1. (Quantum Mechanics)

A particle of mass m in two dimensions is confined by an isotropic harmonic oscillator potential of frequency ω, while subject to a weak and anisotropic perturbation of strength $\alpha \ll 1$. The total Hamiltonian describing the motion of this particle is

$$H = H_0 + V = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}m\omega^2(x^2 + y^2) + \alpha m\omega^2 xy$$

(a) What are the energies and degeneracies of the three lowest-lying unperturbed states?

(b) Use perturbation theory to correct the energies to first order in α.

(c) Find the exact spectrum of H.

(d) Check that the perturbative results in part (b) are recovered.

(e) Assume that two identical electrons are subject to the same anisotropic Hamiltonian. Write down the explicit wave-functions and degeneracies of the two lowest energy states.

Solution: *Solution by Audrey Farrell*

(a)

Clarification: This question wants the three lowest lying states, not energy levels. These three states comprise two energy levels: a non-degenerate ground energy level and a two-fold degenerate excited energy level. Since we use "ground state" and "excited state" to describe these degenerate energies, it's easy to misinterpret this question and do a lot more work than necessary.

The unperturbed Hamiltonian is

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

And the time-independent Schrödinger equation is

$$H\,\psi(x,y) = \left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{1}{2}m\omega^2(x^2+y^2)\right]\psi(x,y) = E\,\psi(x,y)$$

This is a separable differential equation, so we take $\psi(x,y) = \psi_x(x)\psi_y(y)$, and we have two independent one-dimensional harmonic oscillator problems, with $E = E_x + E_y$. For a 1D harmonic oscillator $E_i = \hbar\omega\left(n_i + \frac{1}{2}\right)$, so the total energy is

$$E_{mn} = \hbar\omega\,(m + n + 1)$$

where m gives the state of the 1D harmonic oscillator in x, and n gives the state of the 1D harmonic oscillator in y. The three lowest-energy *states* are then

$$E_0 = E_{00} = \hbar\omega \rightarrow \text{non-degenerate ground state}$$
$$E_1 = E_{10} = E_{01} = 2\hbar\omega \rightarrow \text{2-fold degenerate excited state}$$

(b) *Clarification: The question asks for corrections to the first order in α, the first order correction to the groundstate is zero. You do not need to go to higher orders to find the first nonzero correction, just leave it there.*

The perturbation is $H' = \alpha m\omega^2 xy$. We'll use the ladder operators in each direction: a and $a^\dagger$ in the x-direction, b and $b^\dagger$ in the y-direction. Both sets of operators have the same properties:

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \quad a|n\rangle = \sqrt{n}|n-1\rangle$$

Rewriting x and y in terms of these operators:

$$x = \frac{1}{\sqrt{2\beta}}\left(a + a^\dagger\right), \quad y = \frac{1}{\sqrt{2\beta}}\left(b + b^\dagger\right), \quad \beta = \frac{m\omega}{\hbar}$$

The ground state is nondegenerate, so we can use nondegenerate perturbation theory and the first order correction to the ground state $|mn\rangle = |00\rangle$ is

$$E_0^{(1)} = \langle 00|H'|00\rangle \propto \langle 00|xy|00\rangle \propto \langle 00|(ab + ab^\dagger + a^\dagger b + a^\dagger b^\dagger)|00\rangle = \langle 00|11\rangle = 0$$

You can also use symmetry to show that the first order correction to the ground state has to be zero, since the ground state wave function of a harmonic oscillator potential is symmetric (even), and the x and y operators are antisymmetric (odd), so the expectation value of x and y must be zero (the integral of an odd function over all space is always zero).

The first excited state is degenerate, so we'll use degenerate perturbation theory with the basis $\psi_1 = A|10\rangle + B|01\rangle$, $\psi_2 = C|10\rangle - D|01\rangle$. The perturbation matrix $H_{ij} \propto \langle i|xy|j\rangle$

$$\begin{pmatrix} \langle 10|xy|10\rangle & \langle 10|xy|01\rangle \\ \langle 01|xy|10\rangle & \langle 01|xy|01\rangle \end{pmatrix} = \frac{1}{2\beta}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$H' = \frac{m\omega^2\alpha}{2\beta}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\alpha}{2}\hbar\omega\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \mathcal{E}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathcal{E} = \frac{\alpha}{2}\hbar\omega$$

The first order corrections $E_1^{(1)}$ are the eigenvalues of this matrix:

$$\det\left(H' - \mathbb{I}E_1^{(1)}\right) = \begin{vmatrix} -E_1^{(1)} & \mathcal{E} \\ \mathcal{E} & E_1^{(1)} \end{vmatrix} = 0 \rightarrow E_1^{(1)} = \pm\mathcal{E} = \pm\frac{\alpha}{2}\hbar\omega$$

