

## Solution to written exam in QUANTUM PHYSICS F0047T

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

1. This is a 2 dimensional problem with a Schrödinger equation (where  $V(x, y) = 0$ ) like

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x, y) - \frac{\hbar^2}{2m} \frac{d^2}{dy^2} \Psi(x, y) = E \Psi(x, y)$$

This equation is separable and the ansatz  $\Psi(x, y) = \psi(x) * \psi(y)$  gives the following result

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_x(x) - \frac{\hbar^2}{2m} \frac{d^2}{dy^2} \psi_y(y) = E_x \psi_x(x) + E_y \psi_y(y)$$

ie two independent one dimensional Schrödinger equations one for the variable  $x$  and one for  $y$ . We therefore solve the one dimensional problem first and after that we construct the two dimensional solution. To find the eigenfunctions we need to solve the Schrödinger equation which is (in the region where  $V(x)$  is zero)

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi = E \Psi \rightarrow \frac{d^2}{dx^2} \Psi + k^2 \Psi = 0 \text{ where } k^2 = \frac{2mE}{\hbar^2}$$

Solutions are of the kind:

$$\Psi(x) = A \cos kx + B \sin kx$$

Now we need to take the boundary conditions for the wave function  $\Psi$  ( $\Psi(-\frac{a}{2}) = \Psi(\frac{a}{2}) = 0$ ) into account.

$$A \cos(-\frac{ka}{2}) + B \sin(-\frac{ka}{2}) = 0 \text{ and } A \cos(\frac{ka}{2}) + B \sin(\frac{ka}{2}) = 0$$

Adding the two conditions gives:  $\cos(\frac{ka}{2}) = 0$  and subtracting them gives  $\sin(\frac{ka}{2}) = 0$ . These two conditions cannot be fulfilled at the same time, so either  $A$  or  $B$  has to be zero. We start with  $A = 0$  and we get the following solution: The normalising constant  $B = \sqrt{\frac{2}{a}}$  you get from the condition  $\int_{-a/2}^{a/2} |\Psi|^2 dx = 1$ . The condition  $\sin(\frac{ka}{2}) = 0$  gives  $\frac{ka}{2} = \frac{\pi}{2} * (\text{even} - \text{integer})$ . The solution is:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \text{ with eigenenergies } E_n = \frac{n^2 \pi^2 \hbar^2}{2Ma^2} \text{ where } n = 2, 4, 6, \dots \quad (1)$$

In a similar way the other function is analysed ( $A = 0$ ) which gives: The condition  $\cos(\frac{ka}{2}) = 0$  gives  $\frac{ka}{2} = \frac{\pi}{2} * (\text{odd} - \text{integer})$ . The solution is:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi x}{a}\right) \text{ with eigenenergies } E_n = \frac{n^2 \pi^2 \hbar^2}{2Ma^2} \text{ where } n = 1, 3, 5, \dots \quad (2)$$

The eigenfunctions in the  $y$  direction are the same as for the  $x$  direction as the potential is similar for this direction. Now we have the eigenfunctions of the one dimensional problem and the solution to the 2 dimensional problem is readily produced. The eigenfunctions are:

$$\Psi_{n,m}(x, y) = \psi_n(x) \cdot \psi_m(y) \text{ eigenenergies } E_{n,m} = E_n + E_m \text{ where } n = 1, 2, \dots \text{ and } m = 1, 2, \dots \quad (3)$$

In the area where the potential is infinite the wave function is equal to zero.

