Electron collision excitations in complex spectra of ionized heavy atoms

A. Bar-Shalom
Nuclear Research Centre–Negev, P.O.Box 9001, 84 105 Beer-Sheva, Israel

M. Klapisch
Racah Institute of Physics, The Hebrew University of Jerusalem, 91 904 Jerusalem, Israel

J. Oreg*
Lawrence Livermore National Laboratory, P. O. Box 808, Livermore, California 94550
(Received 8 July 1987; revised manuscript received 28 December 1987)

A theory for calculating a many-transition spectrum of electron-ion collisional excitations in the distorted-wave approximation (DWA) is presented. *First*, it is shown that the collision strength including exchange can be factorized into (i) a radial part, involving one-electron wave functions only, and the summation over partial waves of the continuum electron; and (ii) an angular part, involving the coupling between bound electrons in the target states only, specific to each transition. Factorized representations of the collision strengths are derived in various coupling schemes. *Second*, the computationally involved radial part is shown to be a smooth function of transition energies over a very wide range, allowing easy interpolation. These two results enable one to obtain a complete collisional-excitation array with a drastic reduction of the number of time-consuming radial calculations compared with standard methods. This allows the solution of problems which were heretofore considered impractical. As an illustration, the whole array of excitation rate coefficients for Ni-like Gd XXXVII including the lowest 107 levels (5671 transitions) was calculated in the DWA, and used in a steady-state collisional-radiative model. Resulting population inversions are presented versus plasma density.

I. INTRODUCTION

Cross sections for excitation of ions due to electron-ion collisions are required for calculating level populations and spectral line intensities of non–local-thermodynamic-equilibrium (non-LTE) plasmas. This information is important for diagnostics of plasmas occurring in fusion experiments, x-ray lasers, astrophysics, etc. For a reliable evaluation of the plasma parameters such as temperature, density, and especially level populations, one must know the excitation cross sections accurately, and detailed quantum-mechanical calculations are necessary. A comprehensive review of the theory for such calculation was given by Henry.[1]

Three main methods are commonly used. The first is based on the Coulomb-Born (CB) approximation, where the continuum orbitals are calculated for a free electron in a Coulomb potential.[2] An improved method is the distorted-wave (DW) approximation, in which the continuum orbitals are calculated in a more realistic potential which takes into account the ion structure.[3] These two methods assume independent excitation channels for the various ionic transitions and yield a scattering matrix which is not necessarily unitary. In a few DW models the calculation also treats resonances where the total wave function includes closed channels.[4] The most accurate approach used today is the close-coupling (CC) approximation, which couples the various channels and yields a unitary scattering matrix.[5] This method does take into account resonances as well. The crucial drawback of the CC method is the prohibitively long computational time needed, relative to the other methods.

Fortunately, for highly ionized heavy atoms appearing in hot plasma, the coupling among the various channels is very weak[1] and the DW method is most appropriate. Also, since the cross sections, behaving as $1/Z^2$, are relatively small in this case, the unitarization correction is not needed. Still, the enormous amount of relevant transitions needed to determine the level populations and line intensities in these heavy ions does not enable a direct application of the commonly used DW methods, due to computer time limitations. A simple way to cope with this problem was proposed by Hagelstein,[6] when modeling an x-ray laser of Ni-like Eu XXXVI. He calculated excitation cross sections with the relativistic DW method only for the 106 resonant transitions from the ground state to higher levels, while the less important cross sections of the remaining 5565 transitions among the excited levels were approximated by a classical path model, valid for dipole-allowed transitions.

Why are computations of cross sections so time consuming? It should be realized that the first computations by the DW and other methods were performed for light atoms, which are of great interest to astrophysics. These atoms possess very simple configurations. Moreover, these atoms were often in plasma conditions very close to the corona equilibrium, and few excited states were populated, so that a small number of cross sections were needed. In most of the previously mentioned methods, each collisional transition is computed separately. The physical reason for these separate computations is that the wave functions of the continuum electrons, hence the ra-

dial integrals, depend on the energy of the levels involved in the transition, due to conservation of the total energy of the system.

On the other hand, in the case of ionized heavy atoms, with complex configurations involving d or f electrons, an array of transitions connecting all the levels of two mixed configuration manifolds may include thousands of transitions. Hence the question should be asked whether using methods devised for light atoms and computing each transition separately is efficient, or is some part of the work duplicated?

In this work we develop a relativistic DW method for calculating a whole spectrum of excitations simultaneously, suppressing any redundancy. As a starting point, we noticed while looking through many numerical results that the previously mentioned radial integrals do not depend strongly on the transition energy, so that if one could extract from the total cross section the energy-dependent part, one could greatly simplify the numerical work by interpolation.

This approach is inspired by the central-field model for calculating radiative transition probabilities A_{ij} in complex spectra, where the A_{ij} are factorized as a product of an angular part carrying the coupling between the angular momenta for each fine-structure level, and of radial multipole integrals, which involve only one-electron wave functions, and thus have common values for all the levels in one configuration. In an analogous manner, the present work is concerned with establishing two main points.

The first main point is the analytic factorization of the collision-excitation cross-section formulas, *including exchange and configuration interaction in the target states,* into a radial part, formally common to all the transition array of a configuration manifold because it involves only bound and continuum one-electron wave functions, and an angular part, involving only the coupling between the bound electrons in the target states, specific for each transition, but easily calculated. This idea was first introduced and demonstrated in a few simple pure configuration examples by Sobelman *et al.*[7] In the present work we show that the collisional excitation is represented by an effective one-body operator defined on target states, common to both "direct" and "exchange" bound-continuum integrals, thus achieving the factorization. The latter is applicable to any coupling scheme and to mixed-configuration states and is thus suitable for heavy atoms in realistic plasma conditions.

The second main point of this work concerns the radial part, which is the most time consuming part, of the DW calculations. It involves only one-electron wave functions, but in contradistinction to the case of radiative transitions, the radial integrals depend indirectly on the transition energy ΔE, through the energy loss of the continuum electron and conservation of total energy. We show that this dependence is weak as a function of ΔE, for fixed energy of the outgoing continuum electron. This allows interpolation of the radial part in ΔE, based on a very small number of actual computations.

In Sec. II we introduce the one-transition theory, leading to the factorization of the collision strength for mixed-configuration states in various coupling schemes, and present the effective target operators involved. In Sec. III we deal with the implementation of the results of Sec. II for transition arrays, in conjunction with the interpolation process of the radial part of the collisional strength. A summary and discussion are given in Sec. IV where the results of the Ni-like Gd XXXVII collisional radiative model are presented, showing population inversion. For completeness, we derive in Appendix A the required representations of the collisional interaction and some necessary identities, such as the recoupling of the exchange operators in terms of direct-type operators for various coupling schemes. In Appendix B we give some useful examples for matrix elements of the effective atomic operators.

II. ONE-TRANSITION THEORY

A. Background and notation

The collisional strength for transition between target states Ψ_0 and Ψ_1 in the relativistic DW approximation, without unitarization[6] and with proper normalization of the continuum wave functions, is

$$\Omega_{01}=8\sum_{\tilde{j}_0,\tilde{j}_1}\Omega_{01}(\tilde{j}_0,\tilde{j}_1)\ , \tag{1}$$

where the tilde sets $\tilde{j}_0$ and $\tilde{j}_1$ designate the partial waves of the incoming and outgoing continuum electrons characterized by the individual quantum numbers $\{\tilde{k}_0,\tilde{l}_0,\tilde{j}_0\}$ and $\{\tilde{k}_1,\tilde{l}_1,\tilde{j}_1\}$, respectively, where $\tilde{k}$ is the continuum electron momentum and

$$\Omega_{01}(\tilde{j}_0,\tilde{j}_1)=\sum_{J_T}[J_T]\,|\,K_{01}\,|^2\ , \tag{2}$$

$$K_{01}=-\left\langle\psi_0\left|\sum_{\substack{i,j=1\\(i<j)}}^{N+1}\frac{1}{r_{ij}}\right|\psi_1\right\rangle\ , \tag{3}$$

and

$$[J]=2J+1,\quad [J_1J_2\cdots]=(2J_1+)(2J_2+1)\cdots\ , \tag{4}$$

and where ψ_0 and ψ_1 are the antisymmetrized initial and final states of the complete system of $N+1$ electrons (target and continuum electron),

$$\psi_1=\{\Psi_i(\Gamma_i,J_i),\tilde{j}_i;J_T,M_T\},\quad i=0,1\ . \tag{5}$$

In Eq. (5) J_0 and J_1 are the total angular momentum of the target before and after the collision, respectively, and J_T is the total angular momentum of the complete system. Different target states having the same angular momentum J_i are distinguished by Γ_i. In general, Ψ_0

and Ψ_1 are mixed configuration states,

$$\Psi_i(\Gamma_i,J_i)=\sum_n a_n^{\Gamma_i}(\gamma_n,J_i)\varphi_n(\gamma_n,J_i), \quad i=0,1 \tag{6}$$

where $\varphi_n(\gamma_n,J_i)$ relate to a pure coupling scheme, $a_n^{\Gamma_i}(\gamma_n,J_i)$ are the mixing coefficients, and the index n runs over all the states of the interacting configurations.

