Angular factors for radiative and collisional transitions in complex atoms and ions

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(Submitted 25 July 1994)
Zh. Éksp. Teor. Fiz. **107**, 659–667 (March 1995)

We present explicit expressions for the angular factors of radiative and collisional transitions in complex atoms and ions. *LS*, *jj*, and *jl* coupling are all considered. The formulae derived here are amenable to a simple interepretation, and are given in a form suitable for application to kinetic problems. These expressions automatically incorporate the summation and averaging appropriate to transitions between "effective levels." © *1995 American Institute of Physics.*

1. INTRODUCTION

Interest in the study of collisional and radiative transitions in complex atoms and ions has grown of late, both from the standpoint of a fundamental description of multiparticle systems and in terms of applications to laboratory and astrophysical plasmas (see, e.g., Ref. 1).

Probabilities and cross sections can be cast in terms of sums of products of radial and angular components. The radial part has normally received most of the attention, and a multitude of variational and other methods have been developed in the process (see, e.g., Refs. 2–4). In the present paper, we address the angular part. At the heart of the method for finding the latter are the angular coefficients of the transition amplitudes for some type of "pure" coupling scheme; more often than not, one chooses *LS* coupling. In principle, the angular coefficients can be expressed in terms of Racah coefficients or Wigner *j*-symbols,[4] but they must be rederived in each individual instance. Here we present a simple and physically transparent method for writing such expressions in terms of *M*-functions. These functions[5] can be written in terms of Wigner 9*j* symbols, and make it possible—as will be shown below—to write out the angular transition factor for the various types of coupling (*LS*, *jj*, *jl*) essentially by inspection (i.e., based solely on "general considerations").

Plasma level populations and line intensities are governed by the equations of balance, which incorporate collision rates and radiative transition probabilities. If all of the levels in complex atoms or ions are specified by a complete set of quantum numbers—right on up to the total angular momentum *J*—then there will be an inordinate number of such levels. One way to reduce the number of levels without increasing the errors is to identify blocks of similarly populated levels (i.e., levels whose statistical weight ratios are similar) and replace them with "effective levels."

One can derive the angular factors for transitions between effective levels using general expressions that include summation (or averaging) over the various systems of initial- and final-state quantum numbers, but there are dozens of possibilities. Among these expressions are, for instance, those in which one of the levels is specified by a complete set of quantum numbers (in other words, it is not an "effective level"), while the other is summed over the total angular momentum, or over the total orbital momentum but not the total spin. Likewise, both levels might need to be summed over the total angular momentum, etc. We present below a comprehensive expression that automatically subsumes all possible summation schemes over angular quantum numbers.

2. *M*-FUNCTIONS AND *Q*-FACTORS

In the system of angular quantum numbers describing an atom, let there be a triple $\mathbf{j}$ (j_3, j_2, j_1) such that the angular momentum j_1 corresponds to the sum of j_3 and j_2. An interaction characterized by the triple of multipole orders (q,k,v) sends $\mathbf{j}$ into $\mathbf{j}'$ (j_3', j_2', j_1'). To describe this process, we define the *M*-function:

$$M_{qkv}(\mathbf{j}-\mathbf{j}')=[j_1j_1'v]\begin{Bmatrix} j_3 & j_3' & q \\ j_2 & j_2' & k \\ j_1 & j_1' & v \end{Bmatrix}, \tag{1}$$

where

$$[j_1,j_2\ldots j_n]\equiv[(2j_1+1)(2j_2+1)\ldots(2j_n+1)]^{1/2}, \tag{2}$$

and the expression in braces is the Wigner 9*j* symbol.

