Lec 7: Schrodinger equation

position x-basis $\hat{x}|x\rangle = x|x\rangle$
momentum p-basis $\hat{p}|p\rangle = p|p\rangle$

Schrödinger equation usually given in x-basis

$$\hat{I} = \int dx\, |x\rangle\langle x| \quad \& \quad \langle x'|x\rangle = \delta(x'-x)$$

$$|\psi\rangle = \int dx\, |x\rangle\langle x|\psi\rangle = \int dx\, |x\rangle \psi(x)$$

$\psi(x)$ amplitude to measure particle at x with probability $P(x, x+dx) = |\psi(x)|^2 dx$

$\hat{p}$ is generator of translations in position:

$$\hat{T}(a) \equiv e^{-ia\hat{p}_x/\hbar}$$

$$[\hat{x}, \hat{T}(a)] = i\hbar \frac{\partial}{\partial \hat{p}_x} \hat{T}(a) = a\hat{T}(a)$$

so $$\hat{x}(\hat{T}|x\rangle) = (\hat{T}\hat{x} + [\hat{x}, \hat{T}])|x\rangle$$

$$= (\hat{x} + a)\hat{T}|x\rangle = (x+a)\hat{T}|x\rangle$$

so $\hat{T}|x\rangle = |x+a\rangle$ & $\left\{ \begin{array}{l} \hat{T}^\dagger|x\rangle = |x-a\rangle \\ \langle x|\hat{T} = \langle x-a| \end{array} \right.$

& $\langle x|\hat{T}^\dagger = \langle x+a|$

infinitessimal translation ε

$$\hat{T}(\varepsilon)|\psi\rangle = \left(1 - \frac{i\varepsilon}{\hbar}\hat{p}\right)|\psi\rangle$$

$$\langle x|\hat{T}(\varepsilon)|\psi\rangle = \langle x|\left(1 - \frac{i\varepsilon}{\hbar}\hat{p}\right)|\psi\rangle = \langle x|\hat{T}|\psi\rangle$$

$$= \langle x-\varepsilon|\psi\rangle = \psi(x-\varepsilon)$$

$$= \psi(x) - \varepsilon \frac{\partial\psi}{\partial x}\Big|_x$$

$$\psi(x) - \frac{i\varepsilon}{\hbar}\langle x|\hat{p}|\psi\rangle = \psi(x) - \varepsilon\frac{\partial\psi}{\partial x}\Big|_x$$

$$\langle x|\hat{p}|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\psi\rangle$$

let $|\psi\rangle = |x'\rangle$ get matrix rep. of $\hat{p}$

$$\langle x|\hat{p}|x'\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|x'\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\delta(x-x')$$

$$= \frac{\hbar}{i}\delta(x-x')\frac{\partial}{\partial x'}$$

Then $\langle x|\hat{p}|\psi\rangle = \int dx' \langle x|\hat{p}|x'\rangle\langle x'|\psi\rangle$

$$= \int dx' \frac{\hbar}{i}\delta(x-x')\frac{\partial}{\partial x'}\langle x'|\psi\rangle$$

$$= \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\psi\rangle$$

$$\hat{p} \xrightarrow{x\text{-rep}} \frac{\hbar}{i}\frac{\partial}{\partial x}$$

you can do the same in momentum-space, see homework

Then Schrödinger for single particle in 1-dim, is

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$

$$i\hbar \frac{\partial}{\partial t} \langle x|\psi\rangle = \langle x|\hat{H}|\psi\rangle =$$

$$\int dx' \; \langle x|\hat{H}|x'\rangle \langle x'|\psi\rangle$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

$$\langle x|\hat{H}|x'\rangle = \left[\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 + V(x)\right]\delta(x-x')$$

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

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

In the presence of $\vec{E}, \vec{B}$ fields in 3 Dim.

$$\hat{H} = \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla} - \frac{q}{c}\vec{A}\right)^2 + q\phi$$

$$\vec{E} = -\vec{\nabla}\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t} \quad ; \quad \vec{B} = \vec{\nabla}\times\vec{A}$$

Probability Current (Commins)

$$i\hbar\frac{\partial}{\partial t}\Psi = \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla} - \frac{q}{c}\vec{A}\right)\Psi + q\phi\Psi$$

construct $\Psi^*\left(i\hbar\frac{\partial}{\partial t}\Psi\right) - \Psi\left(i\hbar\frac{\partial}{\partial t}\Psi\right)^*$

$$= i\hbar\left(\Psi^*\frac{\partial}{\partial t}\Psi + \Psi\frac{\partial}{\partial t}\Psi^*\right) = i\hbar\frac{\partial}{\partial t}(\Psi^*\Psi)$$

time rate of change of probability Density.

