P3220 LECTURE 31/32

Spherical harmonics – practical issues.

An angular momentum eigenstate is:

$$\psi(x) = R(r)g(\Theta)h(\phi) = R(r)Y_{lm}(\theta,\phi)$$

Normalization says you have to find the particle somewhere:

$$\int d\vec{r}\,\left|R(r)g(\theta)h(\phi)\right|^2 = 1.$$

$$= \int d\vec{r}\,|R(r)|^2|g(\theta)|^2|h(\phi)|^2 = \iiint dr\,d\theta\,d\phi\; r^2\sin\theta\,|R(r)|^2|g(\theta)|^2|h(\phi)|^2$$

Remember it's all separable:

$$1 = \underbrace{\int_0^\infty dr\,r^2|R(r)|^2}_{=1}\;\underbrace{\int_0^\pi d\theta\,\sin\theta\,|g(\theta)|^2}_{=1}\;\underbrace{\int_0^{2\pi} d\phi\,|h(\phi)|^2}_{=1}$$

Can normalize each part separately.

Concentrate on angular part: $Y_{lm} = \left(\Theta_{lm}(\theta)\right)\left(Ae^{im\phi}\right)$

$$1 = \int_0^\pi d\theta\,\Theta_{lm}(\theta) = A^2\int_0^{2\pi} d\phi\,\underbrace{|e^{im\phi}|^2}_{=1} \Rightarrow A^2 = \frac{1}{2\pi} \Rightarrow Y_{lm} = \frac{1}{\sqrt{2\pi}}\Theta(\theta)e^{im\phi}$$

$$= \frac{1}{\sqrt{2\pi}}\left[\frac{2l+1}{2}\,\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_{lm}(\cos\theta)\,e^{im\phi}$$

General behavior of solutions:

$l = m = 0$: $Y_{00}(\theta, \phi) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2}} P_{00}(\cos\theta) = \frac{1}{\sqrt{4\pi}}$

- Isotropic → no angular dependence (expected since $\vec{L} = 0$)
- Normalized: $\int_{4\pi} |Y_{00}|^2 = 1$.
- "s-wave" state.

$l = 1; m = 1$: $Y_{11} = \frac{1}{\sqrt{2\pi}} \Theta_{11}(\cos\theta)\, e^{i\phi}$

$= -\frac{1}{2}\sqrt{\frac{3}{2\pi}} \sin\theta\, e^{i\phi}$

$l = 1, m = -1$: $Y_{1-1} = +\frac{1}{2}\sqrt{\frac{3}{2\pi}}\, e^{-i\phi}$ only change is sign, + $i\phi$ dependence

$l = 1; m = 0$: $\frac{1}{2}\sqrt{\frac{3}{2\pi}} \cos\theta$ No ϕ dependence!

1-node solutions: "p-waves"

Higher l solutions have more nodes; d, f, etc. waves.
Higher $|m|$ → faster phase rotation about z axis.

$\langle l' m' | l m \rangle = \delta_{l'l}\delta_{m'm}$: states are orthogonal.

What about $\hat{L}_x$? If $l = 1$, then my possible values of L_x are $-\hbar, 0, +\hbar$ sine physically x, z symmetric. But what are probabilities of L_x = each value if I am in an eigenstate of $\hat{L}_z$? Use operator methods!

- Eigenstates of $\hat{L}_x$ are solutions to $L_x|\psi\rangle = m_x\hbar|\psi\rangle$

Remember that $\hat{L}_x = \frac{1}{2}(L_+ + L_-)$ and $|\psi\rangle = \sum_{l,m_z} a_{lm}|l\,m\rangle$.

A useful table of operator relations is on Liboff ~~p. 321~~ Table 9.4

Take $|\psi\rangle = a|1\,{-1}\rangle + b|1\,0\rangle + c|1\,1\rangle$ in $\underline{\hat{L}^2, L_z \text{ basis}}$.

Solve for $|\psi\rangle$ such that $L_x|\psi\rangle = +\hbar|\psi\rangle$ $(m_x = 1)$.

$$\frac{1}{2}(\hat{L}_+ + \hat{L}_-)|\psi\rangle = \hbar|\psi\rangle \Rightarrow$$

$$\frac{1}{2}(\hat{L}_+ + \hat{L}_-)\left[a_1|1\,{-1}\rangle + b_1|1\,0\rangle + c_1|1\,1\rangle\right] = a\hbar|1\,{-1}\rangle + b\hbar|1\,0\rangle + c\hbar|1\,1\rangle$$

$$= \frac{1}{2}\Big[a\hat{L}_+|1\,{-1}\rangle + \cancel{a\hat{L}_-|1\,{-1}\rangle}_{\to 0} + b\hat{L}_+|1\,0\rangle + b\hat{L}_-|1\,0\rangle + $$

$$+ \cancel{c\hat{L}_+|1\,1\rangle} + c\hat{L}_-|1\,1\rangle\Big] \quad \text{(more in homework!)}$$

$\Rightarrow$ so we can construct $|l\,m_x\rangle$ states in m_z basis; thus

for $m_z = 1$, $P(L_x = 1) = \left|\langle l, m_x{=}1 | l, m_z{=}1\rangle\right|$.

