LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in QUANTUM PHYSICS F0047T

Examination date: 2016-08-27
The solutions are just suggestions. They may contain several alternative routes.

1. Note: As the task is 'solve the Schrödinger equation' failing to do so will result in nought points.

   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 on for y. We therefor 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 ($\Psi(0) = \Psi(a) = 0$) into account.
   $$A\cos(0) + B\sin(0) = 0 \text{ and } A\cos(ka) + B\sin(ka) = 0$$

   From the first relation we get $A = 0$. From the second we get $B\sin(ka) = 0$ where $ka = n\pi$ with $n = 1, 2, 3, ...$ and hence $k = \frac{n\pi}{a}$. The normalising constant $B = \sqrt{\frac{2}{a}}$ you get from the condition $\int_{-a/2}^{a/2} |\Psi|^2 \, dx = 1$.

   The solution is:

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

   By analogy the y directions is treated in a similar fasion but with a different size of box.

   The solution is:

   $$\psi_m(y) = \frac{2}{\sqrt{a}}\sin(\frac{2m\pi y}{a}) \;\text{ with eigenenergys } E_m = \frac{2m^2\pi^2\hbar^2}{Ma^2} \;\;\text{ where }\;\; m = 1, 2, 3, ... \qquad (2)$$

   Now we have the eigenfunctions of the one dimensional problem and the solution to the 2 dimensional problem is readily produced. The eigenfunctions are:

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

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

b) The ground state eigenfunction is given by (using eq. (3))

$$\Psi_{n=1,m=1}(x,y) = \psi_1(x) \cdot \psi_1(y) = \sqrt{\frac{2}{a}} \sin(\frac{\pi x}{a}) \cdot \frac{2}{\sqrt{a}} \sin(\frac{2\pi y}{a}) \tag{4}$$

The next lowest state (in energy) eigenfunction is given by (using eq. (1) and (2)). Note there is only one eigenfunction as ($\Psi_{n=1,m=2}(x,y)$) has an higher energy.

$$\Psi_{n=2,m=1}(x,y) = \psi_2(x) \cdot \psi_1(y) = \sqrt{\frac{2}{a}} \sin(2\frac{\pi x}{a}) \cdot \frac{2}{\sqrt{a}} \sin(\frac{2\pi y}{a}) \tag{5}$$

Orthogonality is defined as

$$\int_x \int_y \Psi_{n_1,m_1}(x,y) \Psi_{n_2,m_2}(x,y) = \delta_{n_1,n_2} \, \delta_{m_1,m_2} \tag{6}$$

by explicit calculation

$$\int_{x=0}^{a} \int_{y=0}^{a/2} \left(\frac{2\sqrt{2}}{a} \sin(\frac{\pi x}{a}) \cdot \sin(\frac{2\pi y}{a}) \right) \cdot \left(\frac{2\sqrt{2}}{a} \sin(2\frac{\pi x}{a}) \cdot \sin(\frac{2\pi y}{a}) \right) = \text{calculations} = 0 \tag{7}$$

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) The parity of a hydrogen eigenfunction $\psi_{nlm_l}(\mathbf{r})$ is given by $(-1)^l$. The given wave function $\Psi(\mathbf{r})$ consists of eigenfunctions with the same parity. Hence $\Psi(\mathbf{r})$ has a definite parity.

   (b) The probability is given by the absolute square of the coefficients.
   ($\Psi(\mathbf{r}, t=0) = \frac{1}{\sqrt{15}} (3\psi_{100}(\mathbf{r}) - 2\psi_{200}(\mathbf{r}) + \psi_{320}(\mathbf{r}) - \psi_{322}(\mathbf{r}))$)
   The probabilities are (in order) $\frac{9}{15}, \frac{4}{15}, \frac{1}{15}, \frac{1}{15}$. 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 $< E >= \frac{9}{15}(-\frac{13.56}{1^2}) + \frac{4}{15}(-\frac{13.56}{2^2}) + \frac{1}{15}(-\frac{13.56}{3^2}) + \frac{1}{15}(-\frac{13.56}{3^2}) =$
   $-13.56(\frac{9}{15} + \frac{4}{60} + \frac{1}{135} + \frac{1}{135}) = -9.240889 \approx -9.24$ eV
   The operator $\mathbf{L}^2$ has eigenvalues $\hbar^2 l(l+1)$. The expectation value is given by
   $< \mathbf{L}^2 >= \frac{9}{15} \cdot 0 + \frac{4}{15} \cdot 0 + \frac{1}{15}(\hbar^2 2(2+1)) + \frac{1}{15}(\hbar^2 2(2+1)) = \frac{12}{15}\hbar^2 = \frac{4}{5}\hbar^2$
   The operator L_z has eigenvalues $\hbar m_l$. The expectation value is given by
   $< L_z >= \frac{9}{15} \cdot 0 + \frac{4}{15} \cdot 0 + \frac{1}{15} \cdot 0 + \frac{1}{15}(\hbar 2) = \frac{2}{15}\hbar$

3. The task is to calculate the change of the difference between two 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.

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

The two harmonic oscillator eigenfunctions that are of interest are :

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

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

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

where the integral taken separately will be

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

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.

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

where the integral taken separately 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

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

The difference in the perturbed levels energys will be

$$E_1^1 - E_0^1 = \frac{3}{2}\hbar\omega + \frac{15A}{4\alpha^4} - (\frac{1}{2}\hbar\omega + \frac{3A}{4\alpha^4}) = \hbar\omega + \frac{12A}{4\alpha^4} = \hbar\omega + 3A \left(\frac{\hbar}{m\omega} \right)^2$$

Note that the constant A has dimension.

4. (a) The mean position of the particle is

$$< x >= \int_{-\infty}^{\infty} \psi^*(x) x \psi^*(x) dx = \frac{\gamma}{\sqrt{\pi}} \int_{-\infty}^{\infty} x e^{-\gamma^2 x^2} dx = 0$$

(b) The mean momentum of the particle is

$$< p >= \int_{-\infty}^{\infty} \psi^*(x) \frac{\hbar}{i} (\frac{d}{dx} \psi(x)) dx = \frac{\gamma\hbar}{\sqrt{i\pi}} \int_{-\infty}^{\infty} e^{-\gamma^2 x^2/2} \frac{d}{dx} e^{-\gamma^2 x^2/2} dx = 0$$

(c) The Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\psi(x)$$

can be written as

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = [E - V(x)]\psi(x).$$

As

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}e^{-\gamma^2 x^2/2} = -\frac{\hbar^2}{2m}(-\gamma^2 + \gamma^4 x^2)e^{-\gamma^2 x^2/2}$$

we have

$$E - V(x) = -\frac{\hbar^2}{2m}(-\gamma^2 + \gamma^4 x^2)$$

or

$$V(x) = \frac{\hbar^2}{2m}(-\gamma^2 + \gamma^4 x^2) + \frac{\hbar^2\gamma^2}{2m} = \frac{\hbar^2\gamma^4 x^2}{2m}$$

5. a) There are 4 states the system can have with the energys and (degeneracys) $\hbar\omega$ (1), $2\hbar\omega$ (2) and $3\hbar\omega$ (1). The partition sum is given by:

$$Z = \sum_{n_1=0,n_2=0}^{n_1=1,n_2=1} e^{-(n_1+n_2+1.0)\hbar\omega/k_B T} = e^{-1.0\hbar\omega/k_B T} + 2e^{-2.0\hbar\omega/k_B T} + e^{-3.0\hbar\omega/k_B T}$$

b) There is one state of the lower energy and **two** states with the next higher energy. The probability to find the system in a state of energy is proportional to the Boltzmann factor, we arrive at the following equation.

$$\frac{1e^{-1,0\hbar\omega/k_B T}}{Z} = \frac{2e^{-2,0\hbar\omega/k_B T}}{Z} \tag{8}$$

and $e^{1\hbar\omega/k_B T} = 2$ which evaluates to $T = \frac{1\hbar\omega}{k_B \ln 2}$.

c) The partition sum at this specific temperature is given by: ($k_B T = \frac{1\hbar\omega}{\ln 2}$) ($\frac{1}{k_B T} = \frac{\ln 2}{1\hbar\omega}$) we arrive at the following

$$Z = e^{-1.0\hbar\omega/k_B T} + 2e^{-2.0\hbar\omega/k_B T} + e^{-3.0\hbar\omega/k_B T} = e^{-1.0\ln 2} + 2e^{-2.0\ln 2} + e^{-3.0\ln 2} =$$

$$\frac{1}{2} + 2\frac{1}{4} + \frac{1}{8} = \frac{1}{2} + \frac{1}{2} + \frac{1}{8} = 1 + \frac{1}{8} = \frac{9}{8}$$

The probability P will be (put Z into one of the terms in eq (8).

$$P = \frac{e^{-1,0\ln 2}}{\frac{9}{8}} = \frac{1}{2}\cdot\frac{8}{9} = \frac{4}{9} \approx 0.444...$$

As a check we can calculate for the state with the highest energy

$$P_3 = \frac{e^{-3,0\ln 2}}{\frac{9}{8}} = \frac{1}{8}\cdot\frac{8}{9} = \frac{1}{9} \approx 0.111...$$

and we can easily conclude the probabilities add up to one.

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