Clearly, Eq. (6) is valid also for the case of a single configuration. Due to the antisymmetrization of the states ψ_0 and ψ_1 in Eq. (3), the electrostatic interaction involving $\tilde{\mathbf{j}}_0$ and $\tilde{\mathbf{j}}_1$ may be represented by an operator[8] [see Appendix, Eq. (A12)]

$$V(\tilde{\mathbf{j}}_0,\tilde{\mathbf{j}}_1)\equiv\sum_{\substack{i,j\\(i<j)}}\frac{1}{r_{ij}}=\sum_{\mathbf{j}_0,\mathbf{j}_1}\sum_k[(Z^{(k)}(\mathbf{j}_0,\mathbf{j}_1)\cdot Z^{(k)}(\tilde{\mathbf{j}}_0,\tilde{\mathbf{j}}_1))X^k(\mathbf{j}_0,\tilde{\mathbf{j}}_0;\mathbf{j}_1,\tilde{\mathbf{j}}_1)+(Z^{(k)}(\mathbf{j}_0,\tilde{\mathbf{j}}_1)\cdot Z^{(k)}(\tilde{\mathbf{j}}_0,\mathbf{j}_1))X^k(\mathbf{j}_0,\tilde{\mathbf{j}}_0;\tilde{\mathbf{j}}_1,\mathbf{j}_1)] \ . \tag{7}$$

Here $\mathbf{j}_0$ and $\mathbf{j}_1$ represent sets of individual quantum numbers $\mathbf{j}\equiv\{n,l,j\}$ of bound electrons. The unit tensor operators $Z^{(k)}(\mathbf{j},\mathbf{j}')$ in Eq. (7) are defined by the single-particle reduced matrix elements

$$\langle n_1l_1j_1\|\zeta^{(k)}(\mathbf{j},\mathbf{j}')\|n_2l_2j_2\rangle = \delta(n_1,n)\delta(l_1,l)\delta(j_1,j)\delta(n_2,n')\delta(l_2,l')\delta(j_2,j') \ , \tag{8}$$

with the condition that j_1, k, and j_2 satisfy the triangular inequalities, but without constraint on the parity of orbital angular momenta l, and by

$$Z^{(k)}(\mathbf{j},\mathbf{j}')=\sum_{i=1}^{N+1}\zeta_i^{(k)}(\mathbf{j},\mathbf{j}') \ . \tag{9}$$

Moreover,

$$X^k(a,b;c,d)=\langle j_a\|C^{(k)}\|j_c\rangle\langle j_b\|C^{(k)}\|j_d\rangle \times R^k(a,b;c,d) \ , \tag{10}$$

where $C^{(k)}$ are the spherical harmonics defined on quantum numbers j_a, j_b, etc.,[9] satisfying the usual parity condition on the orbital angular momenta l_a, l_b, etc., with rank k, and $R^k(a,b;c,d)$ are the Slater integrals, which depends on j quantum numbers when the Dirac one-electron wave functions are used. The two terms in the square brackets of Eq. (7) are the "direct" and "exchange" parts, respectively.

B. Direct matrix element

Let us denote by $D^k_{J_T}$ the direct angular matrix element:

$$D^k_{J_T}=\langle\psi_0\,|\,(Z^{(k)}(\mathbf{j}_0,\mathbf{j}_1)\cdot Z^{(k)}(\tilde{\mathbf{j}}_0,\tilde{\mathbf{j}}_1))\,|\,\psi_1\rangle \ . \tag{11}$$

By removing the antisymmetrization between bound and continuum electrons it can be shown that

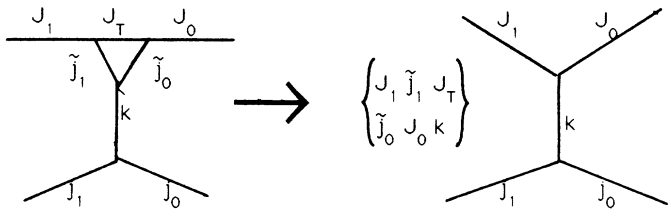
$$D^k_{J_T}=\langle\Psi_0\tilde{\mathbf{j}}_0(N+1)J_T\,|\,(Z^{(k)}(\mathbf{j}_0,\mathbf{j}_1)\cdot\zeta^{(k)}_{N+1}(\tilde{\mathbf{j}}_0,\tilde{\mathbf{j}}_1))\,|\,\Psi_1\tilde{\mathbf{j}}_1(N+1)J_T\rangle \ , \tag{12}$$

where the bound antisymmetrical states and the symmetric operator $Z^{(k)}(\mathbf{j}_0,\mathbf{j}_1)$ are defined for electrons $1,2,\ldots,N$.

Equation (12) can be reduced immediately using the well-known rule for the scalar product of two operators acting on different parts of the wave functions [Eq. (3-36) of Ref. 10 and Eq. (4.169) of Ref. 11]. The result is

$$D^k_{J_T}=(-1)^{J_1+\tilde{J}_0+J_T}\begin{Bmatrix}J_1 & \tilde{J}_1 & J_T\\ \tilde{J}_0 & J_0 & k\end{Bmatrix}\langle\Psi_0(\Gamma_0,J_0)\|Z^{(k)}(\mathbf{j}_0,\mathbf{j}_1)\|\Psi_1(\Gamma_1,J_1)\rangle \ . \tag{13}$$

This reduction to Eq. (13) is described graphically[12,13] by taking out the triangle from the diagrams representing the matrix element, i.e.,



(14)

C. Exchange matrix element

We denote the exchange operator matrix element by

$$E^k_{J_T}=\langle\psi_0\,|\,(Z^{(k)}(\mathbf{j}_0,\tilde{\mathbf{j}}_1)\cdot Z^{(k)}(\tilde{\mathbf{j}}_0,\mathbf{j}_1))\,|\,\psi_1\rangle \ . \tag{15}$$

The factorization of Eq. (15) to separate target and continuum matrix elements is not immediate as for the direct part,

since the operators $Z^{(k)}(\mathbf{j},\tilde{\mathbf{j}})$ mix bound and continuum electrons. For relativistic j-j target states Ψ_i, the exchange matrix element, becomes

$$E^k_{J_T}=\langle \Psi_0\tilde{j}_0(N+1)J_T \,|\, [Z^{(k)}(\mathbf{j}_0,\tilde{\mathbf{j}}_1)\cdot\xi^{(k)}_{N+1}(\tilde{\mathbf{j}}_0,\mathbf{j}_1)] \,|\, \Psi_1\tilde{j}_1(N)J_T\rangle \ , \tag{16}$$

where Ψ_1 is an antisymmetrized state of electrons $1,2,\ldots,N-1,N+1$. The reduction rule of Sec. II C does not apply to Eq. (16).

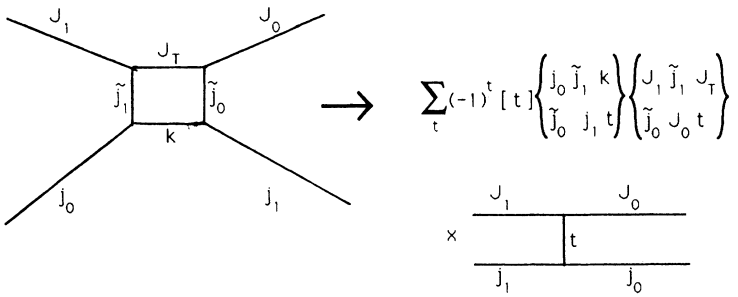
However, it was shown[14,15] that the exchange operator of Eq. (7) can be expressed in terms of direct-type operators which allow the desired factorization. Specifically, the exchange angular operator is expressed as[14] (see Appendix A)

$$(Z^{(k)}(\mathbf{j}_0,\tilde{\mathbf{j}}_1)\cdot Z^{(k)}(\tilde{\mathbf{j}}_0,\mathbf{j}_1))=\sum_t (-1)^{k+t}(2t+1)\begin{Bmatrix} j_0 & \tilde{j}_1 & k \\ \tilde{j}_0 & j_1 & t\end{Bmatrix}(Z^{(t)}(\mathbf{j}_0,\mathbf{j}_1)\cdot Z^{(t)}(\tilde{\mathbf{j}}_0,\tilde{\mathbf{j}}_1)) \ . \tag{17}$$

Substituting Eq. (17) in Eq. (15) and using the reduction rule, as was done for the direct part, we obtain

$$E^k_{J_T}=\sum_t (-1)^{k+t+J_1+\tilde{J}_0+J_T}(2t+1)\begin{Bmatrix} j_0 & \tilde{j}_1 & k \\ \tilde{j}_0 & j_1 & t\end{Bmatrix}\begin{Bmatrix} J_1 & \tilde{j}_1 & J_T \\ \tilde{j}_0 & J_0 & t\end{Bmatrix}\langle \Psi_0(\Gamma_0,J_0)\|Z^{(t)}(\mathbf{j}_0,\mathbf{j}_1)\|\Psi_1(\Gamma_1,J_1)\rangle \ . \tag{18}$$

The graphical description for this reduction is as follows:



(19)

