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Exercise 1: Zeeman and Paschen-Back effects (Oral).


In Exercises 1 and 2 of Assignment 3 we studied the fine structure of the Hydrogen atom resulting from the spin-orbit coupling of the electron. Let us now consider the Hydrogen atom in a uniform magnetic field in the z -direction, $\mathbf{B} = B\hat{\mathbf{z}}$. Taking into account the spin magnetic-moment interaction, the Hamiltonian now reads

$$H = H_0 + H_{LS} + H_m.$$

where $H_m = -\frac{eB}{m_e c}(L_z + 2S_z)$. Using perturbation theory, find the energy correction in first order for the $2p$ orbital in two cases:

- Weak magnetic field (Zeeman effect). Consider here the perturbation to the fine structure levels obtained in Exercise 2 Assignment 3, i.e. $2p_{1/2}$ and $2p_{3/2}$.
- A strong magnetic field (Paschen-Back effect). In this case, the spin orbit coupling H_{LS} can be considered a small perturbation to $H = H_0 + H_m$.

Exercise 2: Electrical dipole transitions in polar molecules (Oral).

Due to their asymmetric structure, heteronuclear molecules  have an electric dipole moment \mathbf{d} along their symmetry axis. In this exercise, we are only concerned with the rotational degree of freedom of such molecules, which is described by the angular momentum \mathbf{J} . The dynamics of such a “rigid rotor” is governed by $H_{\text{rot}} = B \cdot \mathbf{J}^2/\hbar^2$ (why?). Thus, the states $|J, M\rangle$ are eigenstates of H_{rot} with energy $BJ(J+1)$ and degeneracy $2J+1$. The rotational constant B/\hbar is typically of the order of the GHz. Consequently, it is possible to drive microwave transitions between different $|J, M\rangle$ states. In this exercise, we calculate the matrix elements of possible transitions. Electrical dipole transitions are only allowed if the matrix element $\langle J', M' | \mathbf{d} | J, M \rangle$ is different from zero.

- First we describe the dipole operator \mathbf{d} in a spherical basis with components d_q , where $q = 0, \pm 1$. The components are given by $d_0 = d \cos(\theta)$ and $d_{\pm} = \mp d e^{\pm i\phi} \sin(\theta)/\sqrt{2}$. They are proportional to spherical harmonics $d_q \propto Y_1^q$.

Apply the Wigner-Eckart Theorem for the dipole matrix elements in the spherical representation $\langle J', M' | d_q | J, M \rangle$. What is the rank of the tensor d_q ? Which selection rules for $\Delta J \equiv J' - J$ and $\Delta M \equiv M' - M$ can you derive directly from the Clebsch-Gordan coefficients?

- Use a parity argument to show why $\Delta J = 0$ transitions are not allowed. To do this use the above matrix elements and make use of the parity of the spherical harmonics involved.

- c) We have now derived the selection rules $\Delta J = \pm 1$ with $\Delta M = q = 0, \pm 1$. We would like to simplify the dipole matrix elements. The Wigner-Eckart theorem allows us to choose q as well as M and M' freely to determine $\langle J' || d || J \rangle$. In order to do this, solve the equation for this term and choose $M = J$ and $q = 1$ to explicitly compute $\langle J + 1 || d || J \rangle$. How can you use this result to determine the matrix elements for $\Delta J = -1$? (Giving the idea is enough).

Hint: The appearing Clebsch-Gordan coefficient couples two “stretched states” (i.e. those states with $M = J$) to a final state which is also stretched. Think about a general property of such Clebsch-Gordan coefficient. The spherical harmonics for these states are given by equation

$$Y_J^J(\theta, \phi) = \frac{(-1)^J}{2^J J!} \sqrt{\frac{(2J+1)!}{4\pi}} \sin^J(\theta) e^{iJ\phi}.$$

For odd n we have:

$$\int_0^\pi d\theta \sin(\theta)^n = \frac{(\frac{n-1}{2})!(\frac{n+1}{2})!}{(n+1)!} 2^{n+1}.$$

The final result for $\Delta J = +1$ should be

$$\langle J + 1, M + q | d_q | J, M \rangle = d \sqrt{\frac{J+1}{2J+3}} \langle J, M; 1, q | J + 1, M + q \rangle$$

- d) As a simple application we consider a polar molecule in the ground state $|0, 0\rangle$. First, compute the dipole moment for the ground state $\langle 00 | \mathbf{d} | 00 \rangle$. A dipole moment can be induced by an external electric field $\mathbf{E} = E \mathbf{e}_z$ (static). To get an approximate value for this dipole moment we treat the coupling of the dipole moment to the electric field $H_E = -\mathbf{d} \cdot \mathbf{E} = -d_0 E$ as a perturbation (that is, $dE/B \ll 1$). Compute the induced dipole moment (component in z -direction) $\langle \widehat{00} | d_0 | \widehat{00} \rangle$ using the above matrix elements, where $|\widehat{00}\rangle$ stands for the ground state in first order perturbation theory.

Hint: The only appearing Clebsch-Gordan coefficient is again trivial in this case. What happens in general if one of the two angular momenta in the coupling is zero?

Exercise 3: Permutation operator (Written, 3 points).

We consider a system of two particles in one spacial dimension $x \in \mathbb{R}$. Let $\mathcal{H}^{(1)}$ and $\mathcal{H}^{(2)}$ be their respective Hilbert spaces. The operator which exchanges the two particles in the product Hilbert space, $\mathcal{H} = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)}$, can be formally defined by its action on the product basis of two particle states $|x_1 x_2\rangle = |x_1\rangle^{(1)} \otimes |x_2\rangle^{(2)}$ by

$$P_{(12)} |x_1 x_2\rangle := |x_2 x_1\rangle, \quad \forall x_1, x_2 \in \mathbb{R}$$

We call P_p the permutation operator corresponding to the permutation p . Here, we only consider $p = (12)$. Show that

- a) $P_{(12)}^{-1} = P_{(12)}^\dagger = P_{(12)}$;
b) The eigenvalues of $P_{(12)}$ can only be $+1, -1$;
c) The vectors

$$\begin{aligned} |xx\rangle_S &:= |xx\rangle, \\ |x_1x_2\rangle_S &:= \frac{1}{\sqrt{2}} (|x_1x_2\rangle + |x_2x_1\rangle), \quad x_1 < x_2 \\ |x_1x_2\rangle_A &:= \frac{1}{\sqrt{2}} (|x_1x_2\rangle - |x_2x_1\rangle), \quad x_1 < x_2 \end{aligned}$$

are eigenvectors of $P_{(12)}$.