Lecture 38: 04/27/09

- Angular momentum II
  - simultaneous eigenfunctions
- Angular momentum states of central potentials
  - spherical harmonics $Y_\ell^m(\theta,\phi)$

Recap:

VI_4 Orbital Angular Momentum of Particles in QM

$\hat{L} = \hat{r} \times \hat{p} \Rightarrow$ for example:

$$\hat{L}_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = \frac{\hbar}{i}\frac{\partial}{\partial \phi}$$

$$\hat{L}^2 = -\hbar^2\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right\}$$

- eigenfunctions of $\hat{L}^2$:

(1) $$\hat{L}^2 F(\theta,\phi) = \hbar^2\beta F(\theta,\phi) = L^2 \underbrace{F(\theta,\phi)}_{\text{states of definite } L^2}$$

- eigenfunction of $\hat{L}_z$

$$\hat{L}_z \Phi(\phi) = L_z \Phi(\phi) \Rightarrow \Phi(\phi) \propto e^{im\phi}$$

with eigenvalues $L_z = m\hbar$, $m = 0, \pm 1, \pm 2, \ldots$

$\Rightarrow$ quantized! $\Rightarrow$ same for $\hat{L}_x$, and $\hat{L}_y$

→ Simultaneous set of eigenfunctions of angular momentum operators: $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$, $\hat{L}^2$

Question: Are there complete sets of eigenfunctions which are simultaneous eigenfunctions of two of these operators?

Answer: yes, if the two operators commute:

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

no, if the two operators do not commute:

$$[\hat{A}, \hat{B}] \neq 0$$

$\Rightarrow$ $\hat{A}$, $\hat{B}$ are incompartible observables

Proof: If $\hat{A}\Phi_n = a_n \Phi_n$ and $\hat{B}\Phi_n = b_n \Phi_n$

$\Rightarrow \{\Phi_n\}$ is simultaneous set of eigenfunctions of $\hat{A}$ and $\hat{B}$

$\{\Phi_n\}$ is complete $\Rightarrow$ general wave function

$$\psi = \sum_n c_n \Phi_n(x)$$

$$\Rightarrow \hat{A}\hat{B}\psi = \hat{A}\sum_n c_n b_n \Phi_n = \sum_n c_n a_n b_n \Phi_n$$

$$\Rightarrow \hat{B}\hat{A}\psi = \hat{B}\sum_n c_n a_n \Phi_n = \sum_n c_n b_n a_n \Phi_n$$

$$\Rightarrow (\hat{A}\hat{B} - \hat{B}\hat{A})\psi = 0 \quad \Rightarrow [\hat{A}, \hat{B}] = 0$$

$\Rightarrow$ if two operators commute, they have a complete set of simultaneous eigenfunctions

$\Rightarrow$ eigenfunctions have definite eigenvalues for A <u>and</u> B

$\Rightarrow$ can measure A <u>and</u> B for the eigenstates without collapsing the wave function $\Rightarrow$ can know A and B at the same time for a given eigenstate

<u>Note:</u> Not every eigenfunction of $\hat{A}$ is necessarily an eigenfunction of $\hat{B}$, but one can always construct a complete set of simultaneous eigenfunctions by superposition if $[\hat{A}, \hat{B}] = 0$

$\longrightarrow$ start with $[\hat{L}_x, \hat{L}_y]$:

$$\hat{L}_x \hat{L}_y \psi = -\hbar^2 \left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\psi$$

$$= -\hbar^2 \left\{ \underbrace{y\frac{\partial}{\partial x}}_{\text{product rule}} + yz\frac{\partial}{\partial z}\frac{\partial}{\partial x} - yx\frac{\partial}{\partial z^2} - z^2\frac{\partial}{\partial y}\frac{\partial}{\partial x} + zx\frac{\partial}{\partial y}\frac{\partial}{\partial z} \right\}\psi$$

$$\hat{L}_y \hat{L}_x \psi = -\hbar^2 \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\psi$$

$$= -\hbar^2 \left\{ zy\frac{\partial}{\partial x}\frac{\partial}{\partial z} - z^2\frac{\partial}{\partial x}\frac{\partial}{\partial y} - xy\frac{\partial^2}{\partial z^2} + \underbrace{x\frac{\partial}{\partial y}}_{\text{product rule}} + xz\frac{\partial}{\partial z}\frac{\partial}{\partial y} \right\}\psi$$

$$\Rightarrow \left(\hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x\right)\psi = -\hbar^2\left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right)\underline{\psi}$$

$\Rightarrow$ $[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$: do <u>not</u> commute!

