Lecture $\boxed{11}$ (Sept. 25, Fri.)

Outline for today / next week

- $\boxed{\text{SHO}}$: energy eigenkets/values, wavefunctions and expectation values at fixed time via operator/algebraic method
  - time evolution : S & H - pictures
- Finally(!), Schroedinger's $\boxed{\text{wave}}$ equation for ψ (wavefunction) : time-dependent & independent
  - interpretation of ψ (including phase); classical limit
- Solutions to Schroedinger's wave equation : free particle in 3D ; SHO (again : analytic method); linear potential (useful for WKB approximation)

$\boxed{\text{SHO}}$ motivation to study it : pedagogical ; approximates realistic potentials (in molecules, nuclei); technique used in quantum field theory also

- Fixed time first : $\boxed{H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2}$

$\omega = \sqrt{\frac{k \text{ (spring constant)}}{m}}$ is angular frequency of classical version

- $\boxed{a \equiv \sqrt{\frac{m\omega}{2\hbar}} \left(x + i p / m\omega \right)}$; $\boxed{a^{+} \equiv \sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{i p}{m\omega} \right)}$

not Hermitian

(annihilation / lowering & creation / raising)

see below why

Use $[x, p] = i\hbar$

— $\boxed{[a, a^\dagger] = 1}$ see below why

— N (number operator) $\equiv a^\dagger a$ (Hermitian)

$= H/(\hbar\omega) - 1/2$

$\Rightarrow H = \hbar\omega(N + 1/2)$

— common eigenkets: $N|r\rangle = r|r\rangle$ — r real (will show later needs to be integer ≥ 0)

$$H|r\rangle = \underbrace{(r + 1/2)\hbar\omega}_{E_r}|r\rangle$$

— $[N, a] = -a$; $[N, a^\dagger] = a^\dagger$

$\Rightarrow N(a|r\rangle) = (r-1)(a|r\rangle)$ & $N(a^\dagger|r\rangle) = (r+1)(a^\dagger|r\rangle)$

$a, a^\dagger$ decrease/increase energy by $\hbar\omega$,
N eigenvalue by 1

$\Rightarrow a|r\rangle = c|r-1\rangle$ (assume normalized)

$$\langle r|N|r\rangle = \langle r|r|r\rangle = r$$

$$= (\langle r|a^\dagger)\underbrace{(a|r\rangle)}_{c|r-1\rangle} = |c|^2$$

$\Rightarrow a|r\rangle = \sqrt{r}|r-1\rangle$ & $a^\dagger|r\rangle = \sqrt{r+1}|r+1\rangle$

$\Rightarrow \boxed{r \geq 0} \Rightarrow$ lowest allowed E_r is $\frac{1}{2}\hbar\omega$

... but is this "realized"?

Successive application of $\boxed{a}$:

$a^2|r\rangle = \sqrt{r(r-1)}\;|r-2\rangle \dots \Rightarrow$ 2 cases

$\boxed{(a)}$ $r = n$ (≥ 0 integer) : after n steps,

$$a^n|n\rangle = \sqrt{n}\sqrt{n-1}\dots\sqrt{n-(n-1)}\;\underbrace{|n-n\rangle}_{|0\rangle}$$

$|0\rangle$: lowest state is obtained

$$a^{n+1}|n\rangle \propto a|0\rangle = \sqrt{0}\;|0-1\rangle = 0 \text{ (null ket)}$$

... terminates!

$\boxed{(b)}$ r not integer : after m steps,

$$a^m|r\rangle = \sqrt{r}\sqrt{r-1}\underbrace{\sqrt{r-(m-1)}}_{\substack{\text{never } 0 \\ \text{(doesn't stop)}}}\;\underbrace{|r-m\rangle}_{\substack{\text{never } |0\rangle \\ \text{(can't get to it)}}}$$

what's worse : choose $m = [r]+1$, where $[r]$ is greatest integer $< r$

$$\Rightarrow a^{[r]+1}|r\rangle \propto \Big|\underbrace{\underbrace{r-[r]}_{<1}-1}_{<0}\Big\rangle, \text{ i.e.,}$$

state with N eigenvalue < 0 : pathological! $\Rightarrow$ r must be integer

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$E_0 = \frac{1}{2}\hbar\omega$ ground state, $|0\rangle$ ...

$$|n\rangle = \left[(a^+)^n/\sqrt{n!}\right]|0\rangle \qquad E_n = (n+\tfrac{1}{2})\hbar\omega$$

