

PROBLEM SHEET 9

FYS3110

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PROBLEM 6.1

For the harmonic oscillator the potential is $V(x) = \frac{1}{2}kx^2$ and the allowed energies are

$$(1) \quad E_n = \left(n + \frac{1}{2}\right) \hbar\omega, \text{ for } n = 0, 1, 2, \dots$$

where $\omega = \sqrt{\frac{k}{m}}$ is the classical angular frequency.

a. The spring constant is increased slightly from k to $(1 + \epsilon)k$. The exact new allowed energies are

$$(2) \quad E_n = \left(n + \frac{1}{2}\right) \hbar\sqrt{\frac{(1 + \epsilon)k}{m}}.$$

The MacLaurin series¹ of the increased spring constant up to second order is

$$(3) \quad \sqrt{1 + \epsilon} \approx 1 + \frac{\epsilon}{2} - \frac{\epsilon^2}{8} \dots$$

Inserting equation 3 into 2 yields

$$(4) \quad E_n \approx \left(n + \frac{1}{2}\right) \hbar\sqrt{\frac{k}{m}} \left(1 + \frac{\epsilon}{2} - \frac{\epsilon}{8}\right)$$

b. Now to calculate the first-order perturbation in the energy

$$(5) \quad E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle,$$

where $H' = T + V'$ and $V' = \frac{1+\epsilon}{2}kx^2$. The change in change in energy is

$$H' - H = V' - V = \frac{1 + \epsilon}{2}kx^2 - \frac{1}{2}kx^2 = \frac{1}{2}\epsilon kx^2 = \epsilon V,$$

which reduces equation 5 to

$$(6) \quad E_n^1 = \langle \psi_n^0 | \epsilon V | \psi_n^0 \rangle.$$

¹Taylor expansion around zero, from which the power series arises.

This equation can be solved quite easily by employing the virial theorem for a stationary state

$$(7) \quad 2 \langle T \rangle = \left\langle x \frac{dV}{dx} \right\rangle.$$

For the harmonic oscillator

$$\left\langle x \frac{dV}{dx} \right\rangle = k \langle x^2 \rangle \rightarrow \langle T \rangle = k \langle x^2 \rangle \rightarrow \langle T \rangle = \frac{1}{2} k \langle x^2 \rangle = \langle V \rangle = \frac{E_n}{2}.$$

It follows that equation 6 becomes

$$(8) \quad E_n^1 = \frac{\epsilon}{2} E_n^0 = \frac{\epsilon}{2} \left(n + \frac{1}{2} \right) \hbar \omega,$$

which is interesting considering that ω includes the original spring constant.

PROBLEM 6.2

A spin- $\frac{1}{2}$ degree of freedom is influenced by a magnetic field that has a large z -component and a small x -component such that the Hamiltonian is

$$(9) \quad H = -\frac{B}{\hbar} S^z - \frac{g}{\hbar} S^x.$$

The x -component of the field will be treated as a perturbation.

The unperturbed Schrödinger equation reads

$$(10) \quad H |n\rangle = E_n^0 |n\rangle.$$

Employing Pauli matrices for convenience, one must find the eigenvalues of

$$(11) \quad H^0 = -\frac{B}{\hbar} \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = -\frac{B}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

if

$$(12) \quad |\uparrow^0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |\downarrow^0\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix},$$

then it is quite easy to see that the ground state energy eigenvalues must be

$$(13) \quad E_{\uparrow}^0 = -\frac{B}{2}, \quad E_{\downarrow}^0 = \frac{B}{2}$$

a. Now to find the change in energy and due to the perturbation Hamiltonian

$$(14) \quad H' = -\frac{g}{\hbar} \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = -\frac{g}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

The first order shift in ground state is

$$(15) \quad E_{\uparrow}^1 = \langle \uparrow^0 | H' | \uparrow^0 \rangle = -\frac{g}{2} \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 0,$$

which means that there is *no* first-order shift in ground state energy. You will get the same result for $|\downarrow\rangle$ and/or using $S^x = \frac{1}{2}(S^+ + S^-)$ as well.

$$(16) \quad E_{\downarrow}^1 = -\frac{g}{\hbar} \langle \downarrow^0 | S^x | \downarrow^0 \rangle = -\frac{g}{2\hbar} \langle \downarrow^0 | (S^+ + S^-) | \downarrow^0 \rangle = -\frac{g}{2} \langle \downarrow^0 | \uparrow^0 \rangle = 0$$

c. The perturbed first order eigenkets are found by way of the following formula

$$(17) \quad |n\rangle = |n^0\rangle + \sum_m \frac{|m^0\rangle \langle m^0 | H' | n^0 \rangle}{E_n^0 - E_m^0} = |n^0\rangle + |n^1\rangle$$

the first order correction is given by $|n^1\rangle$. This gives us

$$\begin{aligned} |\uparrow\rangle &= \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \frac{\begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} \left(-\frac{g}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right) \begin{bmatrix} 1 \\ 0 \end{bmatrix}}{-\frac{B}{2} - \frac{B}{2}} \\ &= \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \frac{\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \left(-\frac{g}{2} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right)}{-B} \\ &= \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \frac{g}{2B} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |\uparrow^0\rangle + \frac{g}{2B} |\downarrow^0\rangle, \end{aligned}$$

similarly,

$$|\downarrow\rangle = |\downarrow^0\rangle - \frac{g}{2B} |\uparrow^0\rangle$$

b. Using the perturbed first order wave function one can calculate the second-order energy shift due to perturbation using the following formula.

$$(18) \quad E_n^2 = \langle n^0 | H' | n \rangle.$$

We get

$$\begin{aligned} E_{\uparrow}^2 &= \begin{bmatrix} 1 & 0 \end{bmatrix} \left(-\frac{g}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right) \left(\begin{bmatrix} 1 \\ 0 \end{bmatrix} + \frac{g}{2B} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right) = -\frac{g^2}{4B} \\ E_{\downarrow}^2 &= \begin{bmatrix} 0 & 1 \end{bmatrix} \left(-\frac{g}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right) \left(\begin{bmatrix} 0 \\ 1 \end{bmatrix} - \frac{g}{2B} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \right) = \frac{g^2}{4B} \end{aligned}$$