PHY 2D QUIZ 8 SOLUTIONS March 2010

1. (a) Inside box, $U(x,y,z) = 0$ and TISE becomes

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z) = E\,\psi(x,y,z) \quad (1)$$

(Look at your lecture notes or text book to see how to solve this subject to boundary conditions:
$\psi = 0$ at $x=0,\ x=L;\ y=0,\ y=L;\ z=0;\ z=L$)

Solution is of form $\psi(x,y,z) = \psi_1(x)\,\psi_2(y)\,\psi_3(z)$ (2)

Putting this in (1), and dividing by $\psi(x,y,z)$ given by (2) we obtain

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_1(x)}{dx^2}\frac{1}{\psi_1(x)} - \frac{\hbar^2}{2m}\frac{d^2\psi_2(y)}{dy^2}\frac{1}{\psi_2(y)} - \frac{\hbar^2}{2m}\frac{d^2\psi_3(z)}{dz^2}\frac{1}{\psi_3(z)} = E \quad (3)$$

Can only be true if each term on LHS is separately a constant.

Thus $-\frac{\hbar^2}{2m}\frac{d^2\psi_1(x)}{dx^2}\frac{1}{\psi_1(x)} = E_1$ etc. (with $E = E_1 + E_2 + E_3$)

or $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E_1\psi_1(x)$, etc (4)

Eqns. (4) reduce to 3 versions of 1-D Infinite Wall Finite Box problem so solutions are

$$\psi_1(x) = \sqrt{\frac{2}{L}}\sin(k_1 x) \qquad k_1 = \frac{n_1\pi}{L} \qquad n_1 = 1, 2, \ldots$$

$$\psi_2(y) = \sqrt{\frac{2}{L}}\sin(k_2 y) \qquad k_2 = \frac{n_2\pi}{L} \qquad n_2 = 1, 2, \ldots$$

$$\psi_3(z) = \sqrt{\frac{2}{L}}\sin(k_3 z) \qquad k_3 = \frac{n_3\pi}{L} \qquad n_3 = 1, 2, \ldots$$

(5)

Substituting in Eq. (2) gives the solution $\psi(x,y,z)$ properly normalized so $\int_0^L dx \int_0^L dy \int_0^L dz\, |\psi(x,y,z)|^2 = 1$.

ie: $\psi(x,y,z) = \left(\frac{2}{L}\right)^{3/2} \sin(k_1 x) \sin(k_2 y) \sin(k_3 z)$ (6)

(k_1, k_2, k_3 given by eq. (5))

From Eqs. (4). $E_1 = \frac{\hbar^2}{2m} k_1^2$; $E_2 = \frac{\hbar^2}{2m} k_2^2$; $E_3 = \frac{\hbar^2}{2m} k_3^2$

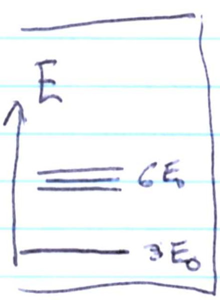
$$\therefore \quad E = E_1 + E_2 + E_3 = \frac{\hbar^2}{2m}\left(n_1^2 \left(\frac{\pi}{L}\right)^2 + n_2^2 \left(\frac{\pi}{L}\right)^2 + n_3^2 \left(\frac{\pi}{L}\right)^2 \right) \quad (7a)$$

$$\text{or} \quad E = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 \left(n_1^2 + n_2^2 + n_3^2\right) \quad (7b)$$

$$= E_0 \left(n_1^2 + n_2^2 + n_3^2\right) \quad \text{say.}$$

Lowest 4 energy levels occur at

$n_1 = n_2 = n_3 = 1$, $E = 3E_0$ $\quad \psi = \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{\pi z}{L}\right)$ (8a)



$n_1 = n_2 = 1$, $n_3 = 2$ $\quad E = 6E_0$ $\quad \psi = \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{2\pi z}{L}\right)$ (8b)

$n_1 = 1$, $n_2 = 2$, $n_3 = 1$ $\quad E = 6E_0$ $\quad \psi = \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{2\pi y}{L}\right) \sin\left(\frac{\pi z}{L}\right)$ (8c)

+ $n_1 = 2$, $n_2 = 1$, $n_3 = 1$ $\quad E = 6E_0$ $\quad \psi = \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{\pi z}{L}\right)$ (8d)

8(a) corresponds to a <u>singlet</u> (non-degenerate) level

8(b), 8(c) + 8(d) correspond to a <u>triplet</u> (triply degenerate) level.

(b) Probability density for finding electron in box is $|\psi(x,y,z)|^2$

$$\text{or} \quad P(x,y,z) = \left(\frac{2}{L}\right)^3 \sin^2\left(\frac{n_1 \pi x}{L}\right) \sin^2\left(\frac{n_2 \pi y}{L}\right) \sin^2\left(\frac{n_3 \pi z}{L}\right) \quad (9)$$

This will be a maximum when <u>each</u> of the $\sin^2(\cdot\cdot)$ factors $= 1$

For $n_1 = n_2 = n_3 = 1$,

This corresponds to: $\sin\left(\frac{\pi x}{L}\right) = \pm 1$, $\sin\left(\frac{\pi y}{L}\right) = \pm 1$, $\sin\left(\frac{\pi z}{L}\right) = \pm 1$

for x, y, z) inside the box, ($0 < x < L$; $0 < y < L$; $0 < z < L$)