An **alternative route** taken by many students has been to present a calculation with the following boundary conditions:  $\Psi$  ( $\Psi(0) = \Psi(a) = 0$ ) into account. In this case the solution is for these boundary conditions:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \text{ with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \text{ where } n = 1, 2, 3, \dots \quad (4)$$

This solution has to be adapted to the boundary conditions related to this exam problem:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}\left(x + \frac{a}{2}\right)\right) \text{ with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \text{ where } n = 1, 2, 3, \dots \quad (5)$$

$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a} + \frac{n\pi}{2}\right) = \sqrt{\frac{2}{a}} \left(\sin\left(\frac{n\pi x}{a}\right) \cdot \cos\left(\frac{n\pi}{2}\right) + \cos\left(\frac{n\pi x}{a}\right) \cdot \sin\left(\frac{n\pi}{2}\right)\right)$ . We see that we recover the solution in eq (??), (??) and (??) as we let  $n$  run from 1 to  $\infty$ .

b) The ground state eigenfunction is given by (using eq. (??))

$$\Psi_{n=1,m=1}(x, y) = \psi_1(x) \cdot \psi_1(y) = \sqrt{\frac{2}{a}} \cos\left(\frac{\pi x}{a}\right) \cdot \sqrt{\frac{2}{a}} \cos\left(\frac{\pi y}{a}\right) \quad (6)$$

The next lowest state eigenfunction is given by (using eq. (??) and (??)). Note there are two eigenfunctions with the same energy ( $\Psi_{n=1,m=2}(x, y)$ ) you may use either one of them.

$$\Psi_{n=2,m=1}(x, y) = \psi_2(x) \cdot \psi_1(y) = \sqrt{\frac{2}{a}} \sin\left(2\frac{\pi x}{a}\right) \cdot \sqrt{\frac{2}{a}} \cos\left(\frac{\pi y}{a}\right) \quad (7)$$

Orthogonality is defined as

$$\int_x \int_y \Psi_{n_1,m_1}(x, y) \Psi_{n_2,m_2}(x, y) = \delta_{n_1,n_2} \delta_{m_1,m_2} \quad (8)$$

by explicit calculation

$$\int_{x=-a/2}^{a/2} \int_{y=-a/2}^{a/2} \left(\frac{2}{a} \cos\left(\frac{\pi x}{a}\right) \cdot \cos\left(\frac{\pi y}{a}\right)\right) \cdot \left(\frac{2}{a} \sin\left(2\frac{\pi x}{a}\right) \cdot \cos\left(\frac{\pi y}{a}\right)\right) = \text{calculations} = 0 \quad (9)$$

this is a separable integral (in  $x$  and  $y$ ), suggestion do the integral in  $x$  first as this will be zero as they belong to different eigenvalues. Thus the calculation ends with a zero as it should.

2. A general time dependent solution is given by

$$\Psi(x, t = 0) = \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar}$$

(a) In the present case with only two eigenstates we have energies  $E_0 = \frac{1}{2}\hbar\omega$  and  $E_1 = \frac{3}{2}\hbar\omega$  and hence :

$$\Psi(x, t) = c_0 \psi_0(x) e^{-iE_0 t/\hbar} + c_1 \psi_1(x) e^{-iE_1 t/\hbar} = \frac{1}{\sqrt{2}} \psi_0(x) e^{-i\frac{1}{2}\hbar\omega t/\hbar} + \frac{1}{\sqrt{2}} \psi_1(x) e^{-i\frac{3}{2}\hbar\omega t/\hbar}$$

and

$$\Psi(x, t) = \frac{1}{\sqrt{2}} \psi_0(x) e^{-i\frac{1}{2}\omega t} + \frac{1}{\sqrt{2}} \psi_1(x) e^{-i\frac{3}{2}\omega t}$$

(b) To calculate the time evolution of the expectation value of the kinetic energy we have to calculate the following.

$$\langle E_k \rangle = \langle \frac{p_{op}^2}{2m} \rangle = \int \frac{1}{\sqrt{2}} (\psi_0^* e^{+i\frac{1}{2}\hbar\omega t/\hbar} + \psi_1^* e^{+i\frac{3}{2}\hbar\omega t/\hbar}) \frac{p_{op}^2}{2m} \frac{1}{\sqrt{2}} (\psi_0 e^{-i\frac{1}{2}\hbar\omega t/\hbar} + \psi_1 e^{-i\frac{3}{2}\hbar\omega t/\hbar}) dx$$

where  $p_{op} = -i\hbar \frac{\partial}{\partial x}$  and for the square we get  $p_{op}^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}$ .

