Mandatory Assignment 3

FYS-2000 - Quantum Mechanics

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Contains 10 pages, frontpage included

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Task 1

Bound state is when an particle is trapped in a potential well and is only to be found in that region, and is also normalized. For scattering state the particle is free and can be found everywhere in space. This makes the wave function non normalizable. In figure 1 we have the two situations.

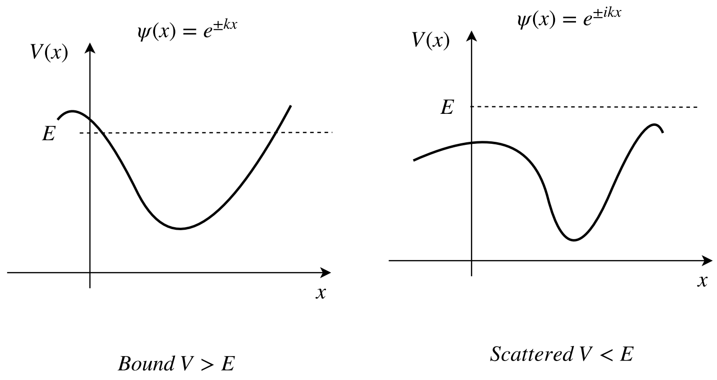

Figure 1

So the conditions we have for bound states is $V(x) > E$, $\lim_{x\to\infty}$ and $\lim_{x\to-\infty}$ Where V is the potential and E is the energy. The wave function also has to be normalizable in the region. For scattered state we have $V(x) < E$, $\lim_{x\to\infty}$ and $\lim_{x\to-\infty}$ and the wave function does extend to infinity and is non-normalizable.

Task 2

For a finite well the potential is zero between $x = 0$ and $x = L$ and some potential V_0(could also be different kinds of potential on either side) outside. Because of this the wave function will be sinusoidal inside the well and exponential outside such that the wave function goes to zero.

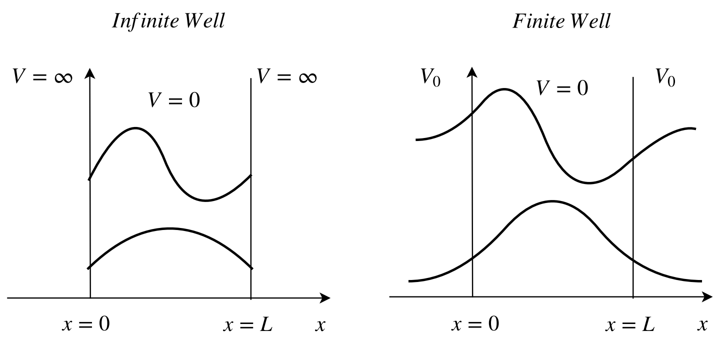

Figure 2

In the finite well the particle can be found outside the walls which it cannot in the infinite well. Here the boundary condition for the finite well are such that $\psi(0)_{inside} = \psi(0)_{outside}$ and $\psi(L)_{inside} = \psi(L)_{outside}$ and the same with the derivatives. The wave function has to continues because it has to obey the **Schrödinger equation**.

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi = E\psi \tag{1}$$

Now for the infinite square well the wave function has to be continues inside the well to obey the **Schrödinger equation**. The potential outside and at the boundary is infinite so at the boundary the wave function cant be continues because as we approach the boundary we have that the integral for the **Schrödinger equation** is

$$\int_{-\epsilon}^{\epsilon} \frac{d^2\psi}{dx^2}dx = -\frac{2m}{\hbar^2}\int_{-\epsilon}^{\epsilon}(E - V)\psi dx$$

We then have,

$$\left.\frac{d\psi}{dx}\right|_{\epsilon} - \left.\frac{d\psi}{dx}\right|_{-\epsilon} = -\frac{2m}{\hbar^2}\left(\int_{-\epsilon}^{0}(E-V)\psi dx + \int_{0}^{\epsilon}(E-V)\psi dx\right)$$

Now as $\lim_{\epsilon\to 0}$ the finite well both sides of the equation goes to zero. As pictured in figure 3 we see that we can close the area infinitely small until its zero.

