F2009

Problem 3: Artificial Atoms (10 points)

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Modern techniques in nanotechnology research can create artificial atoms, man-made structures that confine electrons like real atoms but with properties that can be engineered. In this problem, consider a 2D atom (electrons tightly bound in the z-direction) with a parabolic potential in the x- and y-directions. The Hamiltonian is:

$$H_0 = \frac{p^2}{2m} + \frac{m\omega^2}{2}\left(x^2 + y^2\right). \tag{1}$$

Note: In solving this problem, you might want to use the standard operators:

$$a_x = \frac{1}{\sqrt{2}}\left(\frac{x}{\lambda} + i\frac{\lambda}{\hbar}p_x\right), \quad a_y = \frac{1}{\sqrt{2}}\left(\frac{y}{\lambda} + i\frac{\lambda}{\hbar}p_y\right) \tag{2}$$

and their Hermitian conjugates, where $\lambda = \sqrt{\frac{\hbar}{m\omega}}$.

(a) What are the eigenenergies of this atom? What are the degeneracies of these energy levels? If the separation between adjacent levels is 20 meV (0.02 eV), approximately how large are the low-energy electron states in the atom (the radius)? (2 pts)

b) If the atom is put in a constant electric field, the Hamiltonian H_0 is perturbed by a potential:

$$H_1 = -eE_1 x \tag{3}$$

where E_1 is a constant (the electric field). Prove that to first order in the field, the energy levels of the atom do not change. (2 pts)

c) Next the atom is placed in a more complex field to study its properties. The new potential is:

$$H_2 = \frac{C_2}{\lambda^2}xy \tag{4}$$

To first order in C_2, what are the new eigenenergies of what were the first three energy levels of H_0? Show your work. (4 pts)

d) If a different perturbing potential:

$$H_3 = \frac{C_3}{\lambda^2}x^2 \tag{5}$$

is applied (rather than H_2), how would your answers to part (c) change? No computations should be necessary to answer this question. (2 pts)

(a)

The general expression for the eigenenergies is

$$\boxed{E_{n_x n_y} = (n_x + n_y + 1)\hbar\omega}$$

where $n_x = 0, 1, 2, \ldots$ and $n_y = 0, 1, 2, \ldots$

(b)

The first order energy correction is

$$\begin{aligned}
E^{(1)} &= \langle n_x n_y | H_1 | n_x n_y \rangle \\
&= \langle n_x n_y | -eE_1 x | n_x n_y \rangle \\
&= -eE_1 \langle n_x n_y | x | n_x n_y \rangle \\
&= -eE_1 \langle n_x n_y | \sqrt{\tfrac{\hbar}{2m\omega}} (a_x + a_x^+) | n_x n_y \rangle \\
&= -eE_1 \sqrt{\tfrac{\hbar}{2m\omega}} \langle n_x n_y | a_x + a_x^+ | n_x n_y \rangle \\
&= -eE_1 \sqrt{\tfrac{\hbar}{2m\omega}} \left(\sqrt{n_x} \langle n_x n_y | n_x - 1 \; n_y \rangle + \sqrt{n_x + 1} \langle n_x n_y | n_x + 1 \; n_y \rangle \right) \\
&= 0
\end{aligned}$$

since our states are orthogonal. Thus, our correction to first order is zero and the levels of the atom do not change.

(c)

The first three energy levels are

$$E_{00}^{(0)} = \hbar\omega$$
$$E_{01}^{(0)} = E_{10}^{(0)} = 2\hbar\omega$$
$$E_{11}^{(0)} = E_{20}^{(0)} = E_{02}^{(0)} = 3\hbar\omega$$

$\underline{E_{00}}$

$$E_{00}^{(1)} = \langle 0\,0 | \frac{C_2}{\lambda^2} xy | 0\,0 \rangle$$
$$= \frac{C_2}{\lambda^2}\frac{\hbar}{2m\omega}\langle 0\,0 | a_x a_y + a_x a_y^\dagger + a_x^\dagger a_y + a_x^\dagger a_y^\dagger | 1\,0 \rangle$$
$$= \frac{C_2\hbar}{2\lambda^2 m\omega}\left(0 + 0 + 0 + \langle 0\,0 | 1\,1 \rangle\right)$$
$$= 0$$

So our eigenenergy of the ground state is unchanged,

$$\boxed{E_{00} = \hbar\omega}.$$

$\underline{E_{01} = E_{10}}$

Since this state is degenerate, we must determine the eigenvalues of the two-fold W matrix,

$$W = \begin{pmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{pmatrix},$$

where, in general, $W_{ij} = \langle \psi_i^{(0)} | H' | \psi_j^{(0)} \rangle$. Let $\psi_a = |1\,0\rangle$ and $\psi_b = |0\,1\rangle$.

(c), cont'd...

