

E263: Second order perturbation of an atom in electric field

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The problem:

- (1) Explain why, in a generic way, an electron eigenfunction, in an atom, has a defined parity. How does the above explain that in an electric field the first order correction to the energy is zero. An atom can be described as a two level system with level spacing Δ .
- (2) Write the Hamiltonian of an atom in electric field. Use ϵ for the perturbation strength. What is the connection of ϵ with the strength of the electric field?
- (3) Using the perturbation theory, find the second order correction to the energy of the atom above. Compare the solution to the exact solution from the diagonalization of the Hamiltonian. Be sure you understand the following: An electric field strength can change in different places in space. That is why an atom will feel an effective potential $V(R) \propto |\epsilon(R)|^2$. This potential explains the energy drop caused by the atom's polarization in electric field.
- (4) Define and calculate the polarization using the perturbation theory.

The solution:

- (1) Electron in an atom has $r \rightarrow -r$ symmetry and therefore has definite parity. Consequently $\langle x \rangle = \langle y \rangle = \langle z \rangle = 0$, since $V(x) = -e\mathcal{E}\hat{x}$, it follows that $\langle V(x) \rangle = 0$, that is why the first order correction is zero.
- (2) The Hamiltonian is:

$$H = H_0 + V$$

Where: $V = -e\mathcal{E}\hat{x}$ and $\hat{x} = \frac{a}{2}\sigma_x$.

$$H = \begin{pmatrix} \frac{ea}{2}\mathcal{E} & c \\ c & -\frac{ea}{2}\mathcal{E} \end{pmatrix}$$

Hence we see that

$$\Delta = 2c$$

$$\epsilon = e\mathcal{E}a$$

In the H_0 Basis we have:

$$\mathcal{H} = \frac{\Delta}{2} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{ea}{2}\mathcal{E} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = -\frac{\Delta}{2}\sigma_z + \frac{ea\mathcal{E}}{2}\sigma_x$$

(3) By using:

$$E_0 = E_0^{[0]} + V_{nn} + \sum_{p \neq n} \frac{|V_{np}|^2}{E_n^{[0]} - E_p^{[0]}}$$

We obtain the atom's energy, in the ground state, up to the second order:

$$E_0^{[0]} = -\frac{\Delta}{2}$$

$$E_0^{[1]} = 0$$

$$E_0^{[2]} = -\frac{|ea\mathcal{E}|^2}{4\Delta}$$

So we can write:

$$E_0 = E_0^{[0]} + E_0^{[1]} + E_0^{[2]} = -\frac{\Delta}{2} - \frac{|ea\mathcal{E}|^2}{4\Delta}$$

To compare the result with the exact solution, we first diagonalize the Hamiltonian:

$$\mathcal{H}_{diag} = \begin{pmatrix} -\sqrt{\left(\frac{\Delta}{2}\right)^2 + \left(\frac{ea\mathcal{E}}{2}\right)^2} & 0 \\ 0 & \sqrt{\left(\frac{\Delta}{2}\right)^2 + \left(\frac{ea\mathcal{E}}{2}\right)^2} \end{pmatrix}$$

From here the exact solution for the ground state:

$$E_{exact} = -\sqrt{\left(\frac{\Delta}{2}\right)^2 + \left(\frac{ea\mathcal{E}}{2}\right)^2}$$

By Tylor expending E_{exact} we obtain the same result as the perturbe energy:

$$E_{exact} = -\frac{\Delta}{2} - \frac{|ea\mathcal{E}|^2}{4\Delta}$$

(4) Let us assume that the electron is in the $|1\rangle$ state, and now calculate the wave function corrections using:

$$|\psi_n\rangle = |\phi_n\rangle + \sum_{p \neq n} \frac{\langle \phi_p | V | \phi_n \rangle}{E_n^{[0]} - E_p^{[0]}} |\phi_p\rangle$$

We obtain:

$$|\psi\rangle = |1^{[0]}\rangle + \frac{ea\mathcal{E}}{2\Delta} |2^{[0]}\rangle$$

The polarization is given by the expectation value of \hat{x} (in the H_0 basis):

$$\langle \hat{x} \rangle = \langle \psi | \hat{x} | \psi \rangle = \frac{ea\mathcal{E}}{2\Delta}$$