$\Rightarrow$ no simultaneous complete set of eigenfunctions!

result:

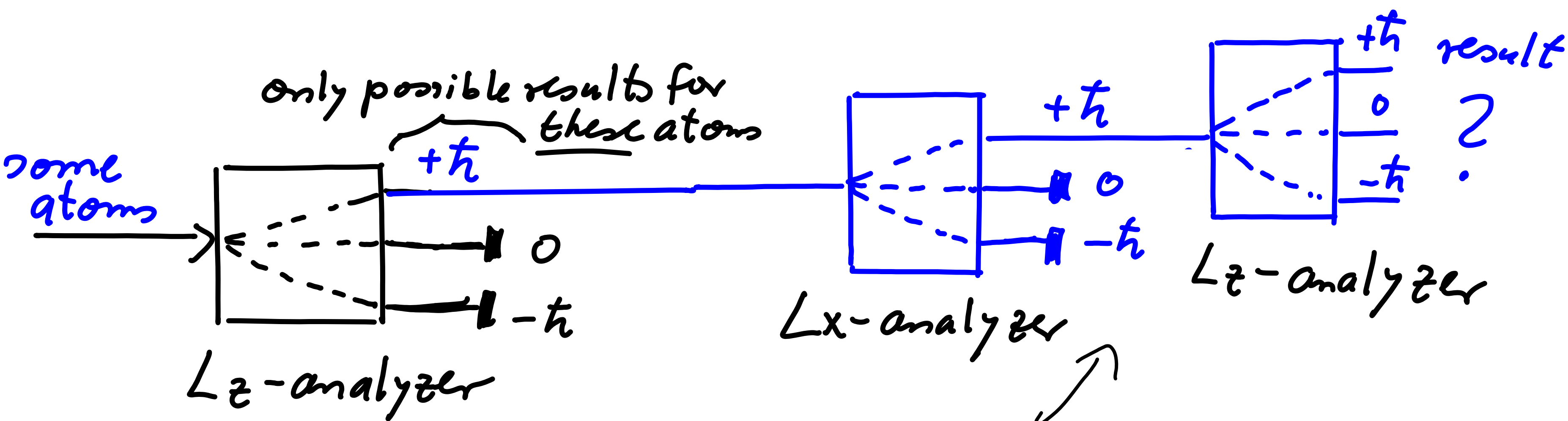
$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$
$$[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$$
$$[\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y$$

by cyclic permutation ($x \to y$, $y \to z$, $z \to x$)

$\Rightarrow$ Conclusion 1:

- $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$ are incompatible observables
- have no simultaneous complete set of eigenfunctions
- in general, can only know L_x, or L_y, or L_z of a state at a given time
- in general, can't write down functions in which L_x, L_y and L_z all have definite values
- particles can have only L_x or L_y, or L_z!
- $\Rightarrow$ uncertainty principle: $\sigma_{L_x}^2 \sigma_{L_y}^2 \geq \left(\frac{1}{2i}\langle i\hbar L_z\rangle\right)^2$

→ "Experiment"



$L_x = +\hbar$ state is a superposition of different L_z-states! (no complete set of simultaneous eigenfunctions!)

$\Rightarrow$ could get $L_z = \hbar$, 0, or $-\hbar$ at the end!

→ do $\hat{L}^2$ and $\hat{L}_z$ commutate?

⇒ yes!

Proof: 1) start with the following commutator identity:

$$[\hat{A}\hat{B},\hat{C}] = \hat{A}\hat{B}\hat{C} - \hat{C}\hat{A}\hat{B} = \hat{A}\hat{B}\hat{C} - \hat{A}\hat{C}\hat{B} + \hat{A}\hat{C}\hat{B} - \hat{C}\hat{A}\hat{B}$$

$$= \hat{A}[\hat{B},\hat{C}] + [\hat{A},\hat{C}]\hat{B}$$

2) $[\hat{L}^2, L_z] = [L_x^2 + L_y^2 + L_z^2, L_z]$

$$= [\hat{L}_x\hat{L}_x,\hat{L}_z] + [\hat{L}_y\hat{L}_y,\hat{L}_z] + \underbrace{[\hat{L}_z\hat{L}_z,\hat{L}_z]}_{\substack{=0 \\ \text{(operator commutes} \\ \text{with itself)}}}$$

$$= \hat{L}_x[\hat{L}_x,\hat{L}_z] + [\hat{L}_x,\hat{L}_z]\hat{L}_x + \hat{L}_y[\hat{L}_y,\hat{L}_z] + [\hat{L}_y,L_z]\hat{L}_y$$

$$= \hat{L}_x(-i\hbar\hat{L}_y) + (-i\hbar\hat{L}_y)\hat{L}_x + \hat{L}_y(i\hbar\hat{L}_x) + (i\hbar\hat{L}_x)\hat{L}_y$$

$$= \underline{\underline{0}}$$

Q.E.D.

$\Rightarrow$ result: $[\hat{L}^2, L_z] = 0$

$$\left.\begin{aligned}[\hat{L}^2, L_x] &= 0\\ [\hat{L}^2, L_y] &= 0\end{aligned}\right\}\text{ by symmetry!}$$

$\Rightarrow$ conclusion?:

- $\hat{L}^2$ is compatible with each component of $\vec{L}$

$\Rightarrow$ can find a complete set of simultaneous eigenfunctions of $\hat{L}^2$ and (for example) $\hat{L}_z$

$\Rightarrow$ can label all simultaneous eigenstates $F(\theta, \phi)$ by their eigenvalues L^2 and L_z

$\Rightarrow$ this is just one of the possible choices. Could use $\hat{L}_x$ or $\hat{L}_y$ instead of $\hat{L}_z$, but $\hat{L}_z$ is the conventional choice.

