

## Solution to written exam in QUANTUM PHYSICS F0047T

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The solutions are just suggestions. They may contain several alternative routes.

1. (a) There are several ways to determine  $A$ . One is to integrate and use the normalization condition to solve for  $A$ . A different path (done here) is to write the given wave function in terms of eigenfunctions (here particle in a box). The eigenfunctions are (PH)  
 $\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$ . We can directly conclude that the given wave function consists of  $n = 1$ ,  $n = 5$  and  $n = 7$  functions, we can write:

$$\begin{aligned} \psi(x, 0) &= \frac{\sqrt{11}}{\sqrt{8 \cdot 2}} \frac{\sqrt{2}}{\sqrt{a}} \sin\left(\frac{\pi x}{a}\right) + \frac{\sqrt{2}}{2\sqrt{2} \cdot a} \sin\left(\frac{4\pi x}{a}\right) + \frac{A\sqrt{2}}{\sqrt{2} \cdot a} \sin\left(\frac{5\pi x}{a}\right) = \\ &= \frac{\sqrt{11}}{\sqrt{16}} \psi_1(x, 0) + \frac{1}{\sqrt{8}} \psi_4(x, 0) + \frac{A}{\sqrt{2}} \psi_5(x, 0) \end{aligned}$$

As all three eigenfunctions are orthonormal the normalisation integral reduces to  $\frac{11}{16} + \frac{1}{8} + \frac{A^2}{2} = 1$  and hence  $A = \sqrt{\frac{3}{8}}$  ( $\approx 0.612$ ).

- (b) The wave function contains only  $n = 1$ ,  $n = 4$  and  $n = 5$  eigenfunctions and therefore the only possible outcome of an energy measurement are  $E_1 = \frac{\hbar^2 \pi^2}{2ma^2}$  with probability  $\frac{11}{16}$  and  $E_4 = \frac{\hbar^2 \pi^2}{2ma^2} 16$  with probability  $\frac{1}{8}$  and  $E_5 = \frac{\hbar^2 \pi^2}{2ma^2} 25$  with probability  $\frac{A^2}{2} = \frac{3}{16}$ .

The average energy is given by

$$\langle E \rangle = \frac{11}{16} E_1 + \frac{1}{8} E_4 + \frac{3}{16} E_5 = \frac{\hbar^2 \pi^2}{2ma^2} \left( \frac{11}{16} + \frac{1}{8} \cdot 16 + \frac{3}{16} \cdot 25 \right) = \frac{118}{16} \cdot \frac{\hbar^2 \pi^2}{2ma^2} = \frac{59}{8} \cdot \frac{\hbar^2 \pi^2}{2ma^2}$$

- (c) The time dependent solution is given by  $\Psi(x, t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}$  and hence

$$\Psi(x, t) = \sqrt{\frac{11}{16}} \psi_1(x, 0) e^{-i \frac{\hbar \pi^2 t}{2ma^2}} + \frac{1}{\sqrt{8}} \psi_4(x, 0) e^{-i \frac{16 \hbar \pi^2 t}{2ma^2}} + \sqrt{\frac{3}{16}} \psi_5(x, 0) e^{-i \frac{25 \hbar \pi^2 t}{2ma^2}}$$

2. Rewrite  $L_x^2 + L_y^2 = L^2 - L_z^2$ , which gives the Hamiltonian

$$H = \frac{L^2 - L_z^2}{2\hbar^2} + \frac{L_z^2}{3\hbar^2}.$$

The eigenfunctions are  $Y_{l,m}$

$$HY_{l,m} = \left( \frac{L^2 - L_z^2}{2\hbar^2} + \frac{L_z^2}{3\hbar^2} \right) Y_{l,m} = \left( \frac{l(l+1)\hbar^2 - m^2\hbar^2}{2\hbar^2} + \frac{m^2\hbar^2}{3\hbar^2} \right) Y_{l,m}.$$

Hence the energies are:

$$E_{l,m} = \left( \frac{l(l+1)}{2} - \frac{m^2}{6} \right).$$

The lowest (ground state) energy is  $E_{0,0} = 0$  ( $l = 0$  no rotation).

$l = 1 \rightarrow m = 0, \pm 1$ , gives  $E_{1,0} = 1\text{eV}$   $E_{1,\pm 1} = \frac{5}{6}\text{eV}$

$l = 2 \rightarrow m = 0, \pm 1, \pm 2$ , gives  $E_{2,0} = 3\text{eV}$   $E_{2,\pm 1} = \frac{17}{6}\text{eV}$   $E_{2,\pm 2} = \frac{7}{3}\text{eV}$

and so on.

