Hyperfine structure of atoms in combined external fields

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Abstract. In order to interpret experimental hyperfine spectra of the resonance lines of the alkali atoms in presence of external electric and magnetic fields in arbitrary direction relative to each other a computer programme has been developed which computes the splitting of hyperfine components of spectral lines and their expected relative transition probabilities. The computed data can be directly compared with experimental spectra taken by laser-atomic-beam spectroscopy. Splitting parameters, like hyperfine structure constants or polarizabilities, can be evaluated with the help of a fitting procedure. The theoretical approach used in the programme has rather general validity, therefore the programme can be utilized, within the validity of the applied theoretical assumptions, for any kind of atom.

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1. Introduction

In the last years laser-atomic-beam spectroscopy experiments performed at our institute were mainly concerned with systematic investigations of the behaviour of the hyperfine components of the alkali resonance lines in external fields. The resonance lines of sodium were studied in magnetic fields up to 1 T [1-3], in electric fields up to 300 kV/cm [4, 5] and in simultaneously applied fields up to 0.03 T and 200 keV/cm [6-8]; other alkalis under study were lithium [9, 10] and potassium [11].

All the experimental spectra of the resonance lines of the alkali atoms in external fields show a rather complex structure. The need for their interpretation led to the development of a computer programme enabling the calculation of the theoretical splitting and of the theoretical relative transition probabilities of the hyperfine line components. The field strength range, the quantum numbers and the splitting parameters (hyperfine structure constants, g-factors, polarizabilities) of the levels involved in the transition are the input parameters. The programme was also used to check or to determine part of the splitting parameters with the help of a fitting procedure, which compares the experimental line splittings with the computed ones.

The following theoretical considerations have rather general validity and may be used, within the validity of the applied assumptions, for any kind of atom. Nevertheless the sodium atom in its first excited level 3p\(^2\)P\(_{3/2}\) has been used as "working horse" for all calculations in combined fields presented in this article due to the availability of a large amount of experimental data, thus enabling us to check the calculations.

2. Splitting of energy levels

In general the influence of external fields on the energy levels |\(\gamma, J M\rangle\) of an atom characterized by a suitable set of quantum numbers \(\gamma, J\) and by the total angular momentum quantum number \(J\) leads to the removal of the energy degeneracy of the levels relative to the projection quantum number \(M\): the levels split according to the value of \(M\) and to the strength of the fields [12, 13]. A simple analytical description of the splitting behaviour can only be given for \(J \leq 1/2\). In all other cases the splitting behaviour is usually numerically calculated with the help of matrix diagonalization programs.

In laser-atomic-beam-spectroscopy experiments [14] the splitting of the levels due to the presence of external fields is indirectly observed as the splitting of the spectral lines observed via laser excitation of the atoms in the atomic beam. In this article only the splitting of the hyperfine structure of fine structure levels \(\gamma, J\) will be considered.

The programme used for calculating the splitting of hyperfine energy levels is a modified version of the programme LEVEL by W. Happer. LEVEL already allows the computation of the eigenvalues and eigenvectors of a nondiagonal, real, symmetric energy matrix

\[
\langle \gamma' \gamma, J' M' \rangle | H_{\text{hf}} + H_{\text{mag}} + H_{\text{sec}} | \gamma, J M \rangle
\]
describing the interaction of an atom with the nuclear quantum numbers \( \gamma_x, I \) and \( M_I \) and the electronic quantum numbers \( \gamma_x, J \) and \( M_J \), with the external fields, both taken parallel to the z-axis. The matrix contains the energy contributions due to the hyperfine interaction \( H_{\text{hf}} \), the Zeeman interaction \( H_{\text{mag}} \) and the Stark interaction \( H_{\text{elec}} \).

Both in LEVEL and in the modified version the matrix elements used for the computation imply several assumptions: Firstly, the nucleus is always in its ground state, therefore the nuclear spin quantum number \( I \) is assumed to be a good quantum number. Secondly, the total electronic angular momentum quantum number \( J \) too is assumed to be a good quantum number, therefore the energy splitting of the fine structure levels due to the external fields has to be much less than the distance between any neighbouring fine structure levels. That means that the matrix elements describing the interactions are diagonal in \( \gamma_x, \gamma_x, I \) and \( J \). The matrices are calculated in the uncoupled basis

\[
| \gamma_x \gamma_x I J M_I M_J \rangle = | \gamma_x I M_I \rangle | \gamma_x J M_J \rangle
\]

for practical reasons, since an external field tends to uncouple the total angular momentum \( F \) of the atom into its constituents \( I \) and \( J \). In LEVEL the directions of both the magnetic and the electric field are assumed to be parallel to the z axis.

