PHSX 461: HW11

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Griffiths 4.12

Work out the radial wave functions of R_{31}, using the recursion formula. Don't bother to normalize them.

$$c_{j+1} = \frac{2(j+l+1-n)}{(j+1)(j+2l+2)} c_j \qquad \text{(Equation 4.76)}$$

$$R_{n,l} = \frac{1}{r}\rho^{l+1} e^{-r/a} V_n\left(\frac{r}{a}\right)$$

$$\Rightarrow R_{3,1} = \frac{1}{r}\left(\frac{r}{3a}\right)^2 \left[c_0 + c_1\left(\frac{r}{3a}\right) + c_2\left(\frac{r}{3a}\right)^2\right]$$

taking a quick break to calculate c's:

$$c_0 = c_0$$

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

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

Plugging these back in:

$$\boxed{R_{3,1} = \frac{c_0 r}{(3a)^2}\left[1 - \frac{1}{2}\left(\frac{r}{3a}\right)\right]}$$

Griffiths 4.15

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.*

$$\langle r \rangle \Rightarrow \langle \psi | r | \psi \rangle = \langle R_{10} | r | R_{10} \rangle = \int (4a^{-3} r \exp(-2r/a)) r^2 \, \mathrm{d}r$$

$$\boxed{\langle r \rangle = 0} \quad \text{(odd)}$$

$$\left\langle r^2 \right\rangle \Rightarrow \langle \psi | r^2 | \psi \rangle = \langle R_{10} | r^2 | R_{10} \rangle = \int_{-\infty}^{\infty} 4a^{-3} r^2 \exp(-er/a) r^2 \, \mathrm{d}r$$

$$= 8a^{-3} \int_0^{\infty} r^4 \exp(-er/a) \, \mathrm{d}r \quad \text{(even)}$$

By using an identity given in Griffiths

$$= 8a^{-3} \left(4! \left(\frac{a}{2} \right)^5 \right)$$

$$\boxed{\left\langle r^2 \right\rangle = 24a^2}$$

b) *Find $\langle x \rangle$ and $\langle x^2 \rangle$ for an electron in the ground state of hydrogen.*

There is no bias in the location for $n = 1$, so the expected r will be a symmetric sphere. Thus, $\boxed{\langle x \rangle = 0}$

We know that $\langle r^2 \rangle = \langle x^2 + y^2 + z^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle$. Since the spherical harmonic is symmetric in θ and ϕ for the $n = 1$ level, then all three components will be equal. Thus:

$$\left\langle r^2 \right\rangle = 3 \left\langle x^2 \right\rangle \to \boxed{\left\langle x^2 \right\rangle = 8a^2}$$

c) *Find $\langle x^2 \rangle$ in the state $n = 2, l = 1, m = 1$.* The quickest way for me to do with, was to just do it.

$$\left\langle x^2 \right\rangle = \langle \psi | x^2 | \psi \rangle = \langle \psi | (r \sin(\theta) \cos(\phi))^2 | \psi \rangle$$

since we are at $n = 2, l = 1, m = 1$, we can just read ψ out of the book.

$$R_{2,1} Y_1^1 = \left[\frac{1}{2\sqrt{6}} a^{-3/2} \left(\frac{r}{a} \right) \exp(-2r/a) \right] \left[- \left(\frac{3}{4\pi} \right)^{1/2} \cos\theta \right]$$

$$\langle x^2 \rangle = \int r^2 \frac{1}{2\sqrt{6}} a^{-3} \left(\frac{r}{a}\right) \exp(-r/a) r^2 \, \mathrm{d}r \cdot$$

$$\int -\left(\frac{3}{4\pi}\right) \cos^2\theta \sin^2\theta \cos^2\phi \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi$$

$$= \left(\frac{3}{4\pi}\right) \frac{1}{24} a^{-3} \left(\frac{1}{a^2}\right) \int r^6 \exp(-r/a) \, \mathrm{d}r \int \cos^2\theta \sin^3\theta cos^2\phi \, \mathrm{d}\theta \, \mathrm{d}\phi$$

