Schrödinger Equation

$$\boxed{\underset{\sim}{H}|\psi\rangle = i\hbar \frac{d}{dt}|\psi\rangle}$$

$\underset{\sim}{H}$? classical $H = T + V$
but written in terms of
x and p, (not $x, \dot{x}$ like L).

Free Particle $V(x) = 0$

$$H = T = \frac{1}{2}m\dot{x}^2 \qquad m\dot{x} = p$$
$$= \frac{1}{2}m\frac{p^2}{m^2} = \frac{p^2}{2m} \qquad \dot{x} = \frac{p}{m}$$

$$\underset{\sim}{H} = \frac{p^2}{2m}.$$

How Eigenkets of $\underset{\sim}{H}$ are Crucial

suppose $\underset{\sim}{H}|E\rangle = E|E\rangle$

for many, many useful cases, $\underset{\sim}{H}$ is <u>time independent</u>! Then $|E\rangle$ itself will be time independent. And, then consider $a(t)|E\rangle$ as a candidate for a solution to the Schrödinger Equation

$$\underset{\sim}{H}\, a(t)|E\rangle = a(t)\underset{\sim}{H}|E\rangle = a(t)E|E\rangle$$

$$i\hbar\frac{d}{dt}\left(a(t)|E\rangle\right) = i\hbar\frac{da}{dt}|E\rangle + i\hbar a(t)\cancel{\frac{d}{dt}|E\rangle}^{\,0}$$ assumed time independent

Schrödinger:

$$i\hbar\frac{d}{dt}|\psi\rangle = \underset{\sim}{H}|\psi\rangle$$

plug in $a(t)|E\rangle$

$$i\hbar\frac{da}{dt}|E\rangle = aE|E\rangle$$

so $$\frac{da}{dt} = \left(\frac{E}{i\hbar}\right)a = -\left(\frac{iE}{\hbar}\right)a$$

and $$\boxed{a(t) = a_0 e^{-\frac{iEt}{\hbar}}}$$

Schrödinger Equation is Easy to Solve, When you know the eigenkets of $\underset{\sim}{H}$!

- at $t=0$, suppose system described by $|\psi(0)\rangle \to t=0$.
- Project $|\psi(0)\rangle$ on to eigenkets of $\underset{\sim}{H}$

$$|\psi(0)\rangle = \sum_{i=1}^{\infty}|E_i\rangle\langle E_i|\psi(0)\rangle$$

$$\underset{\sim}{H}|E_i\rangle = E_i|E_i\rangle$$

a constant

- For later times, each

$$|E_i\rangle\langle E_i|\Psi(0)\rangle \longrightarrow |E_i\rangle e^{\frac{-iE_it}{\hbar}}\langle E_i|\Psi(0)\rangle$$

- So

$$|\Psi(t)\rangle = \sum_{i=1}^{\infty}|E_i\rangle e^{\frac{-iE_it}{\hbar}}\langle E_i|\Psi(0)\rangle$$

sometimes called the propagator, $\underset{\sim}{U}(t,0)$

- $$|\Psi(t)\rangle = \underbrace{\underset{\sim}{U}(t,0)}_{\text{Hurls } |\Psi(0)\rangle \text{ forward in time}}|\Psi(0)\rangle$$

$$\underset{\sim}{U}(t,0) = \sum_{i=1}^{\infty}|E_i\rangle e^{\frac{-iE_it}{\hbar}}\langle E_i|$$

$$= \underset{\sim}{\mathbb{1}} \quad \text{at } t=0.$$

Free Particle in One Dimension

$$\underset{\sim}{H}|\Psi\rangle = i\hbar\frac{d}{dt}|\Psi\rangle$$

with $\underset{\sim}{H} = \frac{\underset{\sim}{P}^2}{2m}$

get eigenkets: $\underset{\sim}{H}|E\rangle = \frac{\underset{\sim}{P}^2}{2m}|E\rangle = E|E\rangle$

try eigenkets of $\underset{\sim}{P}$!

$$\hat{p}|p\rangle = p|p\rangle$$

$$\hat{p}^2|p\rangle = \hat{p}\,p|p\rangle = p\,\hat{p}|p\rangle = p^2|p\rangle$$

so, $\frac{\hat{p}^2}{2m}|p\rangle = \frac{p^2}{2m}|p\rangle$; with $E = \frac{p^2}{2m}$

then there are two degenerate eigenkets of E:

$$|E,+\rangle = |p = \sqrt{2mE}\rangle \quad \text{(moves right)}$$

$$|E,-\rangle = |p = -\sqrt{2mE}\rangle \quad \text{(moves left)}$$

The general eigenstate of $\underset{\sim}{H}$ is linear superposition of these two. A compact way to incorporate both eigenstates in the sum needed for the propagator is to recall:

$$\underset{\sim}{1} = \int_{-\infty}^{\infty} |p\rangle dp \langle p| = \underset{\sim}{U}(0,0)$$