We now return to Eq. (2) and express the contribution of specific continuum partial waves $\tilde{j}_0$ and $\tilde{j}_1$ to the collisional strength by

$$\begin{aligned}\Omega_{01}(\tilde{j}_0,\tilde{j}_1)&=\sum_{J_T}(2J_T+1)\left|\sum_{j_0,j_1}\sum_k D^k_{J_T}X^k(\mathbf{j}_0,\tilde{\mathbf{j}}_0;\mathbf{j}_1,\tilde{\mathbf{j}}_1)+E^k_{J_T}X^k(\mathbf{j}_0,\tilde{\mathbf{j}}_0;\tilde{\mathbf{j}}_1,\mathbf{j}_1)\right|^2 \\ &=\sum_{J_T}(2J_T+1)\left|\sum_{j_0,j_1}\sum_k\langle\Psi_0\|Z^{(k)}(\mathbf{j}_0,\mathbf{j}_1)\|\Psi_1\rangle\begin{Bmatrix} J_1 & \tilde{j}_1 & J_T \\ \tilde{j}_0 & J_0 & k\end{Bmatrix}(2k+1)^{1/2}P^k(\tilde{\mathbf{j}}_0,\tilde{\mathbf{j}}_1;\mathbf{j}_0,\mathbf{j}_1)\right|^2 ,\end{aligned} \tag{20}$$

where

$$P^k(\tilde{\mathbf{j}}_0,\tilde{\mathbf{j}}_1;\mathbf{j}_0,\mathbf{j}_1)=(2k+1)^{-1/2}X^k(\mathbf{j}_0,\tilde{\mathbf{j}}_0;\mathbf{j}_1,\tilde{\mathbf{j}}_1)+\sum_t(-1)^{k+t}(2k+1)^{1/2}\begin{Bmatrix} j_0 & \tilde{j}_1 & t \\ \tilde{j}_0 & j_1 & k\end{Bmatrix}X^t(\mathbf{j}_0,\tilde{\mathbf{j}}_0;\tilde{\mathbf{j}}_1,\mathbf{j}_1) \ . \tag{21}$$

The summation over J_T can now be carried out using the orthogonality relations of $6j$ symbols, yielding for the total collision strength of Eq. (1),

$$\begin{aligned}\Omega_{01}&=8\sum_{\tilde{j}_0,\tilde{j}_1}\Omega_0(\tilde{j}_0,\tilde{j}_1) \\ &=8\sum_k\sum_{\substack{j_0,j_1,\\ j_0'j_1'}}\langle\Psi_0\|Z^{(k)}(\mathbf{j}_0,\mathbf{j}_1)\|\Psi_1\rangle\langle\Psi_0\|Z^{(k)}(\mathbf{j}_0',\mathbf{j}_1')\|\Psi_1\rangle Q^k(\mathbf{j}_0,\mathbf{j}_1;\mathbf{j}_0',\mathbf{j}_1') \ ,\end{aligned} \tag{22}$$

where

$$Q^k(\mathbf{j}_0,\mathbf{j}_1;\mathbf{j}_0',\mathbf{j}_1')=\sum_{\tilde{j}_0,\tilde{j}_1}P^k(\tilde{\mathbf{j}}_0,\tilde{\mathbf{j}}_1;\mathbf{j}_0,\mathbf{j}_1)P^k(\tilde{\mathbf{j}}_0,\tilde{\mathbf{j}}_1;\mathbf{j}_0',\mathbf{j}_1') \ . \tag{23}$$

The target matrix elements in Eq. (22) can be expressed in terms of the pure basis states of Eq. (6) as

$$\langle\Psi_0(\Gamma_0,J_0)\|Z^{(k)}(\mathbf{j}_0,\mathbf{j}_1)\|\Psi_1(\Gamma_1,J_1)\rangle=\sum_{n,m}a_n^{\Gamma_0}(\gamma_{0n},J_0)a_m^{\Gamma_1}(\gamma_{1m}J_1)\langle\varphi_n(\gamma_{0n},J_0)\|Z^{(k)}(\mathbf{j}_0,\mathbf{j}_1)\|\varphi_m(\gamma_{1m},J_1)\rangle \tag{24}$$

and can be calculated by the usual techniques of Racah algebra using standard computer codes.[16] (Analytical formulas for some useful cases are given explicitly in Appendix B).

It is remarkable that the cumbersome continuum dependence of the collisional strength is factorized out analytically in Eq. (22) from the target part, even though the exchange interaction is taken into account, as well as configuration mixing. Moreover, for pure configurations $\mathbf{j}_0=\mathbf{j}_0'$ and $\mathbf{j}_1=\mathbf{j}_1'$ and Eq. (22) reduces to

$$\Omega_{01}=8\sum_{\mathbf{j}_0,\mathbf{j}_1}\sum_{k}\langle\Psi_0\|Z^{(k)}(\mathbf{j}_0,\mathbf{j}_1)\|\Psi_1\rangle^2 Q^k(\mathbf{j}_0,\mathbf{j}_1;\mathbf{j}_0,\mathbf{j}_1)\ , \tag{25}$$

and for excitations between different configurations only one term in the sum over $\mathbf{j}_0$ and $\mathbf{j}_1$ remains. *Thus collisional excitations behave like one-electron multipole transitions,* with a radial part described by $Q^k(\mathbf{j}_0,\mathbf{j}_1;\mathbf{j}_0',\mathbf{j}_1')$. Note that the contribution of the exchange manifests itself by the fact that some values of k might not satisfy the usual parity constraints for electric multipoles, since this role is now played by t in Eq. (21). This result is similar in spirit to the recent formulation of inelastic cross sections by Lee and Fano,[17] albeit without introduction of new quantum numbers. Here we are only interested in total cross sections. We shall now show that similar factorization holds for other coupling schemes used in different physical circumstances.

D. Semirelativistic approximation

A semirelativistic approach approximates the large-component radial part of the continuum electrons by Schrödinger solutions with zero small component, while keeping a full relativistic description of the bound electrons. Furthermore, since these continuum radial solutions are independent of $\tilde{j}_0$ and $\tilde{j}_1$, the summation over these indices in Eq. (23) can be carried out on the angular part using the relation

$$\langle slj\|C^{(k)}\|s'l'j'\rangle=\langle l\|C^{(k)}\|l'\rangle(-1)^{1/2+l'+j+k}(2j+1)^{1/2}(2j'+1)^{1/2}\begin{Bmatrix} j & j' & k \\ l' & l & \frac{1}{2}\end{Bmatrix} \tag{26}$$

and known relations between n-j symbols. The result for the collisional strength is the same as Eq. (22), with

$$Q^k(\mathbf{j}_0,\mathbf{j}_1;\mathbf{j}_0',\mathbf{j}_1')=\sum_{r,t}\sum_{\tilde{l}_0,\tilde{l}_1}P^{rtk}(\tilde{l}_0,\tilde{l}_1;\mathbf{j}_0,\mathbf{j}_1)P^{rtk}(\tilde{l}_0,\tilde{l}_1;\mathbf{j}_0',\mathbf{j}_1')\ , \tag{27}$$

where $\tilde{l}=\{\tilde{k},\tilde{l}\}$ and

$$\begin{aligned}P^{rtk}(\tilde{l}_0,\tilde{l}_1;\mathbf{j}_0,\mathbf{j}_1)=&(2k+1)^{1/2}(2j_0+1)^{1/2}(2j_1'+1)^{1/2}\begin{Bmatrix}\frac{1}{2} & \frac{1}{2} & r\\ l_0 & l_1 & t\\ j_0 & j_1 & k\end{Bmatrix}\\ &\times\left[2(2k+1)^{-1/2}\delta_{r,0}X^k(\mathbf{j}_0,\tilde{l}_0;\mathbf{j}_1,\tilde{l}_1)+(-1)^{t+1}(2r+1)^{1/2}(2t+1)^{1/2}\right.\\ &\left.\times\sum_{k'}(-1)^{k'}\begin{Bmatrix}l_0 & \tilde{l}_1 & k'\\ \tilde{l}_0 & l_1 & t\end{Bmatrix}X^{k'}(\mathbf{j}_0,\tilde{l}_0;\tilde{l}_1,\mathbf{j}_1)\right]\ .\end{aligned} \tag{28}$$

Here the X^k have a slightly different definition than in Eq. (10),

$$\begin{aligned}X^k(a,b;c,d)=&\langle l_a\|C^{(k)}\|l_c\rangle\langle l_b\|C^{(k)}\|l_d\rangle\\ &\times R^k(a,b;c,d)\ .\end{aligned} \tag{29}$$

It should be pointed out that the sum over r and t in Eq. (27) is preferable to the original sum over $\tilde{j}_0,\tilde{j}_1$ for fixed $\tilde{l}_0,\tilde{l}_1$, since r can take values 0 or 1, and t is restricted by the bound electrons' angular momenta, through the triangular conditions of the $9j$ symbol of Eq. (28).

