5. *Quantum Mechanics* (Spring 2005)

An electron moves in a hydrogen atom potential – ignoring spin and relativity – in a state $|\psi\rangle$ that has the wave function

$$\psi(r,\theta,\phi) = NR_{21}(r)\left[2iY_1^{-1}(\theta,\phi) + (2+i)Y_1^0(\theta,\phi) + 3iY_1^1(\theta,\phi)\right]$$

where the $Y_l^m(\theta,\phi)$ are the spherical harmonics, $R_{nl}(r)$ are the normalized hydrogen atom wave functions, and N is a positive real number.

(a) Calculate N.

(b) What is the expectation value of L_z? ($\hbar\mathbf{L} = \mathbf{r}\times\mathbf{p}$)

(c) What is the expectation value of $\mathbf{L}^2$?

(d) What is the expectation value of the kinetic energy in terms of $\hbar, c$, the electron charge e or the fine-structure constant α, and the electron mass m?

Note: The explicit forms of the functions that appear in $\psi(r,\theta,\phi)$ above are

$$R_{21}(r) = \frac{1}{2\sqrt{6}}\frac{r}{a^{5/2}}e^{-r/2a} \quad Y_1^{\pm1}(\theta,\phi) = \mp\sqrt{\frac{3}{8\pi}}\sin(\theta)e^{\pm i\phi} \quad Y_1^0(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos(\theta)$$

a. By normalization, $1 = \langle\psi|\psi\rangle = \int_{-\infty}^{\infty}\int \psi^*(r,\theta,\phi)\psi(r,\theta,\phi)r^2dr\,d\Omega$

$= |N|^2\int_0^\infty R_{21}^*(r)R_{21}(r)r^2dr\,(4+5+9)$ since $\int (Y_{\ell'}^{m'})^* Y_\ell^m d\Omega = \delta_{\ell\ell'}\delta_{mm'}$

$= 18|N|^2\int_0^\infty \frac{1}{24}\frac{r^4}{a^5}e^{-r/a}dr$

$= \frac{3}{4}|N|^2a^{-5}(a^5\,4!) = 18|N|^2 \Rightarrow N = \frac{1}{\sqrt{18}}$ up to a phase

b. $|\psi\rangle = \frac{2i}{\sqrt{18}}|21\,{-1}\rangle + \frac{2+i}{\sqrt{18}}|2\,1\,0\rangle + \frac{3i}{\sqrt{18}}|2\,1\,1\rangle$

and $L_z|n\ell m\rangle = \hbar m|n\ell m\rangle$

$\Rightarrow \langle\psi|L_z|\psi\rangle = \frac{4}{18}\langle 21{-1}|L_z|21{-1}\rangle + \frac{5}{18}\langle 210|L_z|210\rangle$

$+ \frac{9}{18}\langle 211|L_z|211\rangle = -\frac{4}{18}\hbar + \frac{9}{18}\hbar = \frac{5}{18}\hbar$

c. $L^2|n\ell m\rangle = \hbar^2\ell(\ell+1)|n\ell m\rangle$

$\Rightarrow \langle\psi|L^2|\psi\rangle = \frac{4}{18}\langle 21{-1}|L^2|21{-1}\rangle + \frac{5}{18}\langle 210|L^2|210\rangle$

$+ \frac{9}{18}\langle 211|L^2|211\rangle = \frac{8}{18}\hbar^2 + \frac{10}{18}\hbar^2 + \frac{18}{18}\hbar^2 = 2\hbar^2$

d. We know the total energy because this is a Hydrogen atom in an $n=2$ energy eigenstate, so $E = -\frac{me^4}{2\hbar^2(2)^2} = -\frac{me^4}{8\hbar^2}$

So we can use the virial theorem to get the Kinetic energy

$\langle T\rangle = -\langle E\rangle = \frac{me^4}{8\hbar^2}$