Lecture 15 137A

Calculations with Dirac Notation

· Probability Amplitudes

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle$$ Expand in eigenfunctions

$$= \sum_m \sum_n c_m^* c_n \langle \psi_m | \hat{A} | \psi_n \rangle$$

$$= \sum_m \sum_n c_m^* c_n a_n \underbrace{\langle \psi_m | \psi_n \rangle}_{\delta_{mn}}$$

$$= \sum_n |c_n|^2 a_n$$ ← weighted average of eigenvalues

Note: $\sum_n |c_n|^2 = 1$ ← it has to be in some state...

· Probability to observe system with a_n is $|c_n|^2$.

Note: If you have degeneracy:

Eg. a_n is α times degenerate; label wavefunctions as ψ_{nr} with $r = 1, \dots, \alpha$

Then, the probability to find a_n is $P_n = \sum_{r=1}^{\alpha} |C_{nr}|^2 = \sum_{r=1}^{\alpha} |\langle \psi_{nr} | \psi \rangle|^2$

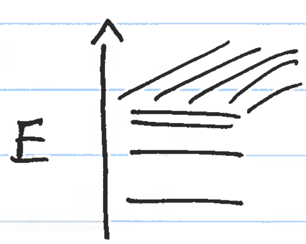
all the α different ways to get a_n.

• After measurement, you end up in one of the α possible wavefunctions

$$|\psi\rangle_{\text{after}} = \sum_{r=1}^{\alpha} C_{nr} |\psi_{nr}\rangle$$

Continuous & Discrete Spectrum of States

Eg. Finite Square well



} continuous $\hat{A}|\psi_a\rangle = a|\psi_a\rangle$

} discrete $\hat{A}|\psi_n\rangle = a_n|\psi_n\rangle$

Most general state has both types of states:

$$|\psi\rangle = \sum_n C_n |\psi_n\rangle + \int c(a) |\psi_a\rangle \, da$$

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$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle$

$\downarrow$ algebra

$= \sum_n |c_n|^2 a_n + \int |c(a)|^2 a \, da$

with $c_n = \langle \psi_n | \psi \rangle$

$c(a) = \langle \psi_a | \psi \rangle$

Commuting Observables

$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ $\quad$ $\hat{A}, \hat{B}$ commute if $[\hat{A}, \hat{B}] = 0$

If $[\hat{A}, \hat{B}] = 0$, then $\hat{A}$ and $\hat{B}$ are compatible and there exists a common set of eigenfunctions for both of them! $(\{\psi_n\})$

$\Rightarrow$ If a system is in $|\psi_n\rangle$, a measurement of $\hat{A}$ will precisely yield a_n without changing $|\psi_n\rangle$. A measurement of $\hat{B}$ will yield b_n without perturbing the state.

e.g. $\hat{x}, \hat{y} \sim \hat{p}_x, \hat{p}_y$

Heisenberg Uncertainty

Consider two observables $\hat{A}, \hat{B}$

$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle$, $\langle \hat{B} \rangle = \langle \psi | \hat{B} | \psi \rangle$

Define:

$$\Delta \hat{A} = \left[\langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle \right]^{1/2}$$ mean square deviation

Can show
$$(\Delta \hat{A})^2 = \langle \hat{A}^2 \rangle - \langle A \rangle^2$$

Similarly, $\Delta \hat{B} = \left[\langle (\hat{B} - \langle B \rangle^2 \rangle \right]^{1/2}$

Can prove: $\Delta \hat{A} \Delta \hat{B} \geq \frac{1}{2} | \langle [\hat{A}, \hat{B}] \rangle |$

eg. $[x, p_x] = i\hbar$, $\Delta \hat{x} \Delta \hat{p}_x \geq \hbar/2$

minimum uncertainty $= \hbar/2$

$\rightarrow$ Gaussian wave packet

Unitary Transformations

- Leave the physical description unchanged
- Suppose $\hat{A}|\psi\rangle = |\chi\rangle$

  ↓ linear, Hermitian

$$\left.\begin{array}{l}|\psi'\rangle = \hat{U}|\psi\rangle \\ |\chi'\rangle = \hat{U}|\chi\rangle\end{array}\right\}$$ describe the action of unitary $\hat{U}$. Calculate $\hat{A}'$

$$\hat{A}'\underbrace{|\psi'\rangle}_{\hat{U}|\psi\rangle} = \underbrace{|\chi'\rangle}_{\hat{U}\underbrace{|\chi\rangle}_{\hat{U}\hat{A}|\psi\rangle}} \implies \hat{A}'\hat{U} = \hat{U}\hat{A}$$

since $\hat{U}\hat{U}^+ = \hat{I} = \hat{U}^+\hat{U}$

$$\rightarrow \quad \hat{A}' = \hat{U}A\hat{U}^+, \quad \hat{U}^+A'\hat{U} = \hat{A}$$

→ looks like a simple change of basis

(i) If $\hat{A}$ is Hermitian, $\hat{A}'$ is Hermitian

(ii) Operator equations and commutators are unchanged

eg. $\hat{A} = c_1\hat{B} + c_2\hat{C}\hat{D}$

$\hat{A}' = c_1\hat{B}' + c_2\hat{C}'\hat{D}'$

(iii) The eigenvalues of $\hat{A}'$ are the same as for $\hat{A}$.

