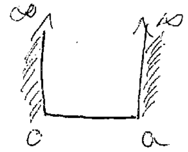
Uitwerking Final exam Kwantumfysica 1
3 November 2011

Problem 1

$$V(x) = \begin{cases} \infty & \text{for } x<0 \text{ or } x>a \\ 0 & \text{for } 0<x<a \end{cases}$$



a) $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

with $V(x) = \begin{cases} \infty & \text{for } x<0 \text{ or } x>a \\ 0 & \text{for } 0<x<a \end{cases}$

The eigenstates are $|\psi_n\rangle = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$

with eigenenergies $\epsilon_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$: $\hat{H}|\psi_n\rangle = \epsilon_n|\psi_n\rangle$

b) $|\Psi(t=0)\rangle = \frac{1}{\sqrt{2}}\left[|\psi_1\rangle + |\psi_2\rangle\right]$

b.1) $\langle\hat{H}\rangle = \langle\Psi(t=0)|\hat{H}|\Psi(t=0)\rangle =$

$$= \left[\frac{1}{\sqrt{2}}\left(\langle\psi_1| + \langle\psi_2|\right)\right]\hat{H}\left(\frac{1}{\sqrt{2}}\left(|\psi_1\rangle + |\psi_2\rangle\right)\right) =$$

$$= \frac{1}{2}\left[\langle\psi_1|\hat{H}|\psi_1\rangle + \langle\psi_1|\hat{H}|\psi_2\rangle + \langle\psi_2|\hat{H}|\psi_1\rangle + \langle\psi_2|\hat{H}|\psi_2\rangle\right]$$

Since $\hat{H}|\psi_n\rangle = \epsilon_n|\psi_n\rangle \Rightarrow \langle\psi_n|\hat{H}|\psi_n\rangle = \epsilon_n$
and $\langle\psi_n|\psi_m\rangle = \delta_{mn}$, we have
$\langle\psi_n|\hat{H}|\psi_m\rangle = \epsilon_m\delta_{mn}$

So:

$$\langle\hat{H}\rangle = \frac{1}{2}\left[\epsilon_{n=1} + 0 + 0 + \epsilon_{n=2}\right]$$

$$= \frac{1}{2}\left[\frac{1\pi^2\hbar^2}{2ma^2} + \frac{2^2\pi^2\hbar^2}{2ma^2}\right]$$

$$\boxed{\langle\hat{H}\rangle = \frac{5\pi^2\hbar^2}{4ma^2}} \text{ or } \boxed{\langle\hat{H}\rangle = \frac{\epsilon_1+\epsilon_2}{2} = \frac{5}{2}\epsilon_1}$$

b.2) $|\Psi(t)\rangle = e^{-\frac{i\hat{H}t}{\hbar}}|\Psi(t=0)\rangle$

$e^{-\frac{i\hat{H}t}{\hbar}}|\psi_n\rangle = e^{-\frac{i\epsilon_n t}{\hbar}}|\psi_n\rangle$, so:

$$|\Psi(t)\rangle = e^{-\frac{i\hat{H}t}{\hbar}}\left[\frac{1}{\sqrt{2}}\left(|\psi_1\rangle + |\psi_2\rangle\right)\right]$$

$$= \frac{1}{\sqrt{2}}\left[e^{-\frac{i\hat{H}t}{\hbar}}|\psi_1\rangle + e^{-\frac{i\hat{H}t}{\hbar}}|\psi_2\rangle\right]$$

$$\boxed{|\Psi(t)\rangle = \frac{1}{\sqrt{2}}\left[e^{-\frac{i\epsilon_1 t}{\hbar}}|\psi_1\rangle + e^{-\frac{i\epsilon_2 t}{\hbar}}|\psi_2\rangle\right]}$$