The two eigenfunctions in question are:  $\psi_0(x) = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} e^{-\frac{1}{2}\alpha^2 x^2}$  and

$\psi_1(x) = \left(\frac{\alpha}{2\sqrt{\pi}}\right)^{1/2} 2\alpha x e^{-\frac{1}{2}\alpha^2 x^2}$  where  $\alpha = \sqrt{m\omega/\hbar}$ .

We can proceed along several routes. The first one make use of that the operator  $p_{op}$  is Hermitian and we calculate the first derivative of the wave function and then identify the result as eigen functions after that calculate  $\langle E_k \rangle$  using the kronecker delta. The second route just makes a brute calculation of the second derivative of the wave function and the identify eigen functions and then calculate  $\langle E_k \rangle$  using the kronecker delta. The third route makes use of the step operators  $a_+$  and  $a_-$ . So non of the routes do calculate any integrals at all!

### The first route:

This makes use of the fact that the operator  $p_{op}$  is Hermitian. First we need to make some derivatives. The results is written in terms of eigen functions. For the ground state eigen function:

$$\frac{\partial}{\partial x} \psi_0(x) = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} (-\alpha^2 x) e^{-\frac{1}{2}\alpha^2 x^2} = -\frac{\alpha}{2} \sqrt{2} \left(\frac{\alpha}{2\sqrt{\pi}}\right)^{1/2} (2\alpha x) e^{-\frac{1}{2}\alpha^2 x^2} = -\frac{\alpha}{\sqrt{2}} \psi_1(x)$$

For the first excited state eigen function:

$$\frac{\partial}{\partial x} \psi_1(x) = \left(\frac{\alpha}{2\sqrt{\pi}}\right)^{1/2} (2\alpha) e^{-\frac{1}{2}\alpha^2 x^2} - \left(\frac{\alpha}{2\sqrt{\pi}}\right)^{1/2} (2\alpha^3 x^2) e^{-\frac{1}{2}\alpha^2 x^2} = \quad (10)$$

$$\sqrt{2}\alpha \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} e^{-\frac{1}{2}\alpha^2 x^2} - \alpha \left(\frac{\alpha}{8\sqrt{\pi}}\right)^{1/2} (4\alpha^3 x^2 - 2) e^{-\frac{1}{2}\alpha^2 x^2} - 2\alpha \left(\frac{\alpha}{8\sqrt{\pi}}\right)^{1/2} e^{-\frac{1}{2}\alpha^2 x^2} = \quad (11)$$

$$\left(\sqrt{2} - \frac{1}{\sqrt{2}}\alpha\psi_0(x) - \alpha\psi_2(x)\right) = \frac{1}{\sqrt{2}}\alpha\psi_0(x) - \alpha\psi_2(x) \quad (12)$$

Now we return to the calculation of  $\langle E_k \rangle$  and make use of the orthonormality of the eigenfunctions.

