

# Assignment 5

Monday, 11 October 2021 10:28 PM

## Problem 9.2

- a. Since a square-well potential in one dimension upscaled to three dimensions (square-well in each direction superimposed on each other), it would follow that the solution to the 3D box potential is the multiplication of the three 1D square potentials for each direction.

$$\psi_{x,y,z}(x,y,z) = A_x A_y A_z f(x) g(y) h(z)$$

where  $A_i$  corresponds to the normalisation factor in each direction. If each of  $\psi_i$  is normalised, then its integral over its coordinate axis is equal to one, and so  $\psi_{x,y,z}$  is normalised to 1 (since three normalised [=1] functions multiplied is just one). The time-independent solution to each coordinate axis is

$$\psi_{n_i}(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n_i \pi}{a} x\right)$$

so the solution is

$$\Psi_{n_x, n_y, n_z}(x, y, z) = \left(\sqrt{\frac{2}{a}}\right)^3 \sin\left(\frac{n_x \pi}{a} x\right) \sin\left(\frac{n_y \pi}{a} y\right) \sin\left(\frac{n_z \pi}{a} z\right)$$

However, each coordinate axis has with it its own energy described by  $E_{n_i} = \frac{n_i^2 \pi^2 \hbar^2}{2ma^2}$

so the energies are added together with

$$E_{n_x, n_y, n_z} = \frac{\pi^2 \hbar^2}{2ma^2} (n_x^2 + n_y^2 + n_z^2)$$

- b. The energy for the  $E_{\{1,2,3\}}$  state is

$$\begin{aligned} E_{\{1,2,3\}} &= \frac{\pi^2 \hbar^2}{2ma^2} (1^2 + 2^2 + 3^2) \\ &= \frac{\pi^2 \hbar^2}{2ma^2} (14) \end{aligned}$$

The permutations for  $\{1,2,3\}$  correspond to

$$\left. \begin{matrix} 1 & 2 & 3 \\ 1 & 3 & 2 \\ 2 & 1 & 3 \\ 3 & 2 & 1 \end{matrix} \right\} 4 \text{ degenerate states}$$

(also 3 1 2 and 2 1 3 which I forgot to handwrite => 6 degeneracy)

Since no combination of other square numbers can give 14, this is the only set of states that are degenerate to this energy.

## Problem 9.3

- a. If the electron is in the ground state  $\{1,0,0\}$ , then

$$\psi_{1,0,0}(r) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$$

Since the expectation value over 1D is

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x,t)|^2 dx$$

since the expectation value over  $\mathcal{W}$  is

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x, t)|^2 dx$$

the extension to 3 dimensions is

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x, t)|^2 dV$$

$$= \int_{\mathbb{R}^3} x |\psi(x, t)|^2 dx dy dz$$

and in spherical coordinates, is

$$\langle r \rangle = \int_0^{\pi} \int_0^{2\pi} \int_0^{\infty} r |\psi(r, \theta, \phi)|^2 r^2 \sin \theta dr d\theta d\phi$$

and for  $\langle r^2 \rangle$ ,

$$\langle r^2 \rangle = \int_0^{\pi} \int_0^{2\pi} \int_0^{\infty} r^2 |\psi(r, \theta, \phi)|^2 r^2 \sin \theta dr d\theta d\phi$$

Substituting in  $\Psi_{100}(r, \theta, \phi)$

$$\begin{aligned} \langle r \rangle &= \int_0^{\pi} \int_0^{2\pi} \int_0^{\infty} r^3 \left( \frac{1}{\pi a^3} e^{-r/a} \right)^2 \sin \theta dr d\theta d\phi \\ &= \frac{1}{\pi a^3} \int_0^{\infty} r^3 e^{-2r/a} dr \int_0^{2\pi} 1 d\phi \int_0^{\pi} \sin \theta d\theta \\ &= \frac{2}{\pi a^3} \int_0^{\infty} r^3 e^{-2r/a} dr \\ &= \frac{4\pi}{\pi a^3} \int_0^{\infty} r^3 e^{-2r/a} dr \end{aligned}$$