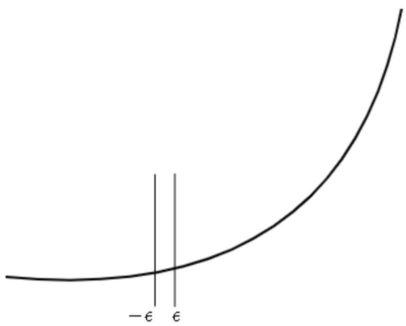

Figure 3

For the infinite well the potential immediately goes to infinity therefore we will always have infinite amount of area no matter how much we squeeze the boundary of the integral. (see figure 4)

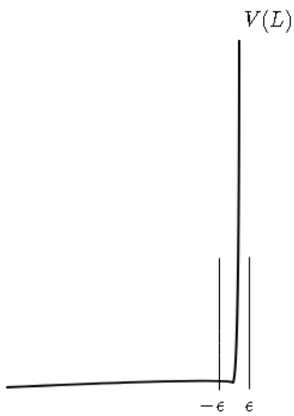

Figure 4

Therefore the wave equation has to be zero so that $\psi(0) = 0$, $\psi(L) = 0$ for the infinite well, and this makes up the difference in boundary condition.
The energy level is also always lower in the finite well because the wavelength is bigger because it stretches over longer distance as seen in figure 2. And since $p = \frac{h}{\lambda}$ by **De Broglie's** and $E_n = \frac{p_n^2}{2m}$ the energy is lower at all energy levels. The finite well also has finite energy levels and for the infinite well it has infinite energy levels.

Task 3

The ground state of the hydrogen atom is where the electron is in it lowest energy state The energy level given in the hydrogen atom is by eq 2 below. (derived from the **Schrödinger equation**)

$$E_n = -\frac{1}{(4\pi\epsilon_0)^2}\frac{m_r e^4}{2n^2\hbar^2} \tag{2}$$

where m_r is the reduced mass of proton and the electron. Putting in known variables gives,

$$E_n = -\frac{13.60}{n^2}eV \tag{3}$$

The ground state is when $n = 1$ therefore the ground level energy is.

$$E_{ground} = -13.60eV$$

Physical part is that the **Lyman series** (which is the ultraviolet spectrum) always goes to this energy level, from $E_n \rightarrow E_1$ as seen in figure 5.

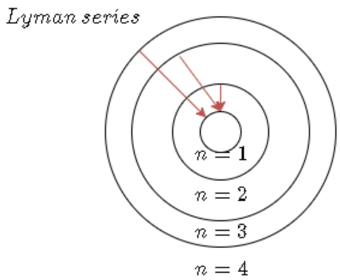

Figure 5

Task 4

For hydrogen like system with Z protons we can alter eq(2) by multiplying with Z, $e^2 \rightarrow Ze^2$ and since the part is squared we now have,

$$E_n(Z) = -Z^2E_n = -\frac{Z^2}{n^2}13.60eV$$

where E_n is the n^{nth} orbit with the atomic number Z.
Looking back to previous task in weekly assignment we solved for the **Bohr radius** by minimizing the energy like this,

$$\frac{d}{da} < E >= 0 \Rightarrow -\frac{\hbar^2}{2m_e a^3} + \frac{e^2}{4\pi\epsilon_0 a^2} = 0$$

where we used the fact that $< E >=< T > + < V >$ and a is the radius, this gave us,

$$a_0 = \frac{4\hbar^2\pi\epsilon_0}{m_e e^2}$$

now by using the fact that we now have a function of protons, $e^2 \rightarrow Ze^2$ we have,

$$a(Z) = \frac{1}{Z}a_0$$

where a_0 is the **Bohr radius**.
So the energy and **Bohr radius** according to $Z = 2$ and $Z = 3$

$$E_1(2) = -4 \cdot 13.60eV$$

$$E_1(3) = -9 \cdot 13.60eV$$

$$a(2) = \frac{1}{2}a_0$$

$$a(3) = \frac{1}{3}a_0$$

The chemical elements for $Z = 2$ is Helium and for $Z = 3$ is Lithium. The difference between these and the hydrogen-like systems are that the hydrogen-like system only contains *one* electron and the other have more then one.