The programme used at our institute has been modified in order to calculate the eigenvalues \( W_e \), \( W_e \), and eigenvectors \( | \Phi \rangle \), \( | \Phi' \rangle \) of the matrices describing the interactions of the hyperfine structure of two given fine structure levels \( \gamma_x J \) and \( \gamma_x J' \) (e.g. \( 3s^2 S_1/2 \) and \( 3p^2 P_3/2 \) in the case of the resonance lines of the sodium atom) with the external fields. Furthermore the matrix elements describing the interaction with an external electric field have been changed in order to allow an arbitrary direction of the electric field relative to the magnetic field, the latter still assumed to be parallel to the z axis.

The eigenvalues \( W_\Phi \), \( W_{\Phi'} \) of each matrix describe the splitting and shift of the hyperfine structure of the corresponding fine structure level. The splitting and shift of the hyperfine components of the line is then given by the difference between the splitting and shift of the two levels involved in the transition (see Sect. 3):

\[
\Delta W_{\Phi, \Phi'} = W_\Phi - W_{\Phi'}.
\]

**2.1. Hyperfine structure**

The hyperfine structure of the energy levels is due to the interaction of the charge distribution of the nucleus (with nuclear spin quantum number \( I \)) with the electromagnetic field generated at the nucleus position by the electron cloud (with total angular momentum quantum number \( J \)). The hyperfine interaction couples the angular momenta \( I \) and \( J \) to the total angular momentum of the atom \( F \). A detailed description of the hyperfine structure interaction is presented in [15–20], while an overview on the hyperfine structure of the alkali atoms is given in [21]. Since the nuclear charge distribution can be expressed in terms of electromagnetic multipole moments, the operator of the hyperfine structure interaction \( H_{\text{hf}} \) itself can be also expressed by a multipole expansion as a sum of scalar products of spherical tensor operators of rank \( k \)

\[
H_{\text{hf}} = \sum_{k > 0} (T^{(k)}_r M^{(k)}_r)
\]

\[
= \sum_{k > 0} \sum_{q = -k}^{+k} (-1)^q T^{(k)}_q M^{(k)}_{-q},
\]

where \( T^{(k)}_q \) is the electronic part of the interaction, describing the electromagnetic field at the nucleus position, and \( M^{(k)}_q \) is the nuclear part, describing the electromagnetic multipole moments of the nucleus. Due to parity considerations the electric interaction is described by terms with even \( k \), the magnetic interaction by terms with odd \( k \). The matrix elements in the uncoupled basis \( | \gamma_x \gamma_x I J M_I M_J \rangle \) are given by

\[
\langle \gamma_x \gamma_x I J M_I M_J | H_{\text{hf}} | \gamma_x \gamma_x I' J' M_I' M_J' \rangle
\]

\[
= \sum_{k > 0} \frac{h A_k(J)}{k!} \left( \begin{array}{ccc} J & k & J \\ -J & 0 & J \end{array} \right) \left( \begin{array}{ccc} I & k & I \\ -I & 0 & I \end{array} \right) \times \sum_{q = -k}^{+k} (-1)^{J + I - M_J - M_I} \times \left( \begin{array}{ccc} J & k & J \\ -M_J & q & M_J \end{array} \right) \left( \begin{array}{ccc} I & k & I \\ -M_I & q & M_I \end{array} \right),
\]

where \( A_k(J) \) are the diagonal hyperfine structure constants [15, 20] defined by

\[
A_k = \left\langle \gamma_x \gamma_x J J | T_0^{(k)}_0 | \gamma_x \gamma_x J J \right\rangle \left\langle \gamma_x I I | M^{(k)}_0 | \gamma_x I I \right\rangle
\]

\[
= \left( \begin{array}{ccc} J & k & J \\ -J & 0 & J \end{array} \right) \left( \begin{array}{ccc} I & k & I \\ -I & 0 & I \end{array} \right) \times \left\langle \gamma_x J | T^{(k)}_0 | \gamma_x J \right\rangle \left\langle \gamma_x I | M^{(k)}_0 | \gamma_x I \right\rangle.
\]

The constants \( A_k(J) \) are directly connected to the traditionally used constants \( a(J), b(J), c(J) \)…[16, 17]:

\[
A_1(J) = I J a(J)
\]

\[
A_2(J) = \frac{1}{2} b(J)
\]

\[
A_3(J) = c(J)
\]

\[
A_4(J) = d(J).
\]

Taking into account contributions up to \( k = 2 \) (\( k = 1 \): magnetic dipole interaction, \( k = 2 \): electric quadrupole interaction) and (6) and (7), we obtain the hyperfine structure matrix elements used in the programme: