A. LHO with Ax^6 potential

The $V = \frac{1}{2}m\omega^2x^2$ potential of linear harmonic oscillator changes to Ax^6, in the first order of the perturbation theory, calculate the energy of the ground state for the new potential.

Solution:

The original Hamiltonian reads

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$$

and in the perturbed Hamiltonian, $V = Ax^6$. The perturbing potential is then

$$V' = Ax^6 - \frac{1}{2}m\omega^2x^2$$

In the first order of perturbation theory, we need to obtain the expectation value of V' for a given state. The ground state wavefunction is $\Psi = (\alpha/\pi)^{\frac{1}{4}}e^{\frac{\alpha x^2}{2}}$, with $\alpha = \frac{m\omega}{\hbar}$. The change of the energy of the ground state is then

$$
\begin{aligned}
\Delta E_0 =& \langle 0|V'|0\rangle \\
=& \sqrt{\frac{\alpha}{\pi}}\int_{-\infty}^{\infty}dx(-\frac{1}{2}m\omega)x^2e^{-\alpha x^2} + \sqrt{\frac{\alpha}{\pi}}\int_{-\infty}^{\infty}dxAx^6e^{-\alpha x^2} \\
=& -\frac{1}{2}m\omega\sqrt{\frac{\alpha}{\pi}}\sqrt{\frac{\pi}{\alpha}}\frac{1}{2\alpha} + A\sqrt{\frac{\alpha}{\pi}}\frac{5}{2\alpha}\frac{3}{2\alpha}\frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}} \\
=& -\frac{1}{2}m\omega\frac{\hbar}{2m\omega} + \frac{15A}{8\alpha^3} \\
=& -\frac{1}{4}\hbar\omega + \frac{15A}{8\alpha^3}
\end{aligned}
$$

The expectation value of the original potential is half of the ground state energy, due to virial theorem.

B. Square well potential with Ax^2 perturbation

A quantum particle is bound in a one-dimensional infinitely deep square well potential of length l. An additional potential starts to act on the particle with the form $V' = Ax^2$, where $0 < A < 1$. What is the first order correction to the ground state energy of the system?

Hint:

The wavefunctions of a particle in a square well potential are

$$\psi_n = \sqrt{\frac{2}{l}}\cos\left(\frac{\pi n}{l}x\right)$$

and the corresponding energies are

$$E_n = \frac{\pi^2\hbar^2}{2ml^2} \, , n = 1, 2, \dots \, .$$

Solution:

The ground state wavefunction of the non-perturbed system is

$$\psi = \sqrt{\frac{2}{l}}\cos\left(\frac{\pi x}{l}\right) \, .$$

In the first order the correction to the ground state energy is given by the matrix element of the perturbation

$$\Delta E = \langle\psi|V'|\psi\rangle = \frac{2}{l}\int_{-l/2}^{l/2}\cos^2\left(\frac{\pi x}{l}\right)Ax^2 dx \, .$$

Using

$$\int dx \cos^2(Bx)x^2 = \frac{x\cos(2Bx)}{4B^2} + \frac{(2B^2x^2 - 1)\sin(2Bx)}{8B^3} + \frac{x^3}{6}$$

we obtain

$$\begin{aligned}
\Delta E &= \frac{2A}{l}\left[\frac{xl^2\cos(2\pi x/l)}{4\pi^2} + \frac{(2\pi^2 x^2/l^2 - 1)\sin(s\pi x/l)}{8\pi^3/l^3} + \frac{x^3}{6}\right]_{-l/2}^{l/2} \\
&= \frac{2A}{l}\left(-\frac{l^3}{4\pi^2} + 0 + \frac{l^3}{24}\right) \\
&= Al^2\left(-\frac{1}{2\pi^2} + \frac{1}{12}\right) \\
&= \frac{Al^2}{12\pi^2}(\pi^2 - 6) \, .
\end{aligned}$$

To within the first order perturbation theory the energy of the new ground state is

$$E_0 = \frac{\pi^2\hbar^2}{2ml^2} + \frac{Al^2}{12\pi^2}(\pi^2 - 6)$$

C.   LHO with doubled potential

Consider a particle with mass m moving in a field of harmonic potential with frequency ω. The frequency changes so that the potential is doubled. Show that the new ground state energy is exactly $E = \sqrt{2}E_0 = \frac{\sqrt{2}}{2}\hbar\omega$. Use perturbation theory to obtain the energy through third order.