The properties of the *M*-functions follow from the corresponding properties of the 9*j* symbols; specifically,

$$\sum_{j_1j_1'} M_{qkv}^2(\mathbf{j},\mathbf{j}')=\frac{[v]^2}{[qk]^2}, \quad \sum_{j_1j_1'v} M_{qkv}^2(\mathbf{j},\mathbf{j}')=1. \tag{3}$$

If one of the multipole orders is zero, the *M*-function can be expressed in terms of a 6*j* symbol. We will also need the following relations:

$$M_{0kk}(\mathbf{j},\mathbf{j}')=(-1)^{j_3+j_2'+j_1+k}\frac{[j_1j_1']}{j_3]} \times\begin{Bmatrix} j_1' & j_1 & k \\ j_2 & j_2' & j_3 \end{Bmatrix}\delta_{j_3j_3'},$$

$$M_{kk0}(\mathbf{j},\mathbf{j}')=(-1)^{j_3'+j_2+j_1+k}\frac{[j_1]}{[k]} \times\begin{Bmatrix} j_3' & j_3 & k \\ j_2 & j_2' & j_1 \end{Bmatrix}\delta_{j_1j_1'}, \tag{4}$$

$$M_{000}(\mathbf{j},\mathbf{j}')=\frac{[j_3]}{[j_1j_2]}\,\delta_{\mathbf{j}\mathbf{j}'}. \tag{5}$$

When the only difference between the first and second triples is that the latter is primed, we omit it for brevity:

$$M_{qkv}(\mathbf{j})\equiv M_{qkv}(j_3j_2j_1)\equiv M_{qkv}(j_3j_2j_1,j_3'j_2'j_1')$$
$$\equiv M_{qkv}(\mathbf{j},\mathbf{j}'). \qquad (6)$$

The Q-factors are angular multipliers that enable one to express the squares of matrix elements (or their sums), which determine the transition probabilities (or cross sections) in complex atoms, in terms of the corresponding quantities for a one-electron atom.

We begin by considering the Q-factors for one-electron transitions. Let the atom be described in the LS coupling scheme by a set of angular quantum numbers γ (S_cL_clSLJ), where S,L,J represents the spin, orbital, and total angular momentum, l is the orbital momentum of the electron making the transition, and S_c,L_c represents the spin and orbital momentum of the atomic core. The probability W_k of an electric radiative transition of multipole order k, for example, can then be written in the form

$$W_k(\gamma\rightarrow\gamma')=Q_kw_k(nl\rightarrow n'l'), \qquad (7)$$

where w is the corresponding transition probability for a one-electron atom. For the case at hand, the expression for Q_k can be found, for example, in the book by Sobel'man.[2] In terms of M-functions,

$$Q_k=\frac{g_o}{g(\gamma)}|[S_c]M_{000}(S_csS)[L_c]M_{0kk}(L_clL)$$
$$\times M_{0kk}(SLJ)|^2, \qquad (8)$$

where $g(\gamma)=[J]^2$ is the statistical weight of the state γ, and $s=1/2$ and $g_o=[sl]^2$ are the spin and statistical weight of the optical electron. Equation (8) gives the transition probability between fine-structure components. For transitions between terms, i.e., probabilities summed over J' and averaged over J, we can replace the J-dependent last M-function with the value 1, by virtue of (3). Finally, then, the statistical weight is $g(\gamma)=[SL]^2$. For transitions between levels, $\gamma=(S_cL_clSL)$, the Q-factor is

$$Q_k=\frac{g_0}{g(\gamma)}\,|[S_cM_{000}(S_csS)[L_c]M_{0kk}(L_clL)|^2. \qquad (8a)$$

Equations (8) and (8a) apply to transitions that do not involve shells containing equivalent electrons. When one of the states (the final state, for instance) actually does, both (8) and (8a) must be multiplied by the number of equivalent electrons m and the square of the fractional parentage coefficient $G^{SL}_{S_cL_c}$.

