

11/21/16 Lecture 16 outline

- Aside:  $Y_{\ell,m}(\theta, \phi)$  asides:  $Y_{\ell,\ell} = c_{\ell} e^{i\ell\phi} \sin^{\ell} \theta$ ,  $Y_{\ell,0} = \sqrt{\frac{2\ell+1}{4\pi}} P_{\ell}(\cos \theta)$ ,

$$Y_{\ell,m} = c_{\ell,m} e^{im\phi} (\sin \theta)^{-m} \frac{d^{\ell-m}}{d(\cos \theta)^{\ell+m}} (\sin \theta)^{2\ell}.$$

In rectangular coordinates, the  $Y_{\ell m}$  are given by appropriate  $F_{\ell}(x, y, z)/r^{\ell}$  which we can understand in terms of addition of angular momentum. E.g.  $r^2 = x^2 + y^2 + z^2$  has  $\ell = m = 0$  whereas  $Q_{ij} = (x_i x_j - \frac{1}{3} r^2)/r^2$  has  $\ell = 2$ , with the five independent components corresponding to  $m = 2, 1, 0, -1, -2$ . This is referred to as an  $\ell = 2$  tensor. Likewise can consider  $Q_{i_1, \dots, i_{\ell}}$  by symmetrizing and subtracting the traces.

- Last time: spherically symmetric  $V(r)$  means that  $[H, L_a] = 0$ , so we can find simultaneous eigenstates  $|E, \ell, m\rangle$ . Writing  $\vec{p}^2 \rightarrow p_r^2 + L^2/r^2$ , we find that  $\vec{x}|E\ell m\rangle = R_{E,\ell}(r)Y_{\ell,m}(\theta, \phi)$ , where  $R_{E,\ell}$  satisfies the radial SE

$$\left( -\frac{\hbar^2}{2mr^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) + \frac{\ell(\ell+1)\hbar^2}{2mr^2} + V(r) \right) R_{E,\ell}(r) = ER_{E,\ell}(r).$$

It looks a little nicer for  $u_{E,\ell}(r) \equiv rR_{E,\ell}(r)$ :

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + V_{eff}(r)u = Eu, \quad V_{eff} = V(r) + \frac{\ell(\ell+1)\hbar^2}{2mr^2}.$$

If we assume that  $r^2 V(r) \rightarrow 0$  for  $r \rightarrow 0$ , then the angular momentum barrier wins and the SE implies  $u(r) \rightarrow Ar^{\ell+1} + Br^{-\ell}$  in this limit, and the condition that  $j_r = \hat{r} \cdot \vec{j} = \frac{\hbar}{m} Im(\psi^* \partial_r \psi) \rightarrow 0$  for  $r \rightarrow 0$  excludes the second term, so  $R_{E,\ell} \rightarrow r^{\ell}$  for  $r \rightarrow 0$ . So wavefunction vanishes at origin except for  $\ell = 0$ ; this is the angular momentum barrier.

- Free particle in spherical coordinates:  $\psi_{E,\ell,m} = R_{E,\ell}(r)Y_{\ell,m}(\theta, \phi)$  has  $R = u/r$  with

$$\left( \frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2} \right) u = 0, \quad \hbar k = \sqrt{2mE}.$$

Function of  $\rho = kr$ . Solutions of the ODE in  $\rho$  are the spherical Bessel functions

$$j_{\ell} = (-\rho)^{\ell} \left( \frac{1}{\rho} \frac{d}{d\rho} \right)^{\ell} \left( \frac{\sin \rho}{\rho} \right).$$

(Replacing  $\sin \rho \rightarrow -\cos \rho$  gives the spherical Neumann functions  $n_{\ell}(\rho)$  which also solve the ODE but have  $n_{\ell} \sim \rho^{-\ell-1}$  for  $\rho \rightarrow 0$  which is badly behaved and thus thrown away. As expected, here  $k$  and  $E$  are continuous. The solutions are delta-function normalizable:

$$\int_0^{\infty} j_{\ell}(kr) j_{\ell'}(k'r) r^2 dr = \frac{\pi}{2k^2} \delta(k - k') \delta_{\ell\ell'}.$$

- Particle in a spherical well of radius  $a$ : need to impose  $j_\ell(ka) = 0$ , leads to quantized  $k \rightarrow k_{\ell,n}$  e.g.  $k_{0,n} = n\pi$ , and thus  $E_{n,\ell}$ . No degeneracy in  $\ell$ .

- SHO:  $r \equiv \sqrt{\hbar/m\omega\rho}$ ,  $u = \rho^{\ell+1}e^{-\rho^2/2}f(\rho)$  gives an eqn for  $f(\rho) \equiv \sum_{n=0}^{\infty} a_n \rho^n$  with recursion relation

$$a_{n+2} = \frac{2n + 2\ell + 3 - 2E/\hbar\omega}{(n+2)(n+2\ell+3)} a_n.$$

For  $n \rightarrow \infty$  this recursion relation gives  $f \sim e^{\rho^2}$ , which would lead to a non-normalizable  $\psi$ , so there has to be some  $n = q$  where it truncates, i.e.  $a_{n>q} = 0$ . This leads to  $E = (2q + \ell + \frac{3}{2})\hbar\omega$ , where  $q = 0, 1, 2, \dots$  is the number of nodes in the radial wavefunction. Compare to rectangular coordinates and 3 decoupled SHOs, where we get  $E = (N + \frac{3}{2})\hbar\omega$ , get  $N = n_1 + n_2 + n_3 = 2q + \ell$ . Note degeneracy with different  $\ell$  having same  $E$ .

- Coulomb potential:  $V = -Ze^2/r$ . Usual to write in terms of  $\alpha = e^2/\hbar c \approx 1/137$ . Coulomb potential: define  $\rho \equiv \kappa r$  where  $\hbar\kappa \equiv \sqrt{2m|E|}$  and  $\rho_0 \equiv \sqrt{2m/|E|}(Ze^2/\hbar)$  and use  $\alpha \equiv e^2/\hbar c \approx 1/137$ . Then  $u_{E,\ell} \equiv \rho^{\ell+1}e^{-\rho}w(\rho)$  solves the radial S.E. if  $w(\rho)$  satisfies an ODE. The solutions can be written in terms of hypergeometric functions. As usual for bound state problems, we find that  $E$  has to be quantized or the solution would be badly behaved for  $r \rightarrow \infty$ , would get  $w(\rho) \rightarrow e^\rho$  for generic  $E$ . To avoid this, the series for  $w(\rho)$  must truncate at finite order  $N$ . This requires  $\rho_0 = 2(N + \ell + 1)$ . Note degeneracy.

Upshot: Find that the radial equation gives  $E_n = -\frac{1}{2}mc^2 Z^2 \alpha^2 / n^2$  where  $n = N + \ell + 1$ , with  $N = 0, 1, 2, \dots$ , i.e.  $\ell = 0, 1, \dots, n-1$ . The degeneracy for fixed  $n$  is  $\sum_{\ell=0}^{n-1} (2\ell+1) = n^2$ . Taking  $a_0 \equiv \hbar^2/me^2$ , (with  $F$  a Hypergeometric function)

$$R_{n,\ell}(r) \propto r^\ell e^{-Zr/na_0} F(-n + \ell + 1; 2\ell + 2; 2Zr/na_0).$$