E. Collision strength in nonrelativistic $(\Gamma J)\tilde{j}J_T$ schemes

In the nonrelativistic case the radial parts of the bound (continuum) electrons depend upon $l\equiv\{n,l\}$ ($\tilde{l}\equiv\{\tilde{k},\tilde{l}\}$) and not upon j ($\tilde{j}$). In this case a single treatment is possible for a general ΓJ scheme such as j-jJ, SLJ, j_1KJ, etc., where the target states Ψ_i are characterized by a total J, which is coupled further with the continuum $\{\tilde{k},\tilde{l},\tilde{j}\}$ electron to J_T as in ψ_i of Eq. (5).

We define the double tensor $Z^{(r,t)}(l,l')$ by the single-particle reduced matrix elements as in Eqs. (8) and (9),

$$\langle n_1l_1\|\zeta^{(r,t)}(l,l')\|n_2l_2\rangle=\delta(n_1,n)\delta(l_1,l)\delta(n_2,n')\delta(l_2,l')\ , \tag{30}$$

where r and t are the tensor ranks with respect to $\hat{S}$ and $\hat{L}$, respectively. The reduced matrix element here is defined by applying the Wigner-Eckart theorem twice with respect to both $\hat{S}$ and $\hat{L}$. It is easily seen that

$$Z^{(0k)}(l,l')=Z^{(0k)k}(l,l')=2^{-1/2}Z^{(k)}(l,l')\ , \tag{31}$$

with

$$\langle n_1 l_1 \| \xi^{(k)}(l,l') \| n_2 l_2 \rangle = \delta(n_1,n)\delta(l_1,l)\delta(n_2,n')\delta(l_2,l') \ . \tag{32}$$

The operator $Z^{(rt)k}(l,l')$ is obtained by recoupling r and t to k.

It is convenient to use in this case the following representation for the collisional interaction of the target and the continuum electrons $\tilde{l}_0,\tilde{l}_1$ (see Appendix A),

$$\sum_{i<j} \frac{1}{r_{ij}}\bigg|_{\{\tilde{l}_0,\tilde{l}_1\}} = \sum_{r,t} \sum_{l_0,l_1} \sum_{k} (-1)^{r+t+k} (Z^{(rt)k}(l_0,l_1)\cdot Z^{(rt)k}(\tilde{l}_0,\tilde{l}_1)) \times \left[2\delta_{r,0}\delta_{t,k} X^t(l_0,\tilde{l}_0;l_1,\tilde{l}_1) + (2r+1)(2t+1) \sum_{k'} (-1)^{k'+t+1} \begin{Bmatrix} l_0 & \tilde{l}_1 & k' \\ \tilde{l}_0 & l_1 & t \end{Bmatrix} X^t(l_0,\tilde{l}_0;\tilde{l}_1,l_1) \right] , \tag{33}$$

where $X^k(l_a,l_b;l_c,l_d)$ are defined by Eq. (29).

Taking the matrix element of Eq. (33) between the states ψ_i of Eq. (5), following the same steps as in the relativistic j-j scheme of Sec. II C, and summing over $\tilde{j}_0,\tilde{j}_1$, we obtain the following result:

$$\Omega_{01} = 8 \sum_{r,t} \sum_{\substack{l_0,l_1, \\ l_0',l_1'}} \left[\sum_k \langle \Psi_0 \| Z^{(rt)k}(l_0,l_1) \| \Psi_1 \rangle \langle \Psi_0 \| Z^{(rt)k}(l_0',l_1') \| \Psi_1 \rangle \right] Q^{rt}(l_0,l_1;l_0',l_1') \ , \tag{34}$$

with

$$Q^{rt}(l_0,l_1;l_0',l_1') = \sum_{\tilde{l}_0,\tilde{l}_1} P^{rt}(\tilde{l}_0,\tilde{l}_1;l_0,l_1) P^{rt}(\tilde{l}_0,\tilde{l}_1;l_0',l_1') \ , \tag{35}$$

and

$$P^{rt}(\tilde{l}_0,\tilde{l}_1;l_0,l_1) = 2\delta_{r,0}(2t+1)^{-1/2} X^t(l_0,\tilde{l}_0;l_1,\tilde{l}_1) + (-1)^{t+1}(2r+1)^{1/2}(2t+1)^{1/2} \sum_{k'} (-1)^{k'} \begin{Bmatrix} l_0 & \tilde{l}_1 & k' \\ \tilde{l}_0 & l_1 & t \end{Bmatrix} X^{k'}(l_0,\tilde{l}_0;\tilde{l}_1,l_1) \ . \tag{36}$$

It should be mentioned that the results of Sec. II D for the semirelativistic approximation may be obtained directly from Eq. (34) using the identity (Appendix A)

$$Z^{(rt)k}(l_0,l_1) = \sum_{j_0,j_1} (2j_0+1)^{1/2}(2j_1+1)^{1/2}(2k+1)^{1/2} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & r \\ l_0 & l_1 & t \\ j_0 & j_1 & k \end{Bmatrix} Z^{(k)}(\mathbf{j}_0,\mathbf{j}_1) \ . \tag{37}$$

For the SLJ coupling scheme it turns out that the summation over k in Eq. (34) can be carried out and the results are expressed in terms of regular double tensors $Z^{(rt)}$. Furthermore, J_0 and J_1 appear only in a $12j$ symbol.

F. Collision strength in the SLM_SM_L coupling scheme

In physical situations where the state vectors of the complete system, target plus continuum electron is in LS coupling scheme, it is convenient to use the representation (A4) of Appendix A for the collisional interaction,

$$\Omega_{01} = \sum_{S_T,L_T} (2S_T+1)(2L_T+1) \left| \left\langle \psi_0 \left| \sum_{\substack{i,j=1 \\ i<j}}^{N+1} \frac{1}{r_{ij}} \right| \psi_1 \right\rangle \right|^2 , \tag{38}$$

where

$$\psi_i = \{ \psi_i(\Gamma_i,S_i,L_i), \tilde{l}_i; S_T,L_T,M_{ST},M_{LT} \}, \quad i=0,1 \ . \tag{39}$$

The same procedure as in the other schemes leads to the desired factorization between the target and the continuum, i.e.,

$$\Omega_{01} = 8 \sum_{r,t} \sum_{l_0,l_1} \langle \Psi_0 \| Z^{(rt)}(l_0,l_1) \| \Psi_1 \rangle \times \langle \Psi_0 \| Z^{(rt)}(l_0',l_1') \| \Psi_1 \rangle \times Q^{rt}(l_0,l_1;l_0',l_1') \ , \tag{40}$$

where Q^{rt} is defined in Eq. (35).

Thus for the nonrelativistic case the collisional excitations behave like one-electron double tensor multipoles with respect to the orbital and spin spaces. The spin dependence originates from the exchange term in the collisional Hamiltonian.

III. TRANSITION ARRAYS AND INTERPOLATION OF THE RADIAL INTEGRALS

In Sec. II we established the factorization of the collision strength into an angular part and a radial part involving the sum over partial waves, thus establishing the first point exposed in the Introduction. However, the expressions considered so far concern the collision strength of a transition between two levels. In this section, we address the problem of a transition array.

Let us consider as an example the case of relativistic wave functions, and for that matter, rewrite Eq. (22), taking into account Eq. (24), in a more compact form,

$$\Omega_{ir}=8\sum_k \left[\sum_{n,s}(i\mid n\rangle\langle n\|Z^k\|s\rangle\langle s\mid r)\right] \times\left[\sum_{n',s'}(i\mid n'\rangle\langle n'\|Z^k\|s'\rangle\langle s'\mid r)\right] \times Q^k(\mathbf{j}_n,\mathbf{j}_s;\mathbf{j}_{n'}\mathbf{j}_{s'}\mid\Delta E_{ir})\ . \tag{41}$$

The transition takes place between the level r, described as a combination of the pure configuration states (PCS) s (s'), with coefficients $\langle s\mid r\rangle$ ($\langle s'\mid r\rangle$) of one configuration manifold, and the level i, a combination of PCS n (n'), with coefficients $(i\mid n\rangle$ ($(i\mid n'\rangle$), of the other one. The radial integrals Q^k are defined through Eqs. (23) and (21). Here their dependence on the transition energy ΔE_{ir} is explicitly stated.

It is clear from Eq. (41) that, indeed, all the dependence on the quantum numbers of the fine-structure levels is separated from the radial wave functions. The matrix elements of the Z operators can thus be computed like ordinary multipole transitions;[9,11] they are independent of the energies, and actually even of the element, so that they can be used for a whole isoelectronic sequence. On the other hand, the Q^k depend on radial wave functions, and on the energy of the transitions *only*.

Equation (41) is analogous to the example, quoted in the introduction, of the radiative transitions. However, there are two fundamental differences with the case of radiative transition integrals, which are given in the following.