$$\begin{aligned} \langle E_k \rangle = \langle \frac{p_{op}^2}{2m} \rangle &= \int \frac{p_{op}^+}{2m} \frac{1}{\sqrt{2}} (\psi_0^* e^{+i\frac{1}{2}\hbar\omega t/\hbar} + \psi_1^* e^{+i\frac{3}{2}\hbar\omega t/\hbar}) \frac{p_{op}}{2m} \frac{1}{\sqrt{2}} (\psi_0 e^{-i\frac{1}{2}\hbar\omega t/\hbar} + \psi_1 e^{-i\frac{3}{2}\hbar\omega t/\hbar}) dx = \\ &= \frac{1}{2} \frac{\hbar^2}{2m} \int \left( i \frac{\alpha}{\sqrt{2}} \psi_1^*(x) e^{+i\frac{1}{2}\hbar\omega t/\hbar} - i \left( \frac{1}{\sqrt{2}} \alpha \psi_0^*(x) - \alpha \psi_2^*(x) \right) e^{+i\frac{3}{2}\hbar\omega t/\hbar} \right) \\ &\quad \cdot \left( -i \frac{\alpha}{\sqrt{2}} \psi_1(x) e^{-i\frac{1}{2}\hbar\omega t/\hbar} + i \left( \frac{1}{\sqrt{2}} \alpha \psi_0(x) - \alpha \psi_2(x) \right) e^{-i\frac{3}{2}\hbar\omega t/\hbar} \right) dx = \\ &= \frac{1}{2} \frac{\hbar^2}{2m} \left( \frac{\alpha^2}{2} + \frac{\alpha^2}{2} + \alpha^2 \right) = \frac{1}{2} \frac{\hbar^2}{2m} 2\alpha^2 = \frac{1}{2} \hbar\omega \end{aligned}$$

### Second route:

This route just takes a second derivative of the wave function and expresses the result in terms of eigen functions. First we need to make some more derivatives as we need second derivatives as well. For the groundstate eigen function:

$$\frac{\partial^2}{\partial x^2} \psi_0(x) = \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2} (-\alpha^2) e^{-\frac{1}{2}\alpha^2 x^2} + \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2} \alpha^4 x^2 e^{-\frac{1}{2}\alpha^2 x^2}$$

For the first excited state eigen function:

$$\frac{\partial^2}{\partial x^2} \psi_1(x) = \left( \frac{\alpha}{2\sqrt{\pi}} \right)^{1/2} (-2\alpha^3 x) e^{-\frac{1}{2}\alpha^2 x^2} - \left( \frac{\alpha}{2\sqrt{\pi}} \right)^{1/2} (4\alpha^3 x) e^{-\frac{1}{2}\alpha^2 x^2} + \left( \frac{\alpha}{2\sqrt{\pi}} \right)^{1/2} (2\alpha^5 x^3) e^{-\frac{1}{2}\alpha^2 x^2}$$

These derivatives can be rewritten in terms of eigenfunctions of the harmonic oscillator:

$$\begin{aligned} \frac{\partial^2}{\partial x^2} \psi_0(x) &= -\alpha^2 \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2} e^{-\frac{1}{2}\alpha^2 x^2} + \alpha^2 \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2} \alpha^2 x^2 e^{-\frac{1}{2}\alpha^2 x^2} = \\ &= -\alpha^2 \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2} e^{-\frac{1}{2}\alpha^2 x^2} + \alpha^2 \frac{\sqrt{8}}{4} \left( \frac{\alpha}{8\sqrt{\pi}} \right)^{1/2} 4\alpha^2 x^2 e^{-\frac{1}{2}\alpha^2 x^2} = \\ &= \frac{\alpha^2}{\sqrt{2}} \psi_2(x) + \frac{\alpha^2}{2} \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2} e^{-\frac{1}{2}\alpha^2 x^2} - \alpha^2 \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2} e^{-\frac{1}{2}\alpha^2 x^2} = \\ &= \frac{\alpha^2}{\sqrt{2}} \psi_2(x) - \frac{\alpha^2}{2} \psi_0(x) \end{aligned}$$

