A heuristic procedure to go from LS to jj expressions in atomic and nuclear spectroscopy

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The expressions for the energy matrix elements and for the radiative transitions in the jj coupling can be obtained from the respective LS expressions by making a few simple changes. The results shown as examples are compared with other treatments, where the two formulations are deduced in parallel, without making use of these simple rules. We emphasize that the rules were found by heuristic reasoning. In all cases the application of the rules are in accordance with published results. This work completes two previous papers published in this journal (References 19 and 20).

Keywords: LS coupling; jj coupling; energy levels; radiative transitions.

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1. Introduction

In Atomic and Nuclear Spectroscopy the concept (or expression) "LS coupling" is clear: it means that we rely on a non-relativistic treatment of atomic and even nuclear theory: the Hamiltonian $\widehat{H}$ explicitly contains the spin-orbit interaction, and works with both the orbital anguar momentum $(l, L_1, L,$ etc.) and spin angular momentum $(s, S_1, S,$ etc.). On the other hand, "jj coupling" can mean both a non-relativistic or a completely relativistic treatment: in the first case, the angular moments are the same as before, whereas in the second case, the spin moments do not appear in the formulation. Some books develop both types of coupling, but this is done independently, regardless of what is discussed in this article: you can go directly from LS expressions to jj ones with a few simple changes. So, if you have a book that deals with the LS case, you can go to jj expressions (relativistic or not) automatically.

A full development of the Atomic Theory based on LS coupling can be found in Cowan's book [1]. This book can be considered as the culmination of previous works, also of great theoretical value, such as those of Slater [2], Shore-Menzel [3], Mizushima [4], Sobelman [5], Weissbluth [6] and Condon-Odabasi [7]. Thus, with the use of the Racah algebra, the calculation of the energy level structure and the radiative transitions (E1, M1 and E2) can be written in terms of closed-form expressions. It should be noted that, beyond the theoretical results, explicit expressions for the energies of the terms of complex configurations appear, to a large extent, only in the Refs. [2, 7]. For the case of nuclear theory, a few simple examples in the jj coupling are given in Ref. [8]**.** On the other hand, in recent years several books have appeared that deal with the Relativistic Theory of Atoms. In this regard, we can mention the books by Johnson [9], Grant [10] and Rudzikas [11].

The purpose of this work is to indicate that both sets of expressions are simply related. Whereas a detailed discussion is necessary for specialists, it may be too much for general physicists. So, for example, in Laboratory Astrophysics, the need arises for a conceptual handling of these topics for people who need to run calculation codes without knowing, necessarily, the finer details of the theory [12, 13]. Also, something similar happens in Collision Physics and Plasma Spectroscopy, where many theoretical and semiempirical expressions for cross sections and rates were published in the LS schema [14]. We ourselves had to apply both formulations when studying the consistency of published levels in various isoelectronic sequences [15–17].

In short, different researchers not specialists in the atomic theory, can find profit in this work. The same goes for graduate students doing their master's work. Those who have taken standard courses in Quantum Mechanics and in Introductory Atomic Physics (*e.g.* Ref. [18]) can use these results.

As we have indicated in the abstract, our results were found by heuristic methods starting from the Cowan treatment [1]. Attending to the question about the final goal of this article, we can answer saying that if one knows the equations written in the LS schema, can translate them to the jj one in a easy form. Several examples are shown in Sec. 7. Therefore this work complements those presented as Refs. [19, 20] in this same Journal.

2. Changes to be made

We will present our work by analyzing the expressions of the atomic theory in the *LS* coupling, since this is the one extensivey and clearly developed in Cowan's book[i]. Furthermore, if we have these expressions in LS coupling, it is easy to go to jj coupling, as we will see below. The reciprocal case is not simple since, in the relativistic jj formulation, the spin angular moments do not appear and, therefore, we would not know how to introduce them later.