(c) The easiest way to solve this system exactly is to switch to a coordinate system oriented along $y = x$, using the transformation

$$X = \frac{x+y}{\sqrt{2}}, \quad Y = \frac{x-y}{\sqrt{2}}$$

$$X^2 = \frac{1}{2}(x^2+y^2+2xy), \quad Y^2 = \frac{1}{2}(x^2+y^2-2xy) \rightarrow X^2+Y^2 = x^2+y^2, \quad X^2-Y^2 = 2xy$$

so that the Hamiltonian is still separable.

$$H = \frac{p_X^2}{2m} + \frac{p_Y^2}{2m} + \frac{1}{2}\left[(1+\alpha)X^2 + (1-\alpha)Y^2\right]$$

Just like in part (a) we have two separate harmonic oscillators, with $E = E_X + E_Y$, but this time the two do not have the same frequency.

$$E = \hbar\omega\sqrt{1+\alpha}\left(m+\frac{1}{2}\right) + \hbar\omega\sqrt{1-\alpha}\left(n+\frac{1}{2}\right)$$

(d) Here we take the approximation $\sqrt{1\pm\alpha} \approx 1 \pm \frac{\alpha}{2}$ since $\alpha \ll 1$.

$$E_{00} = \frac{1}{2}\hbar\omega\left(\sqrt{1+\alpha}+\sqrt{1-\alpha}\right) \approx \frac{1}{2}\hbar\omega\left(1+\frac{\alpha}{2}+1-\frac{\alpha}{2}\right) = \hbar\omega$$

$$E_{10} = \frac{1}{2}\hbar\omega\left(3\sqrt{1+\alpha}+\sqrt{1-\alpha}\right) \approx \frac{1}{2}\hbar\omega\left(3\left(1+\frac{\alpha}{2}\right)+1-\frac{\alpha}{2}\right) = 2\hbar\omega + \frac{\alpha}{2}\hbar\omega$$

$$E_{01} = \frac{1}{2}\hbar\omega\left(\sqrt{1+\alpha}+3\sqrt{1-\alpha}\right) \approx \frac{1}{2}\hbar\omega\left(1+\frac{\alpha}{2}+3\left(1-\frac{\alpha}{2}\right)\right) = 2\hbar\omega - \frac{\alpha}{2}\hbar\omega$$

This matches the results from perturbation theory to first order in α.

(e) Neglecting Coulomb interactions between the two electrons, each can be in a spin up or a spin down state, and can be in one of the 2 eigenstates of the Hamiltonian with lowest energies: $|00\rangle$ with energy $\hbar\omega$ or $|01\rangle$ with energy $2\hbar\omega - \frac{\alpha}{2}\hbar\omega$. The energy states of the two-electron system are then $E = E_1 + E_2$, and the wave functions are the products of the two wave functions of the Hamiltonian $\varphi_{mn}(\vec{r}_1)$ and $\varphi_{mn}(\vec{r}_2)$ with the spin-state wave functions of the two electrons.

The non-degenerate ground state has both electrons in the $|00\rangle$ eigenstate of the Hamiltonian, with one electron spin-up and one spin-down:

$$E_0 = E_{00} + E_{00} = 2\hbar\omega, \quad \psi(\vec{r}_1,\vec{r}_2) = \varphi_{00}(\vec{r}_1)\varphi_{00}(\vec{r}_2)\cdot\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

The first excited state has one electron in the $|00\rangle$ state and one in the $|01\rangle$ state, and each can be either spin up or spin down, so it is a 4-fold degenerate state:

$$E_1 = E_{00} + E_{01} = 3\hbar\omega + \frac{\alpha}{2}\hbar\omega, \quad \psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}\left[\varphi_{00}(\vec{r}_1)\varphi_{01}(\vec{r}_2) + \varphi_{01}(\vec{r}_1)\varphi_{00}(\vec{r}_2)\right] \cdot \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

$$= \frac{1}{\sqrt{2}}\left[\varphi_{00}(\vec{r}_1)\varphi_{01}(\vec{r}_2) - \varphi_{01}(\vec{r}_1)\varphi_{00}(\vec{r}_2)\right] \cdot \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$$

$$= \frac{1}{\sqrt{2}}\left[\varphi_{00}(\vec{r}_1)\varphi_{01}(\vec{r}_2) - \varphi_{01}(\vec{r}_1)\varphi_{00}(\vec{r}_2)\right] \cdot |\uparrow\uparrow\rangle$$

$$= \frac{1}{\sqrt{2}}\left[\varphi_{00}(\vec{r}_1)\varphi_{01}(\vec{r}_2) - \varphi_{01}(\vec{r}_1)\varphi_{00}(\vec{r}_2)\right] \cdot |\downarrow\downarrow\rangle$$