$$\begin{aligned} \frac{\partial^2}{\partial x^2} \psi_1(x) &= \alpha^2 \frac{\sqrt{6}}{2} \left( \frac{\alpha}{48\sqrt{\pi}} \right)^{1/2} (8\alpha^3 x^3) e^{-\frac{1}{2}\alpha^2 x^2} + \left( \frac{\alpha}{2\sqrt{\pi}} \right)^{1/2} (-2-4)\alpha^3 x e^{-\frac{1}{2}\alpha^2 x^2} = \\ &= \alpha^2 \frac{\sqrt{6}}{2} \psi_3(x) + \alpha^2 \frac{\sqrt{6}}{2} \left( \frac{\alpha}{48\sqrt{\pi}} \right)^{1/2} 12\alpha x e^{-\frac{1}{2}\alpha^2 x^2} - \left( \frac{\alpha}{2\sqrt{\pi}} \right)^{1/2} (6)\alpha^3 x e^{-\frac{1}{2}\alpha^2 x^2} = \\ &= \alpha^2 \frac{\sqrt{6}}{2} \psi_3(x) + \left( \frac{\alpha}{2\sqrt{\pi}} \right)^{1/2} (3)\alpha^3 x e^{-\frac{1}{2}\alpha^2 x^2} - \left( \frac{\alpha}{2\sqrt{\pi}} \right)^{1/2} (6)\alpha^3 x e^{-\frac{1}{2}\alpha^2 x^2} = \\ &= \alpha^2 \frac{\sqrt{6}}{2} \psi_3(x) - \alpha^2 \frac{3}{2} \left( \frac{\alpha}{2\sqrt{\pi}} \right)^{1/2} 2\alpha x e^{-\frac{1}{2}\alpha^2 x^2} = \alpha^2 \frac{\sqrt{6}}{2} \psi_3(x) - \alpha^2 \frac{3}{2} \psi_1(x) \end{aligned} \tag{13}$$

Now we return to the calculation of  $\langle E_k \rangle$ .

$$\begin{aligned} \langle E_k \rangle &= \langle \frac{p_{op}^2}{2m} \rangle = \int \frac{1}{\sqrt{2}} (\psi_0^* e^{+i\frac{1}{2}\hbar\omega t/\hbar} + \psi_1^* e^{+i\frac{3}{2}\hbar\omega t/\hbar}) \frac{p_{op}^2}{2m} \frac{1}{\sqrt{2}} (\psi_0 e^{-i\frac{1}{2}\hbar\omega t/\hbar} + \psi_1 e^{-i\frac{3}{2}\hbar\omega t/\hbar}) dx \\ &= \frac{1}{2} \frac{\hbar^2}{2m} \int (\psi_0^* e^{+i\frac{1}{2}\hbar\omega t/\hbar} + \psi_1^* e^{+i\frac{3}{2}\hbar\omega t/\hbar}) \cdot \\ & \quad (-1) \left( \left( \alpha^2 \frac{\sqrt{6}}{2} \psi_3(x) - \alpha^2 \frac{3}{2} \psi_1(x) \right) e^{-i\frac{3}{2}\hbar\omega t/\hbar} + \left( -\frac{\alpha^2}{2} \psi_0(x) + \frac{\alpha^2}{\sqrt{2}} \psi_2(x) \right) e^{-i\frac{1}{2}\hbar\omega t/\hbar} \right) = \end{aligned}$$

To calculate the integrals is simple it is just a matter of applying the kronecker delta.

$$= \frac{1}{2} \frac{\hbar^2}{2m} \left( \alpha^2 \frac{3}{2} + \alpha^2 \frac{1}{2} \right) = \frac{\alpha^2 \hbar^2}{2m} = \frac{\hbar\omega}{2}$$

**The third route:**

This route makes use of the stepping operators. Their action on the eigenfunctions are  $a_+\psi_n(x) = \sqrt{n+1}\psi_{n+1}(x)$  and  $a_-\psi_n(x) = \sqrt{n}\psi_{n-1}(x)$ . The momentum operator in terms of the stepping operators is

$$p = i \sqrt{\frac{\hbar m \omega}{2}} (a_+ - a_-)$$

The operator for the kinetic energy will be:

$$E_k = \frac{p^2}{2m} = \frac{1}{2m} \left( -\frac{\hbar m \omega}{2} \right) (a_+ - a_-)(a_+ - a_-) = -\frac{\hbar \omega}{4} (a_+ a_+ - a_+ a_- - a_- a_+ + a_- a_-)$$