(iv) Matrix elements are unchanged

$$\langle x | \hat{A} | \psi \rangle = \langle x' | \hat{A}' | \psi' \rangle$$

$\longrightarrow$ physical observables are unchanged

eg. momentum space & position space wavefunctions! $\hat{U} = \mathcal{F}$ ← fourier transform operator!

** Expressing Unitary Operators as a function of Hermitian operators:

Can write $\hat{U} = e^{i\hat{A}}$ ← Hermitian!

• Consider an "infinitesimal" unitary, very close to $\hat{I}$.

$$\hat{U} = \hat{I} + i\epsilon\hat{F}$$

$\hat{F}$ ← Hermitian "generator" of the unitary

ϵ ← real, small parameter

$$|\psi'\rangle = |\psi\rangle + |\delta\psi\rangle = (\hat{I} + i\epsilon\hat{F})|\psi\rangle$$

$$\rightarrow \quad |\delta\psi\rangle = i\epsilon\hat{F}|\psi\rangle$$

For operators $\hat{A}' = \hat{A} + \delta\hat{A} =$

$$\underbrace{(\hat{I} + i\epsilon\hat{F})}_{\hat{U}} A \underbrace{(I - i\epsilon\hat{F})}_{\hat{U}^{+}}$$

$$= \hat{A} + i\epsilon\hat{F}\hat{A} - i\epsilon\hat{A}\hat{F} + \mathcal{O}(\epsilon^2)$$

$$= \hat{A} + i\epsilon[\hat{F}, \hat{A}] + \mathcal{O}(\epsilon^2)$$

$$\Rightarrow \delta\hat{A} = i\epsilon[\hat{F}, \hat{A}]$$

- Consider now unitary time evolution

$\hat{U}(t, t_0)$ advances the system from $t_0 \rightarrow t$.

$$\hat{U}(t_0, t_0) = \hat{I}$$

$$|\psi(t)\rangle = \hat{U}(t, t_0)|\psi(t_0)\rangle$$

We can break up into little smaller timesteps:

$$\hat{U}(t, t_0) = \hat{U}(t, t')\,\hat{U}(t', t_0)$$

Also note $\hat{U}^{-1}(t, t_0) = \hat{U}(t_0, t)$ (8)

Let's substitute into SE:

$$i\hbar \frac{\partial}{\partial t} \hat{U}(t, t_0) = \hat{H}\hat{U}(t, t_0)$$

(we're divided by $|\psi(t_0)\rangle$ which is time indep.!)

Formal integration

$$\hat{U}(t, t_0) = \hat{I} - \frac{i}{\hbar} \int_{t_0}^{t} \hat{H} U(t', t_0)\, dt'$$

If we consider a small time step, δt from the SE alone,

$$i\hbar \left[\hat{U}(t_0 + \delta t, t_0) - \underbrace{\hat{U}(t_0, t_0)}_{\hat{I}} \right]$$

$$= \hat{H}\hat{U}(t_0, t_0)\delta t$$

Then, to <u>first</u> order in δt,

$$* \quad \hat{U}(t_0 + \delta t, t_0) = \hat{I} - \frac{i}{\hbar} \hat{H} \delta t$$

causes time translation.

($\hat{p}$ moves in space, $\hat{L}$ rotates)

Case of a time indep. $\hat{H}$: ⑨

Starting with $i\hbar \frac{\partial}{\partial t} \hat{u}(t,t_0) = \hat{H}\hat{u}(t,t_0)$

a solution is $\hat{u}(t,t_0) = \underbrace{\exp\left[\frac{-i}{\hbar}\hat{H}\cdot(t-t_0)\right]}_{\sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{-i}{\hbar}\right)^n \hat{H}^n (t-t_0)^n}$

If ψ were an energy eigenfunction,

$\psi_n(t) = e^{-\frac{i}{\hbar}E_n(t-t_0)}\psi_n(t_0)$ as we've seen!

- Time variation of Expectation values

$$\frac{d}{dt}\langle\hat{A}\rangle = \frac{d}{dt}\langle\psi|\hat{A}|\psi\rangle$$

$$= \left\langle\frac{\partial\psi}{\partial t}\middle|\hat{A}\middle|\psi\right\rangle + \left\langle\psi\middle|\frac{\partial\hat{A}}{\partial t}\middle|\psi\right\rangle + \left\langle\psi\middle|\hat{A}\middle|\frac{\partial\psi}{\partial t}\right\rangle$$

$$= \frac{-1}{i\hbar}\underbrace{\langle\hat{H}\psi|\hat{A}|\psi\rangle}_{\langle\psi|HA|\psi\rangle \text{ since } \hat{H}=\hat{H}^\dagger} + \left\langle\psi\middle|\frac{\partial\hat{A}}{\partial t}\middle|\psi\right\rangle + \frac{1}{i\hbar}\langle\psi|\hat{A}\hat{H}|\psi\rangle$$

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$$\Rightarrow \frac{d}{dt}\langle \hat{A} \rangle = \frac{1}{i\hbar}\langle [\hat{A},\hat{H}] \rangle + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle$$

For a time <u>indep</u> operator $\hat{A}$, $\frac{\partial \hat{A}}{\partial t} = 0$

and $\frac{d}{dt}\langle \hat{A} \rangle = \frac{1}{i\hbar}\langle [\hat{A},\hat{H}] \rangle$

** <u>Note</u>: If $\hat{A}$ commutes with $\hat{H}$,

then $\langle \hat{A} \rangle$ is a constant of motion!