It is very important to remark that the mathematical techniques devoloped by Racah make it possible to completely bypass explicit use of determinantal functions, and to write down formulae for the direct evaluation of matrix elements for coupled basis functions and so, obtain the observables (energy levels, dipole line strengths, etc.). All the coefficients of the theory, corresponding to both the energies and the transition probabilities, are expressed through the following types of quantities: $3n-j$ symbols ($\equiv S_{3nj}$), reduced matrix elements of various tensor operators (*i.e.*: $\left\langle l_1 \left\| C^{(k)} \right\| l_2 \right\rangle$, etc.), fractional parentage coefficients, unit and double angular momentum operators, etc. All these quantities were presented in our previous papers [19, 20].

Let's start by remembering some relationships for various matrix elements of renormalized spherical harmonics $C_q^{(k)} = (4\pi/(2k+1))^{1/2} Y_{kq}$; for non-relativistic functions, let $|l\rangle$ an eigenfunction of the operator $\widehat{\mathbf{l}}^2$; then the relation is

$$\left\langle l_1 \left\| C^{(k)} \right\| l_2 \right\rangle = (-1)^{l_1} [l_1, l_2]^{1/2} \begin{pmatrix} l_1 & k & l_2 \\ 0 & 0 & 0 \end{pmatrix}, \quad (1)$$

results, where the left hand side is a *reduced matrix element* (denoted by a double bar) and the final symbol of the right hand side is a *3-j symbol* [1, 6]. The analogous relation for the relativistic case it is [9]:

$$\left\langle j_1 \left\| C^{(k)} \right\| j_2 \right\rangle = (-1)^{j_1+1/2} [j_1, j_2]^{1/2} \times \begin{pmatrix} j_1 & j_2 & k \\ -1/2 & 1/2 & 0 \end{pmatrix}. \quad (2)$$

In some texts, the matrix element of the first member is often denoted $\left\langle \kappa_1 \left\| C^{(k)} \right\| \kappa_2 \right\rangle$, being $\kappa = (-1)^{l+s+j}(j+1/2) = (l-j)(2j-1)$. With the formulas in the Appendix we can see that, starting from Eqs. (1), $(A.1)$ and $(A.2)$, we can get to Eq. (2).

The above results influence the calculation of the various matrix elements, which are made using the Racah algebra, so that to go from LS formulae (from Ref. [1]) to jj formulae ([9] and/or [11]) we must do certain changes. In the next two subsections we will indicate the changes to be made in the LS expressions.

2.1. Relatively simple changes

1) Ignore all symbols of spin angular momentum type (normally denoted by $s, S,$ etc.) in the factors of type $\delta_{SS'}$ and override the values of $(s, S...)$ in the exponents $(-1)^{\text{something}}$, as well as in the 6j-symbols ($\equiv S_{6j}$) that contain some angular spin momentum ($s, S,$ etc.). If a S_{6j} corresponding to spins has all its elements equal to zero, then $S_{6j} = 1$ (which is a general property of the S_{6j}).

2) Change all the symbols $l, L, \overline{L}...$ by the respective $j, J, \overline{J}...$ keeping their meaning (*i.e.*: if $\overline{L}$ indicates the orbital angular momentum of the parent, $\overline{J}$ will indicate the total angular momentum of the parent, etc.).

3a) If the expression given in the LS coupling contains matrix elements of the form $\left\langle l_1 \left\| C^{(k)} \right\| l_2 \right\rangle$, they are replaced directly by $\left\langle j_1 \left\| C^{(k)} \right\| j_2 \right\rangle$.

3b) Equivalently to 3a, given the relations (1) and (2), if in the text the combination

$$(-1)^{l_1} \begin{pmatrix} l_1 & k & l_2 \\ 0 & 0 & 0 \end{pmatrix},$$

appears, it is replaced (in addition to the above cited changes) by

$$(-1)^{j_1+1/2} \begin{pmatrix} j_1 & j_2 & k \\ -1/2 & 1/2 & 0 \end{pmatrix}.$$

2.2. Relatively complex changes

For the following changes, please refer to the Refs. [19, 20] when necessary (where notions as the Wigner-Eckart theorem, unit and double tensor operators, coefficients of fractional parentage, etc. where introduced).