Ψ^*(left hand side) $-\Psi$(left hand side)* =

$$\Psi^*\frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla} - \frac{q}{c}\vec{A}\right)^2\Psi + q\phi\,\Psi^*\Psi$$

$$-\Psi\frac{1}{2m}\left(\frac{\hbar}{i} + \frac{q}{c}\vec{A}\right)^2\Psi^* + q\phi\,\Psi\Psi^*$$

ϕ, $|\vec{A}|^2$ terms cancel

$$-\frac{\hbar^2}{2m}\left[\Psi^*\nabla^2\Psi - \Psi\nabla^2\Psi^*\right]$$

$$+\frac{1}{2m}\left(\frac{\hbar}{i}\frac{q}{c}\right)(-1)\left[\Psi^*\vec{\nabla}\cdot(\vec{A}\Psi) + \Psi^*\vec{A}\cdot\vec{\nabla}\Psi\right]$$

$$-\frac{1}{2m}\left(\frac{\hbar}{i}\frac{q}{c}\right)\left[\Psi\vec{\nabla}\cdot(A\Psi^*) + \Psi\vec{A}\cdot\vec{\nabla}\Psi^*\right]$$

combine Grad A terms,

$$\Psi^*\vec{\nabla}\cdot(\vec{A}\Psi) + \Psi\vec{\nabla}\cdot(\vec{A}\Psi^*) = \vec{A}\cdot\left(\Psi^*\vec{\nabla}\Psi + \Psi\vec{\nabla}\Psi^*\right) + 2\,\vec{\nabla}\cdot\vec{A}\,(\Psi^*\Psi) = \vec{A}\cdot\vec{\nabla}(\Psi^*\Psi) + 2\,\vec{\nabla}\cdot\vec{A}\,(\Psi^*\Psi)$$

also, ~~of~~ terms $\Psi^* A\cdot\vec{\nabla}\Psi + \Psi\vec{A}\cdot\vec{\nabla}\Psi^* = \vec{A}\cdot\vec{\nabla}(\Psi^*\Psi)$

then adding two $A\cdot\vec{\nabla}$ terms,

$$-\frac{\hbar^2}{2m}\vec{\nabla}\cdot\left(\psi^*\vec{\nabla}\psi-\psi\vec{\nabla}\psi^*\right)$$

$$-\frac{1}{2m}\frac{\hbar}{i}\left(\frac{q}{c}\right)2\left[\vec{A}\cdot\vec{\nabla}(\psi^*\psi)+\vec{\nabla}\cdot\vec{A}\,(\psi^*\psi)\right]$$

factor out overall $\vec{\nabla}$ to get

$$=\vec{\nabla}\cdot\left[-\frac{\hbar^2}{2m}\left(\psi^*\nabla\psi-\psi\nabla\psi^*\right)-\frac{\hbar q}{2mi}\vec{A}(\psi^*\psi)\right]$$

$$=i\hbar\frac{\partial}{\partial t}(\psi^*\psi)$$

$$\frac{\partial}{\partial t}(\psi^*\psi)=-\vec{\nabla}\left[\frac{\hbar}{2mi}\left(\psi^*\vec{\nabla}\psi-\psi\nabla\psi^*\right)-\frac{q}{mc}\vec{A}(\psi^*\psi)\right]$$

with $\frac{1}{i}\left(\psi^*\nabla\psi-\psi\nabla\psi^*\right)=2\,\mathrm{Im}\left(\psi^*\nabla\psi\right)$

get conserved probability density $\psi^*\psi$

$$\frac{\partial}{\partial t}(\psi^*\psi)+\frac{\hbar}{m}\mathrm{Im}\left(\psi^*\vec{\nabla}\psi\right)-\frac{q}{mc}\vec{A}(\psi^*\psi)=0$$

probability current:

$$\vec{J}=\frac{\hbar}{m}\mathrm{Im}\left(\psi^*\vec{\nabla}\psi\right)-\frac{q}{mc}\vec{A}(\psi^*\psi)$$

so $\quad\frac{\partial\rho}{\partial t}+\vec{\nabla}\cdot\vec{J}=0$

Gauge Invariance

$\vec{\mathcal{E}}, \vec{B}$ invariant under

$$\phi \to \phi' = \phi + \frac{1}{c}\frac{\partial \chi}{\partial t}$$

$$\vec{A} \to \vec{A}' = \vec{A} - \vec{\nabla}\chi$$

where $\chi(\vec{x}, t)$ is arbitrary function

if we define $\psi' = \psi \exp\left(-\frac{iq}{\hbar c}\chi\right)$

then Schrödinger equation is invariant.

$$i\hbar \frac{\partial}{\partial t}\psi' = \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla} - \frac{q}{c}\vec{A}'\right)\psi' + q\phi'\psi'$$

and probability is conserved.

In Q.E.D., invariance of ψ under the local gauge transformation requires introduction of $\vec{A}, \phi$.