With the operator for  $E_k$  we can now do the calculation:

$$E_k = -\frac{\hbar \omega}{4} \frac{1}{2} \int (\psi_0^*(x) + \psi_1^*(x)) (a_+ a_+ - a_+ a_- - a_- a_+ + a_- a_-) (\psi_0(x) + \psi_1(x)) dx =$$

the two operators  $a_+ a_+$  and  $a_- a_-$  will step functions out of range and these two integrals will hence be zero so continuing for the results of the two mixed step operators

$$a_+ a_- (\psi_0(x) + \psi_1(x)) = a_- (\psi_1(x) + \sqrt{2}\psi_2(x)) = \psi_0(x) + 2\psi_1(x) \text{ and}$$

$$a_- a_+ (\psi_0(x) + \psi_1(x)) = a_+ \psi_0(x) = \psi_1(x)$$

$$E_k = \frac{\hbar \omega}{4} \frac{1}{2} \int (\psi_0^*(x) + \psi_1^*(x)) (\psi_0(x) + 2\psi_1(x) + \psi_1(x)) dx = \frac{\hbar \omega}{4} \frac{1}{2} (1 + 3) = \frac{\hbar \omega}{2}$$

3. (a) i.  $\hat{\Pi} C \left( \cos\left(\frac{\pi x}{L}\right) + \cos\left(\frac{3\pi x}{L}\right) \right) = C \left( \cos\left(\frac{-\pi x}{L}\right) + \cos\left(\frac{-3\pi x}{L}\right) \right) = +C \left( \cos\left(\frac{\pi x}{L}\right) + \cos\left(\frac{3\pi x}{L}\right) \right)$ , the eigenvalue is +1
- ii.  $\hat{\Pi} C e^{-a\sqrt{x^2+3y^2+z^2}} = C e^{-a\sqrt{(-x)^2+3(-y)^2+(-z)^2}} = C e^{-a\sqrt{x^2+3y^2+z^2}}$ , the eigenvalue is +1
- iii.  $\hat{\Pi} C f(r) (\cos(\theta) + \cos^3(\theta)) e^{i\phi} = C f(r) (\cos(\pi - \theta) + \cos^3(\pi - \theta)) e^{i(\phi+\pi)} = C f(r) (-\cos(\theta) - \cos^3(\theta)) (-e^{i\phi}) = C f(r) (\cos(\theta) + \cos^3(\theta)) e^{i\phi}$ , the eigenvalue is +1
- (b) i.  $\hat{\Pi}(4\psi_+(x, y, z) + 2\psi_-(x, y, z)) = +4\psi_+(x, y, z) - 2\psi_-(x, y, z) \neq \lambda(4\psi_+(x, y, z) + 2\psi_-(x, y, z))$ , not an eigenfunction.
- ii.  $\hat{\Pi}^2(4\psi_+(x, y, z) + 2\psi_-(x, y, z)) = \hat{\Pi}(+4\psi_+(x, y, z) - 2\psi_-(x, y, z)) = 4\psi_+(x, y, z) + 2\psi_-(x, y, z)$ , an eigenfunction with eigenvalue +1.
- iii.  $\hat{\Pi} e^{-\alpha x} = e^{+\alpha x} \neq e^{-\alpha x}$  not an eigenfunction and neither is  $e^{+\alpha x}$ . We can however form linear combinations that have parity. The function  $e^{\alpha x} - e^{-\alpha x}$  has parity  $\hat{\Pi} e^{+\alpha x} - e^{-\alpha x} = e^{-\alpha x} - e^{+\alpha x} = -1(e^{+\alpha x} - e^{-\alpha x})$  with eigenvalue -1. The function  $e^{+\alpha x} + e^{-\alpha x}$  has parity  $\hat{\Pi} e^{+\alpha x} + e^{-\alpha x} = e^{-\alpha x} + e^{+\alpha x} = +1(e^{+\alpha x} + e^{-\alpha x})$  with eigenvalue +1.

