Central Forces Homework 10

Due 6/8/18, 4 pm

Sensemaking: For every problem, before you start the problem, make a brief statement of the form that a correct solution should have, clearly indicating what quantities you need to solve for. This statement will be graded.

PRACTICE:

1. (McIntyre 8.6) Calculate the probability that the electron is measured to be within one Bohr radius of the nucleus for the $n = 2$ states of hydrogen. Discuss the differences between the results for the $l = 0$ and $l = 1$ states.

8.6 The probability is the integral over a sphere of radius a_0:

$$\mathcal{P}_{r\le a_0} = \int_{sphere\ r\le a_0} \mathcal{P}(r,\theta,\phi)\,dV = \int_0^{a_0}\int_0^{2\pi}\int_0^{\pi}\left|R_{n\ell}(r)Y_\ell^m(\theta,\phi)\right|^2 r^2\sin\theta\, d\theta\, d\phi\, dr$$

The angular integral is unity, leaving just the radial integral. For the 2s state we get

$$\mathcal{P}_{r\le a_0} = \int_0^{a_0} r^2\left|R_{n\ell}(r)\right|^2 dr = \int_0^{a_0} r^2\left|2\left(\frac{1}{2a_0}\right)^{3/2}\left[1-\frac{r}{2a_0}\right]e^{-r/2a_0}\right|^2 dr$$

$$= 4\left(\frac{1}{2a_0}\right)^3\int_0^{a_0} r^2\left[1-\frac{r}{a_0}+\frac{r^2}{4a_0^2}\right]e^{-r/a_0}\,dr = \frac{1}{2}\int_0^1 x^2\left[1-x+\frac{x^2}{4}\right]e^{-x}\,dx$$

$$= 1-\frac{21}{8e} \cong 0.0343$$

For the 2p state we get

$$\mathcal{P}_{r\le a_0} = \int_0^{a_0} r^2\left|\frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{3/2}\frac{r}{a_0}e^{-r/2a_0}\right|^2 dr$$

$$= \frac{1}{3}\left(\frac{1}{2a_0}\right)^3\int_0^{a_0} r^2\left[\frac{r^2}{a_0^2}\right]e^{-r/a_0}\,dr = \frac{1}{24}\int_0^1 x^4e^{-x}\,dx = 1-\frac{65}{24e} \cong 0.00366$$

The 2p state is pushed farther from the origin by the centrifugal barrier (see Fig. 8.4). Only s states have a nonzero probability of being found at the origin.

2. Consider the initial state $\frac{1}{\sqrt{2}}(|1,0,0\rangle + |2,1,0\rangle)$. Note, this is **not** an *sp* hybrid orbital such as occurs in chemistry in the study of molecular bonding.

   (a) If you measure the energy of this state, what possible values could you obtain?
   Solution:

   The only possible results of a quantum measurement are the eigenvalues of the operator corresponding to the quantity that is measured. The results of a measurement of energy will yield the energy eigenvalues which depend on the principle quantum number n.

$$E_n = \frac{E_1}{n^2}$$

   In this case, There are two different values of n that contribute to Ψ, $n = 1$ and $n = 2$. Therefore the values of the energy that can be measured are:

$$E_1 = -13.6eV. \tag{1}$$

$$E_2 = \frac{E_1}{4} \tag{2}$$

   (b) What is this state as a function of time?
   Solution:

   This state is made up of two eigenfunctions of the Hamiltonian for the hydrogen atom, with principle quantum numbers $n = 1$ and $n = 2$. This means that the energy of these two eigenstates are different (remember, the energy only depends on the principle quantum number, not ℓ or m) so we must introduce different phase factors for each eigenstate.

$$\begin{array}{ll} e^{-\frac{iE_1}{\hbar}t} & \text{for } n = 1 \\ e^{-\frac{iE_2}{\hbar}t} = e^{-\frac{iE_1}{4\hbar}t} & \text{for } n = 2 \end{array}$$

$$|\Psi(t)\rangle = \left(\frac{1}{\sqrt{2}}\right)\left(|1,0,0\rangle e^{-\frac{iE_1}{\hbar}t} + |2,1,0\rangle e^{-\frac{iE_1}{4\hbar}t}\right)$$