Solution:

The Hamiltonian of the LHO is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \, ,$$

and the corresponding energies are $E_n = \hbar\omega(n + \frac{1}{2})$. When the potential is doubled, the frequency changes to a new frequency ω' which can be obtained as follows

$$\frac{1}{2}m\omega'^2 = 2 \cdot \frac{1}{2}m\omega^2$$
$$\omega'^2 = 2\omega^2$$
$$\omega' = \sqrt{2}\omega \, .$$

We see that the new frequency is $\sqrt{2}$ times the original one. The energies for the new potential are then $E_n' = \hbar\omega'(n + \frac{1}{2}) = \sqrt{2}\hbar\omega(n + \frac{1}{2})$.

The change of the energy in the first order of parturbation theory is given by $\Delta E^1 = \langle\psi|V'|\psi\rangle$. For the ground state this is

$$\begin{aligned}\Delta E_0^1 &= \langle 0|V'|0\rangle \\ &= \langle 0|\frac{1}{2}m\omega^2 x^2|0\rangle \\ &= \frac{1}{4}\hbar\omega \, ,\end{aligned}$$

where in the last step we used the virial theorem which gives for LHO that the mean value of the potential energy is one half of the total energy.

Alternatively, the expectation value can be evaluated using the the raising (a) and lowering a^+ operators for LHO and considering $x = \frac{\alpha}{\sqrt{2}}(a + a^+)$. For x^2 we than obtain

$$x^2 = \frac{\alpha^2}{2}(a + a^+)(a + a^+) = \quad \frac{\alpha^2}{2}(a^2 + a^{+2} + aa^+ + a^+a) = \frac{\alpha^2}{2}(a^2 + a^{+2} + 2a^+a + 1)$$

With $\alpha = \sqrt{\frac{\hbar}{m\omega}}$ The expectation value of the perturbing potential $V' = \frac{1}{2}m\omega^2 x^2$ is then

$$\begin{aligned}\langle 0|V'|0\rangle &= \frac{1}{2}m\omega^2\frac{\hbar}{2m\omega}\langle 0|a^2 + a^{+2} + 2a^+a + 1|0\rangle \\ &= \frac{1}{4}\hbar\omega\langle 0|1|0\rangle \\ &= \frac{1}{4}\hbar\omega \, .\end{aligned}$$

In the last step we used the fact that the terms $\langle 0|a^2|0\rangle$ and $\langle 0|a^{+2}|0\rangle$ are zero as they result in a different state on the right and on the left. Moreover, the term $\langle 0|a^+a|0\rangle$ is zero as

$a|0\rangle = 0$, so that only the identity operator remains. The final result is then identical to the one obtained from the knowledge of the virial theorem. Finally, an explicit integration could be performed as well to obtain the result.

Therefore, in the first order of perturbation theory, we find that the estimated value of the ground state energy for the perturbed system is

$$E_0^1 = \frac{1}{2}\hbar\omega + \frac{1}{4}\hbar\omega = \frac{3}{4}\hbar\omega \,. \tag{1}$$

This is above the exact result of $\frac{2\sqrt{2}}{4}\hbar\omega$.

The correction to the energy in the second order is

$$\Delta E_0^2 = \sum_{j\neq 0}^{\infty} \frac{|\langle j|V'|0\rangle|^2}{\epsilon_0 - \epsilon_j} \,.$$