A. Properties of the $Q^k(\mathbf{j}_n,\mathbf{j}_s;\mathbf{j}_{n'},\mathbf{j}_{s'})$ integrals

A consequence of the factorization is that the $Q^k(\mathbf{j}_n\mathbf{j}_s;\mathbf{j}_{n'},\mathbf{j}_{s'})$ integrals are not squares nor products of integrals, when $n\neq n'$, or $s\neq s'$, that is, when configuration mixing plays a role. Consequently, in the general case, taking into account configuration mixing, Eq. (41) does not describe a product of matrices, or squares of matrix elements, as in the case of radiative transitions, and the number of operations necessary to evaluate a full collisional transition array increases at least as the fifth power of the size of the transition matrix. Also, the number of such integrals increases as the fourth power of the number of bound orbitals involved in the spectrum considered. This is particularly important for the case where a relativistic description of the bound-electron wave functions is necessary, because, as is well known, the departure from pure jj coupling, which is seldom negligible, manifests itself by "relativistic subconfigurations" mixing. In addition, the number of relativistic orbitals is obviously nearly double than that for the nonrelativistic case. However, the products of coefficients $(i\mid n\rangle(i\mid n'\rangle\langle s\mid r)\langle s'\mid r)$ are fourth order in "configuration mixing," and are often small enough to be neglected. Consequently, many Q^k do not practically influence the final results.

When configuration mixing can be neglected, the situation is like radiative transitions. Strictly speaking, the integrals of the type $Q^k(\mathbf{j}_n,\mathbf{j}_s;\mathbf{j}_n,\mathbf{j}_s)$—to which we refer in the sequel as $Q^k(\mathbf{j}_n,\mathbf{j}_s)$—are not squares of integrals neither. However, according to Eq. (23), they are sums of squares, i.e., positive for all partial waves, so that one can write

$$\Omega_{ir}=8\sum_k \left[\sum_{n,s}(i\mid n\rangle\langle n\|Z^k\|s\rangle\langle s\mid r) \times[Q^k(\mathbf{j}_n,\mathbf{j}_s\mid\Delta E_{ir})]^{1/2}\right]^2 . \tag{42}$$

Therefore, the collision strengths are squares of matrix elements. Moreover, it is clear from Eq. (23) that the building blocks for the Q^k are the integrals P^k. The number of these behaves as the square of the number of orbitals only. It is here that the global approach of computing a whole spectrum simultaneously makes a difference, because each P^k is common to several Q^k. This approach is possible, however, only if there is a way to compute all these P^k at the same energies, as described in Sec. III B.

B. Interpolation as a function of transition energies

As suggested by the notation in Eq. (41), the Q^k depend on the transition energy

$$\Delta E_{ir}=\varepsilon_{\text{in}}-\varepsilon_{\text{out}}=E_i-E_r\ , \tag{43}$$

where E_i and E_r are the initial and final target state energies and ε_{in} and ε_{out} are the incoming and the outgoing electron energies. This energy dependence comes from the requirement of energy conservation, and has nothing to do with a possible breakdown of the central field approximation. As a matter of fact, in many cases, simply assuming the Q^k to be energy independent would be a poor approximation.

Now it appears from many numerical computations that the Q^k's are smooth functions of the transition energy, and hence can be interpolated between very few values of ΔE. More precisely, the Q^k's can be represented in terms of any two of the following variables: ε_{in}, ε_{out}, ΔE, $X=\varepsilon_{\text{in}}/\Delta E$, $u=\varepsilon_{\text{out}}/\Delta E$, or any monotonic function of these.

It turns out that except for dipole-allowed transitions, the choice $\Delta E,\varepsilon_{\text{out}}$ is appropriate. In most cases it is even possible to obtain sufficiently accurate Q^k (ΔE_{ir}, ε_{out}) by retaining the *linear term only*. For dipole-allowed transitions, it was found that the linear approximation was better when using the variables $\log(\Delta E)$ and ε_{out}.

This behavior of Q^k is demonstrated for various kinds of transitions in Ni-like Gd XXXVII in Figs. 1–3, using

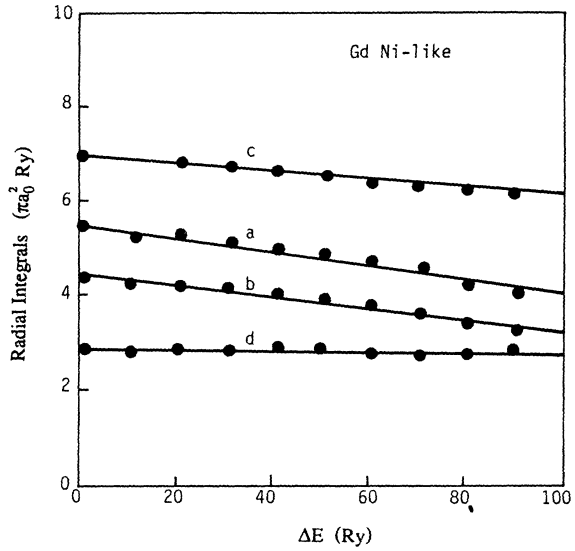


FIG. 1. Linear behavior of the "dipole-forbidden" radial parts Q^k vs ΔE with constant ε_{out} for a Ni-like Gd XXXVII atom. (a) $10^2Q^0(3d_{3/2},4d_{3/2})$; (b) $10^2Q^0(3d_{3/2},4d_{3/2},3d_{5/2},4d_{5/2})$, both cases (direct plus exchange); (c) $10^5Q^1(3d_{3/2},4d_{3/2})$; and (d) $10^5Q^1(3d_{3/2},4d_{3/2},3d_{5/2},4d_{5/2})$ (exchange only).

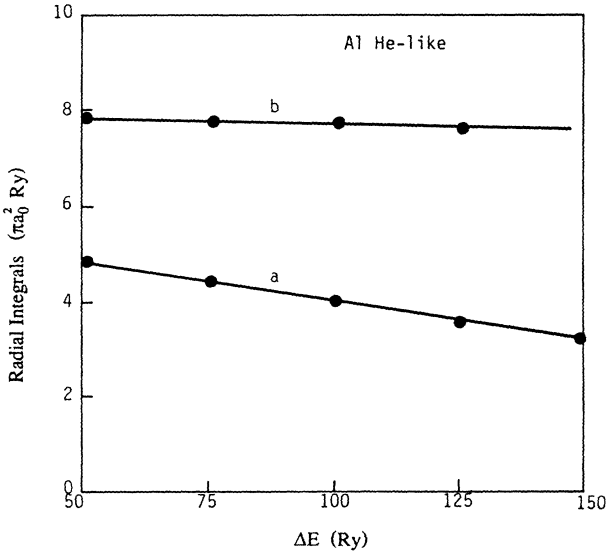


FIG. 3. Linear behavior of the "dipole-forbidden" radial parts Q^k vs ΔE with constant ε_{out} for a He-like Al XII atom. (a) $10Q^0(1s_{1/2},2s_{1/2})$ (direct plus exchange), and (b) $10Q^1(1s_{1/2},2s_{1/2})$ (exchange only).

the short notation $Q^k(a,b)\equiv Q^k(a,b;a,b)$. In Fig. 1 we present the ΔE dependence of $Q^0(3d_j;4d_{j'})$ for different j and j', which correspond to a dipole-forbidden transition and contain both direct and exchange contributions, and of $Q^1(3d_j;4d_{j'})$, corresponding to a dipole-forbidden transition which contains only exchange contributions. In both cases the linear behavior over the whole range of energies, from 0 to 100 Ry is striking. The behavior of the dipole-allowed $Q^1(3d_j;4f_{j'})$ shows linearity versus $\log(\Delta E)$, over a range of 0 to 200 Ry, as displayed in Fig. 2. Examples for much lighter atoms, such as He-like Al are shown in Figs. 3 and 4, for ranges of energies from 50 to 150 Ry. These are just a few selected examples of the wide range linear behavior of the radial integrals Q^k.

In some cases, however, the linear approximation proves to be insufficient for the required accuracy. Then, a simple interpolation with quadratic or higher-order polynomials can be used. In our program, the P^k are computed for the largest, the smallest, and the mean relevant transition energy. If the mean does not fit the linear interpolation within the specified tolerance, two more points are computed, etc. A detailed description of the numerical methods and computer codes are outside the scope of this paper, and will be published elsewhere.

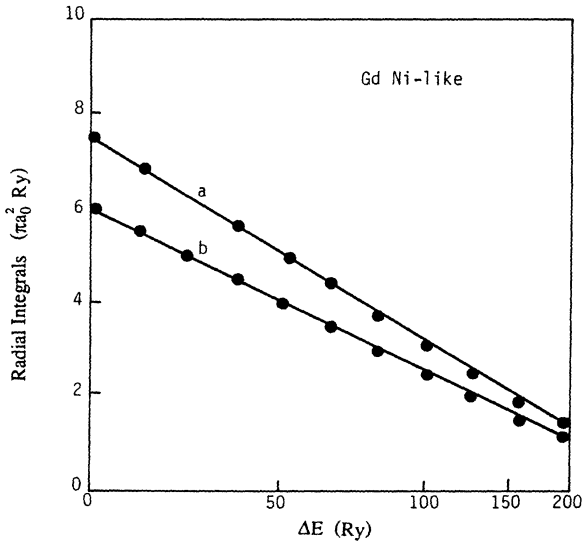


FIG. 2. Linear behavior of the "dipole-allowed" radial part Q^k vs $\log\Delta E$ with constant ε_{out} for a Ni-like Gd XXXVII atom. (a) $10Q^1(3d_{5/2},4f_{7/2})$ and (b) $10Q^1(3d_{3/2},4f_{5/2},3d_{5/2},4f_{7/2})$.