b.3) $\langle\hat{H}(t)\rangle = \langle\Psi(t)|\hat{H}|\Psi(t)\rangle =$

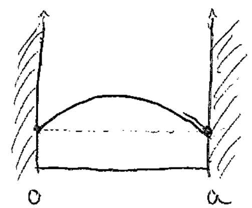
$$= \frac{1}{2}\left[e^{+\frac{i\epsilon_1 t}{\hbar}}\langle\psi_1| + e^{+\frac{i\epsilon_2 t}{\hbar}}\langle\psi_2|\right]\hat{H}\left[e^{-\frac{i\epsilon_1 t}{\hbar}}|\psi_1\rangle + e^{-\frac{i\epsilon_2 t}{\hbar}}|\psi_2\rangle\right]$$

$$= \frac{1}{2}\left[1\langle\psi_1|\hat{H}|\psi_1\rangle + e^{\frac{i(\epsilon_1-\epsilon_2)t}{\hbar}}\cancel{\langle\psi_1|\hat{H}|\psi_2\rangle}^{0} + e^{\frac{-i(\epsilon_1-\epsilon_2)t}{\hbar}}\cancel{\langle\psi_2|\hat{H}|\psi_1\rangle}^{0} + 1\langle\psi_2|\hat{H}|\psi_2\rangle\right]$$

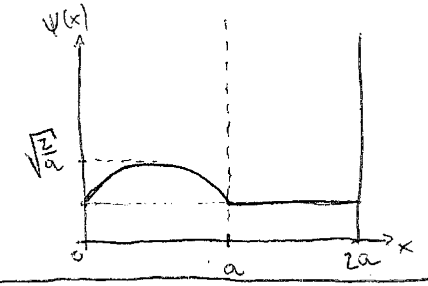
$$= \frac{1}{2}\left[\epsilon_1 + \epsilon_2\right] \Rightarrow \boxed{\langle\hat{H}(t)\rangle = \frac{\epsilon_1+\epsilon_2}{2}}$$

c) $\epsilon = \epsilon_1$ So the particle is at $|\psi_1\rangle$

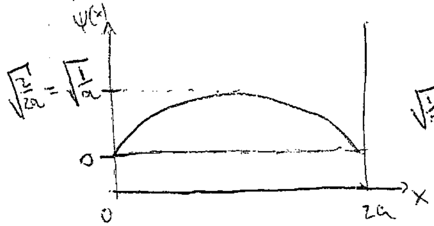
$|\psi\rangle = |\psi_1\rangle = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)$



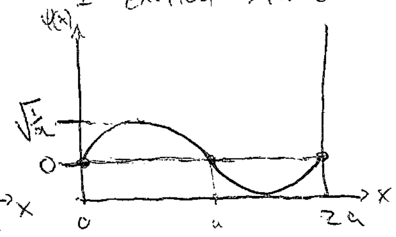
d)



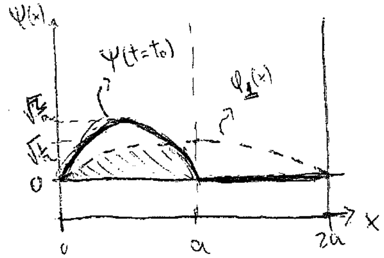
e) Ground state

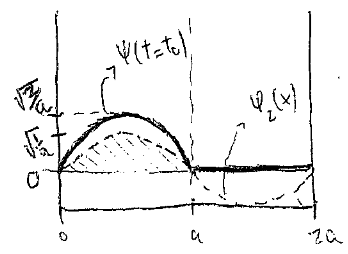


1^{st} excited state



f) The projection of one state into another: $c_n = \langle \Psi | \phi_n \rangle$ represents "how much" of the state $|\phi_n\rangle$ is contained in $|\Psi\rangle$. And the probability of getting $|\phi_n\rangle$ when measuring $|\Psi\rangle$ is $|c_n|^2$. Now let's check the sketches:





The coeficients c_n are proportional to the shaded areas in the graphs above. From this we can see that $c_2 > c_1$. Since the total area under $|\varphi_1(x)|^2 = |\varphi_2(x)|^2 = 1$ we have that $|c_2|^2 = 0.5$ and $|c_1|^2 < 0.5$.