   (c) Calculate the expectation value $\langle \hat{L}^2 \rangle$ in this state, as a function of time. Did you expect this answer? Comment.
   Solution:

$$\begin{aligned} \hat{L}^2|n,\ell,m\rangle &= \ell(\ell+1)\hbar^2|n,\ell,m\rangle \\ &\Rightarrow L^2|n,0,m\rangle = 0\hbar^2|n,0,m\rangle \\ &\Rightarrow L^2|n,1,m\rangle = 2\hbar^2|n,1,m\rangle \end{aligned}$$

$$
\begin{aligned}
\langle \hat{L}^2 \rangle &= \langle \Psi(t) | \hat{L}^2 | \Psi(t) \rangle \\
&= \frac{1}{\sqrt{2}} \Big(\langle 1,0,0| e^{\frac{iE_1}{\hbar}t} + \langle 2,1,0| e^{\frac{iE_1}{4\hbar}t} \Big) \ \hat{L}^2 \ \frac{1}{\sqrt{2}} \Big(|1,0,0\rangle e^{-\frac{iE_1}{\hbar}t} + |2,1,0\rangle e^{-\frac{iE_1}{4\hbar}t} \Big) \\
&= \frac{1}{2} \Big(\langle 1,0,0| \hat{L}^2 |1,0,0\rangle + \langle 1,0,0| \hat{L}^2 |2,1,0\rangle e^{\frac{iE_1}{\hbar}t} e^{-\frac{iE_1}{4\hbar}t} \\
&\quad + \langle 2,1,0| \hat{L}^2 |1,0,0\rangle e^{\frac{iE_1}{4\hbar}t} e^{-\frac{iE_1}{\hbar}t} + \langle 2,1,0| \hat{L}^2 |2,1,0\rangle \Big) \\
&= \frac{1}{2} \Big(\langle 1,0,0| 0\hbar^2 |1,0,0\rangle + \langle 1,0,0| 2\hbar^2 |2,1,0\rangle e^{\frac{iE_1}{\hbar}t} e^{-\frac{iE_1}{4\hbar}t} \\
&\quad + \langle 2,1,0| 0\hbar^2 |1,0,0\rangle e^{\frac{iE_1}{4\hbar}t} e^{-\frac{iE_1}{\hbar}t} + \langle 2,1,0| 2\hbar^2 |2,1,0\rangle \Big) \\
&= \frac{1}{2} \, 2\hbar^2 \Big(\langle 1,0,0|2,1,0\rangle e^{\frac{iE_1}{\hbar}t} e^{-\frac{iE_1}{4\hbar}t} + \langle 2,1,0|2,1,0\rangle \Big) \\
\langle \hat{L}^2 \rangle &= \hbar^2
\end{aligned}
$$

Notice that the time-dependence does not all disappear until the second to the last line. The expectation value of $\hat{L}^2$ is time-independent, which is expected because this operator commutes with the Hamiltonian. The expectation value is also the average between the two possible values of the square of the angular momentum, which follows from the fact that the probability amplitudes for each term in this case happen to be the same.

(d) Write the time-dependent state in wave function notation.

Solution:

The solutions of the hydrogen atom can generally be written as follows:

$$|n, l, m\rangle = R_{nl}(r) \, Y_l^m(\theta, \phi)$$

The specific states we're interested in:

$$
\begin{aligned}
|1,0,0\rangle &= R_{10}(r) \, Y_0^0(\theta, \phi) \\
&= 2 \, a^{-\frac{3}{2}} \, e^{-\frac{r}{a}} \sqrt{\frac{1}{4\pi}} \\
&= \sqrt{\frac{1}{\pi a^3}} \, e^{-\frac{r}{a}} \\
|2,1,0\rangle &= R_{2,1}(r) \, Y_1^0(\theta, \phi)
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{1}{\sqrt{24}}\, a^{-\frac{3}{2}}\, e^{-\frac{r}{2a}} \left(\frac{r}{a}\right) \sqrt{\frac{3}{4\pi}} \cos\theta \\
&= \sqrt{\left(\frac{1}{32\pi a^3}\right)} \left(\frac{r}{a}\right) e^{-\frac{r}{2a}} \cos\theta
\end{aligned}
$$

The eigenstates have different time-dependent phase factors: $e^{-\frac{iE_1}{\hbar}t}$ and $e^{-\frac{iE_1}{4\hbar}t}$, respectively.

