The Schrodinger Eq

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

$\sqrt{-1}$ $\quad \frac{h}{2\pi}$

Particle mass

2 space derivatives

Potential Energy ("Force on particle) $-\frac{dV}{dx}$

Only 1 time derivative

Position & Momentum

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\Psi|^2 dx$$

Note: Not the average of measuring particle many times!

Average x if you measured many particles w/ $\Psi(x,t)$

How does $\langle x \rangle$ change w/ Sch Eq?

$$\frac{d\langle x \rangle}{dt} = \int_{-\infty}^{\infty} x \frac{\partial}{\partial t} |\Psi|^2 dx$$

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

Integration By Parts $\boxed{\text{H.W.}}$

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

More Integration By Parts

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

$$\langle p\rangle = -i\hbar\int_{-\infty}^{\infty}\Psi^*\frac{\partial\Psi}{\partial x}\,dx$$

Knew this would happen

$p \to -i\hbar\frac{\partial}{\partial x}$

or

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

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

The average of $\frac{\partial}{\partial x}$ is telling you how much momentum ($\sim$ KE) the particle has.

All classical dynamical variables can be expressed in terms of x & p.

eg) $KE = \frac{p^2}{2m}$

To calculate the QM expectation value

-) $f(x,p) \longrightarrow f\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right)$

-) Integrate with respect to ψ^* & ψ

eg

$$\langle KE \rangle = -\frac{\hbar^2}{2m}\int \psi^* \frac{\partial^2 \psi}{\partial x^2}\,dx$$

"Stationary States"

For the moment restrict to potential energy to be time independent $V(x,t) = V(x)$

Major Simplification from Separation of variables

$$\psi(x,t) = \psi(x)\,\phi(t)$$

Should really use different symbol for $\psi(x,t)$ & $\psi(x)$ eg $\Psi(x,t)$ vs $\psi(x)$

Proof

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

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

Divide by $\Psi = \psi\phi$

$$\underbrace{-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{\partial^2\psi}{\partial x^2} + V}_{\text{Only cares about } x} = \underbrace{-i\hbar\frac{1}{\phi}\frac{\partial\phi}{\partial t}}_{\text{Only cares abt } t}$$

(iff $V(x,t) = V(x)$)

When this happens each side must be equal to constant

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} + V(x) = C$$

$$-i\hbar\frac{1}{\phi}\frac{d\phi(t)}{dt} = C$$

"Separation Constant"

Now have 2 ordinary differential equations in 1 variable

(Much easier than partial diff eq in 2 variables!)

Deal with time first

- Does not depend on $V(x)$ $\Rightarrow$ time dependence Universal
  (only have to do this once...)

$$\frac{d\phi(t)}{dt} = \frac{-iC}{\hbar}\phi(t) \Rightarrow \phi(t) = e^{-iCt/\hbar}$$

So full solution $\psi(x,t)$ will be oscillating in t w/ frequency $f = \frac{C}{\hbar}$

However, before we saw f given by $f = \frac{E}{\hbar}$ (de Broglie)

$\Rightarrow$ Separation Constant $C = E$ (total energy of particle)

$$\boxed{\phi(t) = e^{-i\frac{E}{\hbar}t}}$$

$\leftarrow$ $\psi(x,t)$ oscillates in t w/ phase given by E.

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

$$\frac{d\langle x\rangle}{dt} = 0$$

- Stationary States don't change with time

eg

$$\langle f(x,p)\rangle = \int \Psi^*(x,t)\, f(x,p)\, \psi(x,t)\, dx$$

$$= \int \cancel{e^{+Et}}\, \psi(x)\, f(x,p)\, \cancel{e^{-Et}}\, \psi(x)\, d$$

- Stationary States have definite Energy

$$H = KE + P.E \qquad H = \frac{p^2}{2m} + V(x)$$

$$\langle H \rangle = \int \psi^* \underbrace{\left(\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \right) \psi}_{= E\psi \text{ (By time-independent Sch Eq)}} dx$$

$$= E \times 1$$

$$\langle H^2 \rangle = E^2 \qquad \Rightarrow \sigma_H = 0$$

-) General Solutions $\Psi(x,t)$ can be constructed from linear combinations of seperable solutions

-) ∞ #, orthogonal & complete

Spatial Equation Now

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

"Time Independant Schr. Eq"

- Normalization condition

$$\int \Psi^*(x,t)\,\Psi(x,t) = \int e^{+i\frac{Et}{\hbar}}\psi^*(x)\,e^{-i\frac{Et}{\hbar}}\psi(x)$$

$$= \int \psi^*(x)\,\psi(x) = 1$$

Reduced solving Schr. eq. to solving only the time independant version for $\psi(x)$ and tacking on $e^{-i\frac{E}{\hbar}t}$

Comments about $\psi(x)$

- $\psi(x)$ depends on form of $V(x)$
  In our toy examples $V(x)$ often discontinuous
  In these cases, we'll solve for ψ in different regions, then require ψ "smooth" across boundaries
- $\psi(x)$ must be continuous. (Prob $\sim \psi^2$ should be continuous)
- Schr. involves 2nd derivatives $\Rightarrow \frac{d\psi}{dx}$ must also be continuous
  (Relaxed if $V \to \infty$)

- Other basic requirements ψ & $\frac{d\psi}{dx}$
  eg finite & single-valued.
- Non-trivial constraint $\int \psi^* \psi \, dx = 1$
  $\Rightarrow \psi(x) \to 0$ as $x \to \pm\infty$
  sufficiently fast

-) E is always real (HW)

-) $E > \min(V(x))$ <u>Proof easy</u>

-) if V symmetric, $(V(x) = V(-x))$
then will have two solutions w/ same E
that can be taken to be even & odd

$$\psi(x) \rightarrow \pm \psi(-x)$$

-) $\psi(x)$ can always be taken to be real