Task 5

The frequency for the **Lyman series** from n = 2 is given by using eq (3),

$$\Delta E_{21} = E_2 - E_1 = -\frac{13.60}{4} + \frac{13.60}{1}$$

Which is,

$$\Delta E_{21} = E_2 - E_1 = 13.60(1 - \frac{1}{4})$$

Which then yields,

$$\Delta E_{21} = E_2 - E_1 = \frac{3}{4}13.60eV$$

By using the relation with energy and frequency given by,

$$\Delta E = hf \tag{4}$$

we then have,

$$f = \frac{\Delta E_{21}}{h} = 2.466 \cdot 10^{15}Hz$$

and for n = 3 we have,

$$\Delta E_{31} = E_3 - E_1 = \frac{8}{9}13.60eV$$

which is,

$$f = \frac{\Delta E_{31}}{h} = 2.923 \cdot 10^{15}Hz$$

Now for solving for the wavelength we use the energy relation,

$$\Delta E = hf = \frac{hc}{\lambda}$$

where c is the speed of light and is the wavelength. Solving this for λ we get,

$$\lambda = \frac{c}{f} \tag{5}$$

Now solving this by using the frequencies we just found,

$$\lambda_{21} = \frac{c}{f_{21}} = 1.216 \cdot 10^{-7}m$$

and for the other frequency we get,

$$\lambda_{31} = \frac{c}{f_{21}} = 1.026 \cdot 10^{-7}m$$

As we can see here we have that $f_{31} > f_{21}$ which means that the excitation to $n = 3$ sends out higher energy then $n = 2$.

Task 6

Here we have the same as task 5, but with some altered energy levels. Using equation in task 4 we have,

$$E_n(Z) = Z^2 E_n$$

and by using eq(4) and eq(5) we have for $Z = 2$,

$$\Delta E_{21}(2) = 2^2(-\frac{13.60}{2^2}) - 2^2(-\frac{13.60}{1^2}) = 40.8eV$$
$$\Delta E_{31}(2) = 2^2(-\frac{13.60}{3^2}) - 2^2(-\frac{13.60}{1^2}) = 48.4eV$$

and for $Z = 3$

$$\Delta E_{21}(3) = 91.8eV$$
$$\Delta E_{31}(3) = 108.8eV$$

And their frequency's are,

$$f_{21}(2) = \frac{\Delta E_{21}(2)}{h} = 9.865 \cdot 10^{15} Hz$$
$$f_{31}(2) = \frac{\Delta E_{21}(2)}{h} = 1.17 \cdot 10^{16} Hz$$

and for $Z = 3$

$$f_{21}(3) = \frac{\Delta E_{21}(2)}{h} = 2.22 \cdot 10^{16} Hz$$
$$f_{31}(3) = \frac{\Delta E_{21}(2)}{h} = 2.63 \cdot 10^{16} Hz$$

and their corresponding wavelength given by eq(5)

$$\lambda_{21}(2) = \frac{\Delta E_{21}(2)}{h} = 3.039 \cdot 10^{-8} m$$
$$\lambda_{31}(2) = \frac{\Delta E_{21}(2)}{h} = 2.562 \cdot 10^{-8} m$$

and for $Z = 3$

$$\lambda_{21}(3) = \frac{\Delta E_{21}(2)}{h} = 1.35 \cdot 10^{-8} m$$
$$\lambda_{31}(3) = \frac{\Delta E_{21}(2)}{h} = 1.14 \cdot 10^{-8} m$$

Task 7

We have the spin vector $\mathbf{S} = \hbar/2\sigma$, where σ is the Pauli spin matrices given by,

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}; \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Now we solve the characteristic equation for solving the eigenvalue, by

$$|(S - \lambda I)| = 0$$

Since we are asked to find the probability for S_z and S_x we solve by using the corresponding Pauli matrix.
For S_x we get the following characteristic equation,

$$\begin{vmatrix} -\lambda & \frac{\hbar}{2} \\ \frac{\hbar}{2} & -\lambda \end{vmatrix} = \lambda^2 - \frac{\hbar^2}{4} = 0$$

Solving yields,

$$\lambda = \pm\frac{\hbar}{2}$$

Now that we have the eigenvalues we put them back in and to the inner product with the eigenvector and solve for the variables, lets put the positive value in first,

$$\frac{\hbar}{2}\begin{bmatrix}-1 & 1\\ 1 & -1\end{bmatrix}\begin{bmatrix}x_1\\ x_2\end{bmatrix} = 0$$

The solution yields $x_1 = x_2$ and therefore the eigenvector or eigenspinor for $\hbar/2$ is,

$$\chi_+^{(x)} = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\ 1\end{bmatrix}$$

The $\frac{1}{\sqrt{2}}$ comes from the fact that it has to be normalized, so for the spinor $\frac{|\chi_+>}{|<\chi_+|\chi_+>|}$.
By doing the same, but substituting with $-\frac{\hbar}{2}$ instead yields $x_1 = -x_2$ and we have the $-\hbar/2$ eigenspinor by,

$$\chi_-^{(x)} = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\ -1\end{bmatrix}$$

By doing the same for S_z we get the eigenspinors,

$$\chi_+^{(z)} = \begin{bmatrix}1\\ 0\end{bmatrix}; \chi_-^{(z)} = \begin{bmatrix}0\\ 1\end{bmatrix}$$

Now for solving the probabilities we take the inner product with each eigenspinor and take the square of the probability amplitude as shown,

$$| < \chi_+^{(z)}|\chi > |^2$$

Since we have,

$$\chi = \frac{1}{\sqrt{6}}\begin{bmatrix}1+i\\ 2\end{bmatrix}$$

we solve the following for $\hbar/2$ with S_x,

$$P_{(x_+)} = \left|\left(\frac{1}{\sqrt{12}}\begin{bmatrix}1 & 1\end{bmatrix}\begin{bmatrix}1+i\\ 2\end{bmatrix}\right)\right|^2$$

This yields,

$$P_{x_+} = |\frac{1}{\sqrt{12}}(3+i)|^2 = \frac{1}{12}\sqrt{(3^2+1^2)}^2 = \frac{5}{6}$$

Which is the probability of observing $\hbar/2$ when measuring S_x.
Doing the same with $-\hbar/2$ eigenspinor we get,

$$P_{(x_-)} = \left|\left(\frac{1}{\sqrt{12}}\begin{bmatrix}1 & -1\end{bmatrix}\begin{bmatrix}1+i\\ 2\end{bmatrix}\right)\right|^2$$

This gives us,

$$P_{(x_-)} = |\frac{1}{\sqrt{12}}(-1+i)|^2 = \frac{1}{12}\sqrt{(1^2+1^2)}^2 = \frac{1}{6}$$

Now if we add both probabilities together we should get 1 if we did properly normalize.

$$\frac{5}{6} + \frac{1}{6} = 1$$

Looks like we did. [1]
By doing the same for S_z and observing $\hbar/2$ we get,

$$P_{(z_+)} = \left| \left(\frac{1}{\sqrt{6}} \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 1+i \\ 2 \end{bmatrix} \right) \right|^2$$

this gives us,

$$P_{(z_+)} = |\frac{1}{\sqrt{6}}(1+i)|^2 = \frac{1}{6}\sqrt{(1^2+1^2)}^2 = \frac{1}{3}$$

Now for $-\hbar/2$,

$$P_{(z_-)} = \left| \left(\frac{1}{\sqrt{6}} \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 1+i \\ 2 \end{bmatrix} \right) \right|^2$$

this gives us,

$$P_{(z_-)} = |\frac{1}{\sqrt{6}}(2)|^2 = \frac{1}{6}\sqrt{(2^2)}^2 = \frac{2}{3}$$

If we add up the probabilities we get,

$$\frac{1}{3} + \frac{2}{3} = 1$$

Task 8

We have the electron in the spin state

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

By solving for the normalization constant we get,

$$< \chi|\chi >= 1$$

which is,

$$A^2 \begin{bmatrix} -3i & 4 \end{bmatrix} \begin{bmatrix} 3i \\ 4 \end{bmatrix} = 1$$

$$A^2(9+16) = 1$$

which gives us,

$$A = \frac{1}{5}$$

or the square which will be more useful,

$$A^2 = \frac{1}{25}$$

Now for solving the spins,

$$< S_x >=< \chi|S_x|\chi >$$

[1]This reminds me of that one time i tried to add up two easy numbers, but took way to long because i did not want to look stupid by getting it wrong.

