6/3/08 Lecture 18 outline

- Last time :

$$L^2|\ell,m\rangle = \hbar^2\ell(\ell+1)|\ell,m\rangle \qquad L_z|\ell,m\rangle = m\hbar|\ell,m\rangle$$

and

$$L_\pm|\ell,m\rangle = \hbar\sqrt{\ell(\ell+1)-m^2\mp m}|\ell,m\pm 1\rangle.$$

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

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

- 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 $\vec{p}\to -i\hbar\nabla$. Converting to spherical coordinates, get

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

and

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

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 $P_\ell^m(u)\sim(1-u^2)^{-m/2}(\frac{d}{du})^{\ell-m}(1-u^2)^\ell$ 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 $\widehat{z}$ axis. And $Y_{\ell,0}$ looks as expected for having $L_z=0$: it's rotation is mostly in a plane including the $\widehat{z}$ axis, so it looks peaked along the $\widehat{z}$ 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 $\ell=0,1,2,3\ldots$ are called the s, p, d, f … orbitals.

• Aside on rotations in a 2d plane. Replace $|\theta\phi\rangle$ with just $|\phi\rangle$ and $|\ell m\rangle$ with $|m\rangle$. Discuss $|\psi\rangle$ in the $|\theta\rangle$ and the $|m\rangle$ basis, and the Fourier transform between these bases, using $\langle\theta|m\rangle = \frac{1}{\sqrt{pi}}e^{im\phi}$.

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

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

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

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

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 $\vec{p}^2 \to -\hbar^2\nabla^2$. In spherical coordinates, this becomes

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

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

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

(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.

• Decoupled systems, e.g. $H = H_1 + H_2$. Energy eigenstates and eigenvalues. Relate to separation of variables.

• Consider spherically symmetric $H = \frac{1}{2m}\vec{p}^2 + V(r)$. Since $[H, L_i] = 0$, we can find simultaneous eigenstates $|E, \ell, m\rangle$ of H, L^2, and L_z. Indeed, note that

$$H = \frac{p_r^2}{2\mu} + \frac{L^2}{2\mu r^2} + V(r)$$

where in position space the first terms correspond to

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

It is common, also in classical mechanics, to note that this looks like a 1d problem now, with $V_{eff}(r) = V(r) + (L^2/2\mu r^2)$. Here μ is the mass, not to be mistaken for the m integer appearing in $|\ell, m\rangle$. The energy eigenvalue equation then becomes

$$\left(\frac{p_r^2}{2\mu} + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} + V(r) \right) |E, \ell, m\rangle = E|E, \ell, m\rangle.$$

In position space, write this equation and discuss solution by separation of variables. We then have $\psi_{E,\ell,m}(r, \theta, \phi) = \langle r, \theta, \phi | E, \ell, m\rangle = R_{n,\ell}(r) Y_{\ell,m}(\theta, \phi)$, where

$$\left(-\frac{\hbar^2}{2\mu}(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}) + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} + V(r) \right) R_{n,\ell}(r) = E_{n,\ell} R_{n,\ell}(r),$$

where n labels the solutions of this equation. The energy is quantized, via n, because we're considering bound states of the potential. Note that the energy eigenvalues $E_{n,\ell}$ don't depend on the L_z eigenvalue m; this is as expected from the spherical symmetry, which implies that $[H, L_\pm] = 0$. The derivative terms become a little simpler if we define $R_{n,\ell}(r) = U_{n,\ell}(r)/r$:

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V(r) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} \right) U_{n,\ell}(r) = E_{n,\ell} U_{n,\ell}(r).$$