g) $c_1 = \langle \Psi | \varphi_1 \rangle = \int_0^a \left[\sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)\right] \cdot \left[\sqrt{\frac{1}{a}} \sin\left(\frac{\pi x}{2a}\right)\right] dx + \int_a^{2a} \emptyset \, dx$

$= \frac{\sqrt{2}}{a} \int_0^a \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{\pi x}{2a}\right) dx =$

$= \frac{\sqrt{2}}{a} \frac{1}{2} \left[\int_0^a \cos\left(\frac{\pi x}{2a}\right) dx - \int_0^a \cos\left(\frac{3\pi x}{2a}\right) dx \right] =$

$= \frac{\sqrt{2}}{2a} \left[\frac{2a}{\pi} \sin\left(\frac{\pi x}{2a}\right)\Big|_0^a - \frac{2a}{3\pi} \sin\left(\frac{3\pi x}{2a}\right)\Big|_0^a \right] =$

$= \frac{\sqrt{2}}{\cancel{2a}} \left[\frac{\cancel{2a}}{\pi}(1-0) - \frac{\cancel{2a}}{3\pi}(-1-0) \right] = \sqrt{2}\left[\frac{3+1}{3\pi}\right] = \frac{4\sqrt{2}}{3\pi}$

$\boxed{P_{n=1} = |c_1|^2 = \frac{32}{9\pi^2} \approx 0.36}$

$c_2 = \langle \Psi | \varphi_2 \rangle = \int_0^a \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) \sqrt{\frac{1}{a}} \sin\left(\frac{2\pi x}{2a}\right) dx + \int_a^{2a} \emptyset \, dx =$

$= \frac{\sqrt{2}}{a} \int_0^a \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{\pi x}{a}\right) dx =$

$= \frac{\sqrt{2}}{a} \frac{1}{2} \left[\int_0^a \cos(0)\, dx - \int_0^a \cos\left(\frac{2\pi x}{a}\right) dx \right] =$

$= \frac{\sqrt{2}}{2a} \left[(a-0) - \frac{a}{2\pi} \sin\left(\frac{2\pi x}{a}\right)\Big|_0^a \right] = \frac{\sqrt{2}}{2a}[a - 0]$

$c_2 = \frac{\sqrt{2}}{2} = \frac{1}{\sqrt{2}} \Rightarrow \boxed{P_{n=2} = |c_2|^2 = \frac{1}{2} = 0.5}$

$c_1 < c_2$ and $|c_2|^2 = 0.5$
$|c_1|^2 < 0.5$ ✓

Problem 2

a) Possible measurement outcomes are determined by the set of <u>eigen values</u> of the associated eigen value equations

<u>For the electron spin</u>

length $\hat{S}^2 |s\, m_s\rangle = \hbar^2 s(s+1) |s\, m_s\rangle$ [Eq 1]

with $s=\frac{1}{2}$, and for any m_s

z-comp. $\hat{S}_z |s\, m_s\rangle = \hbar\, m_s |s\, m_s\rangle$ [Eq 2]

with $s=\frac{1}{2}$ and $m_s = \pm\frac{1}{2}$

<u>For the orbital angular momentum</u>

length $\hat{L}^2 |\ell\, m_\ell\rangle = \hbar^2 \ell(\ell+1) |\ell\, m_\ell\rangle$ [Eq. 3]

with $\ell=2$ and for any m_ℓ

z-comp $\hat{L}_z |\ell\, m_\ell\rangle = \hbar\, m_\ell |\ell\, m_\ell\rangle$ [Eq. 4]

with $\ell=2$ and for $m_\ell = -2, -1, 0, +1, +2$

a1) Using Eq 2 this gives as possible outcomes $S_z = \pm\frac{1}{2}\hbar$

a2) Using Eq 1, this gives only one outcome

$$|\vec{S}| = \hbar\sqrt{\tfrac{1}{2}(1+\tfrac{1}{2})} = \sqrt{\tfrac{3}{4}}\,\hbar$$