3. A measurement of the spin in the direction  $\hat{n} = \sin(\frac{\pi}{4})\hat{e}_y + \cos(\frac{\pi}{4})\hat{e}_z = \frac{1}{\sqrt{2}}\hat{e}_y + \frac{1}{\sqrt{2}}\hat{e}_z$ . The spin operator  $S_{\hat{n}}$  is

$$S_{\hat{n}} = \frac{1}{\sqrt{2}}S_y + \frac{1}{\sqrt{2}}S_z = \frac{\hbar}{2\sqrt{2}} \begin{pmatrix} 1 & -i \\ i & -1 \end{pmatrix}$$

The eigenvalue equation is

$$S_{\hat{n}}\chi = \lambda\chi \Leftrightarrow \frac{\hbar}{2\sqrt{2}} \begin{pmatrix} 1 & -i \\ i & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix} \quad (1)$$

We find the eigenvalues from

$$\begin{vmatrix} \frac{\hbar}{2\sqrt{2}} - \lambda & -i\frac{\hbar}{2\sqrt{2}} \\ i\frac{\hbar}{2\sqrt{2}} & -\frac{\hbar}{2\sqrt{2}} - \lambda \end{vmatrix} = 0 \Rightarrow \lambda = \pm \frac{\hbar}{2}$$

The eigenspinors to  $S_n$  corresponding to the  $+\frac{\hbar}{2}$  we get from

$$\frac{\hbar}{2\sqrt{2}} \begin{pmatrix} 1 & -i \\ i & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = +\frac{\hbar}{2} \begin{pmatrix} a \\ b \end{pmatrix}$$

$$\frac{a}{\sqrt{2}} - \frac{ib}{\sqrt{2}} = a \Leftrightarrow a(\sqrt{2} - 1) = -ib \text{ let } b = 1 \text{ and hence } a = \frac{-i}{\sqrt{2} - 1}$$

This gives the unnormalised spinor

$$\begin{pmatrix} -\frac{i}{\sqrt{2}-1} \\ 1 \end{pmatrix} \text{ and after normalisation we have } \chi_{\hat{n}+} = \frac{1}{\sqrt{2(2+\sqrt{2})}} \begin{pmatrix} -\frac{i}{\sqrt{2}-1} \\ 1 \end{pmatrix}$$

Now we can expand the initial eigenspinor  $\chi_+$  in these eigenspinors to  $S_n$ , the second eigenspinor you can get from orthogonality to the first one.

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = A \frac{1}{\sqrt{2(2+\sqrt{2})}} \begin{pmatrix} -\frac{i}{\sqrt{2}-1} \\ 1 \end{pmatrix} + B \frac{1}{\sqrt{2(2+\sqrt{2})}} \begin{pmatrix} 1 \\ \frac{-i}{\sqrt{2}-1} \end{pmatrix}$$

The coefficients are subjected to the normalisation condition  $|A|^2 + |B|^2 = 1$ . The coefficient  $A$  can be obtained by multiplying the previous equation from the left with  $\chi_{\hat{n}+}^*$ .

$$A = \frac{1}{\sqrt{2(2+\sqrt{2})}} \begin{pmatrix} -\frac{i}{\sqrt{2}-1} & 1 \end{pmatrix} * \begin{pmatrix} 1 \\ 0 \end{pmatrix} = -\frac{i}{\sqrt{2}-1} \cdot \frac{1}{\sqrt{2(2+\sqrt{2})}}$$

The probability (to get  $+\frac{\hbar}{2}$ ) is given by  $|A|^2$ .

$$|A|^2 = \frac{3+2\sqrt{2}}{4+2\sqrt{2}} = 0.8535533906$$

and (to get  $-\frac{\hbar}{2}$ ) for  $|B|^2$ .

$$|B|^2 = \frac{1}{4+2\sqrt{2}} = 0.1464466094$$

To find the probability for  $+\frac{\hbar}{2}$  in the z-direction for the up state of  $S_n$  express the state in the eigenspinors to  $S_z$ .

$$\chi_{\hat{n}+} = \frac{1}{\sqrt{2(2+\sqrt{2})}} \begin{pmatrix} -\frac{i}{\sqrt{2}-1} \\ 1 \end{pmatrix} = -\frac{i}{\sqrt{2}-1} \cdot \frac{1}{\sqrt{2(2+\sqrt{2})}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2(2+\sqrt{2})}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The probability is given by the square of the coefficient:

$$\left| -\frac{i}{\sqrt{2}-1} \cdot \frac{1}{\sqrt{2(2+\sqrt{2})}} \right|^2 = 0.8535533906$$

4. The eigenfunctions of the infinite square well in one dimension are (Here a solution of the S.E. in one dimension is adequate). The width of the well is  $a$ .