Putting these results together, we see that state in the position representation, i.e. the wave function, is given by:

$$
\Psi(t) = \sqrt{\frac{1}{\pi a^3}} \left[\frac{1}{\sqrt{2}} e^{-\frac{r}{a}}\, e^{-\frac{iE_1}{\hbar}t} + \frac{r}{8a} \cos\theta e^{-\frac{r}{2a}}\, e^{-\frac{iE_1}{4\hbar}t} \right]
$$

(e) Calculate the expectation value $\langle \hat{z} \rangle$ as a function of time. Do you expect this answer?

Solution:

Here, it is impossible to use the ket notation for calculating the expectation vale of $\hat{z}$ because the $\hat{z}$ does not commute with the Hamiltonian and therefore the eigenstates $|n\ell m\rangle$ are not eigenstates of $\hat{z}$. Remember that $\hat{z} = r\cos\theta$.

$$
\begin{aligned}
\langle \hat{z} \rangle &= \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \int_{r=0}^{\infty} \Psi(t)^*\ \hat{z}\ \Psi(t)\ r^2 \sin\theta\, dr\, d\theta\, d\phi \\
&= \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \int_{r=0}^{\infty} \Psi(t)^*\ r\cos\theta\ \Psi(t)\ r^2 \sin\theta\, dr\, d\theta\, d\phi \\
&= \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \int_{r=0}^{\infty} \left(\frac{1}{\pi a^3}\right) \left| \frac{1}{\sqrt{2}} e^{-\frac{r}{a}}\, e^{-\frac{iE_1}{\hbar}t} + \frac{r}{8a} \cos\theta e^{-\frac{r}{2a}}\, e^{-\frac{iE_1}{4\hbar}t} \right|^2 \\
&\quad \times r\cos\theta\ \ r^2 \sin\theta\, dr\, d\theta\, d\phi \\
&= \left(\frac{1}{\pi a^3}\right) \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \int_{r=0}^{a} \left[\frac{1}{2} e^{-\frac{2r}{a}} + \frac{r^2}{64a^2} \cos^2\theta e^{-\frac{r}{a}} + \frac{r}{4\sqrt{2}a} \cos\theta e^{-\frac{3r}{2a}} \cos\frac{3E_1}{4\hbar}t \right] \\
&\quad \times r^3 \sin\theta \cos\theta\, dr\, d\theta\, d\phi
\end{aligned}
$$

Use the computer to evaluate the integrals. The θ integrals in the first two terms give zero. The last term yields:

$$
\begin{aligned}
\langle \hat{z} \rangle &= \left(\frac{1}{\pi a^3}\right) 2\pi \left(\frac{128a^4}{243\sqrt{2}} \cos\frac{3E_1}{4\hbar}t \right) \\
&= \frac{256a}{243\sqrt{2}} \cos\frac{3E_1}{4\hbar}t
\end{aligned}
$$

Note the expected time dependence with a frequency that depends on the energy difference between the two energy eigenstates. Note also that the expectation value of $\hat{z}$ is proportional to the Bohr radius a, i.e. it has dimensions of length, as expected.

