

Procedures for improving a relativistic distorted-wave approach for excitation of ions by electron impact

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(Received 4 September 1992)

A simple way to obtain a completely general distorted-wave excitation program in the convenient factorized form of Bar-Shalom, Klapisch, and Oreg [Phys. Rev. A **38**, 1773 (1988)] is described. Procedures for improving numerical accuracy are also discussed, and results obtained by these procedures are compared with other work.

PACS number(s): 34.80.Kw

I. INTRODUCTION

In earlier work [1,2] we and our co-workers developed a rapid relativistic distorted-wave approach for calculating cross sections or, equivalently, collision strengths for excitation of highly charged ions by electron impact. The approach is very well suited for calculating collision strengths for a large portion of an isoelectronic sequence simultaneously, say, all members with

$$Z \geq 2N, \tag{1}$$

where Z is the nuclear charge number and N is the number of bound electrons per ion. The method has been extended to ionization [3,4] and it has been applied to large-scale calculations of atomic data in Refs. [5–10]. The approach uses the same relativistic Hartree-Fock-Slater or Dirac-Fock-Slater (DFS) potential determined using a mean configuration in solving the Dirac equation for all orbitals, bound and free. Hence, all orbitals are automatically orthogonal.

The purpose of the present article is to describe recent work we have done to improve the approach by (1) making the most efficient version of our scattering program completely general with the use of a simple procedure and (2) making modifications that should improve the accuracy and extend the range of validity beyond Eq. (1). The following section deals with the first of these im-

provements and Sec. III describes the second. In Sec. IV some numerical results by these procedures are compared with those by our earlier procedures and recent relativistic distorted-wave results of Qian, Kim, and Desclaux [11]. In the final section a brief summary and conclusions are given.

II. GENERAL FACTORIZATION PROGRAM

The most efficient form of our collisional excitation code [2] uses the factorization method of Bar-Shalom, Klapisch, and Oreg [12], but the code was not initially completely general. Here we describe how it has now been made general in a simple way, which could be applied to essentially any other distorted-wave program as well. In doing this we will make frequent use of equations given in Ref. [4]. Hereafter, Eq. (X) of Ref. [4] will be called Eq. (I-X). In that paper the factorization method was first applied to excitation. Then the result was extended to ionization, for which the very simple, convenient result given by Eq. (I-35) was obtained. For excitation, the results are given by Eqs. (I-28)–(I-32), which we repeat for convenience, except that results are given for the collision strength Ω in place of the cross section Q and a typographical error is corrected by replacing an S'_2 with S'_1 . Specifically, the expression for Ω equivalent to Eq. (I-28) is

$$\Omega(U-U') = 8 \sum_{S,S'} \sum_{\lambda} B^{\lambda}(U,SS_1;U',S'S'_1) Q^{\lambda}(n_a l_a j_a, n'_a l'_a j'_a; n_{a1} l_{a1} j_{a1}, n'_{a1} l'_{a1} j'_{a1}) . \tag{2}$$

Here $n_a l_a j_a$ and $n_{a1} l_{a1} j_{a1}$ indicate initial orbitals of the active electron in the pure jj -coupled states S and S_1 that contribute to the initial level U . An analogous statement applies for corresponding primed quantities contributing to the final level U' . Thus we can write

$$U = \sum_S b(U,S)|S\rangle, \quad U' = \sum_{S'} b(U',S')|S'\rangle, \tag{3}$$

where the b 's are the mixing coefficients. The Q^{λ} in Eq. (2) contain the radial scattering matrix elements and have the summation over initial and final orbital and total angular momenta of the free electron performed within them. In particular,

$$Q^\lambda(n_a l_a j_a, n'_a l'_a j'_a; n_{a1} l_{a1} j_{a1}, n'_{a1} l'_{a1} j'_{a1}) = \sum_{l, l'} P^\lambda(n_a l_a j_a \varepsilon l j; n'_a l'_a j'_a \varepsilon' l' j') P^\lambda(n_{a1} l_{a1} j_{a1} \varepsilon l j; n'_{a1} l'_{a1} j'_{a1} \varepsilon' l' j'), \quad (4)$$