Using integration formula from formula sheet ( $\int_0^{\infty} x^n e^{-ax} dx$ )

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

$$= \frac{24}{a^3 \cdot \frac{16}{a^4}} = \frac{24a}{16} = \frac{3}{2} a$$

And so the expectation radius of a electron of Hydrogen in the ground state is  $\langle r \rangle = \frac{3}{2} a$

Similarly for  $\langle r^2 \rangle$ ,

$$\begin{aligned} \langle r^2 \rangle &= \frac{4\pi}{\pi a^3} \int_0^{\infty} r^4 e^{-2r/a} dr \quad (\text{by working from } \langle r \rangle) \\ &= \frac{4}{a^3} \left( \frac{4!}{(\frac{2}{a})^5} \right) \\ &= \frac{96}{a^3 \cdot \frac{32}{a^5}} = \frac{96}{32} a^2 = 3a^2 \end{aligned}$$

And so the expectation value of  $r^2$  is  $r^2 = 3a^2$

- b. Since the electron probability density is radially symmetric (in the ground state),  $\langle x \rangle$  would be zero since it's equally likely to be  $\langle r \rangle = \frac{3}{2} a$  in every direction.

Again, since it's radially symmetric,

$$\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle \Rightarrow 3\langle x^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle$$

By linearity of expectation values,

$$\begin{aligned} \langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle &= \langle x^2 + y^2 + z^2 \rangle \\ &= \langle r^2 \rangle \quad (\text{since } r^2 = x^2 + y^2 + z^2) \end{aligned}$$

$$\Rightarrow 3\langle x^2 \rangle = \langle r^2 \rangle$$

$$\begin{aligned} \langle x^2 \rangle &= \frac{1}{3} \langle r^2 \rangle \\ &= \frac{1}{3} 3a^2 \\ &= a^2 \end{aligned}$$

The uncertainty is then  $\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{a^2 - 0^2}$

$$\begin{aligned} \text{The uncertainty is then } \sigma_x &= \langle x^2 \rangle - \langle x \rangle^2 \\ &= a^2 - \bar{x}^2 \\ &= a^2 \end{aligned}$$

c. The probability of finding the electron between  $r$  and  $r+dr$  is

$$\begin{aligned}
 P &= \int_0^{\pi} \int_0^{2\pi} \int_r^{r+a} |Y_{100}|^2 r^2 \sin\theta \, dr \, d\phi \, d\theta \\
 &= \int_r^{r+a} \frac{4\pi}{\pi a^3} r^2 e^{-\frac{2r}{a}} dr \quad (\text{as calculated in part a}) \\
 &= p(r) dr \quad (\text{by eq. 1.15 in Griffiths}) \\
 \text{where } p(r) &= \frac{4}{a^3} r^2 e^{-\frac{2r}{a}}
 \end{aligned}$$

The maximum probability occurs when  $\frac{dp}{dr} = 0$

$$\frac{dp}{dr} = \frac{8}{a^3} r e^{-\frac{2r}{a}} - \frac{8}{a^4} r^2 e^{-\frac{2r}{a}} \quad (\text{by product rule})$$

$$= \frac{8r}{a^3} e^{-\frac{2r}{a}} \left(1 - \frac{r}{a}\right)$$

and so  $\frac{dp}{dr} = 0$  only when  $r=0$  (trivial) or  
 when  $1 - \frac{r}{a} = 0 \Rightarrow r=a$

Therefore the most probable  $r$  is the Bohr radius. (for the ground state of Hydrogen)