For the perturbation $x^2 \sim a^2 + a^{+2} + 2a^+a + 1$, only the matrix element between the ground state and the second excited state will be non-zero, as a result of the action of the a^{+2} operator. Therefore, the expression for the energy correction simplifies to

$$\Delta E_0^2 = \frac{m^2\omega^4}{4} \frac{\alpha^4}{4} \frac{|\langle 2|a^{+2}|0\rangle|^2}{\epsilon_0 - \epsilon_2} \,,$$

where the first fraction comes from the square of $\frac{1}{2}m\omega^2$ and the second fraction from the square of the $\frac{\alpha^2}{2}$ coefficient. Using $\alpha^2 = \frac{\hbar}{m\omega}$, $\epsilon_2 = \frac{5}{2}\hbar\omega$, and $a^+|n\rangle = \sqrt{n+1}|n+1\rangle$ we find

$$\begin{aligned} \Delta E_0^2 &= \frac{m^2\omega^4}{4} \frac{\hbar^2}{4m^2\omega^2} \frac{|\sqrt{2}|^2}{\frac{1}{2}\hbar\omega - \frac{5}{2}\hbar\omega} \\ &= \frac{\omega^2\hbar^2}{16} \frac{2}{-2\hbar\omega} \\ &= -\frac{\hbar\omega}{16} \,. \end{aligned}$$

As expected for ground state energy, the second order correction is negative.

The correction to within second order is then

$$E_0^2 = \frac{1}{2}\hbar\omega + \frac{1}{4}\hbar\omega - \frac{\hbar\omega}{16} = \frac{1}{2}\hbar\omega \cdot \frac{11}{8} \,. \tag{2}$$

The factor $\frac{11}{8} = 1.375$ is now closer to the $\sqrt{2} \approx 1.414$.

The correction to the ground state energy in third order can be written as

$$\begin{aligned} \Delta E_0^3 = &\sum_{j\neq 0} \sum_{k\neq 0} \frac{\langle 0|V'|k\rangle\langle k|V'|j\rangle\langle j|V'|0\rangle}{(\epsilon_0 - \epsilon_k)(\epsilon_0 - \epsilon_j)} \\ &- \langle 0|V'|0\rangle \sum_{j\neq 0} \frac{|\langle j|V'|0\rangle|^2}{(\epsilon_0 - \epsilon_j)^2} \,. \end{aligned}$$

For a matrix element of the x^2 perturbation to be non-zero, the quantum number needs to differ by two (in both directions), or needs to stay constant. Considering that neither j nor k can be the ground state in the first expression, a non-zero contribution comes only from $j = k = 2$ in the first expression. In the second expression, $j = 2$, as in the second order. Explicit evaluation of the terms gives $\frac{5}{128}\hbar\omega$ for the first term and $\frac{-\hbar\omega}{128}$ for the latter. Overall, third order contributes $\frac{1}{32}\hbar\omega$ to the energy, giving

$$E_0^3 = 1.4375 \cdot \frac{1}{2}\hbar\omega \,. \tag{3}$$

Comparing the results to sums for $\sqrt{2}$, we find that the formula

$$\sqrt{2} = \sum_{k=0}^{\infty} (-1)^{k+1} \frac{(2k-3)!!}{(2k)!!} \tag{4}$$

$$= 1 + \frac{1}{2} - \frac{1}{2\cdot 4} + \frac{1\cdot 3}{2\cdot 4\cdot 6} - \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6\cdot 8} + \dots \tag{5}$$

gives identical coefficients to those we found using perturbation theory. It is then very likely that the subsequent orders of perturbation theory would follow the series.

D. Free particle and step potential

A "free" particle is restricted to an interval $(0, L)$ with periodic boundary conditions applied. An additional potential is added to the system shifts the initially flat potential by $-V$ on an interval $(0, L/4)$.

- What is the correction to the energy of the ground state within the first order perturbation theory?

- What are the energies of the first excited states in the first order of the perturbation theory?

Solution:

The wavefunctions of a free particle on an interval with length L are

$$\psi_n = \frac{1}{\sqrt{L}} e^{2\pi i x n/L}$$

and the corresponding energies are

$$E_n = \frac{2\pi^2\hbar^2}{mL^2} \,,$$

where n is an integer. All the states, apart from the ground state, are twice degenerate.

To obtain the correction to the ground state level, we need to calculate the matrix element of the perturbation:

$$\Delta E_0^{(1)} = \langle \psi_0 | V' | \psi_0 \rangle = \frac{1}{L} \int_0^{L/4} (-V) dx = -\frac{V}{4} .$$

Here we used the fact that the ground state wavefunction is simply a constant $\psi_0 = \frac{1}{\sqrt{L}}$.

