PROBLEM SHEET 9
FYS3110

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Problem 9.1

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

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

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

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

The MacLaurin series[1] of the increased spring constant up to second order is

$$\sqrt{1+\epsilon} \approx 1 + \frac{\epsilon}{2} - \frac{\epsilon^2}{8} \ldots \tag{3}$$

Inserting equation 3 into 2 yields

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

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

$$E_n^1 = \langle\psi_n^0|\, H'\, |\psi_n^0\rangle, \tag{5}$$

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

$$E_n^1 = \langle\psi_n^0|\, \epsilon V\, |\psi_n^0\rangle. \tag{6}$$

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

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

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

For the harmonic oscillator

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

It follows that equation 6 becomes

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

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

Problem 9.2

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

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

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

The unperturbed Schrdinger equation reads

$$H\left|n\right\rangle = E_n^0\left|n\right\rangle. \tag{10}$$

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

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

if

$$\left|\uparrow^0\right\rangle = \begin{bmatrix}1\\0\end{bmatrix}, \quad \left|\downarrow^0\right\rangle = \begin{bmatrix}0\\1\end{bmatrix}, \tag{12}$$

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

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

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

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

The first order shift in ground state is

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

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.

$$E^1_\downarrow = -\frac{g}{\hbar}\left\langle \downarrow^0\right| S^x \left|\downarrow^0\right\rangle = -\frac{g}{2\hbar}\left\langle \downarrow^0\right| (S^+ + S^-) \left|\downarrow^0\right\rangle = -\frac{g}{2}\left\langle \downarrow^0\middle| \uparrow^0\right\rangle = 0 \tag{16}$$

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

$$|n\rangle = \left|n^0\right\rangle + \sum_m \frac{\left|m^0\right\rangle \left\langle m^0\right| H' \left|n^0\right\rangle}{E^0_n - E^0_m} = \left|n^0\right\rangle + \left|n^1\right\rangle \tag{17}$$

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

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

similarly,

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

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

$$E^2_n = \left\langle n^0\right| H' \left|n\right\rangle. \tag{18}$$

We get

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

Problem 9.3

This is a problem illustrating both first-order non-degenerate and degenerate perturbation theory. Consider the two-dimensional harmonic oscillator with an extra bilinear term gxy, $g \in \mathcal{R}$.

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}m\omega^2 x^2 \frac{1}{2}m\omega^2 y + gxy. \tag{19}$$

For $g = 0$ the exact energy eigenstates are tensor products of one-dimensional harmonic oscillator states: $|n_x, n_y\rangle = |n_x\rangle \otimes |n_y\rangle$, where $n_x, n_y \in \{0, 1, \dots\}$. Their energies are $E_{n_x,n_y} = \hbar\omega(n_x + n_y + 1)$.

a. The two lowest energies are

$$E_{0,0} = \hbar\omega, \quad E_{1,0} = E_{0,1} = 2\hbar\omega,$$

corresponding to the eigenstates

$$|0,0\rangle\,, \quad |1,0\rangle\,, \quad |0,1\rangle\,.$$

We see that the ground state is non-degenerative and the next-lowest energy level has a degeneracy of 2.

b. If $g = 0$ first-order non-degenerate perturbation theory can be used to compute how the ground state energy changes. The first-order energy shift will be

$$\begin{aligned}
E_{00}^1 &= \langle 0,0|\, H \,|0,0\rangle = \langle 0,0|\, qxy \,|0,0\rangle \\
&= g\frac{\hbar}{2}\frac{1}{m\omega}(\langle 0| \otimes \langle 0|)(a_x^\dagger + a_x)(a_y^\dagger + a_y)(|0\rangle \otimes |0\rangle) \\
&= g\frac{\hbar}{2}\frac{1}{m\omega}(\langle 0| \otimes \langle 0|)\left[(a^\dagger + a)\,|0\rangle \otimes (a^\dagger + a)\,|0\rangle\right] \\
&= g\frac{\hbar}{2}\frac{1}{m\omega}(\langle 0| \otimes \langle 0|)(|1\rangle \otimes |1\rangle) \\
&= g\frac{\hbar}{2}\frac{1}{m\omega}\,\langle 0,0|1,1\rangle = 0.
\end{aligned}$$

c. By employing first-order degenerate perturbation theory one can find how the first excited energy splits up when g is finite. The fundamental result of degenerate perturbation theory is the following formula.

