

5/31/07 Lecture 17 outline

- Last time: discussed the eigenkets $|\ell, m\rangle$ of L^2 and L_z . Now consider these kets in position space.

Use spherical coordinates. The $|\ell, m\rangle$ states are independent of the radial coordinate, r ; they depend only on θ and ϕ . To see why, write $\vec{L} = \vec{x} \times \vec{p}$ in position space, by replacing $\vec{p} \rightarrow -i\hbar \nabla$. Converting to spherical coordinates, get

$$L_z \rightarrow -i\hbar \frac{\partial}{\partial \phi} \quad L_{\pm} \rightarrow \hbar e^{\pm i\phi} \left(\pm \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right)$$

and

$$L^2 \rightarrow -\hbar^2 \left[\frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \right].$$

In position space the L^2 and L_z eigenkets become $\langle \theta, \phi | \ell, m \rangle = Y_{\ell, m}(\theta, \phi)$. Their definition in terms of their eigenvalue equations, $L^2 Y_{\ell, m}(\theta, \phi) = \hbar^2 \ell(\ell + 1) Y_{\ell, m}(\theta, \phi)$ and $L_z Y_{\ell, m}(\theta, \phi) = m\hbar Y_{\ell, m}(\theta, \phi)$ are well known equations: the $Y_{\ell, m}(\theta, \phi)$ are the Spherical Harmonics, which always enter in solving problems in spherical coordinates. They are given by $Y_{\ell, m}(\theta, \phi) \sim P_{\ell}^m(\cos \theta) e^{im\phi}$, where $P_{\ell}^m(u) \sim (1 - u^2)^{-m/2} \left(\frac{d}{du}\right)^{\ell - m} (1 - u^2)^{\ell}$ are associated Legendre polynomials. E.g. $Y_{\ell, \ell} \sim \sin^{\ell} \theta e^{i\ell\phi}$. For $m = 0$, they are the ordinary Legendre polynomials, recall $P_0(u) = 1$, $P_1(u) = u$, $P_2(u) = \frac{1}{2}(3u^2 - 1)$, etc. Draw some plots. E.g. $Y_{\ell, \ell}$ looks as expected for having maximum L_z : it's rotation is mostly in the x - y plane, so it's peak is perpendicular to the \hat{z} axis. And $Y_{\ell, 0}$ looks as expected for having $L_z = 0$: it's rotation is mostly in a plane including the \hat{z} axis, so it looks peaked along the \hat{z} axis. Also the $\ell = 1$ is called dipole, as seen from the shape of the $L_{\ell=1, m}$, and $\ell = 2$ is called quadropole, as seen from e.g the shape of $Y_{2, 1}$, etc. Mention names for $\ell = 0, 1, 2, 3 \dots$ are called the $s, p, d, f \dots$ orbitals.

- The $|\theta, \phi\rangle$ form a complete orthonormal basis:

$$\langle \theta', \phi' | \theta, \phi \rangle = \frac{1}{\sin \theta} \delta(\theta - \theta') \delta(\phi - \phi') \quad \int_0^{2\pi} d\phi \int_0^{\pi} \sin \theta d\theta |\theta, \phi\rangle \langle \theta, \phi| = \mathbf{1}.$$

The $|\ell, m\rangle$ similarly form a complete, orthonormal basis:

$$\langle \ell', m' | \ell, m \rangle = \delta_{\ell, \ell'} \delta_{m, m'} \quad \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} |\ell, m\rangle \langle \ell, m| = \mathbf{1}.$$

Combining these give many standard formulae for the spherical harmonics, e.g. a general function of θ and ϕ can be expanded in terms of the spherical harmonics as:

$$f(\theta, \phi) \equiv \langle \theta, \phi | f \rangle = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \langle \theta, \phi | \ell, m \rangle \langle \ell, m | f \rangle \equiv \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} Y_{\ell, m}(\theta, \phi) f_{\ell, m},$$

where $f_{\ell, m} = \langle \ell, m | f \rangle = \int d\Omega \langle \ell, m | \theta, \phi \rangle \langle \theta, \phi | f \rangle = \int d\Omega Y_{\ell, m}(\theta, \phi)^* f(\theta, \phi)$.

- In position space, we replace $\vec{p}^2 \rightarrow -\hbar^2 \nabla^2$. In spherical coordinates, this becomes

$$\vec{p}^2 \rightarrow -\hbar^2 \nabla^2 = -\hbar^2 \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{L^2}{\hbar^2 r^2} \right) \equiv p_r^2 + \frac{L^2}{r^2}.$$

So the angular part of the Laplacian in spherical coordinates is just the L^2 operator. This connects with how the $Y_{\ell, m}(\theta, \phi)$ arise in solving differential equations involving ∇^2 in spherical coordinates (as seen e.g. in evaluating the scalar potential in E& M). Indeed, the general solution of $\nabla^2 \phi = 0$ is

$$\phi = \sum_{\ell=0}^{\infty} \left(A_{\ell, m} r^{\ell} + \frac{B_{\ell, m}}{r^{\ell+1}} \right) Y_{\ell, m}(\theta, \phi).$$

(In problems with azimuthal rotational symmetry around an axis, which can be taken to be \hat{z} , there are only the $m = 0$ terms.) The very particular form of the r dependent terms above, i.e. r^{ℓ} and $1/r^{\ell+1}$ are special to solutions of $\nabla^2 \phi = 0$. For other equations, like the 3d energy eigenvalue equation, the r dependence will be different. But the (θ, ϕ) dependence of any function can be expressed in terms of the $Y_{\ell, m}(\theta, \phi)$: that is the statement that the $|\ell, m\rangle$ form a complete basis.