LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in QUANTUM PHYSICS F0047T

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1. (a) $\langle H\rangle = \frac{1}{2}0.25 + \frac{1}{4}0.95 + \frac{1}{6}2.12 + \frac{1}{24}3.23 + \frac{1}{24}4.79 = 1.05\text{eV}$.
   Uncertainty is defined by: $\langle \Delta H\rangle = \sqrt{\langle H^2\rangle - \langle H\rangle^2}$
   $\langle H^2\rangle = \frac{1}{2}(0.25)^2 + \frac{1}{4}(0.95)^2 + \frac{1}{6}(2.12)^2 + \frac{1}{24}(3.23)^2 + \frac{1}{24}(4.79)^2 = 2.39665 \approx 2.40(\text{eV})^2$.
   $\langle \Delta H\rangle = \sqrt{3.44665 - 1.05^2} = 1.13761 \approx 1.14\text{eV}$

   (b) The expression is not unique as we only know the probabilities which are the squares of the coefficients. In the evaluation of $\langle H\rangle$ and $\langle H^2\rangle$ only the probabilities are important thats why a different sign $\pm$ is of no importance in this calculation.
   One is: $\Psi(z) = \frac{1}{\sqrt{2}}\psi_1(z) + \frac{1}{2}\psi_2(z) + \frac{1}{\sqrt{6}}\psi_3(z) + \frac{1}{\sqrt{24}}\psi_4(z) + \frac{1}{\sqrt{24}}\psi_5(z)$.

   Another is: $\Psi(z) = \frac{1}{\sqrt{2}}\psi_1(z) + \frac{1}{2}\psi_2(z) - \frac{1}{\sqrt{6}}\psi_3(z) + \frac{1}{\sqrt{24}}\psi_4(z) - \frac{1}{\sqrt{24}}\psi_5(z)$.

   (c) Decrease by a factor of 4, or lowered by a factor of 4. (All eigenvalues change by a factor of 4)

2. (a) An appropriate model to use is a **particle in a box** in 1, 2 or 3 dimensions of size $L = 1$ fm$= 1\cdot 10^{-15}$m. Here a calculation of the 3 dimensional version is made. The eigenenergys of the particle in the box in one dimension are given by:

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad \text{where} \quad n = 1, 2, 3, ...$$

   and in three dimensions this will become:

$$E_{n_x,n_y,n_z} = \frac{\pi^2\hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2) \quad \text{where} \quad n_{x,y,z} = 1, 2, 3, ...$$

   Use the ground state to calculate the estimate.

$$E_{1,1,1} = \frac{3\pi^2\hbar^2}{2mL^2} = \frac{3\pi^2(1.054\cdot 10^{-34})^2}{2\cdot 9.1094\cdot 10^{-31}\cdot 1\cdot 10^{-30}\cdot 1.6022\cdot 10^{-19}} = 1.13\cdot 10^{12}\ \text{eV} \approx 1\ \text{TeV}$$

   Note this is a very high energy !

   (b) Another appropriate model you may use is the **spherical box** in 3 dimensions.

   (c) Another appropriate model you may use is the **harmonic oscillator** in 1, 2 or 3 dimensions. This is perhaps not a really good box as the walls are not very hard as box actually will consist of a parabola. The energy of the ground state in 3 dimensions is

$$E_{0,0,0} = \frac{3}{2}\hbar\omega$$

   Now the frequence ω has to be determined. The strenght (and shape of parabola) is determined by ω. To connect the length scale to ω we can use the an appropriate expectation value for x. $< x >= 0$ cannot be used but $< x^2 >= (n + \frac{1}{2})\frac{\hbar}{m\omega}$ with $n = 0$ we have $< x^2 >= \frac{1}{2}\frac{\hbar}{m\omega}$. Now an estimate for $< x^2 >= \frac{1}{4}10^{-30}$.

$$E_{0,0,0} = \frac{3}{2}\hbar\frac{1}{2}\frac{\hbar}{m < x^2 >} = \frac{3(1.054\cdot 10^{-34})^2}{4\cdot 9.1094\cdot 10^{-31}\cdot 0.25\cdot 10^{-30}\cdot 1.6022\cdot 10^{-19}} = 2.28\cdot 10^{11}\ \text{eV}$$

Whatever model one applies the energy will be very high. In the case of the harmonic oscillator also an estimate had to be made for ω. Also the harmonic oscillator does not have as 'hard' walls as the walls of an infinite box. As one can argue for any of these three models an answer in the range of 0.1 - 1 TeV is reasonable.