The first excited states correspond to levels with $n = 1$ and $n = -1$. To obtain the new energies within the first order of the perturbation theory, we need to obtain the partial Hamiltonian of the perturbation for these two states. Therefore, we need to obtain the diagonal matrix elements $\langle 1|V'|1 \rangle$ and $\langle -1|V'|-1 \rangle$ as well as the off-diagonal element $\langle 1|V'|-1 \rangle$ and its conjugate. The first diagonal element can be evaluated as

$$\langle 1|V'|1 \rangle = \frac{1}{L} \int_0^{L/4} e^{-2\pi i x/L} (-V) e^{2\pi i x/L} dx$$
$$= \frac{1}{L} \int_0^{L/4} (-V) dx = -\frac{V}{4} .$$

The matrix element for the state $|-1\rangle$ yields the same value. The result is also identical to the one obtained for the ground state level. This can be understood from the fact that the product of the potential and the density of a given state is integrated to obtain the correction. For free particle, all the states have the same density $\rho = \frac{1}{L}$ and thus will have the same matrix element for the potential V' and, in fact, for any local potential $V'(r)$.

To obtain the partial Hamiltonian of the perturbation we will now obtain the off-diagonal element between the two states:

$$\langle 1|V'|-1 \rangle = \frac{1}{L} \int_0^{L/4} e^{-2\pi i x/L} (-V) e^{-2\pi i x/L} dx$$
$$= -\frac{V}{L} \int_0^{L/4} e^{-4\pi i x/L} dx = -\frac{V}{L} \frac{L}{-4\pi i} e^{-4\pi i x/L} \Big|_0^{L/4}$$
$$= -\frac{iV}{4\pi} \left(e^{-i\pi} - 1 \right) = \frac{iV}{2\pi} .$$

As the off-diagonal elements are complex conjugated to each other, we have $\langle -1|V'|1 \rangle = -\frac{iV}{2\pi}$. The fact that the elements are complex should not worry us as we are using complex orbitals.

Therefore, the partial Hamiltonian of the perturbation reads

$$V' = \begin{pmatrix} -\frac{V}{4} & \frac{iV}{2\pi} \\ -\frac{iV}{2\pi} & -\frac{V}{4} \end{pmatrix} .$$

The off-diagonal matrix elements are non-zero and therefore the two states that were originally degenerate will split. To find the estimates for the energies of the new states, we will solve

$$V'\psi = \lambda\psi$$

in the basis of the two excited states. The determinant of $(V' - \lambda)$ reads

$$\begin{pmatrix} -\frac{V}{4} - \lambda & \frac{iV}{2\pi} \\ -\frac{iV}{2\pi} & -\frac{V}{4} - \lambda \end{pmatrix} = (-\frac{V}{4} - \lambda)^2 - (\frac{iV}{2\pi})(-\frac{iV}{2\pi}) = (-\frac{V}{4} - \lambda)^2 - (\frac{V}{2\pi})(\frac{V}{2\pi}).$$

This is the usual $(A + B)(A - B)$ form and therefore the roots are $\lambda = -\frac{V}{4} \pm \frac{V}{2\pi}$. These are the corrections to the energies of the first excited states $E_1 = \frac{2\pi^2\hbar^2}{mL^2}$.

E. Free particle with Dirac δ

Consider a free particle within periodic boundary conditions on an interval $(0, L)$. What are the wavefunctions, energies, and degeneracies of the states? A perturbing potential of the form $V' = A\delta(x - L/2)$ (periodically repeated) is added. What are the matrix elements between any pair states for the perturbing potential? What is the correction to the energy level for the ground state in the first and second order of perturbation theory? What are the energies and wavefunctions of the first excited states within the first order of perturbation theory? What is the first order change of the wavefunction of the ground state?

Solution:

The states of a particle within periodic boundary conditions are $\Psi_n = \frac{1}{\sqrt{L}}exp(\frac{2\pi inx}{L})$, where L is the length of the box and n is integer. For constant potential equal to zero, only kinetic energy contributes to the total energy, so that $E_n = \frac{2\hbar^2\pi^2}{mL^2}n^2$. The ground state is non-degenerate and all the excited states are twice degenerate, as the states with both positive and negative n occur.