(gets normalization right)

0 to $-\infty$ are "left movers"
0 to $+\infty$ "right movers"

eigenstates of both $\hat{p}$ and $\underset{\sim}{H} = \frac{\hat{p}^2}{2m}$

For later times, multiply by $e^{-\frac{iEt}{\hbar}} = e^{-\frac{ip^2t}{2\hbar m}}$

$$\underset{\sim}{U}(t,0) = \int_{-\infty}^{\infty} |p\rangle e^{-\frac{ip^2t}{2m\hbar}} dp \langle p|$$

diagonal in p-space!

meaning:

$$\langle p''|\underset{\sim}{U}(t,0)|p'\rangle = \int_{-\infty}^{\infty} \langle p''|p\rangle e^{\frac{-ip^2t}{2m\hbar}} dp \underbrace{\langle p|p'\rangle}_{\delta(p-p')}$$

$$= \delta(p''-p')\, e^{\frac{-ip'^2t}{2m\hbar}}$$

meaning:

$$\underset{\sim}{U}(t,0)|\psi\rangle \doteq \langle p|\underset{\sim}{U}(t,0)|\psi\rangle$$

$$\doteq \int \underbrace{\langle p|\underset{\sim}{U}(t,0)|p'\rangle}_{\delta(p-p')\, e^{\frac{-ip'^2t}{2m\hbar}}} dp' \underbrace{\langle p'|\psi\rangle}_{\psi(p')}$$

$$\doteq e^{\frac{-ip^2t}{2m\hbar}}\, \psi(p)$$

$t=0$, have $\psi(p)$; later times have $e^{\frac{-ip^2t}{2m\hbar}}\, \psi(p)$

- Free space Schrödinger equation is really easy to solve in momentum space! (propagator is diagonal)

WHAT ABOUT CO-ORDINATE SPACE?

$\Rightarrow$ not so easy, $\underset{\sim}{U}$ not diagonal (not $\propto \delta(x-x')$)

$$\langle x|\underset{\sim}{U}(t,0)|x'\rangle = \int_{-\infty}^{\infty} \underbrace{\langle x|p\rangle}_{\frac{1}{\sqrt{2\pi\hbar}}e^{+\frac{ipx}{\hbar}}} e^{-\frac{ip^2t}{2m\hbar}}\, dp\, \underbrace{\langle p|x'\rangle}_{\frac{1}{\sqrt{2\pi\hbar}}e^{-\frac{ipx'}{\hbar}}}$$

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp\, e^{\underbrace{\frac{ip}{\hbar}(x-x') - i\frac{p^2t}{2m\hbar}}_{\text{complete the square!}}}$$

$$-\text{"}\alpha\text{"} = \frac{-it}{2m\hbar}\left(p^2 - \frac{2m\hbar(x-x')}{\hbar t}p + \left(\frac{m\hbar(x-x')}{\hbar t}\right)^2 - \left(\frac{m\hbar(x-x')}{\hbar t}\right)^2\right).$$

$$= \frac{1}{2\pi\hbar}\left(\frac{\pi}{\left(\frac{+it}{2m\hbar}\right)}\right)^{1/2} e^{\frac{-it}{2m\hbar}\cdot\left(\frac{m\hbar(x-x')}{\hbar t}\right)^2}$$

$$\boxed{U(x,t;x',0) \text{ or } \langle x|\underset{\sim}{U}(t,0)|x'\rangle = \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} e^{im(x-x')^2/2\hbar t}}$$

⇒ non-zero for $x \neq x'$

⇒ not diagonal

means:

$$\underset{\sim}{U}(t,0)|\psi\rangle \doteq \langle x|\underset{\sim}{U}(t,0)|\psi\rangle$$

$$\doteq \int \underbrace{\langle x|\underset{\sim}{U}(t,0)|x'\rangle}_{\text{function above.}} \underbrace{\langle x'|\psi\rangle}_{\psi(x',0)} dx'$$

$$\boxed{\psi(x,t) = \left(\frac{m}{2\pi\hbar i t}\right)^{1/2}\int_{-\infty}^{\infty} e^{im(x-x')^2/2\hbar t}\,\psi(x',0)\,dx'}$$

Suppose $\psi(x',0)$ is the state that results from a prior measurement of $\underset{\sim}{x}$, that yielded eigenvalue x_0 : $\psi(x',0) = \delta(x'-x_0)$. Then

$$\psi(x,t) = \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} \int_{-\infty}^{\infty} e^{im(x-x')^2/2\hbar t}\, \delta(x'-x_0)\, dx'$$

$$U(x,t;x_0,0) = \underbrace{\left(\frac{m}{2\pi\hbar i t}\right)^{1/2} e^{im(x-x_0)^2/2\hbar t}}_{\text{a rather singular function;}} \Leftarrow \text{the "fate" of a } \delta\text{-function}$$

further physical interpretation is painful.

