Physics 4310 Homework #8

3 problems

Solutions

▷ **1.**

Using the recursion relation for c_j, work out R_{30} and R_{31} for the hydrogen atom.

Answer:

To find the radial functions

$$R_{nl}(r) = \frac{1}{r}\rho^{l+1}e^{-\rho}v(\rho)$$

(where $\rho = r/an$) we need

$$v(\rho) = \sum_{j=0}^{\infty} c_j \rho^j$$

We're given the recursion relation

$$c_{j+1} = \frac{2(j+l+1-n)}{(j+1)(j+2l+2)}c_j$$

For $l = 0$, we have

$$c_1 = \frac{2(0+0+1-3)}{(0+1)(0+2(0)+2)}c_0 = \frac{-4}{2}c_0 = -2c_0$$

$$c_2 = \frac{2(1+0+1-3)}{(1+1)(1+2(0)+2)}c_1 = \frac{-2}{2(3)}(-2c_0) = \frac{2}{3}c_0$$

$$c_3 = \frac{2(2+0+1-3)}{(2+1)(2+2(0)+2)}c_2 = 0$$

and so

$$R_{30}(r) = c_0\frac{1}{r}\left(\frac{r}{3a}\right)e^{-r/3a}\left[1 - 2\left(\frac{r}{3a}\right) + \frac{2}{3}\left(\frac{r}{3a}\right)^2\right]$$

or, to simplify a little,

$$R_{30}(r) = Ce^{-r/3a}\left[1 - 2\left(\frac{r}{3a}\right) + \frac{2}{3}\left(\frac{r}{3a}\right)^2\right]$$

where C is a normalization constant.

For $l = 1$, we have

$$c_1 = \frac{2(0+1+1-3)}{(0+1)(0+2(1)+2)} c_0 = \frac{-2}{4} c_0 = -\frac{1}{2} c_0$$
$$c_2 = \frac{2(1+1+1-3)}{(1+1)(1+2(1)+2)} c_1 = 0$$

and so

$$R_{31}(r) = c_0 \frac{1}{r} \left(\frac{r}{3a}\right)^2 e^{-r/3a} \left[1 - \frac{1}{2}\left(\frac{r}{3a}\right)\right]$$
$$= Cre^{-r/3a} \left[1 - \frac{r}{6a}\right]$$

▷ **2.**

For the following problems, feel free to use the tables in Griffiths; you don't need to work out ψ_{nlm}*. If you want to use Eq. 4.89 and are using Mathematica, note that Mathematica uses a different normalization convention, so*

$$L_a^b(x) = (a+b)!\, \texttt{LaGuerreL}(\texttt{a}, \texttt{b}, \texttt{x})$$

(a) Find $\langle r \rangle$ and $\langle r^2 \rangle$ for an electron in the ground state of hydrogen. Express your answers in terms of the Bohr radius.

(b) Find $\langle z \rangle$ and $\langle z^2 \rangle$ for an electron in the ground state of hydrogen. Hint: This requires no new integration— note that $r^2 = x^2 + y^2 + z^2$, and exploit the fact that the ground state is spherically symmetric.

(c) Find $\langle z^2 \rangle$ for an electron in the state $n = 2$, $l = 1$, and $m = 0$. Note that this state is *not* spherically symmetric, so we do need to integrate. Use $z = r\cos\theta$.

Answer:

We calculate the average of any Q as

$$\langle Q \rangle = \langle \psi | Q | \psi \rangle$$
$$= \int \psi^* Q \psi \, d\tau$$
$$= \int_0^{2\pi} \int_0^{\pi} \int_0^{\infty} R_{nl}(r) Y_{lm}^*(\theta, \phi) Q R_{nl}(r) Y_{lm}(\theta, \phi)\, r^2\, sin\theta \, dr \, d\theta \, d\phi$$

(I used the fact that the radial functions are all real.) Now to specifics:
(a) When we calculate the average $\langle r \rangle$ or $\langle r^2 \rangle$, we can separate the integrals into radial and angular components and exploit the normalization of the spherical harmonics:

$$\begin{aligned}\langle r \rangle &= \int_0^{2\pi} \int_0^{\pi} Y_{lm}^*(\theta, \phi) Y_{lm}(\theta, \phi)\, \sin\theta \, d\theta \, d\phi \int_0^{\infty} R_{nl}(r) r R_{nl}(r)\, r^2 \, dr \\ &= 1 \cdot \int_0^{\infty} r^3 R_{nl}^2(r)\, dr\end{aligned}$$