3. Complete the attached table for the hydrogen atom.

Hydrogen Atom

	Ket Representation	Wave Function Representation	Matrix Representation
Hamiltonian	$\hat{H}$	$\hat{H} \doteq -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r}$ $\doteq -\frac{\hbar^2}{2\mu}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{\hbar^2 r^2}L^2\right) - \frac{e^2}{4\pi\epsilon_0 r}$	$H \doteq \begin{pmatrix} E_{100} & 0 & 0 & 0 & 0 & \cdots \\ 0 & E_{200} & 0 & 0 & 0 & \cdots \\ 0 & 0 & E_{211} & 0 & 0 & \cdots \\ 0 & 0 & 0 & E_{210} & 0 & \cdots \\ 0 & 0 & 0 & 0 & E_{21,-1} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} = -13.6eV \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \cdots \\ 0 & \frac{1}{4} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \frac{1}{4} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \frac{1}{4} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \frac{1}{4} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$
Eigenvalues of Hamiltonian	$E_n = -\frac{1}{2n^2}\frac{e^2}{4\pi\varepsilon_0 a_0} = -13.6eV\frac{1}{n^2}$	$E_n = -\frac{1}{2n^2}\frac{e^2}{4\pi\varepsilon_0 a_0} = -13.6eV\frac{1}{n^2}$	$E_n = -\frac{1}{2n^2}\frac{e^2}{4\pi\varepsilon_0 a_0} = -13.6eV\frac{1}{n^2}$
Normalized Eigenstates of Hamiltonian	$\lvert n\ell m\rangle$	$R_{n\ell}(r)Y_\ell^m(\theta,\phi)$ $= -\sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n\left((n+\ell)!\right)^3}} \left(\frac{2r}{na_0}\right)^\ell e^{\frac{-r}{na_0}} L_{n+\ell}^{2\ell+1}\left(\frac{2r}{na_0}\right) Y_\ell^m(\theta,\phi)$	$\lvert 100\rangle \doteq \begin{pmatrix}1\\0\\0\\0\\\vdots\end{pmatrix}, \lvert 200\rangle \doteq \begin{pmatrix}0\\1\\0\\0\\\vdots\end{pmatrix}, \lvert 211\rangle \doteq \begin{pmatrix}0\\0\\1\\0\\\vdots\end{pmatrix}, \lvert 210\rangle \doteq \begin{pmatrix}0\\0\\0\\1\\\vdots\end{pmatrix}, \ \ldots$
Coefficient of the energy eigenstate with quantum numbers n, ℓ, m	$c_{n\ell m} = \langle n\ell m \vert \psi\rangle$	$c_{n\ell m} = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} R_{n\ell}^*(r)Y_\ell^{m*}(\theta,\phi)\psi(r,\theta,\phi)r^2\sin\theta\, dr\, d\theta\, d\phi$	$c_{n\ell m} = \begin{pmatrix} \cdots & 1 & \cdots \end{pmatrix}\begin{pmatrix}\vdots \\ c_{n\ell m} \\ \vdots\end{pmatrix}$
Probability of measuring E_n	$\mathcal{P}_{E_n} = \sum_{\ell=0}^{n-1}\sum_{m=-\ell}^{\ell}\left\lvert\langle n\ell m\vert\psi\rangle\right\rvert^2$ $= \sum_{\ell=0}^{n-1}\sum_{m=-\ell}^{\ell}\left\lvert c_{n\ell m}\right\rvert^2$	$\mathcal{P}_{E_n} = \sum_{\ell=0}^{n-1}\sum_{m=-\ell}^{\ell}\left\lvert\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} R_{n\ell}^*(r)Y_\ell^{m*}(\theta,\phi)\psi(r,\theta,\phi)r^2\sin\theta\, dr\, d\theta\, d\phi\right\rvert^2$	$\mathcal{P}_{E_n} = \sum_{\ell=0}^{n-1}\sum_{m=-\ell}^{\ell}\left\lvert\begin{pmatrix} \cdots & 1 & \cdots \end{pmatrix}\begin{pmatrix}\vdots \\ c_{n\ell m} \\ \vdots\end{pmatrix}\right\rvert^2$