$$= \frac{1}{32\pi} \left(\frac{1}{a^5}\right) (6!(a)^7) \int_0^\pi (\cos^2\theta - \cos^4\theta) \sin\theta \, \mathrm{d}\theta \int_0^{2\pi} \frac{1}{2}(1 + \cos 2\phi) \, \mathrm{d}\phi$$

$$= \frac{6!}{32\pi} a^2 \left[\frac{1}{3}\cos^3\theta - \frac{1}{5}\cos^5\theta\right] \Big|_0^\pi \left[\frac{1}{2}\phi + \frac{1}{4}\sin 2\phi\right] \Big|_0^{2\pi}$$

$$= \frac{6!}{32\pi} a^2 \left[\frac{4}{16}\right] \pi$$

$$= \frac{45}{8} a^2$$

$$\boxed{\langle x^2 \rangle = \frac{45}{8} x^2}$$

Griffiths 4.16

What is the most probably value of r, in the ground state of hydrogen?

$$\psi \propto R_{1,0} = 2a^{-3/2}\exp(-r/a)$$
$$P = \psi^*\psi \propto 4a^{-3}\exp(-r/a)r^2$$
$$P(r) = \psi^* r\psi \propto \frac{4}{a^3}r^3\exp(-r/a)$$

So, we need to take the derivative to find where that max is:

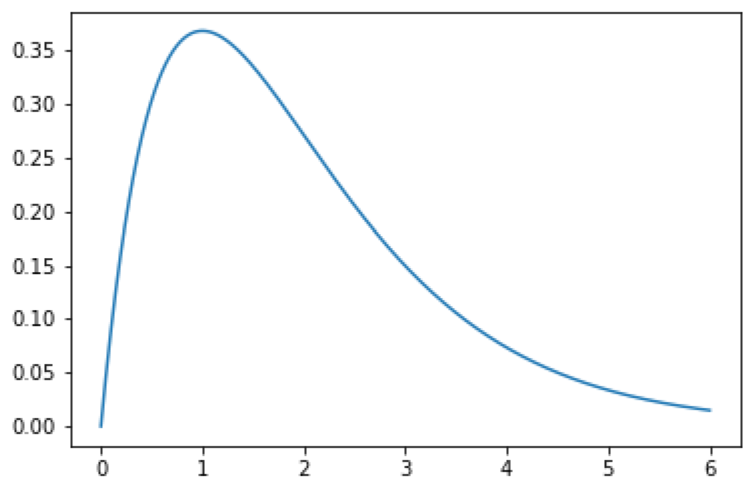

Figure 1: The graph for Question 4.16

$$3r^2\frac{4}{a^3}\exp(-r/a) - \frac{4}{a^3}\frac{r^3}{a}\exp(-r/a) = 0$$

$$\frac{12}{a^3} - \frac{4}{a^4}r = 0$$

$$3 - \frac{1}{a}r = 0$$

$$\boxed{r = 3a}$$

Griffiths 4.27

Two particles (masses m_1 and m_2) are attached to the ends of a massless rigid rod of length a. the system is free to rotate in three dimensions about the (fixed) center of mass.

a) *Show that the allowed energies of this rigid rotor are*

$$E_n = \frac{\hbar^2}{2I} n(n+1) \quad (n = 0, 1, 2, ...) \quad \text{where } I = \frac{m_1 m_2}{m_1 + m_2} a^2$$

is the moment of inertia of the system

Normally $T = \frac{L^2}{2I}$, so the operator is then $\hat{T} = \frac{1}{2I}(\hat{L})^2$.

$$\hat{T} |\psi\rangle = \frac{1}{2I} \hat{L}^2 |\psi\rangle = \frac{1}{2I} \hbar^2 n(n+1) |\psi\rangle$$

Since, we don't have any potential function, then the eigenvalue of the energy is $\boxed{E_n = \frac{\hbar^2}{2I} n(n+1)}$

b) *What are the normalized eigenfunctions for this system? (Let θ and ϕ define the orientation of the rotor axis.) What is the degeneracy of the nth energy level?*