where ε and ε' are the initial and final free-electron energies and

$$P^\lambda(n_a l_a j_a \varepsilon l j; n'_a l'_a j'_a \varepsilon' l' j') = (2\lambda + 1)^{-1/2} D^\lambda(n_a l_a j_a \varepsilon l j; n'_a l'_a j'_a \varepsilon' l' j') \langle j_a \| \underline{C}^\lambda \| j'_a \rangle \langle j \| \underline{C}^\lambda \| j' \rangle \\ + \sum_t (-1)^{\lambda+t} (2\lambda + 1)^{1/2} \begin{Bmatrix} j_a & j' & t \\ j & j'_a & \lambda \end{Bmatrix} E^t(n_a l_a j_a \varepsilon l j; n'_a l'_a j'_a \varepsilon' l' j') \\ \times \langle j_a \| \underline{C}^t \| j' \rangle \langle j \| \underline{C}^t \| j'_a \rangle, \quad (5)$$

in which $\langle j_1 \| \underline{C}^\lambda \| j_2 \rangle$ is given by Eq. (I-11) and the direct and exchange radial matrix elements D^λ and E^λ are given by Eqs. (I-2) and (I-3). The determination of the Q^λ is the lengthy part of the calculation, but as noted in Ref. [2] and used in the large-scale calculations of Refs. [5–10] the Q^λ are smoothly varying functions of Z . Hence, in the consideration of a given class of transitions results for a large portion of an isoelectronic sequence, say, all Z satisfying Eq. (1), can be obtained after making detailed calculations for only a few values of Z by fitting to a power series in Z , as given, for example, by Eq. (22) of Ref. [5] or Eq. (20) of Ref. [9].

Of course, as seen by Eqs. (4) and (5) the Q^λ depend on the initial and final free-electron energies ε and ε' and the difference between these differs with each transition. The procedure we follow is to calculate values for the Q^λ for a fixed set of scattered or final electron energies in units of an effective Z^2 rydbergs [see, for example, Eq. (3) of Ref. [9]] beginning near zero and going out sufficiently far for accurate determination of collision rates for all temperatures of major interest. For each of these final energies we calculate results for three impact-electron energies spanning the range of transition energies for the class of transitions being considered. Then we obtain the results for the exact energy for each transition by Lagrange interpolation, which is generally accurate to within about 1%.

The B^λ in Eq. (2) depend only on the properties of the

ion and require very little computing time to evaluate. The problem is in determining the completely general expression for the f^λ coefficients [see Eq. (7) below]. The purpose of the present section is to indicate how this can be easily done. We can write, as in Eqs. (I-31) and (I-32),

$$B^\lambda(U, SS_1; U', S'S'_1) = F^\lambda(US, U'S') F^\lambda(US_1, U'S'_1), \quad (6)$$

where

$$F^\lambda(US, U'S') = b(U, S) f^\lambda(S, S') b(U', S'). \quad (7)$$

Expressions for the f^λ coefficients were obtained in Ref. [4] for the case that the final orbital $n'_a l'_a j'_a$ is higher than that of the initial orbital and the orbitals of any spectator electrons [see Eq. (I-33) and the discussion following it]. Also, results were obtained as needed for the special cases considered in Refs. [5–10]. However, we now show that the f^λ are really identical to coefficients evaluated in complete generality in the well-known and widely used and tested multiconfiguration Dirac-Fock (MCDHF) relativistic atomic-structure program of Grant and co-workers [13–15], hereafter called the Grant code. In doing this we will outline the derivation of the factorization results for the collision strengths and to simplify this we will initially neglect exchange. The final result with exchange included is then obtained by simply making the substitution

$$(2\lambda + 1)^{-1/2} D^\lambda(\mathbf{j}_a \mathbf{j}; \mathbf{j}'_a \mathbf{j}') \langle j_a \| \underline{C}^\lambda \| j'_a \rangle \langle j \| \underline{C}^\lambda \| j' \rangle \rightarrow P^\lambda(\mathbf{j}_a \mathbf{j}; \mathbf{j}'_a \mathbf{j}'), \quad (8)$$

where P^λ is given by Eq. (5). In writing Eq. (8) we have used the abbreviations $\mathbf{j}_a = n_a l_a j_a$, $\mathbf{j} = \varepsilon l j$, etc.