a3) Using Eq 4 possible outcomes are

$$L_z = -2\hbar,\ -1\hbar,\ 0\hbar,\ +1\hbar,\ +2\hbar$$

a4) Using Eq 3, the only possible outcome is

$$|\vec{L}| = \hbar\sqrt{\ell(\ell+1)} = \sqrt{6}\,\hbar$$

a5) The <u>magnetic dipole moment</u> $\vec{\mu}$ is proportional to the spin

$$\hat{\mu} = \gamma\hat{S} \quad \text{and} \quad \hat{\mu}_z = \gamma\hat{S}_z$$

So, with a1) it follows that the possible outcomes are

$$\mu_z = \pm\frac{1}{2}\gamma\hbar$$

b) Use the rules for <u>addition of angular momentum</u>.

with $\vec{J} = \vec{L} + \vec{S}$, and $\vec{J}$ the total angular momentum of the atom.

$\vec{J}$ obeys the eigenvalue equations

$$\boxed{\begin{aligned} \hat{J}^2 |j\, m_j\rangle &= \hbar^2 j(j+1) |j\, m_j\rangle \quad &[\text{Eq } 5] \\ \hat{J}_z |j\, m_j\rangle &= \hbar\, m_j |j\, m_j\rangle \quad &[\text{Eq } 6] \end{aligned}}$$

with $j = |l+s|, |l+s|-1 \ldots |l-s|+1, |l-s|$

$\Rightarrow j = 2\frac{1}{2}, 1\frac{1}{2}$

and $m_j = -j, -(j-1) \ldots (j-1), j$

b1) Using Eq 5 gives as possible outcomes

$$|\vec{J}| = \hbar\sqrt{\frac{5}{2}\cdot\frac{7}{2}} = \sqrt{\frac{35}{4}}\hbar \text{ and } \hbar\sqrt{\frac{3}{2}\cdot\frac{5}{2}} = \sqrt{\frac{15}{4}}\hbar$$

b2) Listing the outcomes for $j = \frac{5}{2}$ and $\frac{3}{2}$ together, with Eq. 6 gives as possible outcomes

$$J_z = -\frac{5}{2}\hbar, -\frac{3}{2}\hbar, -\frac{1}{2}\hbar, +\frac{1}{2}\hbar, +\frac{3}{2}\hbar, +\frac{5}{2}\hbar$$

Problem 3

a) $\langle \hat{L}_z \rangle = \langle \Psi_1 | \hat{L}_z | \Psi_1 \rangle$

$$= \begin{pmatrix} \sqrt{\frac{1}{5}} & \sqrt{\frac{1}{5}} & -i\sqrt{\frac{3}{5}} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \sqrt{\frac{1}{5}} \\ \sqrt{\frac{1}{5}} \\ +i\sqrt{\frac{3}{5}} \end{pmatrix} \hbar = \begin{pmatrix} \sqrt{\frac{1}{5}} & \sqrt{\frac{1}{5}} & -i\sqrt{\frac{3}{5}} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{1}{5}} \\ 0 \\ -i\sqrt{\frac{3}{5}} \end{pmatrix} \hbar$$

$$= \frac{1}{5}\hbar - \frac{3}{5}\hbar = -\frac{2}{5}\hbar$$

$\langle \hat{L}_x \rangle = \langle \Psi_1 | \hat{L}_x | \Psi_1 \rangle$

$$= \begin{pmatrix} \sqrt{\frac{1}{5}} & \sqrt{\frac{1}{5}} & -i\sqrt{\frac{3}{5}} \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \frac{\hbar}{\sqrt{2}} \begin{pmatrix} \sqrt{\frac{1}{5}} \\ \sqrt{\frac{1}{5}} \\ +i\sqrt{\frac{3}{5}} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{1}{5}} & \sqrt{\frac{1}{5}} & -i\sqrt{\frac{3}{5}} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{1}{5}} \\ \sqrt{\frac{1}{5}} + i\sqrt{\frac{3}{5}} \\ \sqrt{\frac{1}{5}} \end{pmatrix} \frac{\hbar}{\sqrt{2}}$$

$$= +\frac{\sqrt{2}}{5}\hbar$$

b) As for $\hat{L}_z$, the set of eigenvalues for $\hat{L}_x = -\hbar, 0, +\hbar$, and you can directly check that eigen value $+\hbar$ belongs to the eigenvector $|+_x\rangle$.