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \quad \text{and the eigenenergies are } E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \quad \text{where } n = 1, 2, 3, \dots$$

In three dimensions the eigenfunctions and eigenenergies are (Here an argument about separation of variables is needed to justify the structure of the solution)

$\Psi_{n,m,l}(x, y, z) = \psi_n(x) \cdot \psi_m(y) \cdot \psi_l(z)$  and eigenenergies  $E_{n,m} = E_n + E_m + E_l$  where the indices are  $n = 1, 2, 3, \dots$ ,  $m = 1, 2, 3, \dots$  and  $l = 1, 2, 3, \dots$

a) The eigenfunctions inside the box are (note the sidelength is  $a/2$  for one of the sides)

$$\Psi_{n,m,l}(x, y, z) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \cdot \sqrt{\frac{2}{a}} \sin \frac{m\pi y}{a} \cdot \sqrt{\frac{4}{a}} \sin \frac{l\pi 2z}{a} \quad \text{where } n = 1, 2, 3, \dots, m = 1, 2, 3, \dots \text{ and } l = 1, 2, 3, \dots$$

The eigenfunctions outside the box are  $\Psi_{n,m,l}(x, y, z) = 0$

b) The seven lowest eigenenergies are (note the 4 associated to the quantum number  $l$  this is due to that the length of the box along the  $z$  direction is only half of the other two that are of equal length):

$$E_{n,m,l} = \frac{\pi^2 \hbar^2}{2ma^2} (n^2 + m^2 + 4l^2), \quad \text{where the 7 lowest are } (n^2 + m^2 + 4l^2) = 6, 9, 12, 14, 18, \text{ and } 21.$$

c) The seven lowest eigenenergies have degeneracies (different ways to choose  $n, m, l$  to form the same energy) (either one, two or four) as follows:

$$\begin{aligned} E_{1,1,1} &= \text{one state } (n^2 + m^2 + 4l^2 = 6) \\ E_{1,2,1} &= E_{2,1,1} = \text{two states } (n^2 + m^2 + 4l^2 = 9) \\ E_{2,2,1} &= \text{one state } (n^2 + m^2 + 4l^2 = 12) \\ E_{1,3,1} &= E_{3,1,1} = \text{two states } (n^2 + m^2 + 4l^2 = 14) \\ E_{2,3,1} &= E_{3,2,1} = \text{two states } (n^2 + m^2 + 4l^2 = 17) \\ E_{1,1,2} &= \text{one state } (n^2 + m^2 + 4l^2 = 18) \end{aligned}$$

Energy number 7 is special as the degeneracy is 4 but all four are not connected through a symmetry operation, ie some of these states are accidentally degenerated. These four can be grouped in the following way.

$$\begin{aligned} E_{1,2,2} &= E_{2,1,2} = \text{two states } (n^2 + m^2 + 4l^2 = 21) \\ E_{1,4,1} &= E_{4,1,1} = \text{two states } (n^2 + m^2 + 4l^2 = 21) \end{aligned}$$

5. The task is to calculate the change of the energy levels (ground state  $E_0$  and first excited state  $E_1$ ) for a harmonic oscillator due to a perturbation  $H^1$  to the potential.

The two harmonic oscillator eigenfunctions that are of interest are :

$$\psi_0(x) = \sqrt{\frac{\alpha}{\sqrt{\pi}}} e^{-\frac{1}{2}\alpha^2 x^2} \quad \text{and} \quad \psi_1(x) = \sqrt{\frac{\alpha}{2\sqrt{\pi}}} 2\alpha x e^{-\frac{1}{2}\alpha^2 x^2} \quad \text{where} \quad \alpha = \sqrt{\frac{m\omega}{\hbar}}$$

- (a) Here we have a perturbation  $\gamma x^4$  where  $\gamma$  is small in some sense. The first integral to calculate (use integration by parts) will be for the change of the ground state energy

$$\langle 0 | \gamma x^4 | 0 \rangle = \int \psi_0^*(x) \gamma x^4 \psi_0(x) dx = \int \frac{\alpha}{\sqrt{\pi}} \gamma x^4 e^{-\alpha^2 x^2} dx = [\alpha x = y] = \frac{\gamma}{\alpha^4 \sqrt{\pi}} \int y^4 e^{-y^2} dy$$

where the integral taken separately will be

$$\int_{-\infty}^{\infty} y^4 e^{-y^2} dy = \left[ -\frac{y^3}{2} e^{-y^2} \right]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \frac{3y^2}{2} e^{-y^2} dy = \left[ -\frac{3y^1}{4} e^{-y^2} \right]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \frac{3}{4} e^{-y^2} dy = \frac{3}{4} \sqrt{\pi}$$

Hence the shift of the ground state energy will be

$$\langle 0 | \gamma x^4 | 0 \rangle = \frac{\gamma}{\alpha^4 \sqrt{\pi}} \frac{3}{4} \sqrt{\pi} = \frac{3\gamma}{4\alpha^4} = \frac{3\gamma}{4} \left( \frac{\hbar}{m\omega} \right)^2$$

The energy of the unperturbed groundstate is  $E_0 = \frac{\hbar\omega}{2}$ . Hence the energy of the perturbed groundstate is

$$E_0^{\text{perturbed}} = \frac{\hbar\omega}{2} + \frac{3\gamma}{4} \left( \frac{\hbar}{m\omega} \right)^2$$

- (b) Here we have a perturbation  $\epsilon x$  where  $\epsilon$  is small in some sense. The integrals to be calculated are  $\langle 0 | \epsilon x | 0 \rangle$  and  $\langle 1 | \epsilon x | 1 \rangle$ . The squares of both eigenfunctions are even functions and as the perturbation is odd both integrals will be zero.

Hence there is no change in energy to first order.