Hydrogen Atom

	Ket Representation	Wave Function Representation	Matrix Representation
Operator for square of the angular momentum	L^2	$L^2 \doteq -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{d^2}{d\phi^2}\right)$ $\doteq -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\hbar^2\sin^2\theta}L_z^2\right)$	$L^2 \doteq \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 2\hbar^2 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 2\hbar^2 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 2\hbar^2 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$
Eigenvalues of L^2	$\hbar^2\ell(\ell+1)$	$\hbar^2\ell(\ell+1)$	$\hbar^2\ell(\ell+1)$
Normalized Eigenstates of L^2	$\lvert n\ell m\rangle$	$R_{n\ell}(r)Y_\ell^m(\theta,\phi)$ $= -\sqrt{\left(\frac{2}{na_0}\right)^3\frac{(n-\ell-1)!}{2n((n+\ell)!)^3}}\left(\frac{2r}{na_0}\right)^\ell e^{\frac{-r}{na_0}}L_{n+\ell}^{2\ell+1}\left(\frac{2r}{na_0}\right)Y_\ell^m(\theta,\phi)$	$\lvert 100\rangle \doteq \begin{pmatrix}1\\0\\0\\0\\\vdots\end{pmatrix}, \lvert 200\rangle \doteq \begin{pmatrix}0\\1\\0\\0\\\vdots\end{pmatrix}, \lvert 211\rangle \doteq \begin{pmatrix}0\\0\\1\\0\\\vdots\end{pmatrix}, \lvert 210\rangle \doteq \begin{pmatrix}0\\0\\0\\1\\\vdots\end{pmatrix},$
Coefficient of the eigenstates of L^2 with quantum numbers n,ℓ,m	$c_{n\ell m} = \langle n\ell m \vert \psi\rangle$	$c_{n\ell m} = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} R_{n\ell}^*(r)Y_\ell^{m*}(\theta,\phi)\psi(r,\theta,\phi)r^2\sin\theta\,dr\,d\theta\,d\phi$	$c_{n\ell m} = \begin{pmatrix}\cdots & 1 & \cdots\end{pmatrix}\begin{pmatrix}\vdots\\ c_{n\ell m}\\ \vdots\end{pmatrix}$
Probability of measuring $\hbar^2\ell(\ell+1)$ for the square of the angular momentum	$\mathcal{P}_\ell = \sum_{n=\ell+1}^{\infty}\sum_{m=-\ell}^{\ell}\lvert\langle n\ell m\vert\psi\rangle\rvert^2$ $= \sum_{n=\ell+1}^{\infty}\sum_{m=-\ell}^{\ell}\lvert c_{n\ell m}\rvert^2$	$\mathcal{P}_\ell = \sum_{n=\ell+1}^{\infty}\sum_{m=-\ell}^{\ell}\left\lvert\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} R_{n\ell}^*(r)Y_\ell^{m*}(\theta,\phi)\psi(r,\theta,\phi)r^2\sin\theta\,dr\,d\theta\,d\phi\right\rvert^2$	$\mathcal{P}_\ell = \sum_{n=\ell+1}^{\infty}\sum_{m=-\ell}^{\ell}\left\lvert\begin{pmatrix}\cdots & 1 & \cdots\end{pmatrix}\begin{pmatrix}\vdots\\ c_{n\ell m}\\ \vdots\end{pmatrix}\right\rvert^2$