highest eigen value

$$P_{+\hbar} = |\langle +_x | \Psi_1 \rangle|^2 = \left| \begin{pmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{1}{5}} \\ \sqrt{\frac{1}{5}} \\ +i\sqrt{\frac{3}{5}} \end{pmatrix} \right|^2$$

$$= \left| \frac{1}{2}\sqrt{\frac{1}{5}} + \sqrt{\frac{1}{10}} + i\frac{1}{2}\sqrt{\frac{3}{5}} \right|^2 = \frac{3+\sqrt{2}}{10} \simeq 0.44$$

c)

$$P_{+h} = \left| \langle +_z | \psi_2 \rangle \right|^2$$

$$= \left| (1\,0\,0) \left(\sqrt{\tfrac{1}{3}} \begin{pmatrix} \frac{1}{2} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{2} \end{pmatrix} + \sqrt{\tfrac{2}{3}} \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{2} \end{pmatrix} \right) \right|^2$$

$$= \left| \sqrt{\tfrac{1}{3}}\,\tfrac{1}{2} + \sqrt{\tfrac{2}{3}}\,\tfrac{1}{2} \right|^2 = \frac{(1+\sqrt{2})^2}{12} \approx 0.49$$

d) $\langle L_x(t) \rangle = \langle \psi(t) | \hat{L}_x | \psi(t) \rangle$ with $|\psi(t)\rangle = \hat{U} |\psi_3\rangle$

$$\hat{H} \leftrightarrow \begin{pmatrix} E_+ & 0 & 0 \\ 0 & E_0 & 0 \\ 0 & 0 & E_- \end{pmatrix} = \hbar \begin{pmatrix} \omega_+ & 0 & 0 \\ 0 & \omega_0 & 0 \\ 0 & 0 & \omega_- \end{pmatrix} \text{ with } \begin{cases} E_+ = +\gamma B \hbar \\ E_0 = 0 \\ E_- = -\gamma B \hbar \\ \omega_+ = +\gamma B \\ \omega_0 = 0 \\ \omega_- = -\gamma B \end{cases}$$

$$\Rightarrow |\psi(t)\rangle \frac{e^{i\omega_+ t}}{\sqrt{2}} |+_z\rangle + e \frac{-i\omega_0 t}{\sqrt{2}} |0_z\rangle$$

$$\Rightarrow \langle L_x(t) \rangle = \left(e^{+i\omega_+ t}, e^{+i\omega_0 t}, 0 \right) \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} e^{-i\omega_+ t} \\ e^{-i\omega_0 t} \\ 0 \end{pmatrix} \frac{\hbar}{\sqrt{2}} \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}}$$

$$= \frac{\hbar}{2\sqrt{2}} \left(e^{+i(\omega_+ - \omega_0)t} + e^{-i(\omega_+ - \omega_0)t} \right)$$

$$= \frac{\hbar}{\sqrt{2}} \cos\left((\omega_+ - \omega_0) t \right) = \frac{\hbar}{\sqrt{2}} \cos(\gamma B t)$$

The vector $\vec{L}$ precess about the z-axis in the x-y plane ($\langle \hat{L}_y(t) \rangle$ also oscillates like $\langle \hat{L}_x \rangle$, but $\pi/2$ out of phase).
Here we only calculate the full oscillation of $\langle L_x \rangle$ around $L_x = 0$ in a harmonic way.