High Energy Density Physics 5 (2009) 320–327

Contents lists available at ScienceDirect

High Energy Density Physics

journal homepage: www.elsevier.com/locate/hedp

Efficient methods for calculating the number of states, levels and lines in atomic configurations

F. Gilleron*, J.-C. Pain

Commissariat à l'Énergie Atomique, CEA, DIF, F-91297 Arpajon, France

ARTICLE INFO

Article history:
Received 23 April 2009
Accepted 23 April 2009
Available online 5 May 2009

PACS:
05.10.a
02.70.Rr

Keywords:
Angular momentum
Quantum states
Levels
Lines

ABSTRACT

Exact or statistical methods for determining the distribution of the M_J values (projection of total angular momentum J) in an electron configuration are presented. This distribution, noted $P(M_J)$, is used to calculate the allowed values of J and the number of electric-dipolar (E1) lines between two configurations. First, the difficulty to account for the Pauli exclusion principle for equivalent electrons is stressed. Showing the limit of the usual exact approach, a very efficient recursive technique is proposed for determining exactly the distribution $P(M_J)$. Second, the statistical approach of Bauche and Bauche-Arnoult [J. Phys. B Atom. Mol. Opt. Phys. 20 (1987) 1659] is extended in order to account for configurations with a high-ℓ spectator. In this case, identical consecutive values may exist in the center of $P(M_J)$, which can neither be modeled by a Gaussian nor by a Gram–Charlier type function. It is shown that the Generalized Gaussian function, with the exponent constrained by the kurtosis (reduced fourth-order centered moment) of $P(M_J)$, is more suited in these situations. A new analytical formula for the evaluation of the number of E1 lines with a larger range of applicability is then proposed.

1. Introduction

The conservation of angular momentum is an important concept in physics, which is closely related to the rotation symmetries of a system, free of any external torque. In quantum physics, the total angular momentum J of an isolated ion is also a constant of motion, meaning that its projection M_J upon a particular axis is quantized in $2J+1$ values: $-J \le M_J \le +J$. The study of the allowed values of J (or M_J) in quantum states of the ion is of great interest because it plays a role in many concrete problems of atomic physics. For instance, the number of multipolar lines between two configurations is directly linked to the number of J levels in both configurations. Such quantity is obviously important in calculating the opacity coefficient of hot plasmas. The number of E1 lines is a crucial input of the Resolved Transition Array (RTA) model [1,2], which simulates a detailed-line treatment in a statistical manner. In mixed statistical and detailed models [3,4], the number of levels or lines can be used as a criterion in order to decide whether to calculate the spectra with statistical approaches, such as Unresolved Transition Array (UTA) [5] or Super Transition Array (STA) [6], or with detailed line-by-line atomic structure codes. From a practical point of view, the number of levels with a fixed J value in a configuration determines also the size of the Hamiltonian submatrices in most atomic structure codes (for instance in Cowan's code [7]). The determination of these dimensions enables one to estimate the complexity of a calculation, and to extend arrays in the code at the right size if necessary.

Another interest of such study is the calculation of averages for operators which depend only on total angular momenta. The trace of such operators over all $|\alpha J)$ levels can be simplified and evaluated more easily if the distribution of angular momenta is known. For instance, considering the operator $\vec{J}^2$, one has

$$\sum_{\alpha J}\left(\alpha J\left\|\vec{J}^2\right\|\alpha J\right) = \sum_J J(J+1)Q(J), \tag{1}$$

where $Q(J)$ is the number of J levels in the configuration. This averaging technique can be generalized to operators which depend on more angular momenta by calculating the corresponding degeneracy. For the Zeeman operator, $H_z = \vec{B}\mu_0(\vec{J} + (g_s - 1)\vec{S})$, with $\vec{S} = \sum \vec{s}_i$, one must determine the number of levels $|\gamma(SL)J)$ having the same set of values (S, L).

In the first section, exact methods for determining the distribution of the discrete M_J (and J) values in configurations are presented. Showing the usual exact method can be time consuming in the case of equivalent electrons, a more efficient approach based on recursion relations is proposed. In the second section, the study is performed in a statistical framework. It is shown that a continuous representation of the M_J values based on the Generalized Gaussian

* Corresponding author.
E-mail address: franck.gilleron@cea.fr (F. Gilleron).

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doi:10.1016/j.hedp.2009.04.007

function is better suited than the Gram–Charlier expansion series, in particular for configurations having a plateau in the center of this M_J distribution. For that reason, a new compact formula for estimating the number of electric dipolar lines between two configurations is suggested, with a larger range of applicability and an overall better accuracy.

2. Rigorous methods for the study of the total angular momentum

2.1. Generalities

The total angular momentum $\overrightarrow{J}$ of the ion is the addition of the intrinsic angular momenta of each electron:

$$\overrightarrow{J} = \sum_i (\overrightarrow{s}_i + \overrightarrow{\ell}_i), \tag{2}$$

where $\overrightarrow{s}_i$ ($s_i = 1/2$) and $\overrightarrow{\ell}_i$ are respectively the spin and orbital angular momenta of the ith electron. The one-electron states of the ion are defined by $|\ell_i m_{\ell_i} s_i m_{s_i}\rangle$, where m_{ℓ_i} (such that $-\ell_i \le m_{\ell_i} \le +\ell_i$) and m_{s_i} (such that $-1/2 \le m_{s_i} \le +1/2$) are projections of ℓ_i and s_i respectively. Multielectron states of the ion are represented by $|\alpha J M_J\rangle$, where α is an additional set of quantum numbers that describes the way the one-electron states are coupled to give a particular value of J and of its projection M_J. Because the total energy of the ion is independent of the M_J values, it is useful to introduce the $(2J+1)$-degenerated level noted $|\alpha J\rangle$.

