LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

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) $i\hbar\frac{\partial^2}{\partial t^2}\cos\omega t = -i\hbar\omega\frac{\partial}{\partial t}\sin\omega t = -i\hbar\omega^2\cos\omega t$ **YES**

   (b) $\frac{\partial}{\partial x}e^{ikx} = ike^{ikx}$ **YES**

   (c) $\frac{\partial}{\partial x}e^{-ax^2} = -2axe^{-ax^2}$ **NO**

   (d) $\frac{\partial}{\partial x}\cos kx = -k\sin kx$ **NO**

   (e) $\frac{\partial}{\partial x}kx = k$ **NO**

   (f) $\hat{P}\sin(kx) = \sin(-kx) = -\sin(kx)$ **YES**

   (g) $-i\hbar\frac{\partial}{\partial z}C(1+z^2) = -i\hbar C(0+2z)$ **NO**

   (h) $-\frac{\hbar}{2}\frac{\partial}{\partial z}Ce^{-3z} = -\frac{\hbar}{2}C(-3)e^{-3z} \ \propto\ \psi(z)$ **YES**

   (i) $\frac{C}{2}(z^2 - \frac{\partial^2}{\partial z^2})ze^{-\frac{1}{2}z^2} =?$ This has to be done in some steps. Start by doing this derivative first: $-\frac{\partial^2}{\partial z^2}ze^{-\frac{1}{2}z^2} = -\frac{\partial}{\partial z}(e^{-\frac{1}{2}z^2} - z^2e^{-\frac{1}{2}z^2}) = -(-ze^{-\frac{1}{2}z^2} - 2ze^{-\frac{1}{2}z^2} + z^3e^{-\frac{1}{2}z^2}) = 3ze^{-\frac{1}{2}z^2} - z^3e^{-\frac{1}{2}z^2}$.

   Now you go back to the start: $\frac{C}{2}(z^2 - \frac{\partial^2}{\partial z^2})ze^{-\frac{1}{2}z^2} = \frac{C}{2}(z^3e^{-\frac{1}{2}z^2} + 3ze^{-\frac{1}{2}z^2} - z^3e^{-\frac{1}{2}z^2}) = \frac{C}{2}(+3ze^{-\frac{1}{2}z^2}) = \propto\ \psi(z)$ **YES**

2. 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 :

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

   (a) Here we have a perturbation γx^4 where γ is small in some sence. The first integral to calculate (use integration by parts) will be for the change of the ground state energy

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

   where the integral taken separately will be

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

   Hence the shift of the ground state energy will be

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

   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 ϵx where ϵ is small in some sence. The integrals to be calculated are $\langle 0 \mid \epsilon x \mid 0 \rangle$ and $\langle 1 \mid \epsilon x \mid 1 \rangle$. 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.

3. The eigenfunctions and eigenvalues of the free-particle Hamiltonian are found by solving the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} + V(x)u(x) = Eu(x),$$

with $V(x)$ zero everywhere. Thus, the eigenvalue equation reads

$$\frac{d^2u(x)}{dx^2} + k^2u(x) = 0,$$

where $k^2 = 2mE/\hbar^2$. The eigenfunctions are given by the plane waves e^{ikx} and e^{-ikx}, or linear combinations of these, as *e.g.* $\sin kx$ and $\cos kx$.

(a) The wave function of the particle at $t = 0$ is given by

$$\psi(x, 0) = \cos^3(kx) + \sin^3(kx).$$

This is not an eigenfunction in itself but it can be written as sum of eigenfunctions using the Euler relations

$$\psi(x,0) = \left(\frac{e^{ikx} + e^{-ikx}}{2}\right)^3 + \left(\frac{e^{ikx} - e^{-ikx}}{2i}\right)^3 = \tag{1}$$

$$\frac{1}{8}\left(e^{i3kx} + 3e^{ikx} + 3e^{-ikx} + e^{-i3kx}\right) - \frac{1}{8i}\left(e^{i3kx} - 3e^{ikx} + 3e^{-ikx} - e^{-i3kx}\right) = \tag{2}$$

$$\frac{3}{4}\cos(kx) + \frac{1}{4}\cos(3kx) + \frac{3}{4}\sin(kx) - \frac{1}{4}\sin(3kx) \tag{3}$$

Thus, $\psi(x, 0)$ can be written as a superposition of plane waves with two different values of $k_1 = k$ and $k_2 = 3k$.