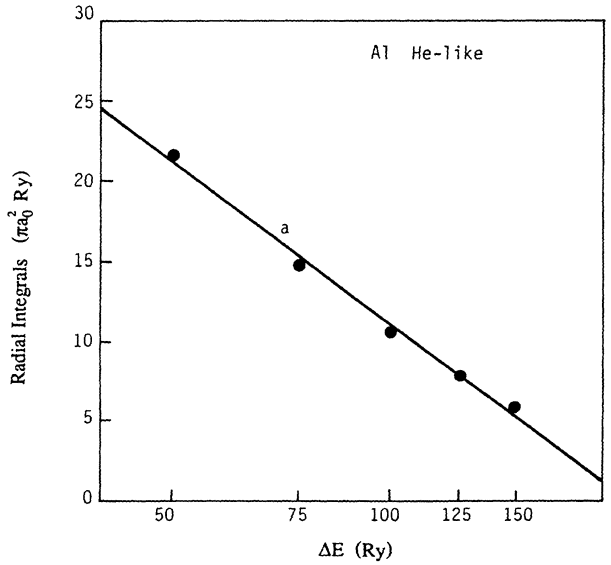


FIG. 4. Linear behavior of the "dipole-allowed" radial part Q^k vs $\log\Delta E$ with constant ε_{out} for a He-like Al XII atom. (a) $Q^1(1s_{1/2},2p_{3/2})$ (direct plus exchange).

IV. SUMMARY AND DISCUSSION

In this work we have developed a method for calculating a complete spectrum of collisional excitations. We have derived factorization formulas where the collision strength including exchange is represented by a one-electron angular operator, acting on target states, which multiplies a radial part containing the dependence on the continuum electrons. The relativistic, semirelativistic (i.e., nonrelativistic continuum wave functions), and nonrelativistic cases were worked out, and the corresponding formulas are given. These factorization rules apply also in the case of configuration interaction. In conjunction with an interpolation procedure for the energy-dependent radial part, those formulas enable a drastic reduction of the number of radial calculations, which are the most time-consuming part of the calculation needed for the complete spectrum analysis.

The theory, in the semirelativistic approach, was implemented in a set of computer codes for calculating populations distribution of complex excitation spectra in non-LTE plasma. In these calculations, collisional excitations as well as radiative spontaneous decay are included. As mentioned earlier, the description of these programs is outside the scope of the present work, but they are mentioned here to compare the results of the factorization-interpolation method with conventional ones.

Numerous computations of cross sections and rate coefficients for collision excitations in various ionized atoms were performed as tests of the method,[18] and compared with results obtained by other authors.[19] Although the numerical methods differ, the cross sections and rate coefficients obtained for similar target states definition are always within a few percent. The gain in computing time was checked at Lawrence Livermore National Laboratory.[20] One standard code in use there (MCDW) requires 10 min of Cray computer time for 36 $\Delta n=1$ transitions in the 37-level Ne-like model, while this one computes all the 663 $\Delta n=1$ and $\Delta n=0$ transitions in 6 min, an improvement of a factor of 30. Other computations have been performed on Ne- and Na- like,[21-23] Mg-like,[24] and Ni-like[25] atoms.

As an example, we report here complete spectrum calculations for the Ni-like Gd XXXVII case mentioned in the preceding, including all the 5565 transitions among excited states. At this stage, since we wish only to illustrate the results of the collisional-excitation cross sections, we have neglected all ionizations and recombinations, and we assume a steady-state equilibrium. The results for the cross sections for excitation from the ground state were compared with those of Hagelstein,[6] also computed in the DW framework, and are within 10% relative difference. No attempt was made to compare our rate coefficients with those obtained by the classical path model. The computations were performed On the Control Data Corporation CDC-855/170 computer of the Computing Center of the Hebrew University in Jerusalem, and took about one hour and a half of central-processing-unit (CPU) time, including the computations of energy levels and radiative transition probabilities.

The populations of some levels, obtained with this approximative model, exhibit relatively large inversions (for optically thin plasma), and are shown versus plasma density for an electronic temperature of 750 eV in Fig. 5. We do not report the values of the expected gains, because obviously, without ionization, recombination proper radiation transport, and a time-dependent model, the numbers are very approximate. But the point here is to show that these lengthy calculations can be performed much quicker with the factorization-interpolation method, even without an access to a supercomputer. A detailed investigation of this system will be described in a forthcoming paper. Analogous transitions in Ni-like Eu XXXVI were previously calculated,[26] and experimental results have been reported recently.[27]

Computations were also performed for the more complex atomic system Co-like Xe XXIX, in order to identify electric quadrupole transitions recorded in a tokamak spectrum. Configurations $3d^9$, $3d^84s$, $3d^84p$, $3d^84d$, $3d^84f$, $3p^53d^{10}$, $3p^53d^94s$, $3p^53d^94p$, and $3p^54d^94d$ were included, summing up to more than 300 levels, i.e., about 45 000 transitions. It should be pointed out that for the Co-like spectrum, the number of radial calculations is not much larger than for the Ni-like case, since it depends only on the number of orbitals involved. The results, obtained at the Hebrew University in about 2 h of computing time, have been reported,[28] and will be published shortly. To the best of our knowledge, this is the first time such a complex spectrum of collisional excitations has been completely computed in the DW framework. Thus the proposed method enables us to obtain the solution of problems which were considered practically impossible until now. It must be clear, however, that the

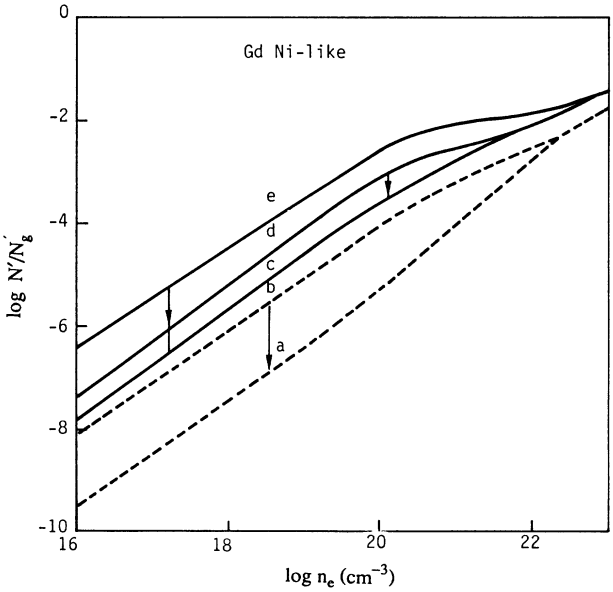


FIG. 5. Normalized reduced-level populations N' vs electronic density for Ni-like Gd XXXVII thin plasma at electron temperature $T_e=750$ eV. $N'=N/(2J+1), N'_g$; reduced population for the ground state. (a) $3d^9(3/2)4d_{5/2}$, $J=1$; (b) $3p^5(3/2)4f_{7/2}$, $J=2$; (c) $3d^9(5/2)4p_{3/2}$, $J=1$; (d) $3d^9(5/2)4d_{5/2}$, $J=2$; and (e) $3d^9(3/2)4d_{3/2}$, $J=0$. Population inversions for a possible x-ray laser are marked by arrows.

gain of time would not be significant for simpler spectra, where the number of fine-structure levels per orbital is small.

In this paper only collisional excitation was mentioned. However, the factorization-interpolation method can be easily applied to other atomic processes in plasmas treated in the DW framework. For radiative recombination, which is a one-electron operator to begin with, there is no angular problem, and the interpolation idea can be used. It is not difficult either to implement the idea of factorization-interpolation for autoionization and electron capture, which are basically two-electron Coulomb interaction, like the collisional excitation discussed in this paper. The extension to collisional direct ionization should be quite simple, since it is a special case of excitation, where the final state has a continuum electron. Thanks to the factorization, the sum over the partial waves of the ejected electron can be performed, and the resulting angular operator is just an annihilation operator. Work is in progress on this subject.

ACKNOWLEDGMENT

This work was accomplished with the partial support of the U. S. Department of Energy through Lawrence Livermore Laboratory under Contract No. W-7405-Eng-48.

APPENDIX A

Representation of the electrostatic interaction operator

The second-quantization form of the electrostatic interaction is

$$\sum_{i<j}\frac{1}{r_{ij}}=\tfrac{1}{2}\sum_{\alpha,\beta,\gamma,\delta}a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta\left\langle\alpha(1)\beta(2)\left|\frac{1}{r_{12}}\right|\delta(1)\gamma(2)\right\rangle , \tag{A1}$$

where α, β, γ, and δ are sets of individual quantum numbers and

$$\left\langle\alpha(1)\beta(2)\left|\frac{1}{r_{12}}\right|\delta(1)\gamma(2)\right\rangle = \sum_{k,q}(-1)^q\langle\alpha\,|\,C_q^{(k)}\,|\,\delta\rangle\langle\beta\,|\,C_{-q}^{(k)}\,|\,\gamma\rangle R^k(\alpha,\beta;\delta,\gamma) . \tag{A2}$$

In Eq. (A2) $C_q^{(k)}$ are the spherical harmonics and $R^k(\alpha,\beta;\delta,\gamma)$ are the radial Slater integrals.