From now, the notation $Q(J)$ (or $P(M_J)$) is introduced to represent the number of levels (or states) having in common the same value of J (or M_J). The study of the distribution of quantum number J in an atomic system is somewhat cumbersome because it is the eigenvalue of no simple operator. But more important, there is no simple rule on J to account for the Pauli exclusion principle in configurations with more than two equivalent electrons. It is usually more comfortable to study the distribution of the projection M_J of J, because M_J is the eigenvalue of the one-electron operator J_z and is thus additive with respect to the magnetic quantum numbers of all the electrons:

$$M_J = \sum_i (m_{s_i} + m_{\ell_i}) \tag{3}$$

The Pauli exclusion principle can be handled through the combinatorics, by searching for all the possibilities to populate the one-electron states. In addition, it is possible to deduce the distribution $Q(J)$ from the $P(M_J)$ by using the following relation [8]:

$$Q(J) = \sum_{M_J=J}^{J+1} (-1)^{J-M_J} P(M_J) = P(J) - P(J+1), \tag{4}$$

and vice versa

$$P(M_J) = \sum_{J \ge |M_J|} Q(J). \tag{5}$$

Obviously, the normalization of both distributions requires

$$\sum_{M_J=-M_{\max}}^{+M_{\max}} P(M_J) = \sum_{J=J_{\min}}^{J_{\max}} (2J+1) Q(J) = g_c, \tag{6}$$

where g_c is the degeneracy of the configuration of interest. The extreme allowed values of M_J or J are defined in the next section. Because the distribution of the M_J values is symmetric, the study can be restricted to positive values:

$$P(M_J) = -P(-M_J). \tag{7}$$

2.2. Extreme values of M_J or J in a configuration

In order to determine the largest value of M_J, it is convenient to sort the values $m_j = m_s + m_\ell$ of the one-electron states by ascending order. Numbering the one-electron states of ℓ^1 from $k=1$ to $k = 4\ell + 2$, the following formula is proposed:

$$m_k = \frac{2k - 4\ell - 3 + (-1)^k}{4} \quad \text{for } 1 \le k \le 4\ell + 2. \tag{8}$$

Now, the largest value of M_J in the subshell ℓ^N is determined by summing the last N values of m_k:

$$\sum_{k=4\ell+3-N}^{4\ell+2} m_k = \frac{1}{8}\left[2N(4\ell + 2 - N) + 1 - (-1)^N\right] \tag{9}$$

For an arbitrary configuration of the type $c = \ell_1^{N_1} \ell_2^{N_2} \ldots \ell_w^{N_w}$, the largest value of M_J is simply the sum of the maxima in each subshell:

$$M_{\max} = \frac{1}{8} \sum_{i=1}^{w} \left[2N_i(4\ell_i + 2 - N_i) + 1 - (-1)^{N_i}\right] \tag{10}$$

The minimum positive value of M_J (noted $M_{\min>0}$) depends on the even or odd number of electrons in the configuration. For an even number, the electrons can be arranged by pairs with opposite values of m_j: the minimum value is zero. For an odd number, the previous arrangement plus one electron with $m_j = 1/2$ gives a minimum value of one half. Finally

$$M_{\min>0} = \frac{1}{4}\left[1 - (-1)^{\sum_{i=1}^{w} N_i}\right] \tag{11}$$

The largest value of J is obviously that of M_J due to Eq. (4), because $Q(M_{\max}) = P(M_{\max})$ and $Q(M_{\max}+1) = 0$. Thus

$$J_{\max} = M_{\max}. \tag{12}$$

The minimum value of J is more cumbersome to determine, because it depends on the type of the configuration. For instance, considering the case ℓ^1 or $\ell^{4\ell+1}$, the result is $J_{\min} = \ell - (1/2)$. For an open subshell ℓ^N with $N > 1$ and $N < 4\ell + 1$, we have $J_{\min} = M_{\min>0}$. More generally, for configurations which contain several open subshells with at least one subshell ℓ^1 (or $\ell^{4\ell+1}$) with a very large value of ℓ, the minimum value of J is between $M_{\min>0}$ and $\ell_> - (1/2)$ ($\ell_>$ is the largest value of the orbital momentum for the electrons). This issue comes from the fact that identical consecutive non-null values (a 'plateau') may exist in the center of the distribution $P(M_J)$ for some configurations (e.g. $3p^2 6h^1$):

$$P(M_{\min>0}) = P(M_{\min>0} + 1) = \cdots P(J_{\min}) \neq 0. \tag{13}$$

The use of Eq. (4) gives $Q(M_{\min>0}) = Q(M_{\min>0}+1) = \cdots = Q(J_{\min}-1) = 0$, and $Q(J_{\min}) \neq 0$. The length of the plateau in $P(M_J)$ (if it exists) thus determines the minimum value of J. This problem of great importance will be discussed in more details in the section related to the statistical approach.

2.3. Case of configuration ℓ^N

As mentioned previously, the difficult part consists in finding the distribution of M_J (or J) values for equivalent electrons. A simple way of doing that in ℓ^N can be found in atomic physics books. This academic method consists, first, in determining the $2(2\ell+1)$