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Problem 10.2:

$$\begin{aligned}
 a. [\hat{L}_x, \hat{L}_y] &= [y\hat{p}_z - z\hat{p}_y, z\hat{p}_x - x\hat{p}_z] \\
 &= ([y\hat{p}_z, z\hat{p}_x] - [y\hat{p}_z, x\hat{p}_z]) - ([z\hat{p}_x, z\hat{p}_x] - [z\hat{p}_y, x\hat{p}_z]) \\
 &= [y\hat{p}_z, z\hat{p}_x] + [z\hat{p}_y, x\hat{p}_z] \quad (\text{since } x_i \text{ with } \hat{p}_{x_i} \text{ doesn't commute}) \\
 &= y\hat{p}_z z\hat{p}_x - z\hat{p}_z y\hat{p}_z + z\hat{p}_y x\hat{p}_z - x\hat{p}_z z\hat{p}_y \\
 &= y[\hat{p}_z, z]\hat{p}_x + [y, z]\hat{p}_z\hat{p}_x + zy[\hat{p}_z, \hat{p}_x] + z[y, \hat{p}_x]\hat{p}_z \\
 &\quad + z[\hat{p}_y, x]\hat{p}_z + [z, x]\hat{p}_y\hat{p}_z + xz[\hat{p}_y, \hat{p}_x] + x[z, \hat{p}_z]\hat{p}_y \\
 &= y[\hat{p}_z, z]\hat{p}_x + 0 + 0 + 0 + 0 + 0 + 0 + x[z, \hat{p}_z]\hat{p}_y \\
 &= x[z, \hat{p}_z]\hat{p}_y - y[z, \hat{p}_z]\hat{p}_x \quad \nwarrow \text{(zeros from canonical commutation relations)} \\
 &= x i\hbar \hat{p}_y - y i\hbar \hat{p}_x = i\hbar (x\hat{p}_y - y\hat{p}_x) \\
 &= i\hbar \hat{L}_z
 \end{aligned}$$

and so the angular momentum operators are cyclic. (since using a different combination of angular momentum operators would involve the exact same process with corresponding operators)

b. Note that  $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$

$$\begin{aligned} \Rightarrow [\hat{L}_z, \hat{L}_x] &= [\hat{L}_x, \hat{L}_x] + [\hat{L}_y, \hat{L}_x] + [\hat{L}_z, \hat{L}_x] \quad (1) \\ &= 0 + L_y [L_y, L_x] + [L_y, L_x] L_y + L_z [L_z, L_x] + [L_z, L_x] L_z \\ &= L_y (-i\hbar L_z) + (-i\hbar L_z) L_y + L_z (i\hbar L_y) + (i\hbar L_y) L_z \\ &= 0 \end{aligned}$$

It follows (by the same reasoning as part a and the symmetry of (1)) that each of the commutator relations are 0.

of (i)) that each of the commutator relations are 0.

$$\text{c. i. } [L_z, x] = [x\hat{p}_y - y\hat{p}_x, x] = [x\hat{p}_y, x] - [y\hat{p}_x, x] \\ = x[\hat{p}_y, x] - y[\hat{p}_x, x] \\ = 0 - ihy \\ = ihy$$

$$\text{ii. } [L_z, y] = [x\hat{p}_y - y\hat{p}_x, y] = [x\hat{p}_y, y] - [y\hat{p}_x, y] \\ = x[\hat{p}_y, y] - y[\hat{p}_x, y] \\ = -ihx - 0 \\ = -ihx$$

$$\text{iii. } [L_z, z] = [x\hat{p}_y - y\hat{p}_x, z] = [x\hat{p}_y, z] - [y\hat{p}_x, z] \\ = x[\hat{p}_y, z] - y[\hat{p}_x, z] \\ = 0 - 0 \\ = 0$$

$$\text{iv. } [L_z, \hat{p}_x] = [x\hat{p}_y - y\hat{p}_x, \hat{p}_x] = [x\hat{p}_y, \hat{p}_x] - [y\hat{p}_x, \hat{p}_x] \\ = \hat{p}_y[x, \hat{p}_x] - y[\hat{p}_x, \hat{p}_x] \\ = ihy$$

$$\text{v. } [L_z, \hat{p}_y] = [x\hat{p}_y - y\hat{p}_x, \hat{p}_y] = [x\hat{p}_y, \hat{p}_y] - [y\hat{p}_x, \hat{p}_y] \\ = x[\hat{p}_y, \hat{p}_y] - \hat{p}_x[y, \hat{p}_y] \\ = 0 - ih\hat{p}_x$$

$$\text{vi. } [L_z, \hat{p}_z] = [x\hat{p}_y - y\hat{p}_x, \hat{p}_z] = [x\hat{p}_y, \hat{p}_z] - [y\hat{p}_x, \hat{p}_z] \\ = x[\hat{p}_y, \hat{p}_z] - y[\hat{p}_x, \hat{p}_z] \\ = 0 - 0 = 0$$