(b) The energy of a plane wave e^{ikx} is given by $E = \hbar^2k^2/2m$. Thus, the energy of e^{ik_1x} (or e^{-ik_1x}) is $E_1 = \hbar^2k^2/2m$ and the energy of e^{ik_2x} (or e^{-ik_2x}) is $E_2 = \hbar^2k_2^2/2m = 9\hbar^2k^2/2m$.

(c) The function $u(x) = e^{ikx}$ is a solution to the the time-independent Schrödinger equation. The corresponding solutions to the time-dependent Schrödinger equation are given by $u(x)T(t)$,with $T(t) = e^{-iEt/\hbar}$. Therefore, $u(x)T(t) = e^{i(kx-Et/\hbar)}$. A sum of solutions of this form is also a solution, since the Schrödinger equation is linear. This means that if $\psi(x, 0)$ is given by equation (3), then the time dependent solution is given by

$$\psi(x,t) = \frac{1}{8}\left(e^{i3kx} + e^{-i3kx}\right)e^{-iE_2t/\hbar} + \frac{3}{8}\left(e^{ikx} + e^{-ikx}\right)e^{-iE_1t/\hbar} + \tag{4}$$

$$\frac{1}{8i}\left(e^{i3kx} - e^{-i3kx}\right)e^{-iE_2t/\hbar} - \frac{3}{8i}\left(e^{ikx} - e^{-ikx}\right)e^{-iE_1t/\hbar} \tag{5}$$

where

$$E_1 = \frac{\hbar^2k^2}{2m} \quad \text{and} \quad E_2 = \frac{9\hbar^2k^2}{2m} \tag{6}$$

4. **a** The strategy is to rewrite the wave function as a series of eigenfunctions. The three harmonic oscillator eigenfunctions (from PH) that are of interest are (evident from the powers of x present in the wave function):

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

$$\psi_2(x) = \sqrt{\frac{\alpha}{8\sqrt{\pi}}}(4\alpha^2x^2 - 2)\ e^{-\frac{1}{2}\alpha^2x^2} \quad \text{where} \quad \alpha = \sqrt{\frac{m\omega}{\hbar}}$$

Start by making a change of variables:

$$y = \sqrt{\frac{m\omega}{\hbar}}x = \alpha x \quad \text{and} \quad \alpha = \sqrt{\frac{m\omega}{\hbar}}$$

With this change the eigenfunctions become:

$$\psi_0(y) = \sqrt{\frac{\alpha}{\sqrt{\pi}}}\ e^{-\frac{1}{2}y^2}\ ;\ \psi_1(y) = \sqrt{\frac{\alpha}{2\sqrt{\pi}}}2y\ e^{-\frac{1}{2}y^2}\ ;\ \psi_2(y) = \sqrt{\frac{\alpha}{8\sqrt{\pi}}}(4y^2 - 2)\ e^{-\frac{1}{2}y^2}$$

Start with the wavefunction:

$$\Psi(x, t = 0) = A\left(1 + 2\sqrt{\frac{m\omega}{\hbar}}x\right)^2 e^{-\frac{m\omega}{2\hbar}x^2} = A(1 - 2y)^2 e^{-y^2/2} = A(1 - 4y + 4y^2)e^{-y^2/2}$$

Start with the y^2 term:

$$\psi_2(y) = \sqrt{\frac{\alpha}{8\sqrt{\pi}}}(4y^2 - 2)\ e^{-\frac{1}{2}y^2} \text{ transforms to } (4y^2 - 2)\ e^{-\frac{1}{2}y^2} = \sqrt{\frac{8\sqrt{\pi}}{\alpha}}\psi_2(y)$$

In a similar way we rewrite the two others

$$2y\ e^{-\frac{1}{2}y^2} = \sqrt{\frac{2\sqrt{\pi}}{\alpha}}\psi_1(y) \quad \text{and} \quad e^{-\frac{1}{2}y^2} = \sqrt{\frac{\sqrt{\pi}}{\alpha}}\psi_0(y)$$

Now we are ready to make an identifacation like: This we can identify in the following manner:

$$\Psi(x, t = 0) = C_0\psi_0(x) + C_1\psi_1(x) + C_2\psi_2(x)$$

$$\Psi(x, t = 0) = A(1 - 4y + 4y^2)e^{-y^2/2} = A(\sqrt{\frac{\sqrt{\pi}}{\alpha}}\psi_0(y) - 2\sqrt{\frac{2\sqrt{\pi}}{\alpha}}\psi_1(y) + \sqrt{\frac{8\sqrt{\pi}}{\alpha}}\psi_2(y) + 2\sqrt{\frac{\sqrt{\pi}}{\alpha}}\psi_0(y))$$

$$\Psi(x, t = 0) = A(3\sqrt{\frac{\sqrt{\pi}}{\alpha}}\psi_0(y) - 2\sqrt{\frac{2\sqrt{\pi}}{\alpha}}\psi_1(y) + \sqrt{\frac{8\sqrt{\pi}}{\alpha}}\psi_2(y))$$

