Homework 10, solutions

problem 1, solution

a) The initial state is $\Phi_0 = \psi_{nem}(\vec{r})\,\phi_i(\vec{r}_1,\vec{r}_2,\cdots\vec{r}_Z)$. The final state is $\Phi_1 = \frac{1}{\sqrt{V}}\, e^{i\vec{k}\cdot\vec{r}}\,\phi_f(\vec{r}_1,\vec{r}_2,\cdots\vec{r}_Z)$. The final state is a plane wave, we use box normalization. We confine the plane wave to a box of volume $V = L^3$ and use periodic boundary conditions.
The matrix element needed to calculate the internal conversion rate is $\langle\Phi_1|W|\Phi_0\rangle = \frac{1}{\sqrt{V}}\int d^3r\, e^{-i\vec{k}\cdot\vec{r}}\langle\phi_f(\vec{r}_1,\cdots\vec{r}_Z)|\sum_{i=1}^{Z}\frac{e^2}{|\vec{r}-\vec{r}_i|}|\phi_i(\vec{r}_1,\cdots\vec{r}_Z)\rangle\,\psi_{nem}(\vec{r})$.

b) We find the internal conversion rate using Fermi's golden rule

$$W_{0\to1} = \frac{2\pi}{\hbar}\,\rho(E_1)\,|W_{10}|^2\,\delta(E_1-E_0),$$ We need to find $\rho(E_1)$.

The energy eigenstates of a free electron confined to a cubical box with periodic boundary conditions are $\phi_{n_xn_yn_z}(x,y,z) = \sqrt{\frac{1}{L^3}}\,e^{i\frac{2\pi}{L}(n_xx+n_yy+n_zz)}$, with $n_x, n_y, n_z = 0, \pm1, \pm2, \cdots$.
We have $k_x = \frac{2\pi}{L}n_x$, $k_y = \frac{2\pi}{L}n_y$, and $k_z = \frac{2\pi}{L}n_z$.

If k is large, then the number of states with a wave vector whose magnitude lies between k and $k+dk$ is $dN = \frac{4\pi k^2dk}{(2\pi/L)^3} = \frac{4\pi V k^2dk}{(2\pi)^3}$,

$$\frac{dN}{dk} = \frac{4\pi Vk^2}{(2\pi)^3}.$$

The density of states is $\frac{dN}{dE} = \frac{dN}{dk}\frac{dk}{dE}$. With $E = \frac{\hbar^2k^2}{2m}$ we have

$$\frac{dN}{dE} = \frac{2mkV}{4\pi^2\hbar^2} = \frac{(2m)^{3/2}}{\hbar^3}\,\frac{1}{4\pi^2}\sqrt{E}\,V.$$

(The problem states to neglect spin. If we do not neglect spin, we multiply this density by 2.)

We therefore have for the internal conversion rate

$$W_{0\to 1} = \frac{2\pi}{\hbar}\ \frac{1}{4\pi^2}\ \left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{E}\ \left| \int d^3r\, e^{-i\vec{k}\cdot\vec{r}} \langle \phi_f | \sum_{i=1}^{Z} \frac{e^2}{|\vec{r}-\vec{r}_i|} | \phi_i \rangle\, \psi_{nem}(\vec{r}) \right|^2 .$$

c) Use $\frac{1}{|\vec{r}-\vec{r}_i|} = \frac{1}{r} + \frac{\vec{r}\cdot\vec{r}_i}{r^3}$.

Then $\langle \phi_f | \sum_{i=1}^{Z} \frac{eZ}{|\vec{r}-\vec{r}_i|} | \phi_i \rangle = \frac{e^2}{r^3}\vec{r}\cdot\langle \phi_f | \sum_{i=1}^{Z} \vec{r}_i | \phi_i \rangle = \frac{e^2}{r^3}\vec{r}\cdot\vec{d}$.

$\vec{d}$ is independent of $\vec{r}$.

We can therefore write

$$W_{0\to 1} = \frac{e^4}{2\pi\hbar}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}\ \left| \vec{d}\cdot \int d^3r\, e^{-i\vec{k}\cdot\vec{r}}\, \frac{\vec{r}}{r^3}\, \psi_{nem}(\vec{r}) \right|^2 .$$

problem 2, solution

For $t<0$ and $t>T$ $\quad V = \frac{1}{2} m\omega^2 x^2.$

For $0<t<T$ $\quad V = \frac{1}{2} m\omega^2 (x-a)^2 = \frac{1}{2} m\omega^2 x^2 - m\omega^2 a x + \frac{1}{2} m\omega^2 a^2.$

For $t<0$ and $t>T$ $\quad H = H_0, \quad H_0|\phi_n\rangle = (n+\frac{1}{2})\hbar\omega|\phi_n\rangle.$