Galilean invariance

Lorentz Boost

$$\begin{pmatrix} t' \\ x' \end{pmatrix} = \begin{pmatrix} \gamma & -\gamma\beta \\ -\gamma\beta & \gamma \end{pmatrix} \begin{pmatrix} x \\ t \end{pmatrix}$$

in limit $\beta = \frac{v}{c} \ll 1$ $\quad \left.\begin{array}{l} x' = x - vt \\ t' = t \end{array}\right\}$ Galilean

Consider Schrödinger w/ velocity independent potential $V(x,t)$

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

in frame moving w/ velocity v w.r.t. this one:
for wave function $\phi(x',t')$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x'^2}\phi + V(x',t')\phi = i\hbar\frac{\partial \phi}{\partial t'}$$

Probability density

$$|\psi|^2 dx = |\phi|^2 dx' \Rightarrow |\psi|^2 = |\phi|^2$$

so $\psi(x,t) = e^{i g(x',t')}\phi(x',t')$

only differ by phase

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial x'} \quad \& \quad \frac{\partial}{\partial t} = \frac{\partial}{\partial t'} - v\frac{\partial}{\partial x'}$$

Then Schrödinger for Ψ becomes

$$LHS = i\hbar\left(\frac{\partial}{\partial t'} - v\frac{\partial}{\partial x'}\right) = i\hbar\left(i\dot{f}\phi + \dot{\phi}\right)e^{if}$$

$$- i\hbar v\left(if'\phi + \phi'\right)e^{if}$$

next, the RHS

$$\frac{\partial}{\partial x'}\left(e^{if}\phi\right) = \left(if'\phi + \phi'\right)e^{if}$$

$$\frac{\partial^2}{\partial x'^2}\left(e^{if}\phi\right) = if'\left(if'\phi + \phi'\right)e^{if}$$

$$+ \left(if''\phi + if'\phi' + \phi''\right)e^{if}$$

$$= \left(-(f')^2\phi + 2if'\phi' + if''\phi + \phi''\right)e^{if}$$

cancelling overall e^{if} we have

$$i\hbar\left(i\dot{f}\phi + \dot{\phi}\right) - i\hbar v\left(if'\phi + \phi'\right)$$

$$= \frac{-\hbar^2}{2m}\left[-f'^2\phi + 2if'\phi' + if''\phi + \phi''\right]$$

$$+ V\phi$$

✓ cancel by Schrodinger in ϕ frame

$$-\hbar \dot{f} \phi + \hbar v f' \phi - i\hbar v \phi'$$

$$= -\frac{\hbar^2}{2m}\left[-f'^2 \phi + 2i f' \phi' + i f'' \phi\right]$$

ϕ' terms must cancel

$$-i\hbar v = -\frac{\hbar^2}{2m}(2if')$$

$$\frac{mv}{\hbar} = f' \ ; \ f'' = 0$$

Using this for f′,f′′ and canceling the common Φ, we get the t′ dependence:

$$-\hbar \dot{f} + mv^2 = \frac{\hbar^2}{2m}\left(\frac{mv}{\hbar}\right)^2$$

$$-\hbar \dot{f} = -\frac{1}{2}mv^2 \Rightarrow \dot{f} = \frac{1}{2}\frac{mv^2}{\hbar}$$

$$f(x',t') = \frac{1}{\hbar}\left(mvx' + \frac{1}{2}mv^2 t'\right)$$

$x' = x - vt$ $\qquad f(x,t) = \frac{1}{\hbar}\left(mvx - \frac{1}{2}mv^2 t\right)$

$t' = t$

Take Ψ to be free particle plane wave

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \exp\left[\frac{i}{\hbar}(px - Et)\right]$$

$$p = mv \ ; \ E = \frac{p^2}{2m}$$

then $\phi(x',t') = e^{-i f(x',t')} \psi(x'+vt', t')$

$$= \exp\left[\frac{-i}{\hbar}\left(m v x' + \frac{1}{2} m v^2 t'\right)\right]$$

$$\times \frac{1}{\sqrt{2\pi\hbar}} \exp\left[\frac{i}{\hbar} p(x'+vt')\right] \exp\left[\frac{-i}{\hbar}\frac{p^2}{2m} t'\right]$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \exp\left[\frac{i}{\hbar}(p - mv)x'\right]$$

$$\times \exp\left[\frac{-i}{\hbar} t' \left(\underbrace{\frac{p^2}{2m} + \frac{1}{2} m v^2 - p v}_{\frac{1}{2m}\left(p^2 + m^2 v^2 - 2mpv\right)}\right)\right]$$

$$= \frac{1}{2m}(p - mv)^2$$

giving

$$\phi(x',t') = \frac{1}{\sqrt{2\pi\hbar}} \exp\left[\frac{i}{\hbar}(p - mv)x'\right]$$

$$\times \exp\left[\frac{-i t'}{2m\hbar}(p - mv)^2\right]$$

We see we get $\phi(x',t')$ with

$$x \to x', \quad t \to t' \quad p \to p - mv$$

Physically, whereas classical wave λ doesn't change under Galilean transformation, in Q.M.

$$\lambda' = \frac{h}{p - mv} = \frac{\lambda}{1 - \frac{mv}{p}}$$

de Broglie wavelength with Galilean transform.

This is just what we expect:

$$x' = x - vt$$

$$\dot{x}' = \dot{x} - v$$

$$m\dot{x}' = m\dot{x} - mv$$