With exchange neglected the collision strength is expressed in terms of the direct component of the reactance matrix by

$$\Omega^d(U - U') = 2 \sum_J (2J + 1) \sum_{\substack{l, l' \\ j, j'}} |R^d(U \varepsilon l j J; U' \varepsilon' l' j' J)|^2 \\ = 2 \sum_J (2J + 1) \sum_{\substack{l, l' \\ j, j'}} | \sum_{S, S'} b(U, S) b(U', S') R^d(S \varepsilon l j J; S' \varepsilon' l' j' J) |^2, \quad (9)$$

where J is the total angular momentum of the system. As in Ref. [4], we use $S = \beta_t J_t$ and $S' = \beta'_t J'_t$, where J_t and J'_t are the initial and final total angular momenta of the target ion, while β_t and β'_t are the additional quantum numbers required to specify the pure jj -coupled states S and S' , respectively. Then using the usual expansion

$$\frac{1}{r_{ij}} = \sum_{r=0}^{\infty} \frac{r_{<}^\lambda}{r_{>}^{\lambda+1}} \underline{C}^\lambda(i) \cdot \underline{C}^\lambda(j), \quad (10)$$

in which $r < (r >)$ is the lesser (greater) of r_i and r_j , one can write

$$R^d(\beta_i J_i \epsilon l j J; \beta'_i J'_i \epsilon' l' j' J) = 2 \sum_{\lambda} \langle \alpha_i J_i l j J | \underline{C}^{\lambda}(1) \cdot \underline{C}^{\lambda}(2) | \alpha'_i J'_i l' j' J \rangle D^{\lambda}(\mathbf{j}_a \mathbf{j}; \mathbf{j}'_a \mathbf{j}'), \quad (11)$$

where the active bound electron and the free electron are indicated by 1 and 2, respectively. Here $|\alpha_i J_i l j J\rangle$ and $|\alpha'_i J'_i l' j' J\rangle$ differ from $|\beta_i J_i \epsilon l j J\rangle$ and $|\beta'_i J'_i \epsilon' l' j' J\rangle$, respectively, only in that the radial functions have been separated out from the latter. Now, using Eq. (C91) of Messiah [16] we obtain

$$\langle \alpha_i J_i l j J | \underline{C}^{\lambda}(1) \cdot \underline{C}^{\lambda}(2) | \alpha'_i J'_i l' j' J \rangle = (-1)^{J+j+J'_i} \begin{Bmatrix} J_i & \lambda & J'_i \\ j' & J & j \end{Bmatrix} \langle \alpha_i J_i | \underline{C}^{\lambda} | \alpha'_i J'_i \rangle \langle j | \underline{C}^{\lambda} | j' \rangle, \quad (12)$$

but we can write

$$\langle \alpha_i J_i | \underline{C}^{\lambda} | \alpha'_i J'_i \rangle = d_{aa'}^{\lambda}(S, S') \langle j_a | \underline{C}^{\lambda} | j'_a \rangle, \quad (13)$$

which is essentially a special case of Eq. (7) of Ref. [17] or Eq. (60) of Ref. [15]. These d^{λ} coefficients are related to the so-called T coefficients in the Grant code by

$$d_{aa'}^{\lambda}(S, S') = \left[\frac{2J_i + 1}{2j_a + 1} \right]^{1/2} T_{aa'}^{\lambda}(S, S'). \quad (14)$$