For $0<t<T$ $\quad H = H_0 + W$

$$P_{if} = \frac{1}{\hbar^2}\left|\int_0^T e^{i\omega_{fi}t'} W_{fi}(t')\, dt'\right|^2$$

use to distinguish from distance a

$$W_{01} = -m\omega^2 a\langle\phi_0|X|\phi_1\rangle = -m\omega^2 a\sqrt{\frac{\hbar}{2m\omega}}\langle\phi_0|\bar{a}^\dagger + \bar{a}|\phi_1\rangle$$

$$= -\sqrt{\frac{\hbar m\omega^3 a^2}{2}}\langle\phi_0|\bar{a}|\phi_1\rangle = -\sqrt{\frac{\hbar m\omega^3 a^2}{2}}.$$

$$P_{10} = \frac{m\omega a^2}{2\hbar} 4\sin^2\left(\frac{\omega T}{2}\right) = \frac{2m\omega a^2}{\hbar}\sin^2\left(\frac{\omega T}{2}\right) = \frac{|W_{01}|^2}{\hbar^2}\frac{\sin^2\left(\frac{\omega T}{2}\right)}{(\omega/2)^2}.$$

$$W_{21} = -m\omega^2 a\langle\phi_2|X|\phi_1\rangle = -m\omega^2 a\sqrt{\frac{\hbar}{2m\omega}}\langle\phi_2|\bar{a}^\dagger + \bar{a}|\phi_1\rangle$$

$$= -\sqrt{\frac{\hbar m\omega^3 a^2}{2}}\langle\phi_2|\bar{a}^\dagger|\phi_1\rangle = -\sqrt{\hbar m\omega^3 a^2}.$$

$$P_{12} = \frac{|W_{21}|^2}{\hbar^2}\frac{\sin^2\left(\frac{\omega T}{2}\right)}{(\omega/2)^2} = 4\frac{m\omega a^2}{\hbar}\sin^2\left(\frac{\omega T}{2}\right)$$

In first order perturbation theory $P_{1n}\ (n>2) = 0$ since $\langle\phi_n|W|\phi_1\rangle = 0$ for $n>2$.

problem 3, solution

a) The perturbation is $\frac{m\omega^2}{2\alpha}\left(1-e^{-\alpha x}\right) - \frac{m\omega^2}{2}x^2 = \frac{(\alpha x^2)^2}{2!} - \frac{(\alpha x^2)^3}{3!} + \cdots = H'$.

The normalized unperturbed ground state energy eigenfunction of the unperturbed harmonic oscillator is

$$\phi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\left(\frac{m\omega}{2\hbar}\right)x^2}.$$

The first order correction to the ground state energy is therefore given by

$$\langle\phi_0|H'|\phi_0\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\int_{-\infty}^{+\infty} dx\, e^{-\frac{m\omega}{\hbar}x^2}\,\frac{m\omega^2}{2}\left[\frac{1-e^{-\alpha x^2}}{\alpha} - x^2\right].$$

$$\left(\int_0^\infty x^n e^{-\lambda x^2}dx = \frac{1}{2}\,\frac{\Gamma\left(\frac{n+1}{2}\right)}{\lambda^{\left(\frac{n+1}{2}\right)}}\ ,\quad \Gamma(x+1) = x\Gamma(x),\ \Gamma(1)=1,\ \Gamma(\tfrac{1}{2}) = \sqrt{\pi}\right)$$

Therefore

$$\langle\phi|H'|\phi_0\rangle = \frac{m\omega^2}{2\alpha}\left[1 - \frac{1}{\sqrt{1+\frac{\alpha\hbar}{m\omega}}}\right] - \frac{\hbar\omega}{4},$$

and the ground state energy is $E = \hbar\omega\left[\frac{1}{4} + \frac{m\omega}{2\hbar\alpha}\left[1 - \frac{1}{\sqrt{1+\frac{\alpha\hbar}{m\omega}}}\right]\right]$ to first order.

b) Use a trial function $e^{-\beta x^2/2}$ and find

$$\langle H\rangle = \frac{\int_{-\infty}^{+\infty} e^{-\frac{\beta x^2}{2}}\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2}{2\alpha}\left(1-e^{-\alpha x^2}\right)\right]e^{-\beta x^2/2}\,dx}{\int_{-\infty}^{+\infty} e^{-\beta x^2}dx}.$$

This yields

$$\langle H\rangle = \hbar\omega\left[\frac{1}{4}\left(\frac{\beta\hbar}{m\omega}\right) + \frac{m\omega}{2\hbar\alpha}\left(1 - \frac{1}{\sqrt{1+\frac{\alpha}{\beta}}}\right)\right].$$

To find β we set $\frac{d\langle H\rangle}{d\beta} = 0$.

$$\frac{d\langle H\rangle}{d\beta} = \frac{\hbar^2}{4m} - \frac{m\omega^2}{4\beta^2\left(1+\frac{\alpha}{\beta}\right)^{3/2}} = 0.$$

$$\beta\left(1+\frac{\alpha}{\beta}\right)^{3/4} = \frac{m\omega}{\hbar}.$$

If $\alpha \ll \frac{m\omega}{\hbar}$, an approximate solution is $\beta = \frac{m\omega}{\hbar}$.

This yields $\langle H\rangle = \hbar\omega\left[\frac{1}{4} + \frac{m\omega}{2\hbar\alpha}\left(1 - \frac{1}{\sqrt{1+\frac{\alpha\hbar}{m\omega}}}\right)\right]$.

This is the same result that we got from first order perturbation theory.

We can now iterate. Using $\beta = \frac{m\omega}{\hbar}$ in the expression $\left(1+\frac{\alpha}{\beta}\right)$

we get: $\beta = \frac{m\omega}{\hbar}\left(1+\frac{\alpha\hbar}{m\omega}\right)^{-3/4}$.

This yields a somewhat lower value for β and somewhat lower estimate of $\langle H\rangle$, our approximate ground state energy.