Physics 115B, Mastery Questions for Section 2 Spring 22

Our goal for today is to build up our intuition for the hydrogen atom, including solutions in spherical coordinates.

The following equations may be useful in solving the problems below.

$$E_n = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2} = -\frac{\mathcal{R}}{n^2} \tag{1}$$

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)Y_\ell^m(\theta,\phi) \tag{2}$$

$$\int_0^{2\pi}\int_0^{\pi}[Y_\ell^m(\theta,\phi)]^*[Y_{\ell'}^{m'}(\theta,\phi)]\sin\theta d\theta d\phi = \delta_{\ell\ell'}\delta_{mm'} \tag{3}$$

$$Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2}, Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta, Y_1^{\pm 1} = \pm\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta e^{\pm i\phi} \tag{4}$$

1. The unit vector $\hat{\mathbf{a}}$ is defined as the vector of unit norm which points in the direction of increasing a. The Cartesian unit vectors $\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}$ are constant; x, y, z always increase in the same direction. In spherical coordinates, however, the unit vectors $\hat{\mathbf{r}}, \hat{\theta}, \hat{\phi}$ depend on the position at which one evaluates them. In general, one can compute a unit vector $\hat{\mathbf{a}}$ by first taking the derivative of the position vector and then normalizing:

$$\hat{\mathbf{a}} = \frac{\partial\vec{r}/\partial a}{|\partial\vec{r}/\partial a|} \tag{5}$$

   In order to become more acquainted with spherical coordinates, use this process to calculate a spherical coordinate unit vector (say $\hat{\theta}$ for definiteness) in terms of Cartesian unit vectors. That is, your answer should take the form

$$f(r,\theta,\phi)\hat{\mathbf{x}} + g(r,\theta,\phi)\hat{\mathbf{y}} + h(r,\theta,\phi)\hat{\mathbf{z}}$$

   for some functions f, g, h which you are to find. Hint: start with the general Cartesian form of the position vector $\vec{r}$, not the spherical form. (Why?) Second hint: make sure to think before you start calculating so you don't do more algebra than necessary.

2. (a) What are the possible values of each of the n, ℓ, m quantum numbers for the hydrogen atom?

   (b) For orbitals sharing the same energy, how many of them share the same quantum number ℓ (angular momentum)? What is the degeneracy of a given hydrogen atom energy level?

3. (a) Recall that, in spherical coordinates, $z = r\cos\theta$. Re-express z in terms of spherical harmonics (it may be useful to define a constant b to contain all of the prefactor constants).

   (b) Considering any of the $\psi_{n\ell m}$, explain why it must be that $\langle z \rangle = 0$.

   (c) Consider the states ψ_{100} and ψ_{210}. From the previous part, we know that $\langle z \rangle = 0$ for both of these states. Now consider the linear combination $\frac{1}{\sqrt{2}}(\psi_{100} + \psi_{210})$. Is $\langle z \rangle$ zero or non-zero?

   (d) The difference between x and z is just a choice we make about how to orient our axes and not any physics content. Consider the states $\psi_{100}, \psi_{210}, \psi_{21\pm1}$. What linear combination of states will have the expectation value of x be the same as the expectation value of z in the state $\frac{1}{\sqrt{2}}(\psi_{100} + \psi_{210})$? You should not need to calculate the exact values of $\langle x \rangle$ and $\langle z \rangle$.