and since $S_x = (\hbar/2)\sigma_x$ we have,

$$\frac{\hbar}{50}\begin{bmatrix}-3i & 4\end{bmatrix}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}3i\\ 4\end{bmatrix} = \frac{\hbar}{50}\begin{bmatrix}-3i & 4\end{bmatrix}\begin{bmatrix}4\\ 3i\end{bmatrix} = 0$$

we have,

$$< S_x >= 0$$

Now for $< S_y >$,

$$\frac{\hbar}{50}\begin{bmatrix}-3i & 4\end{bmatrix}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}\begin{bmatrix}3i\\ 4\end{bmatrix} = -\frac{\hbar}{50}(24)$$

So we have,

$$< S_y >= -\hbar\frac{12}{25}$$

Now for $< S_z >$,

$$\frac{\hbar}{50}\begin{bmatrix}-3i & 4\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\begin{bmatrix}3i\\ 4\end{bmatrix} = -\frac{\hbar}{50}(9-16)$$

We therefore have,

$$< S_z >= -\frac{7}{50}\hbar$$

The standard deviation is solved by using eq(6)

$$\Delta X = \sqrt{< X^2 > - < X >^2} \tag{6}$$

Therefore we have the standard deviations,

$$\Delta S_x = \sqrt{< S_x^2 > - < S_x >^2}$$
$$\Delta S_y = \sqrt{< S_y^2 > - < S_y >^2}$$
$$\Delta S_z = \sqrt{< S_z^2 > - < S_z >^2}$$

We have already solved for $< S_{x,y,z} >$ so we need to solve for $< S_{x,y,z}^2 >$

$$< S_x^2 >= \frac{1}{25}\frac{\hbar^2}{4}\begin{bmatrix}-3i & 4\end{bmatrix}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}3i\\ 4\end{bmatrix}$$

σ_x^2 is,

$$\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} = \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$$

Solving yields,

$$\frac{1}{25}\frac{\hbar^2}{4}\begin{bmatrix}-3i & 4\end{bmatrix}\begin{bmatrix}3i\\ 4\end{bmatrix} = \frac{\hbar^2}{100}(25) = \frac{\hbar^2}{4}$$

By putting in eq(6) we get,

$$\Delta S_x = \sqrt{\frac{\hbar^2}{4} - 0} = \frac{1}{2}\hbar$$

Now for ΔS_y

$$< S_y^2 >= \frac{1}{25}\frac{\hbar^2}{4}\begin{bmatrix}-3i & 4\end{bmatrix}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}\begin{bmatrix}3i\\ 4\end{bmatrix} = \frac{\hbar^2}{4}$$

$$\Delta S_y = \sqrt{\frac{\hbar^2}{4} - (\frac{7\hbar}{50})^2} = \frac{7}{50}\hbar$$

For ΔS_z we also get $< S_z^2 >= \frac{\hbar^2}{4}$
so we get

$$\Delta S_z = \sqrt{\frac{\hbar^2}{4} - \frac{49\hbar^2}{2500}} = \frac{12}{25}\hbar$$

The general equation for the uncertainties is,

$$\Delta A \Delta B \geq \frac{1}{2i} | < [A, B] > | \tag{7}$$

And by using the following identities,

$$[S_x, S_y] = i\hbar S_z; [S_y, S_z] = i\hbar S_x; [S_z, S_x] = i\hbar S_y$$

we have,

$$\Delta S_x \Delta S_y \geq \frac{\hbar}{2} | < S_z > |$$

We already solved for $< S_z >$, therefore we have,

$$\frac{\hbar}{2}\frac{7}{50}\hbar \geq \frac{\hbar}{2}\frac{7}{50}\hbar$$

As we can see the uncertainty principle is satisfied. Doing the same for the others we have,

$$\Delta S_y \Delta S_z \geq \frac{\hbar}{2} | < S_x > |$$

Which gives,

$$\frac{7}{50}\hbar\frac{12}{50}\hbar \geq 0$$

Therefore it is also satisfied.
At last we have,

$$\Delta S_z \Delta S_x \geq \frac{\hbar}{2} | < S_y > |$$

$$\frac{12}{25}\hbar\frac{\hbar}{2} \geq \frac{\hbar}{2}\frac{12}{25}\hbar$$

Which is also satisfied.