**PROBLEM 4: Stationary Perturbation Theory**

Consider a non-relativistic particle of mass $m$ moving in the three dimensional potential:

$$V(x) = \frac{1}{2}k(x^2 + y^2 + z^2)\,.$$

(a) [1 point] What is the ground state energy and first excited state energy for this potential?

Now there is a perturbation applied so the potential becomes

$$V(x) = \frac{1}{2}k(x^2 + y^2 + z^2) + \lambda xy$$

where $\lambda$ is a small parameter.

(b) [1 point] Calculate the ground state energy to first order in $\lambda$.

(c) [4 point] Calculate the ground state energy to second order in $\lambda$.

(d) [4 point] Calculate the first excited state energies to first order in $\lambda$.

(a)

In general, our energy is

$$E = \left(n_x + n_y + n_z + \frac{3}{2}\right)\hbar\omega .$$

So the ground state energy is

$$\boxed{E^{(0)}_{000} = \frac{3}{2}\hbar\omega}$$

and the first excited energy is

$$\boxed{E^{(0)}_{100} = E^{(0)}_{010} = E^{(0)}_{001} = \frac{5}{2}\hbar\omega} .$$

(b)

To first order, we have

$$\begin{aligned}
E^{(1)}_{000} &= \langle n_x n_y n_z | V' | n_x n_y n_z \rangle \\
&= \langle n_x n_y n_z | \lambda x y | n_x n_y n_z \rangle \\
&= \langle 0\,0\,0 | \tfrac{\lambda\hbar}{2m\omega}(a_x + a_x^{+})(a_y + a_y^{+}) | 0\,0\,0 \rangle \\
&= \frac{\lambda\hbar}{2m\omega} \langle 0\,0\,0 | a_x a_y + a_x a_y^{+} + a_x^{+} a_y + a_x^{+} a_y^{+} | 0\,0\,0 \rangle \\
&= \frac{\lambda\hbar}{2m\omega}\Big[\langle 000 | a_x a_y | 000 \rangle + \langle 000 | a_x a_y^{+} | 000 \rangle + \langle 000 | a_x^{+} a_y | 000 \rangle \\
&\qquad + \langle 000 | a_x^{+} a_y^{+} | 000 \rangle\Big] \\
&= \frac{\lambda\hbar}{2m\omega}\left[0 + 0 + 0 + \langle 000 | 110 \rangle\right] \\
&= 0
\end{aligned}$$

So our ground state energy is, to first order,

$$\boxed{E_{000} = \frac{3}{2}\hbar\omega} .$$

(c)

To second order, we have

$$E^{(2)}_{000} = \sum_{\{m\}\neq\{0\}} \frac{|\langle m_x m_y m_z | \lambda x y | 000\rangle|^2}{E^{(0)}_{000} - E^{(0)}_{m}}$$

$$= \left(\frac{\lambda\hbar}{2m\omega}\right)^2 \sum_{\{m\}\neq\{0\}} \frac{|\langle m_x m_y m_z | a_x a_y + a_x a_y^+ + a_x^+ a_y + a_x^+ a_y^+ | 000\rangle|^2}{\frac{3}{2}\hbar\omega - (m_x + m_y + m_z + \frac{3}{2})\hbar\omega}$$

$$= \left(\frac{\lambda\hbar}{2m\omega}\right)^2 \sum_{\{m\}\neq\{0\}} \frac{|\langle m_x m_y m_z | 1\,1\,0\rangle|^2}{-m_x - m_y - m_z}$$

$$= \left(\frac{\lambda\hbar}{2m\omega}\right)^2 \cdot \frac{1}{-(1)-(1)-(0)}$$

$$= -\frac{\lambda^2\hbar^2}{8m^2\omega^2}$$

So our ground state energy to second order is

$$\boxed{E_{000} = \frac{3}{2}\hbar\omega - \frac{\lambda^2\hbar^2}{8m^2\omega^2}}\,.$$

(d)