Problem 10.3:

The  $\hat{L}$  operator is Hermitian (by assumption), so the hermitian conjugate of  $L^\pm$  must be  $L^\mp$  by  $\langle f | L^\pm g \rangle = \langle f | L^\mp | g \rangle$

Note that

$$L^\pm = L_x \pm iL_y$$

$\Rightarrow \langle f | L^\pm g \rangle = \langle f | L_x g \rangle \pm i \langle f | L_y g \rangle$   
Since  $\hat{L}$  is Hermitian and  $\hat{L} = (L_x, L_y, L_z)$ , each component is equal to its Hermitian conjugate.

$$\Rightarrow \langle f | L^\pm g \rangle = \langle L_x f | g \rangle \pm i \langle L_y f | g \rangle \\ = \langle (L_x \pm iL_y) f | g \rangle \\ = \langle L^\mp f | g \rangle$$

so  $L^\mp$  is the Hermitian conjugate of  $L^\pm$

$$\text{Now, using } L^\mp L^\pm = L^2 - L_z^2 + \hbar L_z$$

$$\langle f_\ell^m | L^\mp L^\pm f_\ell^m \rangle = \langle f_\ell^m | (L^2 - L_z^2 + \hbar L_z) f_\ell^m \rangle$$

$$\text{but } L^2 f_\ell^m = \hbar^2 \ell(\ell+1) f_\ell^m \text{ and } L_z f_\ell^m = \hbar m f_\ell^m \\ (\text{by eq 4.118}) \Rightarrow L_z^2 f_\ell^m = \hbar^2 m^2 f_\ell^m$$

$$\Rightarrow \langle f_\ell^m | L^\mp L^\pm f_\ell^m \rangle = \langle f_\ell^m | (\hbar^2 \ell(\ell+1) - \hbar^2 m^2 + \hbar^2 m) f_\ell^m \rangle \\ = \hbar^2 (\ell(\ell+1) - m^2 + m) \langle f_\ell^m | f_\ell^m \rangle \\ = \hbar^2 (\ell(\ell+1) - m^2 + m)$$

and by  $L^\pm$  being the Hermitian conjugate of  $L^\mp$ ,

$$\langle f_\ell^m | L^\mp L^\pm f_\ell^m \rangle = \langle L^\pm f_\ell^m | L^\pm f_\ell^m \rangle$$

$$\Rightarrow \langle f_\ell^m | L^\mp L^\pm f_\ell^m \rangle = \langle (A_\ell^m) f_\ell^{m \pm 1} | (A_\ell^m) f_\ell^{m \pm 1} \rangle \\ = (A_\ell^m)^2 \langle f_\ell^{m \pm 1} | f_\ell^{m \pm 1} \rangle \\ = (A_\ell^m)^2 = \hbar^2 (\ell(\ell+1) - m^2 + m)$$

$$\begin{aligned} \langle \psi_{l+1} | \psi_{l+1} \rangle &= \langle \psi_l | \psi_{l+1} \rangle^* \\ &= (A_l^m)^2 \langle \psi_l^{m+1} | \psi_l^{m+1} \rangle \\ &= (A_l^m)^2 = h^2(l(l+1) - m^2 + m) \end{aligned}$$

$$\Rightarrow A_l^m = h \sqrt{l(l+1) - m^2 + m}$$

I really didn't understand much of this assignment. For the most part, I knew what I was doing but I didn't know why I was doing it (apart to arrive at an answer). This was very difficult and made me pessimistic for the course.