In order to calculate the expecation value of the energy we need to normalize the wavefunction.

$$A^2(3^2\frac{\sqrt{\pi}}{\alpha} + 2^2\frac{2\sqrt{\pi}}{\alpha} + \frac{8\sqrt{\pi}}{\alpha}) = 1$$

$$A^2(9 + 8 + 8) = A^2 25 = \frac{\alpha}{\sqrt{\pi}}$$

Solving for A gives

$$A = \sqrt{\frac{\alpha}{25\sqrt{\pi}}}$$

$$\Psi(x, t = 0) = \sqrt{\frac{\alpha}{25\sqrt{\pi}}} \left(3\sqrt{\frac{\sqrt{\pi}}{\alpha}} \psi_0(y) - 2\sqrt{\frac{2\sqrt{\pi}}{\alpha}} \psi_1(y) + \sqrt{\frac{8\sqrt{\pi}}{\alpha}} \psi_2(y) \right)$$

And finally the wavefunction is expressed in terms of eigenfunctions

$$\Psi(x, t = 0) = \frac{3}{5}\psi_0(y) - \sqrt{\frac{8}{25}}\psi_1(y) + \sqrt{\frac{8}{25}}\psi_2(y)$$

Now we can calculate the expecation value of the energy as

$$E = \langle H \rangle = \frac{9}{25}\frac{\hbar\omega}{2} + \frac{8}{25}\frac{3\hbar\omega}{2} + \frac{8}{25}\frac{5\hbar\omega}{2} = \frac{73\hbar\omega}{50}$$

b The general expresssion for $\Psi(x, t)$ is $\Psi(x, t) = \sum_{n=0}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}$ as $E_n = (n + \frac{1}{2})\hbar\omega$ we get

$$\Psi(x, t) = \frac{3}{5}\psi_0(y)e^{-i\omega t/2} - \sqrt{\frac{8}{25}}\psi_1(y)e^{-i3\omega t/2} + \sqrt{\frac{8}{25}}\psi_2(y)e^{-i5\omega t/2} =$$

$$e^{-i\omega t/2} \left(\frac{3}{5}\psi_0(y) - \sqrt{\frac{8}{25}}\psi_1(y)e^{-i\omega t} + \sqrt{\frac{8}{25}}\psi_2(y)e^{-i2\omega t} \right)$$

The important issue is to change the negative sign to a positive ie. $e^{-i\omega t} = 1$ and hence $\omega T = m\pi$ and the smallest non zero time is therefore $T = \pi/\omega$. (The second term $e^{-i2\omega t}$ is allways 1 under this condition. The smallest time is

$$T = \frac{\pi}{\omega}$$

5. (a) $\langle H \rangle = \frac{1}{2}0.25 + \frac{1}{4}0.95 + \frac{1}{6}2.12 + \frac{1}{24}3.23 + \frac{1}{24}4.79 = 1.05000 \approx 1.05\text{eV}$.
   Uncertainty is defined by: $\langle \Delta H \rangle = \sqrt{\langle H^2 \rangle - \langle H \rangle^2}$
   $\langle H^2 \rangle = \frac{1}{2}0.25^2 + \frac{1}{4}0.95^2 + \frac{1}{6}2.12^2 + \frac{1}{24}3.23^2 + \frac{1}{24}4.79^2 = 2.39665 \approx 2.40\text{eV}^2$.
   $\langle \Delta H \rangle = \sqrt{2.39665 - 1.05^2} = 1.1376 \approx 1.14\text{eV}$

   (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: $\Psi(z) = \frac{1}{\sqrt{2}}\psi_1(z) + \sqrt{\frac{1}{4}}\psi_2(z) + \frac{1}{\sqrt{6}}\psi_3(z) + \frac{\sqrt{1}}{24}\psi_4(z) + \frac{1}{24}\psi_5(z)$.
   Another is: $\Psi(z) = \frac{1}{\sqrt{2}}\psi_1(z) + \sqrt{\frac{1}{4}}\psi_2(z) - \frac{1}{\sqrt{6}}\psi_3(z) - \frac{\sqrt{1}}{24}\psi_4(z) + \frac{1}{24}\psi_5(z)$.

   (c) It would be lowered by a factor of 9. (All eigenvalues change by a factor of 9)