It can be shown by direct calculation that (8) and (8a) retain the same structure under other coupling schemes as well. Thus, for jj coupling, where the atom is described by the set of quantum numbers $\gamma=(S_cL_cJ_c,ljJ)$, where j and J_c are the total angular momentum of the optical electron and the atomic core, respectively, we have

$$Q_k=\frac{g_0}{g(\gamma)}\,|M_{0kk}(slj)[J_c]M_{0kk}(J_cjJ)|^2. \qquad (9)$$

Likewise, for jl coupling with $\gamma=(S_cL_cJ_clKJ)$ (K corresponds to the sum of J_c and l),

$$Q_k=\frac{g_o}{g(\gamma)}\,|[J_c]M_{0kk}(J_clK)M_{0kk}(sKJ)|^2. \qquad (10)$$

3. MATRIX ELEMENTS OF BINARY OPERATORS

Consider a system consisting of an atom (ion) in the state αS_1L_1 and an external electron in the state sl_e:

$$\Gamma=\alpha(S_1L_1)sl_eS_TL_TJ_T, \qquad (11)$$

where S_T,L_T,J_T represents the spin, orbital, and total angular momentum of the atom + electron system. In the present paper, we use a different order of addition, $\mathbf{S}+\mathbf{L}=\mathbf{J}$, from that used in Ref. 2, $\mathbf{L}+\mathbf{S}=\mathbf{J}$. This results in a sign change in certain amplitude expressions. In the scheme adopted here for transitions with no spin flip, the invariant angular momentum S sits in the first slot of SLJ. The corresponding angular factor is analogous to the factors for the triples L_clL and others.

We consider the off-diagonal matrix element corresponding to a transition of the external electron l_e, and of an atomic electron to the state m with angular momentum l_m:

$$\alpha S_1L_1=\alpha_c(S_cL_c)l_m(S_mL_m)l_{m-1}$$
$$\times(S_{m-1}L_{m-1})\ldots(S_2L_2)l_1S_1L_1. \qquad (12)$$

From this point on, we assume that the atomic state has no equivalent electrons beyond m. In terms of the total projected system angular momentum, the matrix element of the rank-r_0 operator $\mathbf{T}^{r_0}$ in the LS coupling scheme is[6]

$$\langle\Gamma|\mathbf{T}^{r_0}|\Gamma'\rangle=p(r_0r)M_{r_sr_lr_0}(S_TL_TJ_T)$$
$$\times\sum_{k_2k_1q_2q_1}BY_{q_2q_1k_2k_1}(l_ml_e),$$

$$B=[S_cL_c]M_{0q_2q_2}(S_csS_m)M_{0k_2k_2}(L_cl_mL_m)$$
$$\times B_{\kappa_20\kappa_2}M_{q_2q_1r_s}(S_1sS_T)M_{k_2k_1r_1}(L_1l_eL_T),$$

$$B_{\kappa_20\kappa_2}=\prod_{i=1}^{m+1}\{M_{q_20q_2}(S_{i+1}sS_i)\times M_{k_20k_2}(L_{i+1}l_iL_i)$$
$$\times[sl_i]\},\quad \kappa=(k,q), \qquad (14)$$

where Y is the radial part, which depends on the radial wave functions and the one-electron quantum numbers $n_ml_ml_e$. The factor $p(r_0r)$ is equal to

$$p(r_0r)=1,\quad r_0\neq 0;\quad p(r_0r)=(-1)^r[r],\quad r_0=0. \qquad (15)$$

We have asumed in (13)–(14) that $\mathbf{T}$ can be represented as a tensor product,

$$\mathbf{T}^{r_0}=\sum_{j>i}[\mathbf{T}_S^{r_s}(ji)\times\mathbf{T}_L^{r_l}(ji)]^{r_0}, \qquad (16)$$

while the binary operator $\mathbf{T}_L^{r_l}(ji)$ can be represented as a sum of tensor products of the operators $\mathbf{t}_L^{k_2}(j)$ and $\mathbf{t}_L^{k_1}(i)$, and likewise $\mathbf{T}_S^{r_s}(ji)$ can be represented in terms of $\mathbf{t}_s^{q_2}(j)$ and $\mathbf{t}_s^{q_1}(i)$.