→ Path toward full solution of the H-atom:

To find stationary state wavefunctions of electron in H-atom:

1) Find complete set of angular eigenfunctions of $\hat{L}^2$ and $\hat{L}_z$: $F(\theta, \phi)$

   ⇒ these have definite values of L^2 and L_z

2) $\hat{L}^2$ and $\hat{L}_z$ also commute with:

$$\hat{E} = \frac{\hat{p}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2} + V(r)$$

for central potentials (only!)

⇒ can find complete set of simultaneous eigenfunctions of $\hat{L}^2$, $\hat{L}_z$, and $\hat{E}$!

⇒ label these eigenstates $\psi(r, \theta, \phi)$ according to their definite energy, (angular momentum)^2, L_z

⇒ 3 quantum numbers (n, ℓ, m)

⇒ need one more quantum number (m_s) to include spin

VI_5 Solution of the angular momentum equation 1 for *any* central potential $\Rightarrow$ spherical harmonics

(1) $\hat{L}^2 F(\theta,\phi) = \hbar^2 \beta F(\theta,\phi)$

with: $\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right]$

$\Rightarrow$ since $\hat{L}^2$ and $\hat{L}_z$ commute: look for simultaneous eigenfunctions:

recall: $\hat{L}_z = \frac{\hbar}{i} \frac{\partial}{\partial\phi}$ with eigenfunctions $\Phi(\phi) \propto e^{im\phi}$

$m = 0, \pm 1, \pm 2, \ldots$

$$\hat{L}_z \Phi(\phi) = \underbrace{\hbar m}_{L_z} \Phi(\phi)$$

$\Rightarrow$ try $F(\theta,\phi) = \underbrace{P(\theta)}_{\text{depends on } \theta \text{ only}} e^{im\phi}$ to solve ①

$\Rightarrow$ insert into ①

$$-\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial P(\theta)}{\partial\theta}\right)e^{im\phi} - \frac{m^2}{\sin^2\theta}P(\theta)e^{im\phi}\right]$$

$$= \hbar^2\beta\, P(\theta)e^{im\phi}$$

- subset of solutions:

$$P(\theta) \propto \sin^l\theta \quad , \quad l = \text{integer}$$

$$\Rightarrow \sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{dP(\theta)}{d\theta}\right) + \left(\beta\sin^2\theta - m^2\right)P(\theta) = 0$$

function of θ only

$\underline{\text{try:}}$ $\sin\theta \frac{d}{d\theta} P(\theta) = \sin\theta \left\{ \ell \sin^{\ell-1}\theta \cos\theta \right\}$

$\Rightarrow \sin\theta \left(\ell^2 \sin^{\ell-1}\theta \cos^2\theta - \ell \sin^{\ell}\theta \sin\theta \right)$

$+ \beta \sin^2\theta \sin^{\ell}\theta - m^2 \sin^{\ell}\theta = 0$

$= \ell^2 \sin^{\ell}\theta \underbrace{\cos^2\theta}_{1-\sin^2\theta} - \ell \sin^{\ell+2}\theta + \beta \sin^{\ell+2}\theta - m^2 \sin^{\ell}\theta$

$= \sin^{\ell}\theta (\ell^2 - m^2) - \sin^{\ell+2}\theta (\ell^2 + \ell - \beta) = 0$ for $\underline{\underline{\text{all}}}$ θ

$\Rightarrow$ solution, if: $\underline{m = \pm \ell}$ and $\underline{\beta} = \ell^2 + \ell = \underline{\underline{\ell(\ell+1)}}$

$\Rightarrow$ $\underline{\text{subset}}$ of solutions:

$F(\theta,\phi) \propto \sin^{\ell}\theta \, e^{\pm i\ell\phi} \equiv \underbrace{Y_{\ell}^{m=\pm\ell}(\theta,\phi)}_{\text{spherical harmonics}}$

with eigenvalues:

quantized! $\begin{cases} L^2 = \beta \hbar^2 = \ell(\ell+1)\hbar^2 \\ L_z = \pm \ell \hbar \end{cases}$ $\ell = 0, 1, 2, \ldots$

- complete set of solutions: spherical harmonics:

$$Y_\ell^m(\theta,\phi) = \epsilon \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}\, P_\ell^m(\underbrace{\cos\theta}_{=\text{"}x\text{"}})\, e^{im\phi}$$

with $\epsilon = (-1)^m$ for $m \geq 0$ and $\epsilon = 1$ for $m < 0$

$P_\ell^m(x) =$ Legendre function, defined by:

$$P_\ell^m(x) \equiv (1-x^2)^{|m|/2}\left(\frac{d}{dx}\right)^{|m|} P_\ell(x)$$

where $P_\ell(x)$ is the ℓ^{th} Legendre polynomial:

$$P_\ell(x) \equiv \frac{1}{2^\ell\, \ell!}\left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell$$