hat{p}$

$$H = \frac{p^2}{2m} + V = -\frac{\hbar^2}{2m}\frac{\partial}{\partial x} + V$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi}$$

$\downarrow$

$$\hat{H}\psi = E\psi$$

$$\langle H\rangle = \int \Psi^* \hat{H}\Psi\, dx = \int \psi^*(x) e^{\frac{i}{\hbar}Et} \hat{H}\psi(x) e^{-\frac{i}{\hbar}Et}\, dx$$

$$= \int \psi^*(x)\hat{H}\psi(x)\, dx = E\int \psi^*(x)\psi(x)\, dx = \underline{E}$$

$$\langle H\rangle = \underline{E}$$