4) In the matrix elements of the *unit tensor operator* $U^{(k)}$, $\left\langle l^N \left\| U^{(k)} \right\| l^N \right\rangle$, which is expressed in terms of 6j-symbols and coefficients of fractional parentage (cfp), the above changes 1-3 are made and the LS-cfp $\left(l_i^{n-1} \overline{\alpha_i L_i}\ \overline{S_i} \| l_i^n \alpha_i L_i S_i\right)$ are replaced by the jj-cfp $\left(j^{n-1} \overline{\alpha}\ \overline{J} \| j^n \alpha J\right)$, to obtain $\left\langle j^N \left\| U^{(k)} \right\| j^N \right\rangle$.

5) In the case of the matrix elements of the *double tensor operators* $\left\langle l^N \left\| V^{(k1)} \right\| l^N \right\rangle$ (basic to evaluate the spin-orbit interaction in LS coupling), keep in mind that if the "S" are removed, then the $\left\langle l^N \left\| V^{(k1)} \right\| l^N \right\rangle$ are transformed into $\left\langle l^N \left\| U^{(k)} \right\| l^N \right\rangle$, which is replaced by matrix elements of the form $\left\langle j^N \left\| U^{(k)} \right\| j^N \right\rangle$.

6) For the calculation of radiative transitions (transition probabilities A_{ij}, or oscillator strengths f_{ij}), we will find a fundamental expression, given by the reduced matrix element $\mathbf{P}^{(1)}_{\alpha\alpha'}$ where, with the indices α, α' we will indicate, for brevity, the values $n, l, j,$ etc., so we will write $\mathbf{P}^{(1)\text{no-rel}}_{\alpha\alpha'}$ or $\mathbf{P}^{(1)\text{rel}}_{\alpha\alpha'}$, as appropriate:

$$\mathbf{P}^{(1)\text{no-rel}}_{\alpha\alpha'} \equiv \langle nl \,||\mathbf{r}||\, n'l' \rangle \equiv \left\langle l \left\| C^{(k)} \right\| l' \right\rangle I^{(1)\text{no-rel}}_{\alpha\alpha'}, \quad (3)$$

with

$$I^{(1)\text{no-rel}}_{\alpha\alpha'} \equiv \int_0^\infty P_{nl}\, r\, P_{n'l'}\, dr. \quad (4)$$

With the above rules, we can write directly

$$\mathbf{P}^{(1)\text{rel}}_{\alpha\alpha'} \equiv \langle nlj \,||\mathbf{r}||\, n'l'j' \rangle \equiv \left\langle j \left\| C^{(k)} \right\| j' \right\rangle I^{(1)\text{rel}}_{\alpha\alpha'}, \quad (5)$$

being $I^{(1)\text{rel}}_{\alpha\alpha'}$ the relativistic generalization of $I^{(1)\text{no-rel}}_{\alpha\alpha'}$.

For brevity, in this work we will not give the results on radiative transitions, which can be the subject of another presentation.

3. Energy expressions

To exemplify compliance with the previous rules, we start with the case of energies in the simplest cases. We use atomic units, where the electron charge e, the electron mass m_e, the Dirac constant $\hbar$ are unity and the energy is measured in rydbergs (1Ry$\equiv$ 13.6 eV). Theoretical treatment of an atom of atomic number Z with N electrons requires to solve the Schröedinger equation $\widehat{H}\Psi = E\Psi$, with the Hamiltonian

$$\widehat{H} = -\sum_i \nabla_i^2 - \sum_i \frac{2Z}{r_i} + \sum\sum_{i>j} \frac{2}{r_{ij}} + \sum_i \xi_i\left(r_i\right)\left(\mathbf{l}_i\cdot\mathbf{s}_i\right), \tag{6}$$

where the different operators are: ∇_i^2 for the kinetic energy, $2Z/r_i$ for the electron-nucleus interaction, $2/r_{ij}$ for electrostatic interactions between the electrons and $\xi_i\left(r_i\right)\left(\mathbf{l}_i\cdot\mathbf{s}_i\right)$ for the spin-orbit interaction.