We start with the scheme of the individual quantum numbers $\{n,s,l,m_s,m_l\}$. It has been shown[12] that the $(2s+1)(2l+1)$ components of

$$a^\dagger_{nslm_sm_l}[\text{and of } \tilde{a}_{nslm_sm_l}\equiv(-1)^{l-m_l+s-m_s}a_{nsl-m_s-m_l}]$$

form an irreducible double tensor set of ranks s and l with respect to $\hat{s}$ and $\hat{l}$.

Since the Slater integrals are independent of m_s and m_l, the summation over these indices recouples the pairs

$$a_\alpha^\dagger a_\delta,\ a_\beta^\dagger a_\gamma,\ \text{and}\ a_\alpha^\dagger a_\delta$$

of

$$a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma = a_\alpha^\dagger a_\delta a_\beta^\dagger a_\gamma - \delta_{\beta\gamma}a_\alpha^\dagger a_\gamma , \tag{A3}$$

where the recoupling coefficients

$$(ll'm_lm_{l'}\,|\,kq),\quad (\tfrac{1}{2}\tfrac{1}{2}m_sm_{s'}\,|\,00)$$

are supplied from the matrix elements of the operators $C_q^{(k)}$ using the Wigner-Eckart theorem. The result is

$$\sum_{i<j}\frac{1}{r_{ij}}=\frac{1}{2}\sum_{\substack{l_\alpha,l_\beta,\\ l_\gamma,l_\delta}}\sum_k[Z^{(k)}(l_\alpha,l_\gamma)\cdot Z^{(k)}(l_\beta,l_\delta)-\delta_{l_\beta l_\gamma}(2l_\alpha+1)^{-1/2}Z^{(0)}(l_\alpha,l_\delta)]X^k(l_\alpha,l_\beta;l_\gamma,l_\delta) , \tag{A4}$$

where

$$l\equiv\{n,s,l\} , \tag{A5}$$

$$X^k(l_\alpha,l_\beta;l_\gamma,l_\delta)=\langle l_\alpha\|C^{(k)}\|l_\gamma\rangle\langle l_\beta\|C^{(k)}\|l_\delta\rangle R^k(l_\alpha,l_\beta;l_\gamma,l_\delta) , \tag{A6}$$

$$Z^{(k)}(l,l')=2^{1/2}Z^{(0k)}(l,l') , \tag{A7}$$

and

$$Z^{(\kappa k)}_{\pi q}(l,l')\equiv-(2\kappa+1)^{-1/2}(2k+1)^{-1/2}\{a_l^\dagger\times\tilde{a}_{l'}\}^{(\kappa k)}_{\pi q} = -(2\kappa+1)^{-1/2}(2k+1)^{-1/2}\sum_{\substack{m,m',\\ \mu,\mu'}}(ll'mm'\,|\,kq)(\tfrac{1}{2}\tfrac{1}{2}\mu\mu'\,|\,\kappa\pi)a^\dagger_{nsl\mu m}\tilde{a}_{n's'l'\mu'm'} . \tag{A8}$$

It can be easily shown that the operator $Z^{(\kappa k)}(l,l')$ is the second-quantization form of the symmetric operator

$$\sum_i\zeta_i^{(\kappa k)}(l,l') \tag{A9}$$

with the single-particle reduced matrix element

$$\langle n_1 s_1 l_1 \| \zeta^{(\kappa k)}(l,l') \| n_2 s_2 l_2 \rangle = \langle n_1 l_1 \| \zeta^{(k)}(l,l') \| n_2 l_2 \rangle = \delta(n_1,n)\delta(l_1,l)\delta(n_2,n')\delta(l_2,l') \ , \tag{A10}$$

where for double tensors the matrix elements are reduced with respect to both $\hat{s}$ and $\hat{l}$.

In the relativistic case the Slater integrals depend on the individual quantum numbers j but not on m_j. In this case we define

$$a^{\dagger}_{nsljm} \text{ and } \tilde{a}_{nsljm}$$

by

$$a^{\dagger}_{nsljm} = \sum_{m_s, m_l} (slm_s m_l \mid jm) a^{\dagger}_{nslm_s m_l} \ , \tag{A11}$$

yielding the representation (A1) in the *nsljm* scheme.

We can now recouple $a^{\dagger}_{nsljm}$ and

$$\tilde{a}_{nsljm} = (-1)^{j-m} a_{nslj-m}$$

of Eq. (A1) in a similar manner as in the *SL* case. The result is

$$\sum_{i<j} \frac{1}{r_{ij}} = \tfrac{1}{2} \sum_{\substack{\mathbf{j}_\alpha, \mathbf{j}_\beta, \\ \mathbf{j}_\gamma, \mathbf{j}_\delta}} \sum_k (Z^{(k)}(\mathbf{j}_\alpha, \mathbf{j}_\gamma) \cdot Z^{(k)}(\mathbf{j}_\beta, \mathbf{j}_\delta) - (-1)^{j_\alpha + j_\beta + 1} \delta_{\mathbf{j}_\beta \mathbf{j}_\gamma} (2j_\alpha + 1)^{-1/2} Z^{(0)}(\mathbf{j}_\alpha, \mathbf{j}_\delta)) X^k(\mathbf{j}_\alpha, \mathbf{j}_\beta; \mathbf{j}_\gamma, \mathbf{j}_\delta) \ , \tag{A12}$$

where

$$\mathbf{j} \equiv \{n, s, l, j\} \ , \tag{A13}$$

$$X^k(\mathbf{j}_\alpha, \mathbf{j}_\beta; \mathbf{j}_\gamma, \mathbf{j}_\delta) = \langle \tfrac{1}{2} l_\alpha j_\alpha \| C^{(k)} \| \tfrac{1}{2} l_\gamma j_\gamma \rangle \langle \tfrac{1}{2} l_\beta j_\beta \| C^{(k)} \| \tfrac{1}{2} l_\delta j_\delta \rangle R^k(\mathbf{j}_\alpha, \mathbf{j}_\beta; \mathbf{j}_\gamma, \mathbf{j}_\delta) \ , \tag{A14}$$

$$\langle slj \| C^{(k)} \| s'l'j' \rangle = \langle l \| C^{(k)} \| l' \rangle (-1)^{1/2 + l' + j + k} (2j+1)^{1/2} (2j'+1)^{1/2} \begin{Bmatrix} j & j' & k \\ l' & l & \frac{1}{2} \end{Bmatrix} \ , \tag{A15}$$

[Eq. (3-38) of Ref. 9] and

$$Z^{(k)}_q(\mathbf{j}, \mathbf{j}') = -(2k+1)^{-1/2} \{ a^{\dagger}_j a_{j'} \}^{(k)}_q \ . \tag{A16}$$

$Z^{(k)}$ is the second-quantization form of the symmetric operator whose single-particle reduced-matrix element is

$$\begin{aligned} &\langle n_1 l_1 j_1 \| \zeta^{(k)}(\mathbf{j}, \mathbf{j}') \| n_2 l_2 j_2 \rangle = \delta(n_1,n)\delta(l_1,l)\delta(j_1,j)\delta(n_2,n')\delta(l_2,l')\delta(j_2,j') \ , \\ &Z^{(k)}(\mathbf{j}, \mathbf{j}') = \sum_{i=1}^{N+1} \zeta^{(k)}_1(\mathbf{j}, \mathbf{j}') \ , \end{aligned} \tag{A17}$$

Taking the matrix element of (A12) between the states Ψ_0 and Ψ_1 of Eq. (3), we obtain the collisional interaction as

$$V(\tilde{\mathbf{j}}_0, \tilde{\mathbf{j}}_1) \equiv \sum_{i<j} \frac{1}{r_{ij}} = \sum_{\mathbf{j}_0, \mathbf{j}_1} \sum_k [(Z^{(k)}(\mathbf{j}_0, \mathbf{j}_1) \cdot Z^{(k)}(\tilde{\mathbf{j}}_0, \tilde{\mathbf{j}}_1)) X^k(\mathbf{j}_0, \tilde{\mathbf{j}}_0; \mathbf{j}_1, \tilde{\mathbf{j}}_1) + (Z^{(k)}(\mathbf{j}_0, \tilde{\mathbf{j}}_1) \cdot Z^{(k)}(\tilde{\mathbf{j}}_0, \mathbf{j}_1)) X^k(\mathbf{j}_0, \tilde{\mathbf{j}}_0; \tilde{\mathbf{j}}_1, \mathbf{j}_1)] \ . \tag{A18}$$

The two terms in the square brackets are the "direct" and "exchange" parts, respectively.

The contribution of the term $Z^{(0)}$ in (A12) vanishes for collisional interaction, since the factor $\delta_{\beta\gamma}$ ($\delta_{\mathbf{j}_1 \tilde{\mathbf{j}}_0}, \delta_{\mathbf{j}_1 \tilde{\mathbf{j}}_0}$) (for the direct and exchange part, respectively) can be made to vanish if we choose an orthogonal basis for radial wave function. Furthermore, the factor $\frac{1}{2}$ in (A12) is canceled since each radial integral appears twice in the sum. For the nonrelativistic case the collisional-interaction operator has the same form as Eq. (A18) with individual l's instead of j's.