– matrix elements : $\langle n'|a|n\rangle = \sqrt{n}\;\delta_{n',n-1}$

& $\langle n'|a^+|n\rangle = \sqrt{n+1}\;\delta_{n',n+1}$

$$\langle n'|x|n\rangle = \sqrt{\hbar/(2m\omega)}\left(\sqrt{n}\;\delta_{n',n-1} + \sqrt{n+1}\;\delta_{n',n+1}\right)$$

$$\langle n' | p | n \rangle = i\sqrt{\frac{m\hbar\omega}{2}} \left(-\sqrt{n}\, \delta_{n', n-1} + \sqrt{n+1}\, \delta_{n', n+1} \right)$$

Wavefunction in position space :

$$\langle x' | a | 0 \rangle = 0 = \sqrt{\frac{m\omega}{\hbar}} \langle x' | \left(x + \frac{ip}{m\omega} \right) | 0 \rangle$$

x'

use $\langle x' | p | \alpha \rangle = -i\hbar \partial/_{\partial x} \langle x' | \alpha \rangle$

$\Rightarrow$ 1st order DE for $\psi_0(x') = \langle x' | 0 \rangle$:

$$\left(x' + x_0^2 \, d/_{dx'} \right) \psi_0(x') = 0 \qquad \boxed{x_0 = \sqrt{\frac{\hbar}{m\omega}}}$$

$$\Rightarrow \boxed{\psi_0(x') = \left(\frac{1}{\pi^{1/4}\sqrt{x_0}} \right) \exp\left[-\frac{1}{2} \left(\frac{x'}{x_0} \right)^2 \right]} \quad \text{(even)}$$

$$\psi_1(x') = \langle x' | 1 \rangle = \langle x' | a^\dagger | 0 \rangle = \frac{1}{\sqrt{2}\, x_0} \underbrace{\left(x' - x_0^2 \frac{d}{dx'} \right)}_{\text{(odd)}} \underbrace{\langle x' | 0 \rangle}_{\psi_0(x')}$$

— expectation values $\langle n | (x \text{ or } p) | n \rangle = 0$ (simply based on above matrix elements!)

$$\left[\sim \int dx' \, \underbrace{\psi_n(x')}_{\text{even/odd}}{}^{*} \underbrace{\left(x' \text{ or } \partial/_{\partial x'} \right) \psi_n(x')}_{\text{odd/even}} = 0 \right]$$

a bit more involved!

Onto $\langle n | (x^2 \text{ or } p^2) | n \rangle$ [for $|0\rangle$ here; $|n\rangle$ is informal HW]

— In fact, $\langle (\Delta x)^2 \rangle \langle (\Delta p)^2 \rangle$ for $|0\rangle$ $= \hbar^2/4$ (Gaussian)

$$\langle (\Delta x)^2 \rangle = \langle x^2 \rangle - \cancel{\langle x \rangle^2}^{\,0} = \langle x^2 \rangle \ldots \quad \boxed{\langle x^2 \rangle \langle p^2 \rangle = \hbar^2/4}$$

$\langle 0 | x^2 = \frac{\hbar}{2m\omega}\left(a^2 + a^{+2} + a^+a + aa^+\right)|0\rangle$

$\underbrace{a^2}_{0}$, $\underbrace{a^{+2}}_{0}$, $\underbrace{a^+a}_{0}$

(verify using a, a^+ vs. wavefunction)

$= \hbar/(2m\omega) = x_0^2/2$; $\langle p^2\rangle = \hbar m\omega/2$

$\Rightarrow \langle x^2\rangle\langle p^2\rangle = \hbar^2/4$ (agrees)

$\boxed{\text{virial theorem (HW 4.4)}}$: $\left\langle \frac{p^2}{2m}\right\rangle = \hbar\omega/4 = \langle H\rangle/2$ ← kinetic energy

$\left\langle \frac{m\omega^2 x^2}{2}\right\rangle = \hbar\omega/4 = \langle H\rangle/2$ $\boxed{\text{equal}}$

↳ potential energy

$\boxed{\text{Time}}$ evolution

$\boxed{\text{S - picture}}$ $|n\rangle \longrightarrow \exp\left(-\frac{iE_nt}{\hbar}\right)|n\rangle$

x, p ... fixed

$\langle n|(x \text{ or } p)|n\rangle$ at $\boxed{t}$ $= \langle n|(x \text{ or } p)|n\rangle$ at $t=0$