This will occur for $\boxed{x = \frac{L}{2},\ y = \frac{L}{2},\ z = \frac{L}{2}.}$ only one maximum at center of box

For $n_1 = 1, n_2 = 1, n_3 = 1$ we must have

$$\sin\left(\frac{\pi x}{L}\right) = \pm 1, \quad \sin\left(\frac{\pi y}{L}\right) = \pm 1, \quad \sin\left(\frac{2\pi z}{L}\right) = \pm 1$$

This will occur for $\boxed{x = \frac{L}{2},\ y = \frac{L}{2},\ z = \frac{L}{4}}$ or $\boxed{x = \frac{L}{2},\ y = \frac{L}{2},\ z = \frac{3L}{4}}$ 2 maxima

Similarly for other 2 states of triplet, by symmetry

maxima will be for $\boxed{x = \frac{L}{2},\ y = \frac{L}{4},\ z = \frac{L}{2}}$ $\boxed{x = \frac{L}{2},\ y = \frac{3L}{4},\ z = \frac{L}{2}}$

and $\boxed{x = \frac{L}{4},\ y = \frac{L}{2},\ z = \frac{L}{2}}$ $\boxed{x = \frac{3L}{4},\ y = \frac{L}{2},\ z = \frac{L}{2}}$ (10)

(c) If y-side of box is changed to $2L$, ie $0 < y < 2L$, then for Eqn (5) above, Expression for k_2 becomes

$$k_2 = \frac{n_2 \pi}{(2L)} \qquad (n_2 = 1, 2, \ldots\ldots)$$

$$\& \quad E_2 = \frac{\hbar^2}{2m} k_2^2 = \frac{\hbar^2}{2m}\left(\frac{n_2^2}{4}\right)\left(\frac{\pi}{L}\right)^2$$

so Expression 7(?) for E changes to

$$E = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2\left(n_1^2 + \frac{n_2^2}{4} + n_3^2\right)$$

$$= E_0\left(n_1^2 + \frac{n_2^2}{4} + n_3^2\right) \qquad (11)$$

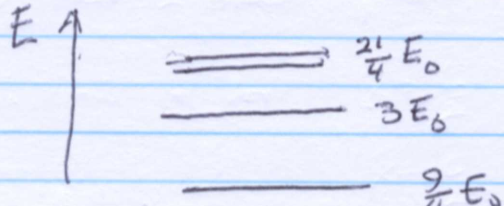
so lowest level becomes (for $n_1 = n_2 = n_3 = 1$)

$$E_{111} = \frac{9}{4} E_0$$

While $E_{112} = E_{211} = E_0 \left(\frac{21}{4}\right)$. (putting corresponding values of n_1, n_2, n_3 into Eq. (1))

but $E_{121} = 3E_0$.

so energy levels get lowered & triplet splits into a singlet and a doublet.



2(a) Let $\psi(x) = xe^{-\alpha x^2}$

Operate on it with $\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2\right] \equiv \mathcal{O}$, say

1st term: $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left[xe^{-\alpha x^2}\right] = -\frac{\hbar^2}{2m}\frac{d}{dx}\left[e^{-\alpha x^2} - 2\alpha x^2 e^{-\alpha x^2}\right]$

$$= -\frac{\hbar^2}{2m}\left[-2\alpha x e^{-\alpha x^2} + 4\alpha^2 x^3 e^{-\alpha x^2} - 4\alpha x e^{-\alpha x^2}\right]$$

$$= -\frac{\hbar^2}{2m}\left[-2\alpha + 4\alpha^2 x^2 - 4\alpha\right] x e^{-\alpha x^2}$$

$$= -\frac{\hbar^2}{2m}\left[-6\alpha + 4\alpha^2 x^2\right] x e^{-\alpha x^2}$$

2nd Term is $\frac{1}{2}kx^2\left(xe^{-\alpha x^2}\right)$

adding, we get $\mathcal{O}\psi(x) = \left[-\frac{\hbar^2}{2m}(-6\alpha + 4\alpha^2 x^2) + \frac{1}{2}kx^2\right]\psi(x)$

Thus $\psi(x)$ will be an eigenfunction if term in $[\cdots]$ is constant (independent of x). That constant will be the eigenvalue

This will be true if coeff. of x^2 term in $[\cdots]$ vanishes,

i.e. $-\frac{\hbar^2}{2m}4\alpha^2 + \frac{1}{2}k = 0$

or $\alpha^2 = \frac{mk}{4\hbar^2}$ or $\alpha = \frac{(mk)^{\frac{1}{2}}}{2\hbar}$.

Eigenvalue is $\frac{3\hbar^2}{m}\alpha = \frac{3\hbar^2 (mk)^{\frac{1}{2}}}{m\, 2\hbar} = \frac{3}{2}\hbar\left(\frac{k}{m}\right)^{\frac{1}{2}}$

(b) $\mathcal{O}$ is the total energy operator for the Harmonic Oscillator.

$\therefore$ Energy level is $\frac{3}{2}\hbar\omega_0$ ($\omega_0 = \sqrt{\frac{k}{m}}$ = Classical angular frequency for Harmonic Oscillator)

& wave function $\psi(x)$ (with normalization constant inserted) is corresponding eigenstate.