By recoupling the creation and annihilation operators of the continuum electron (and bound electron) separately using Eqs. (1-21), (3-13), and (3-29) of Ref. 9 and the anticommutation relations of these operators, we obtain for the exchange angular part the relations,

$$(Z^{(k)}(\mathbf{j}_0, \tilde{\mathbf{j}}_1) \cdot Z^{(k)}(\tilde{\mathbf{j}}_0, \mathbf{j}_1)) = \sum_t (-1)^{k+t} (2t+1) \begin{Bmatrix} j_0 & \tilde{j}_1 & k \\ \tilde{j}_0 & j_1 & t \end{Bmatrix} (Z^{(t)}(\mathbf{j}_0, \mathbf{j}_1) \cdot Z^{(t)}(\tilde{\mathbf{j}}_0, \tilde{\mathbf{j}}_1)) \tag{A19}$$

and

$$(Z^{(k)}(l_0, \tilde{l}_1) \cdot Z^{(k)}(\tilde{l}_0, l_1)) = \sum_t (-1)^{k+t} (2t+1) \begin{Bmatrix} l_0 & \tilde{l}_1 & k \\ \tilde{l}_0 & l_1 & t \end{Bmatrix} \sum_r (2r+1) (Z^{(rt)}(l_0, l_1) \cdot Z^{(rt)}(\tilde{l}_0, \tilde{l}_1)) \ . \tag{A20}$$

Another useful representation of (A20) is

$$(Z^{(k)}(l_0,\bar{l}_1)\cdot Z^{(k)}(\bar{l}_0,l_1))=\sum_t(-1)^{k+1}(2t+1)\begin{Bmatrix} l_0 & \bar{l}_1 & k \\ \bar{l}_0 & l_1 & t \end{Bmatrix}\sum_r(2r+1)\sum_x(-1)^{x+r}(Z^{(rt)x}(l_0,l_1)\cdot Z^{(rt)x}(\bar{l}_0,\bar{l}_1)) , \tag{A21}$$

where the operators $Z^{(rt)x}(l,l')$ are obtained by recouping r and t to x.

Equations (A19), (A20), and (A21) represent the exchange angular operators in terms of direct-type operators which allow the factorization of the matrix element in terms of separate target and continuum matrix elements. Substitution of (A21) in (A4) yields the representation (33) of the collisional interaction. The following useful identity,

$$Z^{(rt)k}(l_0,l_1)=\sum_{j_0,j_1}(2j_0+1)^{1/2}(2j_1+1)^{1/2}(2k+1)^{1/2}\begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & r \\ l_0 & l_1 & t \\ j_0 & j_1 & k \end{Bmatrix}Z^{(k)}(\mathbf{j}_0,\mathbf{j}_1) , \tag{A22}$$

is obtained from the definitions (A11) and (A16) and from the recoupling coefficient [Eq. (3-13) of Ref. 9].

APPENDIX B

Analytical formulas for the matrix elements of the operator $Z^{(k)}$ are obtained easily for the following two useful cases, by Eq. (A8), Eqs. (3-35) and (3-39) of Ref. 9, and Eqs. (31) and (32) of Ref. 12. The results are as follows:

$$\begin{aligned}\langle \mathbf{j}_1^{n_1}(\Gamma_1,J_1),\mathbf{j}_2^{n_2}(\Gamma_2,J_2),J\|Z^{(k)}(\mathbf{j}_1,\mathbf{j}_2)\|\mathbf{j}_1^{n_1-1}(\Gamma_1',J_1'),\mathbf{j}_2^{n_2+1}(\Gamma_2',J_2'),J'\rangle \\ =[n_1(n_2+1)]^{1/2}(\mathbf{j}_1^{n_1}\Gamma_1J_1\{\,|\,\mathbf{j}_1^{n_1-1}\Gamma_1'J_1')(\mathbf{j}_2^{n_2}\Gamma_2J_2\,|\,\}\mathbf{j}_2^{n_2+1}\Gamma_2'J_2')(-1)^{n_1+n_2+J_2-J_2'-j_2} \\ \times(2k+1)(2J_1+1)^{1/2}(2J_2'+1)^{1/2}(2J+1)^{1/2}(2J'+1)^{1/2}\begin{Bmatrix} J_1 & J_1' & j_1 \\ J_2 & J_2' & j_2 \\ J & J' & k \end{Bmatrix} ,\end{aligned} \tag{B1}$$

$$\begin{aligned}\langle \mathbf{j}^n\Gamma J\|Z^{(k)}(\mathbf{j},\mathbf{j})\|\mathbf{j}^n\Gamma'J'\rangle=(-1)^{J-j+k}n(2J+1)^{1/2}(2J'+1)^{1/2} \\ \times\sum_{\Gamma'',J''}(-1)^{J''}\begin{Bmatrix} j & k & j \\ J & J'' & J' \end{Bmatrix}(\mathbf{j}^n\Gamma J\{\,|\,\mathbf{j}^{n-1}\Gamma''J'')(\mathbf{j}^{n-1}\Gamma''J''\,|\,\}\mathbf{j}^n\Gamma'J') .\end{aligned} \tag{B2}$$

---

*Permanent address: Nuclear Research Centre–Negev, P. O. Box 9001, 84 105 Beer-Sheva, Israel.

[1]R. J. W. Henry, Phys. Rep. **68**, 1 (1981).
[2]A. Burgess, D. G. Hummer, and J. A. Tully, Philos. Trans R. Soc. London, Ser. A **266**, 225 (1970).
[3]M. S. Pindzola, A. K. Bhatia, and A. Temkin, Phys. Rev. A **15**, 35 (1977).
[4]W. Eissner and M. J. Seaton, J. Phys. B **5**, 2187 (1972).
[5]M. J. Seaton, Adv. Atom. Mol. Phys., **11**, 83 (1975).
[6]P. L. Hagelstein, Phys. Rev. A **34**, 874 (1986).
[7]I. I. Sobelman, L. A. Vainshtein, and E. A. Yukov, *Excitation of Atoms and Broadening of Spectral Lines* (Springer-Verlag, Berlin, 1981), p. 30.
[8]J. Oreg, J. Math. Phys. **12**, 1018 (1971).
[9]I. P. Grant, J. Phys. B **7**, 1458 (1974); Eq. (4.183) of Ref. 11.
[10]B. R. Judd, *Operator Techniques in Atomic Spectroscopy* (McGraw-Hill, New York, 1963).
[11]I. I. Sobelman, *Atomic Spectra and Radiative Transitions* (Springer-Verlag, Berlin, 1979).
[12]B. R. Judd, *Second Quantization in Atomic Spectroscopy* (Johns Hopkins Press, Baltimore, MD, 1967).
[13]I. Lindgren and J. Morrison, *Atomic Many Body Theory* (Springer-Verlag, Berlin, 1982).
[14]J. Oreg, Ph.D. thesis, The Hebrew University, Jerusalem, 1973.
[15]L. A. Vainshtein, Phys. Scr. **33**, 336 (1986).
[16]A. Hibbert, Comput. Phys. Commun. **8**, 329 (1974); N. C. Pyper, I. P. Grant, and N. Beatham, *ibid.* **15**, 387 (1978).
[17]C. W. Lee and U. Fano, Phys. Rev. A **33**, 981 (1986); **34**, 959 (1986); **36**, 66 (1987); **36**, 74 (1987).
[18]A. Bar-Shalom, Ph.D. thesis, The Hebrew University, Jerusalem, 1983.
[19]A. L. Merts, J. B. Mann, W. D. Robb, and N. H. Magee, Jr., Los Alamos National Laboratory Report No. LA-8267-MS (unpublished).
[20]W. H. Goldstein (private communication).
[21]W. H. Goldstein and R. S. Walling, Phys. Rev. A **36**, 3482 (1987).
[22]W. H. Goldstein, B. L. Whitten, A. U. Hazi, and M. H. Chen, Phys. Rev. A **36**, 3607 (1987).
[23]W. H. Goldstein, R. S. Walling, J. Bailey, M. H. Chen, R. Fortner, M. Klapisch, T. Phillips, and R. E. Stewart, Phys. Rev. Lett. **58**, 2300 (1987).
[24]M. Finkenthal, B. C. Stratton, H. W. Moos, A. Bar-Shalom, and M. Klapisch, Phys. Lett. **108A**, 71 (1985).
[25]J. F. Wyart, C. Bauche-Arnoult, J. C. Gauthier, J. P. Geindre, P. Monier, M. Klapisch, A. Bar-Shalom, and A. Cohn, Phys. Rev. A **34**, 701 (1986).
[26]S. Maxon, P. L. Hagelstein, J. H. Scofield, and Y. Lee, J. Appl. Phys. **59**, 293 (1986).
[27]B. J. McGowan, S. Maxon, P. L. Hagelstein, C. J. Keane, R. A. London, D. L. Matthews, M. D. Rosen, J. H. Scofield, and D. A. Wheelan, Phys. Rev. Lett. **59**, 2157 (1987).
[28]M. Klapisch, A. Cohn, and A. Bar-Shalom (unpublished).