For an electrostatic interaction with $r_0=r_s=r_l=0$, $S_T'L_T'J_T'=S_TL_TJ_T$, $q_2=q_1=q$, and $k_2=k_1=k$, the matrix element (13) becomes

$$\langle\Gamma|\mathbf{T}|\Gamma'\rangle=\sum_{kq} B_{qk}(S_TL_TJ_T)Y_{qk}(l_ml_e),$$

$$B_{qk}(S_TL_TJ_T)=\frac{[J_T]}{[L_TS_T]}B_{qk}(S_TL_T), \tag{17}$$

$$B_{qk}(S_TL_T)=[S_cL_c]M_{0qq}(S_csS_m)M_{0kk}(L_cl_mL_m)$$
$$\times B_{\kappa 0\kappa}M_{qq0}(S_1sS_T)M_{kk0}(L_1l_eL_T),$$

$$Y_{qk}=(-1)^{q+k+l_m+l_e}[qk](2\delta(q)R_k'-[q]^2R_k''), \tag{18}$$

where R' and R'' are the direct and exchange integrals (see Appendix for more details). The factor $B_{\kappa 0\kappa}$ is defined in (14). In the more important transition of an electron l_1 from an inner atomic shell with $m=1$, we have $B_{\kappa 0\kappa}=1$.

Neither Eqs. (13) and (17) nor the total LS-coupling scheme are suitable for transitions between SLJ atomic levels, for which one must use the Jj scheme:

$$\Gamma=\alpha(S_1L_1J),sl_ej_e,J_T. \tag{19}$$

A similar derivation yields the appropriate matrix element:

$$\langle Jj_eJ_T|\mathbf{T}|J'j_e'J_T\rangle=\sum_{kq} B_{qk}(JjJ_T)Y_{qk}(l_ml_e), \tag{20}$$

$$B_{qk}(Jj_eJ_T)=\sum_v \frac{[v]}{[qk]}[S_cL_c]M_{0qq}(S_csS_m)M_{0kk}$$
$$\times(L_cl_mL_m)B_{\kappa 0\kappa}M_{qkv}(S_1L_1J)M_{qkv}(sl_eJ_e)$$
$$\times M_{vv0}(Jj_eJ_T).$$

4. *Q*-FACTORS FOR ELECTRON-INDUCED EXCITATION CROSS SECTIONS

The effective cross section for the $\gamma-\gamma'$ transition in an atom (ion) impacted by an electron can be expressed in terms of the **S**-matrix[3]

$$\sigma(\gamma-\gamma')=\pi a_0^2\frac{2\mathrm{R_y}}{g(\gamma)E}\sum|\mathbf{S}(\Gamma,\Gamma')-\mathbf{I}(\Gamma,\Gamma')|^2, \tag{21}$$

where I is the identity matrix, a_0 is the Bohr radius, E is the electron energy, and the sum is taken over quantum numbers Γ that do not enter into γ. In perturbation theory it is convenient to express the unitary **S**-matrix in terms of the hermitian **K**-matrix:

$$\mathbf{S}=(\mathbf{I}+i\mathbf{K})/(\mathbf{I}-i\mathbf{K}). \tag{22}$$

In this paper we are concerned with transition cross sections in atoms impacted by electrons as given by first-order perturbation theory in the interaction between the external (incident) electron and the atomic electrons. Then

$$S(\Gamma,\Gamma')-I(\Gamma,\Gamma')=2iK(\Gamma,\Gamma'),$$

$$K(\Gamma,\Gamma')=\left\langle\Gamma\left|\sum_{j>i}\frac{1}{|\mathbf{r}_j-\mathbf{r}_i|}\right|\Gamma'\right\rangle. \tag{23}$$