3. The Carbon ion has $Z = 6$ and hence energys $E_n = -\frac{488.16}{n^2}$eV. Try to find a start of the series. The energy of $\lambda = 207.80$nm is $E = h\nu = \frac{hc}{\lambda} = \frac{6.626\cdot10^{-34}\cdot2.9979\cdot10^{8}}{207.80\cdot10^{-9}\cdot1.6022\cdot10^{-19}} = 5.9663$eV A similar calculation gives the energys for the other lines in the series: 9.56395, 11.8989 and 13.4997 eV.

   As the Balmer series in Hydrogen is for transitions down to level n=2 we have to go higher up for the Carbon ion as the energys for the level $n = 2$ in Carbon would be far to large.

   Using the fact that can assume levels are adjecent we let n be the quantum number for the lower level and m for a level above, we have no knowledge of how n and m relate. We know however that for the next level (higher in energy) we have n and $m + 1$. One can form the following two equations 5.9663eV=488.16($\frac{1}{n^2} - \frac{1}{m^2}$)eV and 9.56395eV=488.16($\frac{1}{n^2} - \frac{1}{(m+1)^2}$)eV ie we only need two of the lines to form an appropriate set of equations. (You can use the other pairs of lines as well to form two equations.) Subtracting one equation from the other to eliminat n you get 3.59765=488.16($\frac{1}{m^2} - \frac{1}{(m+1)^2}$) and $\frac{1}{m^2} - \frac{1}{(m+1)^2} = 0.007369817273025237627$ solving for m you arrive at $m = 6$. Now we use the result for m in 5.9663eV=488.16($\frac{1}{n^2} - \frac{1}{6^2}$)eV to solve for n and we arrive at $n = 5$.

   Then there is the tour of brute force ie just trial and error: If we try n=5 we have transitions from m=6, 7, 8, 9, etc. The corresponding energys will be: 488.16($\frac{1}{5^2} - \frac{1}{6^2}$)=5.97 eV, the next one will be: 488.16($\frac{1}{5^2} - \frac{1}{7^2}$)=9.56 eV, 488.16($\frac{1}{5^2} - \frac{1}{8^2}$)=11.899 eV and so on. So these are down to n=5 from level m=6, 7, 8 and 9.

4. 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 Ψ $\left(\Psi(-\frac{a}{2}) = \Psi(\frac{a}{2}) = 0\right)$ 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 $\int_{-a/2}^{a/2} \mid \Psi \mid^2 dx = 1$. The condition $\sin(\frac{ka}{2}) = 0$ gives $\frac{ka}{2} = \frac{\pi}{2} * (even - integer)$. The solution is:

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

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

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

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:

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

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: Ψ ($\Psi(0) = \Psi(a) = 0$) into account. In this case the solution is for these boundary conditions:

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

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

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

$\psi_n(x) = \sqrt{\frac{2}{a}} \sin(\frac{n\pi x}{a} + \frac{n\pi}{2}) = \sqrt{\frac{2}{a}} \left(\sin(\frac{n\pi x}{a}) \cdot \cos(\frac{n\pi}{2}) + \cos(\frac{n\pi x}{a}) \cdot \sin(\frac{n\pi}{2})\right)$. We see that we recover the solution in eq (1), (2) and (3) as we let n run from 1 to ∞.

b) Now we turn to the question of **parity**, ie whether the wave function is *odd* or *even* under a change of coordinates from (x, y) to $(-x, -y)$. The one dimensional eigenfunctions in eq (1) and (2) have a definite parity. The functions in (1) are odd whereas the functions in (2) are even. As the eigenstates for the 2 dimensional system are formed from eq (3) ie products of functions that are even or odd the total function itself will be either even or odd as well.