Both in the non-relativistic case and in the electrostatic part of the relativistic case, the average energy of a configuration l^N (or a sub-configuration j^N) can be written as a sum over the N electrons or over the q shells:

$$E_{av} = \sum_{i=1}^{q} w_i \left\{ E_k^i + E_n^i + \frac{1}{2}\left(w_i - 1\right)E^{ii} + \frac{1}{2}\sum_{j\neq i} w_j E^{ij} \right\}, \tag{7}$$

where w_i is the occupation number of the subshell. In standard notation, E_k^i is the kinetic energy, E_n^i is the electron-nuclear energy and the electron-electron Coulomb energy is calculated between two-electron product functions

$$E^{ij} = \langle ij\left|2/r_{12}\right|ij\rangle_{av} - \langle ij\left|2/r_{12}\right|ji\rangle_{av}. \tag{8}$$

Equation (8) can be written in term of the so called Slater integrals (see below, Eq. (10) and the pedagogical works [19, 20]). As an example, we take the case of the neutral Carbon (C I). It is a common notation to use $I_k^a \equiv E_k^a + E_n^a$ for the energies arising from the one-electron operators, such that

$$E_{av} = 2I_{1s} + 2I_{2s} + 2I_{2p} + E_{1s,1s} + E_{2s,2s} + E_{2p,2p} + 4E_{1s,2s} + 4E_{1s,2p} + 4E_{2s,2p}.$$

With respect to this E_{av}, we have to deal with inter-electronic interaction in order to have the *terms*. Por example, in the case of C I, they are ^1S, ^3P and ^1D. These terms are splitted with respect to the E_{av} : as follow: ^1S : $E_{av} + 12F^2\left(pp\right)/25$, $^3P : E_{av} - 3F^2\left(pp\right)/25$, $^1D : E_{av} + 3F^2\left(pp\right)/25$. Many cases can be found in Ref. [7]. In the following subsection we specialize to the case of two electrons outside closed shells.

3.1. Simple configurations (two electrons outside closed shells)

The fundamental result for two electrons outside closed shells is, in general

$$\langle ij\left|2/r_{12}\right|tu\rangle = \sum_k r_k R^k\left(ij,tu\right), \tag{9}$$

where $R^k\left(ij,tu\right)$ is the generalized Slater integral, calculated in terms of the radial wave functions:

$$R^k\left(ij,tu\right) \equiv \int_0^\infty\int_0^\infty \frac{2r_<^k}{r_>^{k+1}} P_i\left(r\right) \times P_j\left(s\right)P_t\left(r\right)P_u\left(s\right)\, dr\, ds. \tag{10}$$

When $i = t$ and $j = u$**,** we have the direct integrals $F^k\left(ij\right) \equiv R^k\left(ij,ij\right)$ whereas when $i = u$ and $j = t$ we have the exchange integrals $G^k\left(ij\right) \equiv R^k\left(ij,ji\right)$ [20]. The expressions for the coefficients f_k and g_k of the direct and exchange Slater integrals, respectively, will be presented after Eqs. (11) to (12) (so as not to repeat similar expressions that can be confused). Examples for many cases of two electrons outside closed shells can be found in Ref. [7] for LS coupling. For jj cases, the appropriate Ref. [8] about Nuclear Shell Theory.

3.2. Complex configurations

Following Cowan, we will indicate that the cases treated correspond to:

a) the integrals for equivalent electrons $\left(l_j^{w_j}\right)$; the Coulomb contribution to the Hamiltonian matrix element (over and above E_{av}) has the form $\sum_j\sum_{k>0} f_k\left(l_jl_j\right)F^k\left(l_jl_j\right)$,

b) direct integrals for non-equivalent electrons $\left(l_i^{w_i}l_j^{w_j}\right)$ where the contribution is $\sum_{i<j}\sum_{k>0} f_k\left(l_il_j\right)F^k\left(l_il_j\right)$, and

c) exchange integrals, also for the case $\left(l_i^{w_i}l_j^{w_j}\right)$, where the contribution is $\sum_{i<j}\sum_{k>0} g_k\left(l_il_j\right)G^k\left(l_il_j\right)$.