Here $K(\Gamma,\Gamma')$ is given directly by Eqs. (17) and (20) of Sec. 3. We limit attention to a transition involving an external atomic electron l_1 (so that $B_{\kappa 0\kappa}=1$), and omit the subscript 1 from the state labels:

$$\gamma=\alpha SLJ=\alpha_c(S_cL_c)nlSLJ,\quad \Gamma=\gamma,sl_e,j_eJ_T,$$

$$K(\Gamma,\Gamma')=\sum_{kq} B_{qk}(JjJ_T)Y_{qk}(l_ml_e), \tag{24}$$

$$B_{qk}(JjJ_T)=[S_cL_c]\sum_v \frac{[v]}{[qd]}M_{0qq}(S_csS)M_{0kk}(L_clL)$$
$$\times M_{qkv}(SLJ)M_{qkv}(sl_ej_e)M_{vv0}(Jj_eJ_T).$$

In the partial-wave representation, the $\gamma-\gamma'$ transition cross section is

$$\sigma(\gamma-\gamma')=\sum_{l_el_e'}\sigma(\gamma l_e-\gamma' l_e'),$$

$$\sigma(\gamma l_e-\gamma' l_e')=\pi a_0^2\frac{2\mathrm{R_y}}{E[J]^2}\sum_{j_ej_e'J_T}|K(\Gamma,\Gamma')|^2, \tag{25}$$

where l_e and l_e' are the orbital angular momenta of the external electron. Summing over momenta $j_ej_e'J_T$, we obtain the partial-wave cross section

$$\sigma(\gamma l_e-\gamma' l_e')=\pi a_0^2\frac{2\mathrm{R_y}}{E[J]^2}\sum_{qkv}|[S_cL_c]M_{0qq}(S_csS)M_{0kk}$$
$$\times(L_cl_eL)M_{qkv}(SLJ)[qk]^{-2}Y_{qk}(ll_e)|^2. \tag{26}$$

Call the one-electron cross section $\sigma_k^{(p)}(l-l')$. Then

$$\sigma_k^{(1)}(l-l')=\pi a_0^2\frac{4R_y}{[l]^2E}\sum_{l_el_e'}[k]^{-2}R_k(R_k-R_k''),$$
$$\sigma_k^{(2)}(l-l')=\pi a_0^2\frac{4R_y}{[l]^2E}\sum_{l_el_e'}[k]^{-2}(R_k'')^2. \tag{27}$$

Here $p=1$ corresponds to the sum of the "direct" and "interference" parts of the cross section, and $p=2$ corresponds to the pure "exchange" part. From (25), (26), and the expression for Y_{qk} presented in the Appendix, we have that for $S_c=L_c=0$,

$$\sum_{jj'}[J]^2\sigma(\gamma-\gamma')=g_o\sum_{k,p}\sigma_k^{(p)},\quad g_o=[sl]^2. \tag{28}$$

In general, the the $\gamma-\gamma'$ transition cross section can be written in the form

$$\sigma(\gamma-\gamma')=\sum_{k,p}\left\{Q_k^{(p)}\sigma_k^{(p)}(l-l')\right\},\quad p=1,2. \tag{29}$$

The angular factor $Q_k^{(p)}$ is

$$Q_k^{(p)}=\frac{g_o}{g(\gamma)}\sum_{qv}|[S_cL_c]M_{0qq}(S_csS)\times M_{0kk}(L_clL)M_{qkv}(SLJ)|^2C(p,q),$$

$$C(1,q)=\delta(q,0),\quad C(2,q)=\tfrac{1}{4}[q]^2. \tag{30}$$

It has been assumed in these formulae that the atom can be described in the LS coupling scheme. The appropriate expressions for other coupling schemes are given in Sec. 5.

5. Q-FACTORS FOR TRANSITIONS BETWEEN EFFECTIVE LEVELS

The formulae for transitions between levels summed over the various quantum numbers can be obtained from the expressions given above, making use of Eq. (3) with subsequent division by the required statistical weight for the purpose of averaging. For example, summing over the total angular momenta J and J' of the initial and final states reduces simply to deleting the appropriate M-factor from the product. Likewise, summing over J' leads to an additional relationship between the statistical weights. Since general kinetic problems require three different types of summation over the momenta of the initial state (J, L, and S in the case of LS coupling), and correspondingly three different types of averaging over the momenta of the final state, we expect at least 2^6 different possibilities. We now show that the factorization of the dependence on quantum numbers demonstrated by the foregoing formulae for the Q-factors can be supplemented by factorization of the constraints, automatically yielding the required summation (averaging).

Let

$$(J)\equiv(2J+1), \tag{31}$$

and assume that $(J)=0$ denotes summation over the corresponding quantum number. Next, define the transition function $P_{qk}(SLJ)$:

$$P_{qk}(SLJ)\equiv P_{qk}(SLJ-S'L'J')=\begin{cases}\sum_v M_{qkv}^2(SLJ), & \text{if } (J)>0 \text{ and } (J')>0,\\ w(SLJ)w(S'L'J'), & \text{if } (J)=0 \text{ or } (J')=0,\end{cases} \tag{32}$$

where the statistical weighting factor w is

$$w(SLJ)=\begin{cases}1, & (J)=0,\\ (J)/(S)(L), & (J)>0.\end{cases} \tag{33}$$

It is easy to see that the sum of P_{qk} over J and J' is 1. The expression for the angular factor, which automatically allows for all possible averaging and summation over the angular quantum numbers of the optical electron, can be written in the form

$$Q_k^{(p)}(\gamma-\gamma')=\frac{g_0}{g(\gamma)}PY\sum_q \mathfrak{Q}_{qk}(\gamma-\gamma')C(p,q). \tag{34}$$

For LS coupling, the factor $\mathfrak{Q}_{qk}$ is

$$\mathfrak{Q}_{qk}(S_cL_clSLJ-S_cL_cl'S'L'J')=(S_c)P_{0q}(S_csS)(L_c)P_{0k}(L_clL)P_{qk}(SLJ). \tag{35}$$

For jj coupling, $\mathfrak{Q}_{qk}$ can be obtained by means of the familiar transformation formulae

$$\mathfrak{Q}_{qk}(J_c,ljJ-J_c,l'j'J')=P_{qk}(slj)(J_c)P_{0k}(J_cjJ), \tag{36}$$

where j is the angular momentum of the optical electron. Similarly, for jl coupling,

$$\mathfrak{Q}_{qk}(J_clKJ-J_cl'K'J')=(J_c)P_{0k}(J_clK)P_{kq}(KsJ). \tag{37}$$

The multipole order k of the interaction specifies the range over which the orbital angular momenta can vary; q acts like a "spin multipole order." A value of 0 for q or k signifies a transition with no change in the corresponding angular momentum. The value of k ranges from $|l-l'|$ to $l+l'$, and q takes the values 0 and 1.

We have $q=0$ for radiative transitions or collisional transitions with no exchange term (for example, excitation of atoms and ions by heavy particles), and the angular factor, which automatically takes account of possible summation for LS coupling [cf. (8) and (8a)], takes the form

$$Q_k=\frac{g_o}{g(\gamma)}(S_c)P_{00}(S_csS)(L_c)P_{0k}(L_clL)P_{0k}(SLJ). \tag{38}$$

Analogous formulae for jj and jl coupling follow directly from (36) and (37).

Equation (34) yields an expression for the general angular factor Q_k in terms of the quantities $\mathfrak{Q}_{qk}$, which are symmetric with respect to the initial and final states. Equations (35)–(37) show that the $\mathfrak{Q}_{qk}$ are products of the factors $P_{qk}(j_3j_2j_1)$ or $(j_3)P_{0m}(j_3j_2j_1)$, which describe transitions among triples of angular momentum $j_3j_2j_1$. A single such factor corresponds to each such transition. The subscript 0 in the second factor corresponds to a conserved momentum (one that does not take part in the interaction), rather than to an accidentally vanishing value of q or k.

The sum over all transitions yields the statistical weight of the atomic core. One can therefore simply write $\mathfrak{Q}_{qk}$ as the statistical weight of the core multiplied by the product of factors P_{qk} that describe transitions among the appropriate triple of momenta.

Note that just like the indicated prescriptions, Eqs. (36)–(38) hold only for transitions in which the momentum coupling scheme is unaltered.

This work was supported by the Soros International Scientific Foundation (Grant MQ-7000), the Russian Fund for Fundamental Research (Grant 94-02-05371-a), and the International Science and Engineering Center (Contract 076-95).

APPENDIX

We have from (17) that for an electrostatic interaction, the radial part is[5]

$$Y_{qk}=\rho_q\rho_k-\rho''_q\rho''_k, \tag{A1}$$

where ρ corresponds to the direct interaction and ρ'' to the exchange interaction.

The orbital part is

$$\rho_k=\rho_k(ll_e,l'l'_e)=(-1)^k[k](l\|C^k\|l')(l_e\|C^k\|l'_e)\tilde{R}_k, \tag{A2}$$

where

$$\tilde{R}_k(ll_e,l'l'_e)=\int_0^\infty F_{l_e}(r')P_l(r'')\frac{2r_<^k}{r_>^{k+1}}P_{l'}(r'')\times F_{l'_e}(r')dr''dr'. \tag{A3}$$

Here P and F are the radial wave functions of the atomic and external electrons. Replacing the matrix elements with $3j$ symbols, we can write ρ_k and ρ''_k in the form

$$\rho_k=(-1)^{k+l+l_e}[k]R_k, \quad \rho''_k=(-1)^{k+l+l_e}[k]R''_k. \tag{A4}$$

The radial integral R_k is

$$R_k(ll_e,l'l''_e)=[ll'l_el'_e]\begin{pmatrix} l & k & l' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_e & k & l'_e \\ 0 & 0 & 0 \end{pmatrix}\tilde{R}_k(ll_e,l'l''_e). \tag{A5}$$

The exchange integral R''_k can be expressed in terms of R_k by interchanging the functions $P_{l'}$ and $F_{l'_e}$:

$$R''_k\equiv R'_k(ll_e,l'l'_e) = \sum_{k''}(-1)^{k+k''}[k]^2\begin{Bmatrix} k & l & l' \\ k'' & l_e & l'_e \end{Bmatrix}R_{k''}(ll_e,l'_el'). \tag{A6}$$

The spin part ρ_q can be obtained from (A2) at $q=0$ and $\tilde{R}_q=\delta(q,0)$. Clearly, then, $\rho_q=2\delta(q,0)$. Similarly, for ρ''_q we may use (A2) and (A6) with $q''=0$, whence $q=0$ or 1 and $\rho''_q=[q]^2$.

Combining the orbital and spin parts then yields Eq. (18).

[1] E. Silver and S. Kahn (eds.), *UV and X-Ray Spectroscopy of Laboratory and Astrophysical Plasmas*, Cambridge University Press, New York (1993).

[2] I. I. Sobel'man, *Introduction to the Theory of Atomic Spectra*, Nauka, Moscow (1977).

[3] L. A. Vaĭnshteĭn, I. I. Sobel'man, and E. A. Yukov, *Atomic Excitation and Spectral Line Broadening*, Nauka, Moscow (1979).

[4] A. A. Nikitin and Z. B. Rudzikas, *Theoretical Foundations of Atomic and Ionic Spectra*, Nauka, Moscow (1983).

[5] L. A. Vaĭnshteĭn, Phys. Scr. **33**, 336 (1986).

[6] V. P. Shevelko and L. A. Vaĭnshteĭn, *Atomic Physics for Hot Plasmas*, IOP Publishing Ltd, London (1993).

Translated by Marc Damashek