These have the same eigenvalues of $\hat{L}^2$, so the eigenfunctions will be the spherical harmonics: $\boxed{Y_1^1(\theta, \phi)}$. If we think of the spherical harmonics, there is kinda a hidden m value here, that can go from $-n, -n+1, ...n-1, n$. There are 2n+1 values here. So, it is this is $\boxed{2n + 1 \text{ degenerate}}$

c) *What spectrum would you expect for this system?*

Let's take two consecutive energies, n and $n + 1$

$$\nu = \frac{E_{n+1} - E_n}{2\pi} = \frac{1}{2\pi}\Big(\frac{\hbar}{2I}(n+1)(n+2) - \frac{\hbar}{2I}n(n+1)\Big) = \frac{\hbar}{2\pi I}(n+1)(n+2-n)$$

$$\boxed{\nu = \frac{\hbar}{2\pi I} j \text{ where } j = n + 1}$$

d) *According to the figure given in the text, what is the frequency separation between adjacent lines? Look up the masses of ^{12}C and ^{16}O, and from m_1, m_2, and $\Delta\nu$ determine the distance between the atoms.*

There are 5 lines between 30 and 50, so $\Delta\nu \approx 4\text{cm}^{-1}$. By "googling", ${}^{12}C \to m_1 \approx 1.9927e^{-23}\text{g}$ and ${}^{16}O \to m_2 = 2.6593e^{-23}\text{g}$. Solving for a:

$$a = \sqrt{\frac{8\pi}{\hbar}\left(\frac{1}{m_1} + \frac{1}{m_2}\right)}$$

$$\boxed{a \approx 1.9193\mu\text{m}}$$

Griffiths 4.64

the electron in a hydrogen atom occupies the combined spin and position state

$$R_{21}(\sqrt{1/3}Y_1^0\chi_+ + \sqrt{2/3}Y_1^1\chi_-)$$

a) *If you measured the orbital angular momentum squared, what values might you get, and what is the probability of each?*

The magnitude of angular momentum is only dependent on l,

$$L^2 |l,m\rangle = l(l+1)\hbar^2 |l,m\rangle$$

So there is only one value possible, with value $\boxed{2\hbar^2}$

b) *Same for the z component of angular momentum.*

Same kinda thing as above:

$$L_z |l,m\rangle = m\hbar |l,m\rangle$$

$$\boxed{0 \text{ with probability } \frac{1}{3}, \hbar \text{ with probability } \frac{2}{3}}$$

c) *Same for the spin angular momentum squared.*

$$S^2 |s,m_s\rangle = s(s+1)\hbar^2 |s,m_s\rangle$$

$$\boxed{\text{One possible value } \frac{3}{4}\hbar^2}$$

d) *Same for the z component of spin angular momentum.*

$$S_z |s,m_s\rangle = m_s\hbar |s,m_s\rangle$$

$$\boxed{\frac{\hbar}{2} \text{ with probability } \frac{1}{3}, -\frac{\hbar}{2} \text{ with probability } \frac{2}{3}}$$

e) *Same for the energy of the electron.*

$$\hat{H}|n\rangle = -\left[\frac{m_e}{2\hbar}\left(\frac{e^2}{4\pi\varepsilon_0}\right)\right]\frac{1}{n^2}|n\rangle$$

$$\text{Since } n = 1 \rightarrow \boxed{E_1 = -\frac{m_e}{2\hbar}\frac{1}{4}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2}$$

Griffiths 4.30

An electron is in the spin state

$$\chi = A\begin{pmatrix} 3i & 4 \end{pmatrix}$$

a) *Determine the normalization constant A*

$$(9+16)A^2 = 1 \rightarrow \boxed{A = \frac{1}{5}}$$

b) *Find the expectation values of S_x, S_y, and S_z*

Since our spin state is given in the z basis, we can just read those off:

$$\frac{9}{25}\frac{\hbar}{2} - \frac{16}{25}\frac{\hbar}{2} = -\frac{7}{25}\frac{\hbar}{2}$$