For physical interpretation, start from:

$$\psi(x',0) = e^{\frac{ip_0 x'}{\hbar}} \frac{e^{-\frac{x'^2}{2\Delta^2}}}{(\pi\Delta^2)^{1/4}}$$

mean momentum or expectation value of $\underset{\sim}{p}$ is p_0

mean position is $x' = 0$
"width" $\simeq \Delta$
(FWHM $= 2.35\Delta$)

$$\psi(x,t) = \left(\frac{1}{\pi\Delta^2}\right)^{1/4} \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} \int_{-\infty}^{\infty} \underbrace{e^{im(x-x')^2/2\hbar t}\, e^{ip_0 x'/\hbar}\, e^{-x'^2/2\Delta^2}\, dx'}_{\text{"just" a gaussian integral}}$$

... TRUST BOOK RESULT, p. 154, 5.1.15
5.1.16

$$\Psi(x,t) = \frac{1}{\sqrt{\pi^{1/2}\left(\Delta + \frac{i\hbar t}{m\Delta}\right)}} \, e^{\left[\frac{-\left(x-\frac{p_0 t}{m}\right)^2}{2\Delta^2\left(1+\frac{i\hbar t}{m\Delta^2}\right)}\right]} \times$$

$$e^{\left[\frac{i p_0}{\hbar}\left(x - \frac{p_0 t}{2m}\right)\right]} \quad \text{"Phase"}$$

to get $|\Psi(x,t)|^2$, multiply by $\Psi^*(x,t)$, which is just like $\Psi(x,t)$ but with every i replaced by $-i$. This will be:

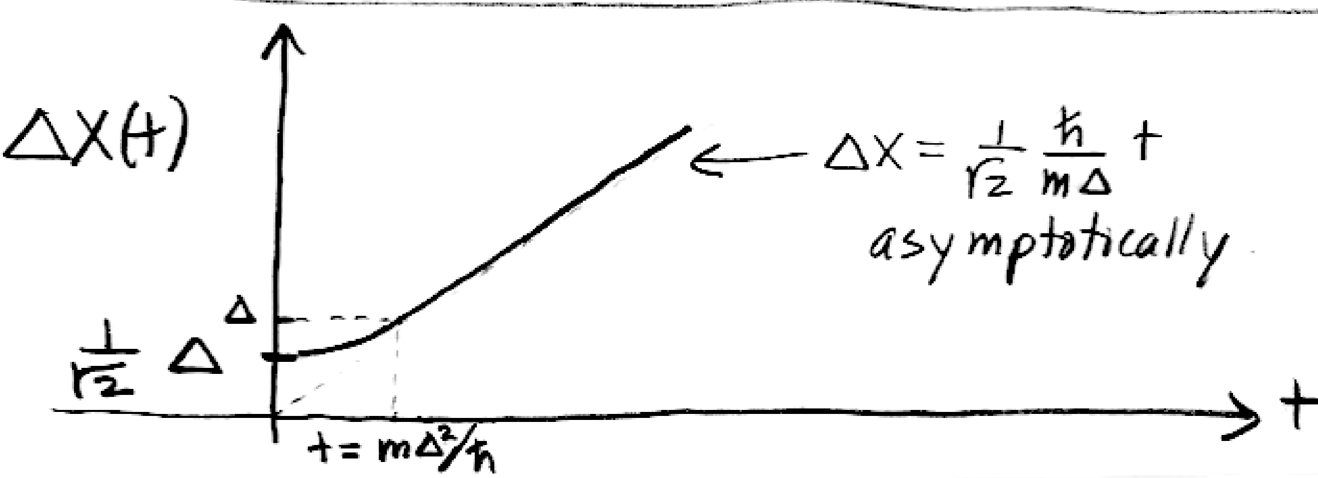
$$|\Psi(x,t)|^2 = \frac{1}{\sqrt{\pi^{1/2}\pi^{1/2}\left(\Delta+\frac{i\hbar t}{m\Delta}\right)\left(\Delta-\frac{i\hbar t}{m\Delta}\right)}} \, e^{\left[\frac{-\left(x-\frac{p_0 t}{m}\right)^2}{2\Delta^2\left(1+\frac{i\hbar t}{m\Delta^2}\right)} - \frac{\left(x-\frac{p_0 t}{m}\right)^2}{2\Delta^2\left(1-\frac{i\hbar t}{m\Delta^2}\right)}\right]} \times$$