The theoretical expressions for f_k and g_k are too long to write down explicitly, but can be tested in a homemade computer program; a pedagogical work was published in Ref. [19]. In all cases the correspondence has been verified, comparing Ref. [1] with Refs. [9, 11]. Many concrete examples are in Ref. [7] for LS; for jj cases we can cite [15–17].

3.3. Relation between the relativistic and the non-relativistic jj expressions

In the relativistic case, we must consider the average energy of the *sub-configurations* j^N distinguishing, for example, $E_{av}\left(p_-^2\right)$ from $E_{av}\left(p_+^2\right)$ and from $E_{av}\left(p_-p_+\right)$. To reduce them to the non-relativistic jj case, we simply equate them:

$$E_{av}\left(p_-^2\right) = E_{av}\left(p_+^2\right) = E_{av}\left(p_-p_+\right).$$

In nonrelativistic expressions, Slater integrals have the form $F^k\left(n_1l_1, n_2l_2\right)$ and $G^k\left(n_1l_1, n_2l_2\right)$ as, for example, $F^2\left(2p, 2p\right)$, etc. In the relativistic case, we will have expressions of the form $F^k\left(n_1l_1j_1, n_2l_2j_2\right)$ as $F^2\left(2p_+, 2p_+\right) \equiv F^2\left(2p_{3/2}, 2p_{3/2}\right)$, $F^2\left(2p_-, 2p_-\right) \equiv F^2\left(2p_{1/2}, 2p_{1/2}\right)$, etc. To go from relativistic jj to non-relativistic jj expressions, the direct integrals are set equal, for example:

$$F^2\left(nl_+, nl_+\right) = F^2\left(nl_-, nl_-\right) = F^2\left(nl_+, nl_-\right),$$

as well as exchange integrals.

4. Configuration interaction and the breakdown of the jj-coupling

This subject, of fundamental importance in Atomic and Nuclear Spectroscopy, is extremely complex in the most general case, and is expressed through the integrals $R^k\left(ij;tu\right)$ and the respective coefficients r_k (Eq. (9)). Simple examples are the configuration interaction $3p4s - 3p3d$, $3p^2 - 3s4d$, etc. A complete treatment for the LS case appears in the Ref. [1], where the author identifies 13 cases.

A simple case is that of two electrons outside closed shells; indicating the closed-shells by (cs)

$$(cs)\, n_\rho l_\rho n_\sigma l_\sigma - (cs)\, n'_\rho l'_\rho n'_\sigma l'_\sigma,$$

the coefficients for direct and exchange terms are given by Eqs. $(13.22-23)$ of Ref. [1], and are called $r^k_{d,LS}$ y $r^k_{e,LS}$:

$$r^k_{d,LS} = \delta_{LS,L'S'}\left(-1\right)^{l'_\rho+l_\sigma+L}\left\langle l_\rho\left\|C^{(k)}\right\|l'_\rho\right\rangle \times\left\langle l_\sigma\left\|C^{(k)}\right\|l'_\sigma\right\rangle\left\{\begin{array}{ccc} l_\rho & l_\sigma & L \\ l'_\sigma & l'_\rho & k\end{array}\right\}, \qquad (11)$$

and

$$r^k_{e,LS} = \delta_{LS,L'S'}\left(-1\right)^{l'_\rho+l_\sigma+S}\left\langle l_\rho\left\|C^{(k)}\right\|l'_\sigma\right\rangle \times\left\langle l_\sigma\left\|C^{(k)}\right\|l'_\rho\right\rangle\left\{\begin{array}{ccc} l_\rho & l_\sigma & L \\ l'_\rho & l'_\sigma & k\end{array}\right\}. \qquad (12)$$