The matrix elements of the perturbing potential are

$$\begin{aligned} \langle m|V'|n\rangle &= \frac{A}{L}\int_0^L e^{-\frac{2\pi i}{L}mx}\delta(x - \frac{L}{2})e^{\frac{2\pi i}{L}nx} \\ &= \frac{A}{L}e^{\frac{2\pi i}{L}\frac{L}{2}(n-m)} \\ &= \frac{A}{L}e^{i\pi(n-m)}. \end{aligned}$$

The matrix element is thus $\frac{A}{L}$ for pairs of states with $(n-m)$ even and $-\frac{A}{L}$ for $(n-m)$ odd. The first order correction to the energy of the ground state $n=m=0$ is then $\Delta E_0^1 = \frac{A}{L}$. This means that for $A > 0$ the potential is repulsive and the energy increases while for $A < 0$, the potential is attractive and the energy is lowered.

In the second order we need to evaluate

$$\Delta E_0^{(2)} = \sum_{j \in \{Z-0\}} \frac{|\langle j|V'|0\rangle|^2}{\epsilon_0 - \epsilon_j}.$$

In this case the matrix elements of the perturbation between the ground state and the excited states are all non-zero. Fortunately, they are all $\pm\frac{A}{L}$ so that their squares are simply $\frac{A^2}{L^2}$. The energy of the unperturbed ground state is zero ($\epsilon_0 = 0$) and the energies of the excited states are $E_n = \frac{2\hbar^2\pi^2}{mL^2}n^2$. We thus find for the correction

$$\Delta E_0^{(2)} = \sum_{j \in \{Z-0\}} \frac{\frac{A^2}{L^2}}{0 - \frac{2\hbar^2\pi^2n^2}{mL^2}}$$

$$= -\frac{A^2m}{2\hbar^2\pi^2} \sum_{j \in \{Z-0\}} \frac{1}{j^2}$$

$$= -\frac{A^2m}{\hbar^2\pi^2} \sum_{j=1}^{\infty} \frac{1}{j^2}.$$

The summation over inverse squares is known as the "Basel problem", posed in 1644 and was first derived by Leonhard Euler almost a hundred years later. The sum equals $\pi^2/6$. The final correction is thus

$$\Delta E_0^{(2)} = -\frac{A^2m}{\hbar^2\pi^2}\frac{\pi^2}{6}$$

$$= -\frac{A^2m}{6\hbar^2}$$

As expected for the second order energy correction to the ground state, $\Delta E_0^{(2)}$ is negative and always lowers the energy.

The excited states are twice degenerate, we therefore need to diagonalise the partial Hamiltonian of the perturbation corresponding to these states to find their energies in the first order of perturbation theory. The partial Hamiltonian contains the diagonal matrix elements $\langle n|V'|n\rangle$ as well as the elements of type $\langle n|V'|-n\rangle$. In both cases, the matrix elements are A/L and the matrix to diagonalise is

$$V'_{\text{sub}} = \frac{A}{L}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

The eigenvalues of this matrix are 0, for the state $\frac{1}{\sqrt{2}}(|n\rangle - |-n\rangle)$, and $\frac{2A}{L}$ for the state $\frac{1}{\sqrt{2}}(|n\rangle + |-n\rangle)$. This result can be simply explained considering that

$$\frac{1}{\sqrt{2}}(|n\rangle - |-n\rangle) = i\sqrt{\frac{2}{L}}sin(2\pi nx/L)\,,$$

which equals zero for $x = L/2$ and thus is not affected by the potential. The second state is then

$$\frac{1}{\sqrt{2}}(|n\rangle + |-n\rangle) = \sqrt{\frac{2}{L}}cos(2\pi nx/L)\,,$$

which has a non-zero value for $x = L/2$.

We now calculate the correction to the ground state wavefunction. The first order correction reads

$$|i^{(1)}\rangle = |i^{(0)}\rangle + \sum_{j\in\{Z-i\}} \frac{|j\rangle\langle j|V'|i\rangle}{\epsilon_i - \epsilon_j}\,.$$

Inserting the matrix element of the perturbation

$$|i^{(1)}\rangle = |i^{(0)}\rangle + \sum_{j\in\{Z-i\}} \frac{|j\rangle\frac{A}{L}e^{i\pi(j-i)}}{\epsilon_i - \epsilon_j}\,.$$

For the ground state $i = 0$ and we obtain

$$|0^{(1)}\rangle = \frac{1}{\sqrt{L}} + \sum_{j\in\{Z-0\}} \frac{\frac{1}{\sqrt{L}}e^{\frac{2\pi ijx}{L}}\frac{A}{L}e^{i\pi j}}{-\frac{2\hbar^2\pi^2 j^2}{mL^2}}$$

$$= \frac{1}{\sqrt{L}} - \frac{mL^2}{2\hbar^2\pi^2}\frac{1}{\sqrt{L}}\frac{A}{L}\sum_{j\in\{Z-0\}} \frac{e^{\frac{2\pi ijx}{L}}e^{i\pi j}}{j^2}$$

$$= \frac{1}{\sqrt{L}} - \frac{mA\sqrt{L}}{2\hbar^2\pi^2}\sum_{j\in\{Z-0\}} \frac{e^{\frac{2\pi ijx}{L}}e^{i\pi j}}{j^2}\,.$$

We now change the summation from all integers, except for zero, to summation over natural numbers (1 to ∞), putting the $-j$ term together with the $+j$ term

$$|0^{(1)}\rangle = \frac{1}{\sqrt{L}} - \frac{mA\sqrt{L}}{2\hbar^2\pi^2}\sum_{j=1}^{\infty} \frac{e^{i\pi j}[e^{\frac{2\pi ijx}{L}} + e^{-\frac{2\pi ijx}{L}}]}{j^2} = \frac{1}{\sqrt{L}} - \frac{mA\sqrt{L}}{\hbar^2\pi^2}\sum_{j=1}^{\infty} \frac{(-1)^j cos(\frac{2\pi jx}{L})}{j^2}\,.$$

We see that all excited states contribute to the first order correction to the wavefunction.

For the interesting point of $x = L/2$ we obtain

$$\psi_0^{(1)}(L/2) = \frac{1}{\sqrt{L}} - \frac{mA\sqrt{L}}{\hbar^2\pi^2}\sum_{j=1}^{\infty} \frac{(-1)^j cos(\frac{2\pi jL}{2L})}{j^2}$$

$$= \frac{1}{\sqrt{L}} - \frac{mA\sqrt{L}}{\hbar^2\pi^2}\sum_{j=1}^{\infty} \frac{(-1)^j cos(\pi j)}{j^2}\,.$$

Since $cos(\pi j) = (-1)^j$, we get

$$
\begin{aligned}
\psi_0^{(1)}(L/2) &= \frac{1}{\sqrt{L}} - \frac{mA\sqrt{L}}{\hbar^2\pi^2} \sum_{j=1}^{\infty} \frac{(-1)^{2j}}{j^2} \\
&= \frac{1}{\sqrt{L}} - \frac{mA\sqrt{L}}{\hbar^2\pi^2} \sum_{j=1}^{\infty} \frac{1}{j^2} \\
&= \frac{1}{\sqrt{L}} - \frac{mA\sqrt{L}}{\hbar^2\pi^2} \frac{\pi^2}{6} \\
&= \frac{1}{\sqrt{L}} - \frac{mA\sqrt{L}}{6\hbar^2} .
\end{aligned}
$$

The sign of the correction is correct – when $A > 0$, a repulsive potential is present and the density will be reduced, for the opposite case of an attractive potential, the density will increase.

Interestingly, one can see that the second derivative becomes infinite. This agrees with the fact that for the δ potential, the exact wavefunction contains a jump in the derivative in the point of the potential. We try to model this potential with smooth functions which can reach the exact result only in the infinite limit. An exactly the same problem of slow convergence of the wavefunction with the number of excited states considered is encountered when using perturbation theory for the many-electron problem in atoms, molecules, and solids.

F.   LHO with Ax^2y^2 perturbation

A particle with mass m moves in the x-y plane in a 2D isotropic linear harmonic oscillator potential with a frequency ω and centered at origin. The particle is subject to an additional perturbing potential of the form $V' = Ax^2y^2$. What is the energy of the ground state to within second order perturbation theory? What are the energies of the first and second excited states in the first order of perturbation theory?

Solution:

The unperturbed Hamiltonian is

$$
H_0 = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}m\omega(x^2 + y^2),
$$

the corresponding eigenstates are $\psi_n(x) \otimes \psi_m(y) = |nm\rangle$ and the eigenenergies $E_{nm} = \hbar\omega(n + m + 1)$.

The corrections to the original energies can be simply evaluated when the perturbing potential is rewritten using the lowering and raising operators for the LHO. As $x = \frac{\alpha}{\sqrt{2}}(a + a^+)$, we obtain

$$V' = A\frac{\alpha^4}{4}(a^2 + a^{+2} + 2a^+a + 1) \otimes (b^2 + b^{+2} + 2b^+b + 1) \,,$$

where a acts in the x space and b in the y space. We see that non-zero matrix elements between different states occur when the quantum number n is either lowered or decreased by two or stays constant. The same (but independent) requirement holds for the quantum number m. This means that, for example, the diagonal matrix elements will be non-zero as both indices stay constant (e.g., matrix elements of the type $\langle nm|V'|nm\rangle$).

The first order correction to the ground state energy is obtained as the matrix element of the perturbation

$$\begin{aligned}
\langle 00|V'|00\rangle =& A\frac{\alpha^4}{4}\langle 00(a^2 + a^{+2} + 2a^+a + 1) \otimes (b^2 + b^{+2} + 2b^+b + 1)|00\rangle \\
=& A\frac{\alpha^4}{4}\langle 0|2a^+a + 1|0\rangle \otimes \langle 0|2b^+b + 1|0\rangle \\
=& A\frac{\alpha^4}{4}\langle 0|1|0\rangle \otimes \langle 0|1|0\rangle \\
=& A\frac{\alpha^4}{4} \,,
\end{aligned}$$

where we used that $a|0\rangle = 0$ and that the matrix elements of the squares of lowering or raising operators are zero.

In the second order correction to the ground state energy, only states $|20\rangle$, $|02\rangle$, and $|22\rangle$ will contribute as for V' all the other states have zero matrix elements with the ground state. The contributions are

$$\begin{aligned}
\Delta E(|20\rangle) =& \frac{|\langle 00|V'|20\rangle|^2}{\epsilon_0 - \epsilon_{20}} \\
=& A^2\frac{\alpha^8}{16}\frac{|\langle 00|a^2 \otimes (2b^+b + 1)|20\rangle|^2}{\hbar\omega - 3\hbar\omega} \\
=& A^2\frac{\alpha^8}{16}\frac{(\sqrt{2} \cdot 1)^2}{-2\hbar\omega} \\
=& -A^2\frac{\alpha^8}{16\hbar\omega} \,,
\end{aligned}$$

where we wrote only the relevant operators of the perturbation on the second line. The contribution of the state $|02\rangle$ will be identical.

The correction to the energy from the state $|22\rangle$ is

$$\begin{aligned}
\Delta E(|22\rangle) =& \frac{|\langle 00|V'|22\rangle|^2}{\epsilon_0 - \epsilon_{22}} \\
=& A^2 \frac{\alpha^8}{16} \frac{|\langle 00|a^2 \otimes b^2|22\rangle|^2}{\hbar\omega - 5\hbar\omega} \\
=& A^2 \frac{\alpha^8}{16} \frac{(\sqrt{2} \cdot \sqrt{2})^2}{-4\hbar\omega} \\
=& -A^2 \frac{\alpha^8}{16\hbar\omega} ,
\end{aligned}$$

Hence the same correction is found also here, so that the total ground state energy through second order is

$$E_{00}^{(2)} = \hbar\omega + A\frac{\alpha^4}{4} - 3A^2 \frac{\alpha^8}{16\hbar\omega} .$$