The ground state of hydrogen has $R_{10}(r) = 2a^{-3/2} e^{-r/a}$, so

$$\begin{aligned}\langle r \rangle &= \int_0^{\infty} r^3 \frac{4}{a^3} e^{-2r/a}\, dr \\ &= \int_0^{\infty} (\frac{1}{2} q a)^3 \frac{4}{a^3} e^{-q}\, (\frac{1}{2} a\, dq) \qquad (q = 2r/a) \\ &= \frac{4}{16} a \int_0^{\infty} q^3 e^{-q}\, dq \\ &= \frac{1}{4} a (3!) = \boxed{\frac{3}{2} a} \qquad \left(\int_0^{\infty} q^n e^{-q}\, dq = n! \right)\end{aligned}$$

Similarly,

$$\begin{aligned}\langle r^2 \rangle &= \int_0^{\infty} r^4 \frac{4}{a^3} e^{-2r/a}\, dr \\ &= \int_0^{\infty} (\frac{1}{2} q a)^4 \frac{4}{a^3} e^{-q}\, (\frac{1}{2} a\, dq) \qquad (q = r/a) \\ &= \frac{4}{32} a^2 \int_0^{\infty} q^4 e^{-q}\, dq \\ &= (4!) \frac{1}{8} a^2 = \boxed{3a^2}\end{aligned}$$

(b) Because the ground state is symmetric, x is going to positive as often as it is negative, so $\boxed{\langle x \rangle = 0}$. We can write $\langle r^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle$, but because of the spherical symmetry of the ground state all three of these terms should be identical. Therefore

$$\langle r^2 \rangle = 3 \langle x^2 \rangle \implies \langle x^2 \rangle = \frac{1}{3} \langle r^2 \rangle = \boxed{a^2}$$

(c) Here the average is

$$
\begin{aligned}
\langle z^2 \rangle &= \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} R_{nl}(r)Y^*_{lm}(\theta,\phi)r^2\cos^2\theta R_{nl}(r)Y_{lm}(\theta,\phi)\, r^2\, sin\theta\, dr\, d\theta\, d\phi \\
&= \int_0^{2\pi}\int_0^{\pi} Y^*_{10}(\theta,\phi)\cos^2\theta Y_{10}(\theta,\phi)\sin\theta\, d\theta\, d\phi \int_0^{\infty} R^2_{21}(r)r^4\, dr \\
&= \int_0^{2\pi}\int_0^{\pi} \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta\cos^2\theta\left(\frac{3}{4\pi}\right)^{1/2}\cos\theta\sin\theta\, d\theta\, d\phi \int_0^{\infty}\frac{1}{24a^3}\frac{r^2}{a^2}e^{-r/a}r^4\, dr \\
&= \frac{3}{4\pi}\frac{1}{24a^5}\left[\int_0^{2\pi}\int_0^{\pi}\cos^4\theta\sin\theta\, d\theta\, d\phi\right]\left[\int_0^{\infty} r^6 e^{-r/a}\, dr\right] \\
&= \frac{3}{4\pi}\frac{1}{24a^5}2\pi\left[\int_0^{\pi}\cos^4\theta\sin\theta\, d\theta\right]\left[\int_0^{\infty} r^6 e^{-r/a}\, dr\right] \\
&= \frac{1}{2}\frac{1}{8a^5}\left[\frac{2}{5}\right]\left[720a^7\right] \\
&= \boxed{18a^2}
\end{aligned}
$$

▷ **3.**
Consider the equation

$$x^2 v'''(x) + x^2 v''(x) + v'(x) + \lambda v(x) = 0$$

(a) Using the power-law method we used for the hydrogen atom, write $v(x) = \sum_{j=0}^{\infty} c_j x^j$, and find a recursion relation for the coefficients c_j.
(b) What is the recursion relation when $j \gg 1$? Prove that $v(x) \approx e^x$ unless the series terminates.
(c) What has to be true about λ if the series terminates?

Answer:______________________________________

(a) Given that $v(x) = \sum_{j=0}^{\infty} c_j x^j$ we also have

$$v'(x) = \sum j c_j x^{j-1} \qquad v''(x) = \sum j(j-1)c_j x^{j-2} \qquad v'''(x) = \sum j(j-1)(j-2)c_j x^{j-3}$$

(All sums are from 0 to ∞ here.) Plugging this into the equation gives us

$$
\begin{aligned}
0 &= x^2 \sum_{j=0}^{\infty} j(j-1)(j-2)c_j x^{j-3} + x^2 \sum_{j=0}^{\infty} j(j-1)c_j x^{j-2} + \sum_{j=0}^{\infty} jc_j x^{j-1} + \lambda \sum_{j=0}^{\infty} c_j x^j \\
&= \sum_{j=0}^{\infty} j(j-1)(j-2)c_j x^{j-1} + \sum_{j=0}^{\infty} j(j-1)c_j x^j + \sum_{j=0}^{\infty} jc_j x^{j-1} + \lambda \sum_{j=0}^{\infty} c_j x^j \\
&= \sum_{j=-1}^{\infty} (j+1)j(j-1)c_{j+1} x^j + \sum_{j=0}^{\infty} j(j-1)c_j x^j + \sum_{j=-1}^{\infty} (j+1)c_{j+1} x^j + \lambda \sum_{j=0}^{\infty} c_j x^j
\end{aligned}
$$

where I adjusted the indices in the first and third sums so that all sums have x^j in them. The first and third sums now run from $j = -1$ to ∞, but in both cases the summand is zero when $j = -1$ (because of the $j + 1$ factor in each), so we can run those sums from $j = 0$ with no change in the final answer. Thus we can combine this into one giant sum:

$$
0 = \sum_{j=0}^{\infty} \left[(j+1)j(j-1)c_{j+1} + j(j-1)c_j + (j+1)c_{j+1} + \lambda c_j\right] x^j
$$

The long factor inside must be zero for this to be true for all values of x, so

$$
\begin{aligned}
0 &= (j+1)j(j-1)c_{j+1} + j(j-1)c_j + (j+1)c_{j+1} + \lambda c_j \\
\implies c_{j+1}\left[-(j+1)j(j-1) - (j+1)\right] &= \left[j(j-1) + \lambda\right] c_j \\
c_{j+1} &= -\frac{j(j-1) + \lambda}{j^3 + 1} c_j
\end{aligned}
$$

(b) If $j \gg 1$, then $c_{j+1} \approx \frac{1}{j} c_j$, which means that $c_j \approx \frac{1}{j!}$ and $v(x) \approx \sum_{j=0}^{\infty} \frac{1}{j!} x^j = e^x$. If this is impossible (if $v(x)$ is a wavefunction, for instance, and can't blow up), then the series must terminate before j gets big.

(c) For the series to terminate, we need that $\lambda = -j(j-1)$ for some integer $j = 0, 1, 2, \ldots$. For example, if $j = 2$, then $\lambda = -2(2-1) = -2$, then we have the differential equation

$$
x^2 v'''(x) + x^2 v''(x) + v'(x) - 2v(x) = 0
$$

The coefficients are

$$
\begin{aligned}
c_1 &= -\frac{0(0-1)-2}{0^3+1}c_0 = 2c_0 \\
c_2 &= -\frac{1(1-1)-2}{1^3+1}c_1 = \frac{2}{2}(2c_0) = 2c_0 \\
c_3 &= -\frac{2(2-1)-2}{2^3+1}c_2 = 0
\end{aligned}
$$

and so the solution is $v(x) = c_0\left[1 + 2x + 2x^2\right]$. Let's try it out with $c_0 = 1$:

$$
\begin{aligned}
&x^2 v'''(x) + x^2 v''(x) + v'(x) - 2v(x) \\
&= x^2(0) + x^2(4) + (2 + 4x) - 2(1 + 2x + 2x^2) \\
&= 4x^2 + 2 + 4x - 2 - 4x - 4x^2 = 0
\end{aligned}
$$

Hey it works!