When

$$n_\rho l_\rho = n'_\rho l'_\rho \quad \text{and} \quad n_\sigma l_\sigma = n'_\sigma l'_\sigma, \quad \text{then}$$
$$r^k_{d,LS} \equiv f^{LS}_k \quad \text{and} \quad R^k\left(\rho\sigma,\rho\sigma\right) \equiv F^k\left(\rho\sigma\right).$$

When

$$n_\rho l_\rho = n'_\sigma l'_\sigma \quad \text{and} \quad n_\sigma l_\sigma = n'_\rho l'_\rho \quad \text{then}$$
$$r^k_{e,LS} \equiv g^{LS}_k \quad \text{and} \quad R^k\left(\rho\sigma,\sigma\rho\right) \equiv G^k\left(\rho\sigma\right).$$

With the changes mentioned in Sec. 3, Eqs. $(11-12)$ become:

$$r^k_{d,jj} = \delta_{JJ'}\left(-1\right)^{j'_\rho+j_\sigma+J}\left\langle j_\rho\left\|C^{(k)}\right\|j'_\rho\right\rangle \times\left\langle j_\sigma\left\|C^{(k)}\right\|j'_\sigma\right\rangle\left\{\begin{array}{ccc} j_\rho & j_\sigma & J \\ j'_\sigma & j'_\rho & k\end{array}\right\}, \qquad (13)$$

and

$$r^k_{e,jj} = \delta_{JJ'}\left(-1\right)^{j'_\rho+j_\sigma}\left\langle j_\rho\left\|C^{(k)}\right\|j'_\sigma\right\rangle \times\left\langle j_\sigma\left\|C^{(k)}\right\|j'_\rho\right\rangle\left\{\begin{array}{ccc} j_\rho & j_\sigma & J \\ j'_\rho & j'_\sigma & k\end{array}\right\}, \qquad (14)$$

respectively, as indicated in Eq. (4.132) of Ref. [9]. Analogously to the LS case we will have, when $n_\rho l_\rho = n'_\rho l'_\rho$ and $n_\sigma l_\sigma = n'_\sigma l'_\sigma$, then $r^k_{d,jj} \equiv f^{jj}_k$ and, when $n_\rho l_\rho = n'_\sigma l'_\sigma$ and $n_\sigma l_\sigma = n'_\rho l'_\rho$, we will have $r^k_{e,jj} \equiv g^{jj}_k$. It is important to remark that in the relativistic case we must add, to the Coulombian interaction, the Breit interaction [9, 21].

Relatively simple cases are that of *single-configuration-like* interactions (*i.e.*: $l_1^{w_1}l_2l_3^{w_3} - l_1^{w_1}l'_2l_3^{w_3}$) and *Rydberg-series* interactions (*i.e.*: $n_m l_m^{w_m} n_\sigma l_\sigma - n_m l_m^{w_m} n'_\sigma l_\sigma$). The more general case of *arbitrary configuration interactions* is treated in all generality in the Ref. [1]; various particular cases of interest are in Ref. [11]. In all cases we have verified compliance with the rules mentioned in Sec. 3.

5. Examples

The energy of an atom (or ion) is given by the average value $\langle\Psi|\widehat{H}|\Psi\rangle$, being $\widehat{H}$ the hamiltonian given by Eq. (6) (or its relativistic counterpart) and Ψ the wave function constructed in the LS or jj scheme. In the non-relativistic case, the spin-orbit integrals ζ_{nl} appear in both the LS and jj coupling. On the other hand, in the relativistic hamiltonian there is no explicit operator for this interaction, so the ζ_{nl} will not appear in the relativistic jj scheme. Instead, the integrals R^k appear, which has been called the breakdown of the jj-coupling.

As an example, we will consider the sp configuration in the three cases mentioned above [15]. Explicit expressions in the cases np^2 and np^3 can be seen in the Refs. [16, 17]. It should be emphasized that the cases of pure couplings are rarely found in practice, so in general the levels must be obtained by diagonalizing the entire matrix $(H_{bb'} - E^k\delta_{bb'})$, with $H_{bb'} \equiv \langle\Psi_b|\widehat{H}|\Psi_{b'}\rangle$.