$$\boxed{\langle S_z \rangle = -\frac{7}{25}\frac{\hbar}{2}}$$

$$\langle S_y \rangle = \chi^\dagger S_y \chi = \frac{1}{5}\begin{pmatrix} -3i & 4 \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\frac{1}{5}\begin{pmatrix} 3i \\ 4 \end{pmatrix}$$

$$\boxed{\langle S_y \rangle = -\frac{24}{25}\frac{\hbar}{2}}$$

$$\langle S_x \rangle = \chi^\dagger S_x \chi = \frac{1}{5}\begin{pmatrix} -3i & 4 \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\frac{1}{5}\begin{pmatrix} 3i \\ 4 \end{pmatrix}$$

$$\boxed{\langle S_x \rangle = 0}$$

c) *Find the "uncertainties" σ_{S_x}, σ_{S_y}, and σ_{S_z}*

We know that $\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2$. Sp, now we just need to know $\hat{S_z}^2$, etc.

$$S_z^2 = S_z S_z = \left(\frac{\hbar}{2}\right)^2\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \left(\frac{\hbar}{2}\right)^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$S_y^2 = S_yS_y = \left(\frac{\hbar}{2}\right)^2\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} = \left(\frac{\hbar}{2}\right)^2\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

$$S_x^2 = S_xS_x = \left(\frac{\hbar}{2}\right)^2\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \left(\frac{\hbar}{2}\right)^2\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

Since $S_x^2 = S_y^2 = S_z^2 \Longrightarrow \langle S_x^2\rangle = \langle S_y^2\rangle = \langle S_z^2\rangle$.

$$\langle S_z|\chi|S_z\rangle \Rightarrow \frac{1}{5}\begin{pmatrix}-3i & 4\end{pmatrix}\left(\frac{\hbar}{2}\right)^2\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\frac{1}{5}\begin{pmatrix}3i\\ 4\end{pmatrix} = \left(\frac{\hbar}{2}\right)^2$$

$$\boxed{\sigma_{S_z} = \sqrt{\langle S_z^2\rangle - \langle S_z\rangle^2} = \frac{\hbar}{2}\sqrt{1-\left(-\frac{7}{25}\right)^2}}$$

$$\boxed{\sigma_{S_y} = \sqrt{\langle S_y^2\rangle - \langle S_y\rangle^2} = \frac{\hbar}{2}\sqrt{1-\left(-\frac{24}{25}\right)^2}}$$

$$\boxed{\sigma_{S_x} = \sqrt{\langle S_x^2\rangle - \langle S_x\rangle^2} = \frac{\hbar}{2}\sqrt{1-0} = \frac{\hbar}{2}}$$

d) *Confirm that your results are consistent with all three uncertainty principles.*
The one they are referring to is

$$\sigma_{L_x}\sigma_{L_y} \geq \frac{\hbar}{2}|\langle L_z\rangle|$$

$$\sigma_{S_x}\sigma_{S_x} = \left(\frac{\hbar}{2}\right)^2\sqrt{1-\left(\frac{24}{25}\right)^2} = 0.28\left(\frac{\hbar}{2}\right)^2 \geq \frac{\hbar}{2}\left|-\frac{7}{25}\frac{\hbar}{2}\right| = 0.28\left(\frac{\hbar}{2}\right)^2 \quad \checkmark$$

$$\sigma_{S_y}\sigma_{S_z} = \left(\frac{\hbar}{2}\right)^2\sqrt{1-\left(\frac{24}{25}\right)^2}\sqrt{1-\left(\frac{7}{25}\right)^2} = 0.269\left(\frac{\hbar}{2}\right)^2 \geq \frac{\hbar}{2}|0| = 0 \quad \checkmark$$

$$\sigma_{S_z}\sigma_{S_x} = \left(\frac{\hbar}{2}\right)^2\sqrt{1-\left(\frac{7}{25}\right)^2} = 0.96\left(\frac{\hbar}{2}\right)^2 \geq \frac{\hbar}{2}\left|-\frac{24}{25}\frac{\hbar}{2}\right| = 0.96\left(\frac{\hbar}{2}\right)^2 \quad \checkmark$$