The first excited state is three-fold degenerate, so we want to determine the eigenvalues for the W matrix

$$W = \begin{pmatrix} W_{aa} & W_{ab} & W_{ac} \\ W_{ba} & W_{bb} & W_{bc} \\ W_{ca} & W_{cb} & W_{cc} \end{pmatrix},$$

where, in general, $W_{ij} = \langle \psi_i^{(0)} | H' | \psi_j^{(0)} \rangle$. Let $\psi_a = |100\rangle$, $\psi_b = |010\rangle$, and $\psi_c = |001\rangle$. Then

$$\begin{aligned} W_{aa} &= \langle \psi_a | \lambda xy | \psi_a \rangle \\ &= \langle 100 | \lambda xy | 100 \rangle \\ &= \frac{\lambda\hbar}{2m\omega} \langle 100 | a_x a_y + a_x a_y^\dagger + a_x^\dagger a_y + a_x^\dagger a_y^\dagger | 100 \rangle \\ &= 0 \end{aligned}$$

$$\begin{aligned} W_{bb} &= \langle 010 | \lambda xy | 010 \rangle \\ &= 0 \end{aligned}$$

$$\begin{aligned} W_{cc} &= \langle 001 | \lambda xy | 001 \rangle \\ &= 0 \end{aligned}$$

$$\begin{aligned} W_{ab} &= \langle \psi_a | \lambda xy | \psi_b \rangle \\ &= \langle 100 | \lambda xy | 010 \rangle \\ &= \frac{\lambda\hbar}{2m\omega} \langle 100 | a_x a_y + a_x a_y^\dagger + a_x^\dagger a_y + a_x^\dagger a_y^\dagger | 010 \rangle \\ &= \frac{\lambda\hbar}{2m\omega} \left( 0 + 0 + \langle 100 | 100 \rangle + 0 \right) \\ &= \frac{\lambda\hbar}{2m\omega} \end{aligned}$$

$$\begin{aligned} W_{ba} &= \langle \psi_b | \lambda xy | \psi_a \rangle \\ &= \langle 010 | \lambda xy | 100 \rangle \\ &= \frac{\lambda\hbar}{2m\omega} \end{aligned}$$

(d), cont'd...

$$W_{ac} = \langle \psi_a | \lambda xy | \psi_c \rangle$$
$$= \langle 100 | \lambda xy | 001 \rangle$$
$$= 0$$

$$W_{ca} = \langle \psi_c | \lambda xy | \psi_a \rangle$$
$$= \langle 001 | \lambda xy | 100 \rangle$$
$$= 0$$

$$W_{bc} = \langle \psi_b | \lambda xy | \psi_c \rangle$$
$$= \langle 010 | \lambda xy | 001 \rangle$$
$$= 0$$

$$W_{cb} = \langle \psi_c | \lambda xy | \psi_b \rangle$$
$$= \langle 001 | \lambda xy | 010 \rangle$$
$$= 0.$$

So our matrix is

$$W = \begin{pmatrix} 0 & \frac{\lambda\hbar}{2m\omega} & 0 \\ \frac{\lambda\hbar}{2m\omega} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The eigenvalues are

$$\begin{vmatrix} -\lambda' & \frac{\lambda\hbar}{2m\omega} & 0 \\ \frac{\lambda\hbar}{2m\omega} & -\lambda' & 0 \\ 0 & 0 & -\lambda' \end{vmatrix} = 0$$

$$(-\lambda')^3 - (-\lambda')\left(\frac{\lambda\hbar}{2m\omega}\right)^2 = 0$$

$$\lambda'^2 = \left(\frac{\lambda\hbar}{2m\omega}\right)^2$$

$$\lambda' = \pm \frac{\lambda\hbar}{2m\omega}.$$

(d), cont'd...

Then our corrected first excited energies are

$$\boxed{E_{100} = E_{010} = E_{001} = \frac{5}{2}\hbar\omega \pm \frac{\lambda\hbar}{2m\omega}}.$$