LS case

The energies for $J = 0, 2$ are given by:

$$E\left({}^3P_0\right) = E_0\left(sp\right) - \frac{G^1\left(sp\right)}{3} - \zeta_p,$$
$$E\left({}^3P_2\right) = E_0\left(sp\right) - \frac{G^1\left(sp\right)}{3} + \frac{\zeta_p}{2},$$

while for $J = 1$ the matrix

	$^3P_1$	$^1P_1$
$^3P_1$	$E_0(sp) - G^1(sp)/3 - \zeta_p/2$	$\zeta_p/\sqrt{2}$
$^1P_1$	$\zeta_p/\sqrt{2}$	$E_0(sp) + G^1(sp)/3$

must be diagonalized. Being the matrix of dimensions 2×2 we could obtain analytical results, but this will not be possible for larger dimensions. We see that only when $\zeta_p \ll G^1(sp)$ are the levels grouped as singlet and triplet; this occurs in light and few times ionized elements.

Non relativistic jj case

Now the energies will be

$$E\left(^3P_0\right) \equiv (1/2, 1/2)_0 = E_0(sp) - \frac{G^1(sp)}{9} - \zeta_p,$$

$$E\left(^3P_2\right) \equiv (1/2, 3/2)_2 = E_0(sp) - \frac{G^1(sp)}{9} + \frac{\zeta_p}{2},$$

while for $J = 1$ we must to diagonalize the matrix

	$^3P_1 \equiv (1/2, 1/2)_1$	$^1P_1 \equiv (1/2, 3/2)_1$
$^3P_1 \equiv (1/2, 1/2)_1$	$E_0(sp) - G^1(sp)/9 - \zeta_p$	$\zeta_p/\sqrt{2}$
$^1P_1 \equiv (1/2, 3/2)_1$	$\zeta_p/\sqrt{2}$	$E_0(sp) + G^1(sp)/9 + \zeta_p/2$

;

now, only when $\zeta_p \gg G^1(sp)$ the $(j1, j2)$ manifolds are ordered as the single-particle energies: $(1/2, 1/2)$ and $(1/2, 3/2)$.

Relativistic jj case

Now the spin-orbit integrals ζ_p do not enter into the formulation and we will have the following results (where we must note the difference between the p_+ and p_- orbitals and the differences between the energies $E_0(sp_-)$, $E_0(sp_+)$, etc.):

$$E\left(^3P_0\right) \equiv (1/2, 1/2)_0 = E_0(sp_-) - \frac{G^1(sp_-)}{9},$$

$$E\left(^3P_2\right) \equiv (1/2, 3/2)_2 = E_0(sp_+) - \frac{G^1(sp_+)}{9},$$

while for $J = 1$ we must to diagonalize the matrix

	$^3P_1 \equiv (1/2, 1/2)_1$	$^1P_1 \equiv (1/2, 3/2)_1$
$^3P_1 \equiv (1/2, 1/2)_1$	$E_0(sp_-) - G^1(sp_-)/9$	$\sqrt{8}R^1(sp_-, sp_+)/9$
$^1P_1 \equiv (1/2, 3/2)_1$	$\sqrt{8}R^1(sp_-, sp_+)/9$	$E_0(sp_+) + G^1(sp_+)/9$

where the integrals $R^1(ij, tu)$ appear. If we want to go from these expressions to the non-relativistic ones, then we must cancel the $R^1(ij, tu)$ integral and do $E_0(sp_-) = E_0(sp_+) = E_0(sp)$, $G^1(sp_-) = G^1(sp_+) = G^1(sp)$, etc., and add the corresponding integrals ζ_p.