Hydrogen Atom

	Ket Representation	Wave Function Representation	Matrix Representation
Operator for z-component of angular momentum	L_z	$L_z \doteq -i\hbar \frac{\partial}{\partial \phi}$	$L_z \doteq \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & \hbar & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & -\hbar & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$
Eigenstates of L_z	$m\hbar$	$m\hbar$	$m\hbar$
Normalized Eigenstates of L_z	$\lvert n\ell m\rangle$	$R_{n\ell}(r)Y_\ell^m(\theta,\phi)$ $= -\sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n((n+\ell)!)^3}} \left(\frac{2r}{na_0}\right)^\ell e^{\frac{-r}{na_0}} L_{n+\ell}^{2\ell+1}\left(\frac{2r}{na_0}\right) Y_\ell^m(\theta,\phi)$	$\lvert 100\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \lvert 200\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \lvert 211\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}, \lvert 210\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix},$
Coefficient of m^{th} eigenstates of L_z	$c_{n\ell m} = \langle n\ell m \vert \psi\rangle$	$c_{n\ell m} = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} R_{n\ell}^*(r)Y_\ell^{m*}(\theta,\phi)\psi(r,\theta,\phi) r^2 \sin\theta \, dr\, d\theta\, d\phi$	$c_{n\ell m} = \begin{pmatrix} \cdots & 1 & \cdots \end{pmatrix} \begin{pmatrix} \vdots \\ c_{n\ell m} \\ \vdots \end{pmatrix}$
Probability of measuring $m\hbar$ for z-component of angular momentum	$\mathcal{P}_m = \sum_{n=\lvert m\rvert+1}^{\infty} \sum_{\ell=\lvert m\rvert}^{\infty} \lvert\langle n\ell m \vert \psi\rangle\rvert^2$ $= \sum_{n=\lvert m\rvert+1}^{\infty} \sum_{\ell=\lvert m\rvert}^{\infty} \lvert c_{n\ell m}\rvert^2$	$\mathcal{P}_m = \sum_{n=\lvert m\rvert+1}^{\infty} \sum_{\ell=\lvert m\rvert}^{\infty} \left\lvert \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} R_{n\ell}^*(r)Y_\ell^{m*}(\theta,\phi)\psi(r,\theta,\phi) r^2 \sin\theta \, dr\, d\theta\, d\phi \right\rvert^2$	$\mathcal{P}_m = \sum_{n=\lvert m\rvert+1}^{\infty} \sum_{\ell=\lvert m\rvert}^{\infty} \left\lvert \begin{pmatrix} \cdots & 1 & \cdots \end{pmatrix} \begin{pmatrix} \vdots \\ c_{n\ell m} \\ \vdots \end{pmatrix} \right\rvert^2$

REQUIRED:

4. McIntyre 8.14

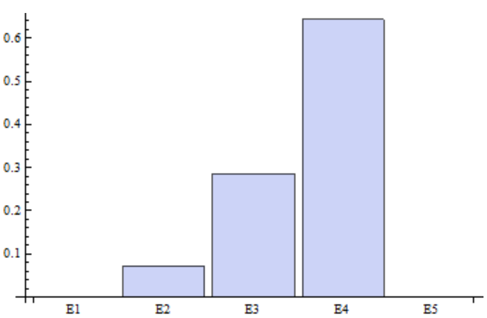
   A hydrogen atom is initially in the superposition state
   $|\psi(0)\rangle = \frac{1}{\sqrt{14}}|2,1,1\rangle - \frac{2}{\sqrt{14}}|3,2,-1\rangle + \frac{3}{\sqrt{14}}|4,2,2\rangle$.

   (a) What are the possible results of a measurement of the energy and with what probabilities would they occur? Plot a histogram of the measurement results. Calculate the expectation value of the energy. **Solution:**

   The form of our answer should be a list of values for the quantity of interest (E, L^2, L_z) and the corresponding probabilities, which can also be presented in graphical form.

   The possible results of a measurement of energy correspond to the values of n represented in the superposition. These are $n = 2, 3, 4$, where $E_n = -13.6eV/n^2$ The probabilities are found by taking appropriate inner products that collapse to the coefficients of the relevant terms, followed by taking the modulus square.

$$\wp_{E_2} = 1/14$$
$$\wp_{E_3} = 4/14$$
$$\wp_{E_4} = 9/14$$

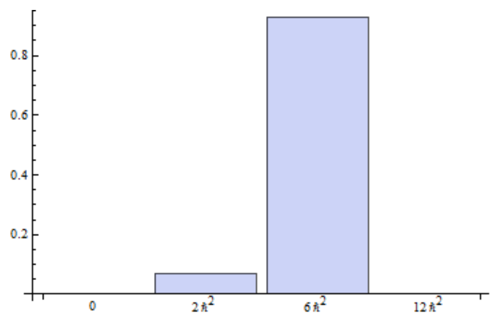


   The expectation value is the weighted average of the eigenvalues, which for this system gives:
   $\langle E\rangle = -13.6eV(1/14(1/4) + 4/14(1/9) + 9/14(1/16) = -13.6eV(181/144)$

   (b) What are the possible results of a measurement of the angular momentum operator L^2 and with what probabilities would they occur? Plot a histogram of the measurement results. Calculate the expectation value of L^2. **Solution:**

   The possible results of a measurement of L^2 correspond to the values of ℓ represented in the superposition. These are $\ell = 1, 2$, where $L^2 = \hbar^2\ell(\ell+1)$ The probabilities are found by taking appropriate inner products that collapse to the coefficients of the relevant terms, followed by taking the modulus square. Because the superposition contains more than one term with the same value of ℓ, it is necessary to sum probabilities corresponding to degenerate states.

$$\wp_{2\hbar^2} = 1/14$$
$$\wp_{6\hbar^2} = 13/14$$



The expectation value is the weighted average of the eigenvalues, which for this system gives:
$\langle L^2\rangle = 1/14(2\hbar^2) + 13/14(6\hbar^2) = 40\hbar^2/7$

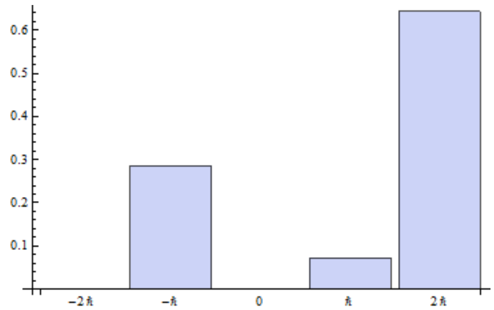
(c) What are the possible results of a measurement of the angular momentum component operator L_z and with what probabilities would they occur? Plot a histogram of the measurement results. Calculate the expectation value of L_z. **Solution:**

The possible results of a measurement of L_z correspond to the values of m represented in the superposition. These are $m = -1, 1, 2$, where $L_z = \hbar m$ The probabilities are found by taking appropriate inner products that collapse to the coefficients of the relevant terms, followed by taking the modulus square.

$$\wp_{-\hbar} = 4/14$$
$$\wp_{\hbar} = 1/14$$
$$\wp_{2\hbar} = 9/14$$

The expectation value is the weighted average of the eigenvalues, which for this system gives:
$\langle L_z\rangle = 5/14(-\hbar) + 1/14\hbar + 9/14(3\hbar) = 23\hbar/14$

5. (McIntyre 8.7) Calculate the probability that the electron is measured to be in the classically forbidden region for the $n = 2$ states of hydrogen. Discuss the differences between the results for the $l = 0$ and $l = 1$ states.



Solution:

The form of our answer should be a probability (a number between zero and one) calculated for each of the four $n = 2$ states of hydrogen. Note that all numerical estimates in this problem are very rough approximations, with radii in terms of a_0, the Bohr radius.

First, we must identify the classical turning points for each case. For $\ell = 0$, there is no angular contribution to the effective potential, so there is only one classical turning point, when the total energy is equal to the potential energy. Since we have $n = 2$, $E_2 = -13.6/4 = -3.4eV$.

$-\frac{e^2}{4\pi\epsilon_0 r_{ctp}} = -3.4eV$ gives $r_{ctp} \approx 8a_0$

For $\ell = 1$, there are two classical turning points (regardless of m value, since the effective potential depends only on ℓ), described by:

$-\frac{e^2}{4\pi\epsilon_0 r} + \hbar^2\ell(\ell+1)/(2mr^2) = -3.4eV$ gives $r_1 \approx a_0$ and $r_2 \approx 6.5a_0$

We can also restrict our integral to covering only the radial wave functions and the radial coordinate, as the angular integrals will cover all angular space over normalized functions of θ and ϕ, which automatically yield 1.

$P(n = 2, l = 0) = \int_{r_{ctp}}^{\infty} |R_2^0(r)|^2 r^2 dr \approx 0.19$

$P(n = 2, l = 1) = \int_0^{r_1} |R_2^1(r)|^2 r^2 dr + \int_{r_2}^{\infty} |R_2^1(r)|^2 r^2 dr \approx 0.23$