Addition of angular momentum: What is the total angular momentum of a system of two particles?

i.e. adding the orbital $\vec{L}$ of 2 electrons in a He atom

or adding orbital $\vec{L}$ and spin $\vec{S}$ of one electron

Assume subsystems independent: $\hat{\vec{J}}_1$ operates on particle 1, $\hat{\vec{J}}_2$ on 2. $[\hat{\vec{J}}_1, \hat{\vec{J}}_2] = 0$

OK, what is $\hat{\vec{J}}^2 = |\hat{\vec{J}}_1 + \hat{\vec{J}}_2|^2$?

$\hat{J}^2 = \hat{J}_1^2 + \hat{J}_2^2 + 2\hat{\vec{J}}_1 \cdot \hat{\vec{J}}_2$. If we are in state $|j_1 m_1\rangle|j_2 m_2\rangle = |\psi\rangle$ then:

$$\hat{\vec{J}}^2|\psi\rangle = \hbar^2 j_1(j_1+1)|\psi\rangle + \hbar^2 j_2(j_2+1)|\psi\rangle + 2\hat{\vec{J}}_1 \cdot \hat{\vec{J}}_2|\psi\rangle$$

So the problem of finding total ang. mom. $\hat{J}^2$ reduces to finding the eigenvalues/eigenstates of $(\hat{\vec{J}}_1 \cdot \hat{\vec{J}}_2) = \hat{J}_{1x}\hat{J}_{2x} + \hat{J}_{1y}\hat{J}_{2y} + \hat{J}_{1z}\hat{J}_{2z}$

Note that $|\psi\rangle$ is <u>not</u> necessarily an eigenstate of $\hat{J}_{1x}, \hat{J}_{2x}, \hat{J}_{1y}, \hat{J}_{2y}$ (unless $j_1 = j_2 = 0$ in which case it's a trivial problem.)

Evidently $\hat{J}^2$, $\hat{J}_z$ are not compatible with $\hat{J}_1^2, \hat{J}_2^2, \hat{J}_{1z}, \hat{J}_{2z}$.

So we are looking at two different bases or representations:

"uncoupled" representation: commuting observables are $\hat{J}_1^2, \hat{J}_{1z}, \hat{J}_2^2, \hat{J}_{2z}$ $\Rightarrow$ corresponding good quantum numbers are j_1, m_1, j_2, m_2: $(2j_1+1)(2j_2+1)$ basis states.

"coupled representation": commuting observables are obviously $\hat{J}^2, \hat{J}_z$. But this seems to indicate fewer distinguishable states. More commuting observables? Yes: it turns out that $[\hat{J}^2, \hat{J}_1^2] = [\hat{J}^2, \hat{J}_2^2] = 0$, so good quantum numbers are actually $\underline{j, m, j_1, j_2}$.

What are the allowed ranges for j, m?

Look at a # of states argument: Need same number of available states in coupled, uncoupled rep.:

$$(2j_1+1)(2j_2+1) = \sum_{J_{min}}^{J_{max}} (2j+1).$$

So given j_1, j_2, j can take values from $|j_1 - j_2|$ to $j_1 + j_2$.

Since $\hat{J}_z = \hat{J}_{1z} + \hat{J}_{2z}$, and $[J_{1z}, J_{2z}] = 0$, $[J_z, J_{1z}]$

$= [J_z, J_{2z}] = 0 \Rightarrow m = m_1 + m_2$.

so $$|j\, m\, j_1 j_2\rangle = \sum_{m_1}\sum_{m_2} \Big(|j_1 m_1\rangle |j_2 m_2\rangle \langle j_1 m_1| \langle j_2 m_2|\Big) |j\, m\, j_1 j_2\rangle$$

only has nonzero coefficients where $m_1 + m_2 = m$.

rewrite: $$|j\, m\, j_1 j_2\rangle = \sum_{m_2 = m - m_1} \sum_{m_1} C_{m_1 m_2} |j_1 m_1\rangle |j_2 m_2\rangle$$

where $$C_{m_1 m_2} \equiv \langle j_1 j_2 m_1 m_2 | j\, m\, j_1 j_2\rangle$$

$C_{m_1 m_2}$ are Clebsch-Gordan coefficients.