$= 0$

(general result: $\langle B\rangle$ in stationary state is constant)

$\Rightarrow$ $\boxed{\text{no}}$ oscillations in $\langle x\rangle, \langle p\rangle$ for $\boxed{\text{single}}$ stationary state

$\neq$ classical oscillator

($\langle x\rangle, \langle p\rangle$ should oscillate)

must do a superposition of stationary states (HW 5.1)

For stationary state, check Ehrenfest theorem

$\underbrace{d\langle p\rangle/dt}_{=0 \text{ (as per above)}} = -\langle \partial V/\partial x\rangle \propto \langle x\rangle = 0$ (agrees)

at time t

$\boxed{\text{H-picture}}$ state fixed; $x, p, a, a^\dagger$ change

$$dp/dt = -\partial V/\partial x \quad (\text{H's EOM}) = -m\omega^2 x$$

$$\& \; dx/dt = p/m \;\ldots \Rightarrow \boxed{\begin{array}{l} da/dt = -i\omega a \\ \& \; da^\dagger/dt = +i\omega a^\dagger \end{array}}$$

$$\Rightarrow a^{(\dagger)}(t) = a^{(\dagger)}(0)\exp(\mp i\omega t) \;\ldots$$

$$\boxed{\begin{array}{l} x(t) = x(0)\cos\omega t + \dfrac{p(0)}{m\omega}\sin\omega t \\ p(t) = -m\omega\, x(0)\sin\omega t + p(0)\cos\omega t \end{array}} \Big\} \text{ like classical}$$

$$\ldots \text{ but } \langle n|\underbrace{(x(t) \text{ or } p(t))}_{\text{contains } x(0)\,\&\,p(0)}|n\rangle = 0$$

$$\ldots \langle n|\, x(0) \text{ or } p(0) |n\rangle = 0$$

x

$\boxed{\text{S's wave equation}}$ for $\psi_\alpha(x', t) = \langle x'|\alpha, t_0; t\rangle$

$$\underbrace{\langle x'|}_{\text{fixed}}$$

$$H = p^2/(2m) + V(x)$$

move

$$\langle x'| i\hbar\, \partial/\partial t\, |\alpha, t_0; t\rangle = \langle x'| H |\alpha, t_0; t\rangle$$

use $\langle x'|p^n|\alpha\rangle = (-i\hbar)^n \partial^n/\partial x'^n \langle x'|\alpha\rangle$

$$\& \quad \langle x'|\, V(x)\, |\alpha, t_0; t\rangle$$

$$\langle x'| V(x')$$

time-dependent

$$\boxed{i\hbar\, \partial/\partial t\, \underbrace{\langle x'|\alpha, t_0; t\rangle}_{\psi_\alpha(x', t)} = -\frac{\hbar^2}{2m}\nabla'^2 \langle x'|\alpha, t_0; t\rangle + V(x')\langle x'|\alpha, t_0; t\rangle}$$

$\boxed{\text{Classical}}$ limit ($\hbar \to 0$)

— Alternative (to Schroedinger's equation) approach to QM: Feynman's path integral (PI) (will do it "soon"!) $\Rightarrow$ phase of wavefunction (when only classical path contributes) is indefinite action: $\boxed{\int^{t} L \, dt}$ ...

... but $\int^{t} L \, dt$ is Hamilton's principal function (classically), which satisfies Hamilton-Jacobi equation (Phys 601 or Goldstein ...)

... indeed, starting from Schroedinger's equation (QM), we can show that phase of wavefunction satisfies Hamilton-Jacobi equation in $\hbar \to 0$ limit (consistency check)

Summary of "various" Schroedinger equations (all related)

(1). for U (time evolution operator):

$$\boxed{i\hbar \, \partial/_{\partial t} \, U(t, t_0) = H \, U(t, t_0)} \Rightarrow$$

$$U(t, t_0) = \exp[-iH(t-t_0)/\hbar]$$

(2). for $|\alpha\rangle$, using $|\alpha, t_0; t\rangle = U \, \overbrace{|\alpha, t_0\rangle}^{\text{fixed}}$ in above:

$$\boxed{i\hbar \, \partial/_{\partial t} \, |\alpha, t_0; t\rangle = H \, |\alpha, t_0; t\rangle}$$