The four lowest eigenenergies are given by

$$E_{n,m} = \frac{\pi^2\hbar^2}{2Ma^2}(n^2 + m^2), \quad \text{where the 4 lowest are} \quad (n^2 + m^2) = 2, 5, 8, 10.$$

When we form the eigenstates we need to keep track of the parity of the $\psi_n(x)$ and $\psi_m(y)$. It is therefore necessary to have the functions in the form like in eq (1) and (2) to identify the parity as odd or even. This is difficult if you try with functions like eq (5) even though it is a correct eigenstate it is hard to identify their parity.

$$E_{1,1} = \text{ one state } \ (n^2+m^2=2) \qquad \text{even * even = even}$$
$$E_{1,2} = E_{2,1} = \text{ two states } \ (n^2+m^2=5) \qquad \text{even * odd = odd}$$
$$E_{2,2} = \text{ one state } \ (n^2+m^2=8) \qquad \text{odd * odd = even}$$
$$E_{1,3} = E_{3,1} = \text{ two states } \ (n^2+m^2=10) \qquad \text{even * even = even}$$

So of the four states only one is odd and three where even.

5. The task is to calculate the change of the difference between to 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.

$$E_1^1 - E_0^1 = E_1^1 + \langle 1 \mid H^1 \mid 1\rangle - \left(E_0^1 + \langle 0 \mid H^1 \mid 0\rangle\right)$$

The two harmonic oscillator eigenfunctions that are of interest are :

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

The first integral to calculate (use integration by parts) will be for the change of the ground state energy

$$\langle 0 \mid H^1 \mid 0\rangle = \int \psi_0^*(x)H^1\psi_0(x)dx = \int \frac{\alpha}{\sqrt{\pi}}Ax^4\ e^{-\alpha^2x^2}dx = [\alpha x = y] = \frac{A}{\alpha^4\sqrt{\pi}}\int y^4\ e^{-y^2}dy$$

where the integral taken separatelly will be

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

Hence the shift of the ground state energy will be

$$\langle 0 \mid H^1 \mid 0\rangle = \frac{A}{\alpha^4\sqrt{\pi}}\frac{3}{4}\sqrt{\pi} = \frac{3A}{4\alpha^4} = \frac{3A}{4}\left(\frac{\hbar}{m\omega}\right)^2$$

The second integral to calculate (use integration by parts) will be for the change of the energy of the lowest excited state.

$$\langle 1 \mid H^1 \mid 1\rangle = \int \psi_1^*(x)H^1\psi_1(x)dx = \int \frac{\alpha}{2\sqrt{\pi}}Ax^4\ 4\alpha^2x^2e^{-\alpha^2x^2}dx = [\alpha x = y] = \frac{4A}{\alpha^4\sqrt{\pi}}\int y^6\ e^{-y^2}dy$$

where the integral taken separatelly will be

$$\int_{-\infty}^{\infty} y^6\ e^{-y^2}dy = [-\frac{y^5}{2}e^{-y^2}]_{-\infty}^{\infty} + \int_{-\infty}^{\infty}\frac{5y^4}{2}e^{-y^2} = [-\frac{5y^3}{4}e^{-y^2}]_{-\infty}^{\infty} + \int_{-\infty}^{\infty}\frac{15y^2}{4}e^{-y^2} =$$
$$= [-\frac{15y^1}{8}e^{-y^2}]_{-\infty}^{\infty} + \int_{-\infty}^{\infty}\frac{15}{8}e^{-y^2} = \frac{15}{8}\sqrt{\pi}$$

Hence the shift of the energy of the lowest excited state will be

$$\langle 1 \mid H^1 \mid 1\rangle = \frac{4A}{\alpha^4\sqrt{\pi}}\frac{15}{8}\sqrt{\pi} = \frac{15A}{8\alpha^4} = \frac{15A}{8}\left(\frac{\hbar}{m\omega}\right)^2$$

The difference in the perturbed energys will be

$$E_1^1 - E_0^1 = \frac{3}{2}\hbar\omega + \frac{15A}{8\alpha^4} - (\frac{1}{2}\hbar\omega + \frac{3A}{4\alpha^4}) = \hbar\omega + \frac{9A}{8\alpha^4} = \hbar\omega + \frac{9A}{8}\left(\frac{\hbar}{m\omega}\right)^2$$

Note that the constant A has dimension.