E621: Stark effect in Hydrogen atom

Submitted by: Naama Shukrun, Ella Yonai

The problem:
The electron in the Hydrogen atom is a particle of mass M and charge e with potential of V (r) = -$\frac{r}{\alpha}$.
Assume that we can neglect the probability to find the particle in an energy level n¿2 so we have a five dimensional space for the particle's states, two spherical and three polaric orbitals so the basis for the representation is : $|s1\rangle$,$|s2\rangle$,$|px\rangle$,$|py\rangle$,$|pz\rangle$.
We also neglect spin orbit interaction so we can ignore the spin.
The atom is placed in constant electric field in the z direction , this causes the atom to polarize.

(1) Write the Hamiltonian in the standard form using the dynamic variables: $\mathcal{H}\left(p_r, L, r, \theta, \mathcal{E}\right)$

(2) Write the two matrices that represent the unperturbed

Hamiltonian and the interaction with the electric field.

(3) Find the expression for the ground state energy $E_{gr}(\mathcal{E})$ in the second order of perturbation theory.

(4) Find the expression for the first excited state energy $E_{ex}(\mathcal{E})$ in the second order of perturbation theory.

(5) Write the expression for the polarization $\widetilde{P} = e\left\langle z\right\rangle$ of the atom that was prepared in the ground state.

(6) Write the expression for the polarization of the atom that was prepared in the excited state.

Guidance:
(a) The solutions should be expressed with (M,a,e,c_1,c_2)

(b) $a = \frac{1}{\alpha M}$ the Bohr atom radius, $c_1 = \frac{8\sqrt{2}}{9}$,$c_2 = 3\sqrt{3}$ constants that represent the solution of the radial integral.

(c) The radial functions $\frac{1}{a^{3/2}}R^{l\nu}$are: $R^{01} = 2e^{-x}$, $R^{02} = \sqrt{\frac{1}{6}}(\frac{x}{2})e^{-\frac{x}{2}}$,
$R^{11} = \sqrt{\frac{1}{2}}(1 - \frac{x}{2})e^{-\frac{x}{2}}$.

(d) Solution will include c1, c2 and other factors.

(e) Solution to clauses 5-6 may be derived without complicated calculations.

The solution:

(1) In the $|\upsilon lm\rangle$basis the Hamiltonian is :

$$\mathcal{H} = \frac{P_r^2}{2M} + \frac{L^2}{2mr^2} - \frac{\alpha}{r} - e\mathcal{E}rcos\theta$$

when the last term stands for the perturbation caused by the electric field in the z direction.

(2) The Eigenvalues for the unperturbed Hydrogen atom are:

$$E_{\upsilon lm} = \frac{1}{2Ma^2\left(l+\upsilon\right)^2}$$

$$\mathcal{H} = \mathcal{H}_0 + V$$

The unperturbed Hamiltonian:

$$\mathcal{H}_0 = -\frac{1}{2Ma^2}\begin{pmatrix} 1 & & & & \\ & \frac{1}{4} & & & \\ & & \frac{1}{4} & & \\ & & & \frac{1}{4} & \\ & & & & \frac{1}{4} \end{pmatrix}$$

the interaction with the electric field:

$$V = -e\mathcal{E}\left\langle \nu' l' m' \mid cos\theta \mid \upsilon lm \right\rangle = -e\mathcal{E}\int_0^\infty R^{l'\nu' *} r^3 R^{l\nu} dr \int_0^{4\pi} Y^*_{l'm'} Y_{lm} cos\theta d\Omega$$

$$cos\theta = \sqrt{\frac{4\pi}{3}} Y_{10}$$

$$V = -\sqrt{\frac{4\pi}{3}} e\mathcal{E}\int_0^\infty R^{l'\nu' *} r^3 R^{l\nu} dr \int_0^{4\pi} Y^*_{l'm'} Y_{lm} Y_{10} d\Omega$$

from parity considerations we see that the only case in which the expression is nonzero is when the function is odd, meaning $l' \neq l$ and $m' = m = 0$.

$$-a\left\langle s1 \mid \mathcal{E}e\frac{r}{a}cos\theta \mid pz\right\rangle = -\sqrt{\frac{4\pi}{3}}\mathcal{E}ea\int R^{01*} x^3 R^{11} dx \int_0^{4\pi} Y^*_{00} Y_{10} Y_{10} d\Omega = \frac{-\mathcal{E}ea}{\sqrt{3}} c_1$$

$$-a\left\langle s2 \mid \mathcal{E}e\frac{r}{a}cos\theta \mid pz\right\rangle = \frac{-\mathcal{E}ea}{\sqrt{3}} c_2$$

$$V = -\frac{\mathcal{E}ea}{\sqrt{3}}\begin{pmatrix} 0 & 0 & 0 & 0 & c_1 \\ 0 & 0 & 0 & 0 & c_2 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ c_1 & c_2 & 0 & 0 & 0 \end{pmatrix}$$

(3) The expression for the ground state energy with second order correction:

$$E_{gr}\left(\mathcal{E}\right) = E_{10} - \frac{\left|\langle s1 \mid V \mid pz\rangle\right|^2}{\left|E_{10} - E_{11}\right|} = -\frac{1}{2Ma^2} - \frac{8c_1^2 e^2 \mathcal{E}^2 M a^4}{9}$$

(4) The expression for the lowest excited state energy will be obtained after using degenerate perturbation theory:

$$\begin{pmatrix} -\frac{1}{8Ma^2} & -\frac{\mathcal{E}ea}{\sqrt{3}}c_2 \\ -\frac{\mathcal{E}ea}{\sqrt{3}}c_2 & -\frac{1}{8Ma^2} \end{pmatrix}$$

$$E_{ex}\left(\mathcal{E}\right) = -\frac{1}{8Ma^2} - \frac{\mathcal{E}ea}{\sqrt{3}}c_2$$

(5) The polarization can be simply obtain from the concept of generalized forces: $\mathcal{F} = \text{-}\frac{\partial \mathcal{H}}{\partial X}$

$$\left\langle \widetilde{\mathcal{P}_{\text{gr}}} \right\rangle = \text{-}\frac{\partial E_{gr}}{\partial \mathcal{E}} = \frac{16c_1^2 e^2 \mathcal{E} M a^4}{9}$$

(6) For the first excited state due to degenerate perturbation theory the energy has different dependence on the electric field:

$$\left\langle \widetilde{\mathcal{P}_{\text{ex}}} \right\rangle = \text{-}\frac{\partial E_{ex}}{\partial \mathcal{E}} = \frac{ea}{\sqrt{3}}c_2$$

Thus the polarization for this state will be constant.