6. Some applications of the present results

6.1. Analysis of the consistency of the published levels of isoelectronic sequences

In the works [15–17] we show that many isoelectronic sequences, of the types $ns\ np$, $ns\ nf$, p^2, p^3 and p^4, whose experimental energy levels are in the NIST repository [22], can be analyzed with advantage using the jj representation more than the LS one. This is due, in part, to the existence of more Slater parameters in jj than in LS couplings: for example, $F^2(nl_+, nl_+)$, $F^2(nl_-, nl_-)$ and $F^2(nl_+, nl_-)$ in place of $F^2(nl, nl)$, and so on.

6.2. Radiative transitions, cross sections and rate coefficients

As we have expressed above, in this work we will not give the results on radiative transitions, which can be the subject of another presentation. If any reader is interested, they can request the expressions from the authors. In all cases the application of the rules are in accordance with Ref. [11]. The same type of angular factors that appear in the theory of radiative transitions are necessary for the calculation of cross sections and rates. The main goal of theoretical plasma spec-

troscopy is the calculation of cross sections and rate coefficients responsible for the excitation and formation of atomic spectra. To this end, efficient and comparatively simple approximate methods for the calculation of cross sections and rate coefficients are of paramount importance. The general theory as well as the approximation of cross sections and rate coefficients by analytic formulas is presented in Ref. [14] using the LS schema. All the machinery of Racah's algebra is present in the final expressions and they are easily translated to jj schema.

7. Conclusions

The substitutions introduced in Section 3 were verified in many circumstances: calculation of the coefficients of the Slater integrals $R^k(ab, cd)$, of transition probabilities A_{if} and in the calculation of cross sections and rate coefficients using semi-theoretical expressions [14]. We have started from the LS-coupling treatment by Cowan [1]; however, until equation (11.47) in his book the treatment is quite general. Only in its Sec. 11-9 it calls for expansion in term of the LS coefficients of fractional parentage

$$|l^w \alpha LS\rangle = \sum_{\overline{\alpha}\overline{LS}} \left|\left(l^{w-1}\overline{\alpha}\overline{LS}, l\right) LS\right\rangle \times \left(l^{n-1}\overline{\alpha}\overline{L}\ \overline{S}\|l^n \alpha LS\right), \quad (15)$$

and from there he develops only the LS formalism. Surely, a similar expansion, using the jj-cpf $\left(j^{n-1}\overline{\alpha}\ \overline{J}\|j^n \alpha J\right)$ allows to obtain the corresponding results in the jj formalism.

Therefore, attending to the question about the final goal of this article, we can answer saying that if one knows the equations written in the LS schema, can translate them to the jj one in a easy form. Several examples were shown in Sec. 7. At the risk of boring the reader, we emphasize that the rules were found by heuristic reasoning. In all cases the application of the rules are in accordance with published results.

Appendix A

Of special interest to the treatment of Section 3 are two results that can be seen in Refs. [3] [10] [8]. The first one refers to the relationship between the matrix elements for LS and jj functions (with $s = 1/2$) :

$$\left\langle (ls)\, j \left|\left| C^k \right|\right| (l's')\, j' \right\rangle = (-1)^{l+j'+k+s} \left[j, j'\right]^{1/2} \times \left\{ \begin{array}{ccc} j & j' & k \\ l' & l & s \end{array} \right\} \left\langle l \left|\left| C^k \right|\right| l' \right\rangle ; \quad (A.1)$$

the other result is a relationship between the following 3j symbols:

$$(-1)^{j+j'+k+1} \left(\begin{array}{ccc} j & k & j' \\ 1/2 & 0 & 1/2 \end{array} \right) = \left[l, l'\right]^{1/2} \times \left(\begin{array}{ccc} l & k & l' \\ 0 & 0 & 0 \end{array} \right) \left\{ \begin{array}{ccc} j & j' & k \\ l' & l & s \end{array} \right\}. \quad (A.2)$$

The important fact is that, starting from Eqs. (1), $(A.1)$ and $(A.2)$, we obtain Eq. (2).

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i. In the middle of the year 2021, there have been more than 5500 citations to Cowan's book and codes, and each year adds about 150 citations to this list.

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