Then

$$W_{aa} = \langle \psi_a | \frac{c_2}{\lambda^2} xy | \psi_a \rangle$$

$$= \frac{c_2 \hbar}{2\lambda^2 m\omega} \langle 1\,0 | a_x a_y + a_x a_y^\dagger + a_x^\dagger a_y + a_x^\dagger a_y^\dagger | 1\,0 \rangle$$

$$= \frac{c_2 \hbar}{2\lambda^2 m\omega} \left[0 + \langle 1\,0 | 0\,1 \rangle + 0 + \sqrt{2} \langle 1\,0 | 2\,1 \rangle \right]$$

$$= 0$$

$$W_{bb} = \langle \psi_b | \frac{c_2}{\lambda^2} xy | \psi_b \rangle$$

$$= \frac{c_2 \hbar}{2\lambda^2 m\omega} \langle 0\,1 | a_x a_y + a_x a_y^\dagger + a_x^\dagger a_y + a_x^\dagger a_y^\dagger | 0\,1 \rangle$$

$$= \frac{c_2 \hbar}{2\lambda^2 m\omega} \left[0 + 0 + \langle 0\,1 | 1\,0 \rangle + \sqrt{2} \langle 0\,1 | 1\,2 \rangle \right]$$

$$= 0$$

$$W_{ab} = \langle \psi_a | \frac{c_2}{\lambda^2} xy | \psi_b \rangle$$

$$= \frac{c_2 \hbar}{2\lambda^2 m\omega} \langle 1\,0 | a_x a_y + a_x a_y^\dagger + a_x^\dagger a_y + a_x^\dagger a_y^\dagger | 0\,1 \rangle$$

$$= \frac{c_2 \hbar}{2\lambda^2 m\omega} \left[0 + 0 + \langle 1\,0 | 1\,0 \rangle + \sqrt{2} \langle 1\,0 | 1\,2 \rangle \right]$$

$$= \frac{c_2 \hbar}{2\lambda^2 m\omega}$$

$$W_{ba} = \langle \psi_b | \frac{c_2}{\lambda^2} xy | \psi_a \rangle$$

$$= \frac{c_2 \hbar}{2\lambda^2 m\omega} \langle 0\,1 | a_x a_y + a_x a_y^\dagger + a_x^\dagger a_y + a_x^\dagger a_y^\dagger | 1\,0 \rangle$$

$$= \frac{c_2 \hbar}{2\lambda^2 m\omega} \left[0 + \langle 0\,1 | 0\,1 \rangle + 0 + \sqrt{2} \langle 0\,1 | 2\,1 \rangle \right]$$

$$= \frac{c_2 \hbar}{2\lambda^2 m\omega}$$

(c), cont'd...

So

$$W = \begin{pmatrix} 0 & \frac{c_2 \hbar}{2\lambda^2 m\omega} \\ \frac{c_2 \hbar}{2\lambda^2 m\omega} & 0 \end{pmatrix}.$$

Then our eigenvalues are

$$\begin{vmatrix} -\lambda' & \frac{c_2 \hbar}{2\lambda^2 m\omega} \\ \frac{c_2 \hbar}{2\lambda^2 m\omega} & -\lambda' \end{vmatrix} = 0$$

$$(-\lambda')(-\lambda') - \left(\frac{c_2 \hbar}{2\lambda^2 m\omega}\right)^2 = 0$$

$$\lambda' = \pm \frac{c_2 \hbar}{2\lambda^2 m\omega}$$

and so our first excited energies are

$$\boxed{E_{10} = E_{01} = 2\hbar\omega \pm \frac{c_2 \hbar}{2\lambda^2 m\omega}}.$$

(c), cont'd...

$E_{11} = E_{20} = E_{02}$

Now our W matrix is

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

Let $\psi_a = |1\,1\rangle$, $\psi_b = |2\,0\rangle$, and $\psi_c = |0\,2\rangle$. Then

$$W_{aa} = \langle \psi_a | \frac{c_2}{\lambda^2} xy | \psi_a \rangle$$
$$= \langle 1\,1 | \frac{c_2}{\lambda^2} \frac{\hbar}{2m\omega} (a_x a_y + a_x a_y^\dagger + a_x^\dagger a_y + a_x^\dagger a_y^\dagger) | 1\,1 \rangle$$
$$= 0$$

$$W_{bb} = \langle \psi_b | \frac{c_2}{\lambda^2} xy | \psi_b \rangle$$
$$= \frac{c_2}{\lambda^2} \frac{\hbar}{2m\omega} \langle 2\,0 | a_x a_y + a_x a_y^\dagger + a_x^\dagger a_y + a_x^\dagger a_y^\dagger | 2\,0 \rangle$$
$$= 0$$