$$e^{\left[\frac{i p_0}{\hbar}\left(x-\frac{p_0 t}{2m}\right) - \frac{i p_0}{\hbar}\left(x - \frac{p_0 t}{2m}\right)\right]}$$

Packet moves, speed $= \frac{p_0}{m}$

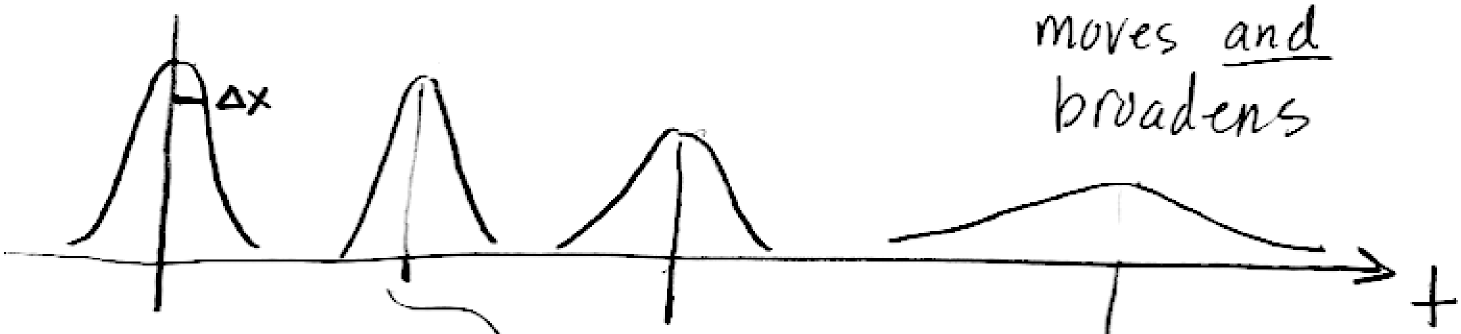
$$= \frac{1}{\sqrt{\pi\left(\Delta^2 + \left(\frac{\hbar t}{m\Delta}\right)^2\right)}} \cdot e^{\left[\frac{-\left(x-\frac{p_0 t}{m}\right)^2}{\Delta^2\left(1+\left(\frac{\hbar t}{m\Delta^2}\right)\right)^2}\right]}$$

$$\boxed{\Delta X(t) = \left[\frac{1}{2}\Delta^2\left(1+\left(\frac{\hbar t}{m\Delta^2}\right)\right)^2\right]^{1/2} = \frac{1}{\sqrt{2}}\sqrt{\Delta^2 + \left(\frac{\hbar t}{m\Delta}\right)^2}}$$



Pictures :

moves and broadens



$$\langle x \rangle = \frac{p_0}{m} t$$

How long? (Before broadening significant)

Case A $\quad 1\ \text{gm} = 10^{-3}\ \text{kg}, \quad \Delta = 1\ \text{cm} = 10^{-2}\ \text{m}$

$$t = \frac{10^{-3}\ \text{kg} \cdot 10^{-4}\ \text{m}^2}{\hbar = 10^{-34}\ \frac{\text{kg}\cdot\text{m}^2}{\text{s}^2}\cdot \text{s}} \cong 10^{27}\ \text{s}$$

$(\text{J} \cdot \text{s})$

age of universe $\simeq 14 \cdot 10^9$ years

1 year $\simeq 3 \cdot 10^7$ s

so age of universe $\simeq 42 \cdot 10^{16}\ \text{s} \sim 4 \cdot 10^{17}\ \text{s}$

→ time to spread macroscopic objects ≫ age of universe

Case B $\quad 1\ \text{electron} \simeq 10^{-30}\ \text{kg} \quad \Delta \simeq 10^{-8}\ \text{cm} \simeq 10^{-10}\ \text{m}$

$$t \simeq \frac{10^{-30}\ \text{kg} \cdot 10^{-10}\ \text{m}}{10^{-34}\ \text{J}\cdot\text{s}} \simeq 10^{-6}\ \text{s}$$

→ the electrostatic attraction of proton holds hydrogen together; electrons rarely free.