(3). for $\psi_\alpha(x', t) = \langle x' | \alpha, t_0; t\rangle$ by $\langle x'|$ ...above:

$$i\hbar \, \partial/_{\partial t} \, \psi_\alpha(x', t) = \langle x' | H | \alpha, t_0; t\rangle$$

$$= -\frac{\hbar^2}{2m} \underset{\substack{\uparrow \\ \text{from } p^2}}{\nabla'^2} \psi_\alpha + V(x')\psi$$

(4). (time-independent) for energy eigenstate:

$$\boxed{-\frac{\hbar}{2m} \nabla'^2 u_E(x') + V(x') \, u_E = E \, u_E}$$

$\boxed{\text{Time independent}}$: $[A, H] = 0$; system initially in eigenstate of A (& H)

$$\langle x' | a', t_0; t\rangle = \langle x' | a\rangle \exp(-iE_{a'}t/\hbar)$$

$$\Rightarrow -\frac{\hbar^2}{2m} \nabla'^2 \underbrace{\langle x' | a'\rangle}_{\psi_{a'}(x')} + V(x')\langle x' | a'\rangle = E_{a'}\langle x' | a'\rangle$$

choose $\boxed{A = H}$ itself : $\langle x' | a'\rangle = u_E(x') \Rightarrow$

$$\boxed{-\hbar^2/(2m)\, \nabla'^2 u_E(x') + V(x')\, u_E(x') = E\, u_E(x')}$$

$\boxed{\text{Boundary condition}}$: if $E < \lim_{|x'| \to \infty} V(x')$, then

$u_E(x') \to 0$ as $x' \to \infty$ $\Rightarrow$ $\boxed{\text{bound state}}$

$\Rightarrow$ non-trivial solutions only for discrete E

e.g., SHO : finite $E < V(x') \to \infty$ as $x' \to \infty$ (already saw E quantized)

Coulomb potential $\propto -1/r$: bound states, discrete spectrum for $E < 0$, since $V(x') \to 0$ as $x' \to \infty$

Probability density, $\boxed{\rho(x', t)} = |\psi_\alpha(x', t)|^2$

(e.g. of general idea: probability given by expansion coefficient in relevant basis) $= |\langle x' | \alpha, t_0; t\rangle|^2$

$\rightarrow$ $\boxed{\text{what about phase}}$?

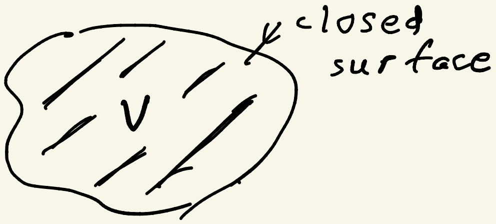
Continuity equation : $\boxed{\partial\rho/\partial t + \vec{\nabla}\cdot\vec{j} = 0}$

$\boxed{\vec{j}}$ (probability flux) $= -\frac{i\hbar}{2m}\left[\psi^* \nabla\psi - (\nabla\psi^*)\psi\right]$

$$\int_V d^3x\, (\vec{\nabla}\cdot\vec{j}) = -\frac{d}{dt}\int_V \rho\, d^3x$$

rate of change

total probability inside V



$$= \oint_{\substack{\text{closed}\\ \text{surface}}} \bar{j} \cdot d\bar{A}$$

$\bar{j} \rightarrow$ rate of "flow" per unit area

- expect j related to momentum :

$$\int d^3x \, j(x,t) = -\frac{i\hbar}{2m} \int d^3x \left[\psi^* \partial \psi - \partial \psi^* \psi \right]$$

i.b.p. : boundary term : $|\psi|^2 \Big]_{-\infty}^{\infty} \sim 0$

$$= -\frac{i\hbar}{m} \int d^3x \left(\psi^* \partial \psi \right)$$

$$\langle p \rangle_t / m = \frac{1}{m} \int d^3x' \underbrace{\langle \alpha | x' \rangle}_{\psi_\alpha(x')} \langle x' | p | \alpha \rangle \rightarrow -i\hbar \frac{\partial}{\partial x'} \psi_\alpha(x')$$

$|x'\rangle\langle x'| \rightarrow \mathbb{1}$

... $\Rightarrow$ $\boxed{\int d^3x \, j(x,t) = \langle p \rangle_t / m}$

- Re-write : $\psi(x,t) = \sqrt{\rho(x,t)} \exp\left[i \frac{S(x,t)}{\hbar} \right]$ ← phase

... to find : $\boxed{\bar{j} = \rho \bar{\nabla} S / m}$ (spatial variation of phase gives probability flux)

- Also, connection to classical mechanics (see next slide / offline discussion)