$$W_{cc} = \langle \psi_c | \frac{c_2}{\lambda^2} xy | \psi_c \rangle$$
$$= \frac{c_2}{\lambda^2} \frac{\hbar}{2m\omega} \langle 0\,2 | a_x a_y + a_x a_y^\dagger + a_x^\dagger a_y + a_x^\dagger a_y^\dagger | 0\,2 \rangle$$
$$= 0$$

$$W_{ab} = \langle \psi_a | \frac{c_2}{\lambda^2} xy | \psi_b \rangle$$
$$= \langle 1\,1 | \frac{c_2}{\lambda^2} \frac{\hbar}{2m\omega} (a_x a_y + a_x a_y^\dagger + a_x^\dagger a_y + a_x^\dagger a_y^\dagger) | 2\,0 \rangle$$
$$= \frac{c_2 \hbar}{2\lambda^2 m\omega} \left[0 + \sqrt{2} \langle 1\,1 | 1\,1 \rangle + 0 + 0 \right]$$
$$= \frac{c_2 \hbar}{\sqrt{2}\lambda^2 m\omega}$$

$$W_{ba} = \langle \psi_b | \frac{c_2}{\lambda^2} xy | \psi_a \rangle$$
$$= \frac{c_2 \hbar}{\sqrt{2}\lambda^2 m\omega}$$

(c), cont'd...

$$W_{bc} = \langle \psi_b | \frac{c_2}{\lambda^2} xy | \psi_c \rangle$$

$$= \frac{c_2 \hbar}{2\lambda^2 m\omega} \langle 20 | a_x a_y + a_x a_y^+ + a_x^+ a_y + a_x^+ a_y^+ | 02 \rangle$$

$$= 0$$

$$W_{cb} = \langle \psi_c | \frac{c_2}{\lambda^2} xy | \psi_b \rangle$$

$$= 0$$

$$W_{ac} = \langle \psi_a | \frac{c_2}{\lambda^2} xy | \psi_c \rangle$$

$$= \frac{c_2 \hbar}{2\lambda^2 m\omega} \langle 11 | a_x a_y + a_x a_y^+ + a_x^+ a_y + a_x^+ a_y^+ | 02 \rangle$$

$$= \frac{c_2 \hbar}{2\lambda^2 m\omega} \left[0 + 0 + \sqrt{2} \langle 11 | 11 \rangle + 0 \right]$$

$$= \frac{c_2 \hbar}{\sqrt{2}\lambda^2 m\omega}$$

$$W_{ca} = \langle \psi_c | \frac{c_2}{\lambda^2} xy | \psi_a \rangle$$

$$= \frac{c_2 \hbar}{\sqrt{2}\lambda^2 m\omega}$$

and our matrix is

$$W = \begin{pmatrix} 0 & \frac{c_2 \hbar}{\sqrt{2}\lambda^2 m\omega} & \frac{c_2 \hbar}{\sqrt{2}\lambda^2 m\omega} \\ \frac{c_2 \hbar}{\sqrt{2}\lambda^2 m\omega} & 0 & 0 \\ \frac{c_2 \hbar}{\sqrt{2}\lambda^2 m\omega} & 0 & 0 \end{pmatrix}$$

(c), cont'd...

Our eigenvalues are then

$$\begin{vmatrix} -\lambda & \frac{c_2\hbar}{\sqrt{2}\lambda^2 m\omega} & \frac{c_2\hbar}{\sqrt{2}\lambda^2 m\omega} \\ \frac{c_2\hbar}{\sqrt{2}\lambda^2 m\omega} & -\lambda & 0 \\ \frac{c_2\hbar}{\sqrt{2}\lambda^2 m\omega} & 0 & -\lambda \end{vmatrix} = 0$$

$$(-\lambda)^3 - (-\lambda)\left(\frac{c_2\hbar}{\sqrt{2}\lambda^2 m\omega}\right)^2 - (-\lambda)\left(\frac{c_2\hbar}{\sqrt{2}\lambda^2 m\omega}\right)^2 = 0$$

$$\lambda^2 - \left(\frac{c_2\hbar}{\lambda^2 m\omega}\right)^2 = 0$$

$$\lambda = \pm \frac{c_2\hbar}{\lambda^2 m\omega}.$$

Thus, our corrected second excited energies are

$$\boxed{E_{11} = E_{20} = E_{02} = 3\hbar\omega \pm \frac{c_2\hbar}{\lambda^2 m\omega}}.$$

(d)

Now we let our perturbing potential be

$$H' = \frac{C_3}{\lambda^2} x^2$$

$$= \frac{C_3 \hbar}{2\lambda^2 m\omega}\left(a_x a_x + a_x a_x^\dagger + a_x^\dagger a_x + a_x^\dagger a_x^\dagger\right)$$

We would get the same result for the corrected ground state energy.

For the degenerate states, I would expect the energy splitting to be asymmetric since the perturbing potential only involves x and not y.