$$E_\pm^1 = \frac{1}{2}\left(W_{aa} + {}''_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab}|^2}\right) \tag{20}$$

where $W_{ij} = \langle \psi_i^0 \big|\, H' \,|\psi\rangle$. Setting $|0,1\rangle = \psi_a^0$ and $|1,0\rangle = \psi_b^0$ gives

$$\begin{aligned}
W_{ab} &= \langle 0,1|\, H' \,|1,0\rangle \\
&= \frac{g\hbar}{2m\omega}\,\langle 0,1|\,(a_x^\dagger + a_x)(a_y^\dagger + a_y)\,|1,0\rangle \\
&= \frac{g\hbar}{2m\omega}\,\langle 0,1|0,1\rangle = \frac{g\hbar}{m\omega},
\end{aligned}$$

similarly

$$W_{ba} = \frac{g\hbar}{2m\omega}, \quad W_{aa} = 0, \quad W_{bb} = 0.$$

Inserting into equation 20 yields

$$E_\pm^1 = \frac{1}{2}\left(0 + 0 \pm \sqrt{0 + \frac{4}{4}\frac{q^2\hbar^2}{m^2\omega^2}}\right) = \pm\frac{g\hbar}{2m\omega}$$

d. Introducing the reflection operator

$$R\,|n_1\rangle \otimes |n_2\rangle = |n_2\rangle \otimes |n_1\rangle \tag{21}$$

For $g = 0$ I will find eigenstates of R that also are eigenstates of H, all with energies $2\hbar\omega$, id est they belong to the first excited energy level.

By setting

$$|0,1\rangle = \begin{bmatrix}0\\1\end{bmatrix} \quad |1,0\rangle = \begin{bmatrix}1\\0\end{bmatrix}$$

then

$$R = \begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$$

R is a unitary matrix and therefore has eigenvalues ± 1. This means that the eigenstates of R can be

$$\begin{bmatrix}1\\1\end{bmatrix} = \begin{bmatrix}0\\1\end{bmatrix} + \begin{bmatrix}1\\0\end{bmatrix}$$
$$\begin{bmatrix}1\\-1\end{bmatrix} = \begin{bmatrix}1\\0\end{bmatrix} - \begin{bmatrix}0\\-1\end{bmatrix}$$

Normalising these we end up with

$$\psi^0_{\pm} = \frac{1}{\sqrt{2}}(|1,0\rangle \pm |0,1\rangle) \tag{22}$$

e. With the "good" states from the previous sub-problem, one can apply non-degenerate first order perturbation theory.

$$\begin{aligned}
E^1_+ &= \langle\psi^0_+|\, H'\, |\psi^0_+\rangle \\
&= \frac{g}{2}(\langle 1,0| + \langle 0,1|)xy(|1,0\rangle + |0,1\rangle) \\
&= \frac{g\hbar}{4m\omega}(\langle 1,0| + \langle 0,1|)(a_x^\dagger + a_x)(a_y^\dagger + a_y)(|1,0\rangle + |0,1\rangle) \\
&= \frac{g\hbar}{4m\omega}(\langle 1,0| + \langle 0,1|)(|0,1\rangle + |1,0\rangle) = \frac{g\hbar}{2m\omega}
\end{aligned}$$

$$\begin{aligned}
E^1_- &= \langle\psi^0_-|\, H'\, |\psi^0_-\rangle \\
&= \frac{g}{2}(\langle 1,0| - \langle 0,1|)xy(|1,0\rangle - |0,1\rangle) \\
&= \frac{g\hbar}{4m\omega}(\langle 1,0| - \langle 0,1|)(a_x^\dagger + a_x)(a_y^\dagger + a_y)(|1,0\rangle - |0,1\rangle) \\
&= \frac{g\hbar}{4m\omega}(\langle 1,0| - \langle 0,1|)(|0,1\rangle - |1,0\rangle) = -\frac{g\hbar}{2m\omega}
\end{aligned}$$

We see that we get the same results using the "good" states for non-degenerate perturbation as for degenerate perturbation. Neat!