There are two first excited states, namely $|10\rangle$ and $|01\rangle$, each with energy $2\hbar\omega$. For degenerate states we need to diagonalise the partial Hamiltonian within the subspace of the degenerate states. However, in this case one can see that $\langle 10|V'|01\rangle = 0$ since each quantum number changes by one and such states are not coupled by the perturbation. Therefore, the energies of both the states will remain degenerate and will shift by $\langle 10|V'|10\rangle$, which is

$$\begin{aligned}
\langle 10|V'|10\rangle =& A\frac{\alpha^4}{4}\langle 10|(a^2 + a^{+2} + 2a^+a + 1) \otimes (b^2 + b^{+2} + 2b^+b + 1)|10\rangle \\
=& A\frac{\alpha^4}{4}\langle 1|2a^+a + 1|1\rangle \otimes \langle 0|2b^+b + 1|0\rangle \\
=& A\frac{\alpha^4}{4}\langle 1|2a^+a + 1|1\rangle \otimes \langle 0|1|0\rangle \\
=& 3A\frac{\alpha^4}{4} .
\end{aligned}$$

There are three excited states, $|20\rangle$, $|02\rangle$, and $|11\rangle$. The state $|11\rangle$ has zero matrix elements of the perturbation with the other two states and will shift by

$$\begin{aligned}
\langle 11|V'|11\rangle =& A\frac{\alpha^4}{4}\langle 11|(a^2 + a^{+2} + 2a^+a + 1) \otimes (b^2 + b^{+2} + 2b^+b + 1)|11\rangle \\
=& A\frac{\alpha^4}{4}\langle 1|2a^+a + 1|1\rangle \otimes \langle 1|2b^+b + 1|1\rangle \\
=& A\frac{\alpha^4}{4}3 \cdot 3 \\
=& 9A\frac{\alpha^4}{4} .
\end{aligned}$$

The matrix element of the perturbation is non-zero between states $|20\rangle$ and $|02\rangle$ so we need to calculate and diagonalise the partial Hamiltonian. For this, we need $\langle 20|V'|20\rangle$ which

will be identical to $\langle 02|V'|02\rangle$ due to the symmetry of the perturbation, and the coupling element $\langle 20|V'|02\rangle$, which is again identical to the conjugate $\langle 02|V'|20\rangle$. We obtain

$$
\begin{aligned}
\langle 20|V'|20\rangle =& A\frac{\alpha^4}{4}\langle 20(a^2 + a^{+2} + 2a^+a + 1) \otimes (b^2 + b^{+2} + 2b^+b + 1)|20\rangle \\
=& A\frac{\alpha^4}{4}\langle 2|2a^+a + 1|2\rangle \otimes \langle 0|1|0\rangle \\
=& A\frac{\alpha^4}{4}5 \cdot 1 \\
=& 5A\frac{\alpha^4}{4},
\end{aligned}
$$

for the diagonal part and

$$
\begin{aligned}
\langle 20|V'|02\rangle =& A\frac{\alpha^4}{4}\langle 20(a^2 + a^{+2} + 2a^+a + 1) \otimes (b^2 + b^{+2} + 2b^+b + 1)|02\rangle \\
=& A\frac{\alpha^4}{4}\langle 2|a^{+2}|0\rangle \otimes \langle 0|b^2|2\rangle \\
=& A\frac{\alpha^4}{4}\sqrt{2} \cdot \sqrt{2} \\
=& A\frac{\alpha^4}{2}.
\end{aligned}
$$

for the coupling element. The partial Hamiltonian is then

$$
H_{02,20} = A\frac{\alpha^4}{4}\begin{pmatrix} 5 & 2 \\ 2 & 5 \end{pmatrix},
$$

which has eigenvalues $(5 \pm 2)A\frac{\alpha^4}{4}$. For $A > 0$, the lower energy state with $E = 3A\frac{\alpha^4}{4}$ corresponds to a combination $\frac{1}{\sqrt{2}}(|20\rangle - |02\rangle)$ and the higher energy state with $E = 7A\frac{\alpha^4}{4}$ is the combination $\frac{1}{\sqrt{2}}(|20\rangle + |02\rangle)$.