4. The eigenfunctions of the infinite square well are (Physics handbook)

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

The correction to the eigenenergies due to perturbation is given by:

$$E_n^1 = \langle H_1 \rangle \text{ where } H_1 \text{ is the deviation in the potential from the infinite square well.}$$

$$E_n^1 = \int_0^{a/2} \frac{2\epsilon}{a} \sin^2 \frac{n\pi x}{a} dx = \int_0^{a/2} \frac{2\epsilon}{a^2} \left(1 - \cos \frac{2n\pi x}{a}\right) dx = \frac{\epsilon}{a} \left[x - \frac{a}{2n\pi} \sin \frac{2n\pi x}{a}\right]_0^{a/2} = \frac{\epsilon}{2}$$

This is the same for all  $n$ . The corrections for  $n=1$  and  $n=2$  are of interest (**answer to a**).

$$E_1^1 = E_2^1 = \frac{\epsilon}{2} = 0.0465\text{eV}.$$

The two lowest eigenenergies are

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2} = \frac{n^2 \hbar^2}{8ma^2} \quad [n = 1] \quad E_1 = 6.02465 \cdot 10^{-20}\text{J} = 0.376028\text{eV} \quad \text{and} \quad E_2 = 1.504114\text{eV}$$

The new energies for the two lowest levels are:

$$E_1^* = 0.376028 + 0.0465 = 0.422528 \approx 0.4225\text{eV} \quad \text{and} \quad E_2^* = 1.504114 + 0.0465 = 1.550614 \approx 1.551\text{eV}$$

The case of  $\epsilon = 1.09$  eV. This energy is much higher than the groundstate energy of the unperturbed model. You cannot use perturbation here. The model is more like a square well of width  $a/2$ . The answer of such a perturbation calculation would not give a trustworthy result.

5. (a) The total wave function has to be normalised which implies that the sum of the squared coefficients equals one.  $A^2(2^2 + 3^2 + 1^2 + 1^2) = 1$  resulting in  $A^2 = \frac{1}{15}$  and hence  $A = \frac{1}{\sqrt{15}}$ .

- (b) The probability is given by the absolute square of the coefficients.

$$(\Psi(\mathbf{r}, t = 0) = \frac{1}{\sqrt{15}} (2\psi_{100}(\mathbf{r}) - 3\psi_{211}(\mathbf{r}) + \psi_{320}(\mathbf{r}) - \psi_{322}(\mathbf{r})))$$

The probabilities are (in order)  $\frac{4}{15}, \frac{9}{15}, \frac{1}{15}, \frac{1}{15}$ . as a check they sum up to 1 as they should do.

- (c) The energy of a single eigenstate is given by:  $E_n = -\frac{13.56}{n^2}$  eV. The expectation value is given by  $\langle E \rangle = \frac{4}{15}(-\frac{13.56}{1^2}) + \frac{9}{15}(-\frac{13.56}{2^2}) + \frac{1}{15}(-\frac{13.56}{3^2}) + \frac{1}{15}(-\frac{13.56}{3^2}) = -13.56(\frac{4}{15} + \frac{9}{60} + \frac{1}{135} + \frac{1}{135}) = -13.56 \frac{233}{540} = -5.807868 \approx -5.81$  eV

The operator  $\mathbf{L}^2$  has eigenvalues  $\hbar^2 l(l+1)$ . The expectation value is given by  $\langle \mathbf{L}^2 \rangle = \frac{4}{15} \cdot 0 + \frac{9}{15} \cdot (\hbar^2 1(1+1)) + \frac{1}{15} (\hbar^2 2(2+1)) + \frac{1}{15} (\hbar^2 2(2+1)) = \frac{30}{15} \hbar^2 = 2\hbar^2$

The operator  $L_z$  has eigenvalues  $\hbar m_l$ . The expectation value is given by  $\langle L_z \rangle = \frac{4}{15} \cdot 0 + \frac{9}{15} \cdot 1\hbar + \frac{1}{15} \cdot 0 + \frac{1}{15} (2\hbar) = \frac{11}{15} \hbar$