Thus, collecting results and applying them to Eq. (9), one can neglect the phase factor of Eq. (12) because $J + j + J'_i$ involves “good” quantum numbers and is an integer. Also, one can perform the summation over J using the well-known formula [16]

$$\sum_J (2J+1) \begin{Bmatrix} J_i & \lambda & J'_i \\ j' & J & j \end{Bmatrix} \begin{Bmatrix} J_i & \lambda' & J'_i \\ j' & J & j \end{Bmatrix} = \frac{\delta_{\lambda\lambda'}}{2\lambda+1}. \quad (15)$$

The result can be written in a form like Eq. (2):

$$\Omega^d(U - U') = 8 \sum_{S, S'} \sum_{\lambda} B^{\lambda}(U, SS_1; U', S' S'_1) \times Q^{\lambda d}(\mathbf{j}_a \mathbf{j}'_a; \mathbf{j}_{a1} \mathbf{j}'_{a1}), \quad (16)$$

where $Q^{\lambda d}(\mathbf{j}_a \mathbf{j}'_a; \mathbf{j}_{a1} \mathbf{j}'_{a1})$ is given by Eqs. (4) and (5) with E' set to zero and B^{λ} is given by Eq. (6) with

$$F^{\lambda}(US, U'S') = b(U, S) d_{aa'}^{\lambda}(S, S') b(U', S'). \quad (17)$$

Although the techniques used by Bar-Shalom, Klapisch, and Oreg [12] may not be completely clear to some readers, the essential key in applying the factorization method with inclusion of exchange is to arrange the angular part of R^e so that it also contains a $6j$ factor of the form

$$\begin{Bmatrix} J_i & C & J'_i \\ j' & J & j \end{Bmatrix} \quad (18)$$

as, for example, in Eqs. (I-21) and (I-22). Then the summation over J can still be performed using the analog of Eq. (15). This leads to a large reduction in the angular part of the calculation and the result is then given by the right-hand side of Eq. (16) with $Q^{\lambda d}$ replaced by Q^{λ} given by Eqs. (4) and (5). Thus, comparing this with Eqs. (2), (6), and (7), one sees that

$$f^{\lambda}(S, S') = d_{aa'}^{\lambda}(S, S'). \quad (19)$$

These d coefficients are defined in Ref. [17] and are very readily obtained in complete generality using the MCT module of the Grant code. We note that the subscript aa' was omitted from f^{λ} because it is nonvanishing only when a single orbit, which we will call a and a' , differs in S and S' due to the orthogonality properties of the orbital functions.

In order to avoid any phase-factor errors resulting from use of different conventions it is advisable to use the same angular package for both the atomic-structure and scattering programs. This is insured in our own codes because the angular package from the Grant code was used in our Dirac-Fock-Slater atomic-structure program, as well as in evaluating the coefficients of Eq. (19). Also, as described in the next section, we now have an option in our scattering program to use the atomic structure data obtained from the Grant code.

III. MODIFICATIONS FOR IMPROVED ACCURACY

We now consider ways in which the accuracy of our procedures for relativistic calculations have been improved. First we note that the relativistic DFS atomic-structure program of Ref. [1] was modified to use a non-point nuclear charge and to include the generalized Breit interaction and other QED corrections. This was discussed in Ref. [18] and in Ref. [9], where it was applied in calculations of collision strengths for excitation of F-like ions. However, as noted in Ref. [9], even with these modifications the program of Ref. [1] introduces some slight numerical error in treating transitions involving s orbitals in ions with very large Z . This appears to have essentially a negligible effect on line strengths and collision strengths, but introduces a significant error in transition energies for $\Delta n = 0$ transitions at high Z . For this reason energies obtained from the Grant code [13–15] were used for these transitions in Ref. [9]. The error appears to arise from using a linear grid for small r rather than a logarithmic grid. The Grant code is quite fast and efficient, especially the latest version, GRASP [15], using the “average level” option. Also, the principal computing time in obtaining collision strengths tends to go into the scattering part of the calculation rather than the structure part. Hence, instead of going through the work of modifying the program of Ref. [1] to use a logarithmic grid we choose to include an option in our collisional-excitation program to use atomic-structure data from the Grant code. This program is generally accepted as being

very accurate for highly charged ions. Use of it has the additional, more significant advantage that the results obtained for low Z are also probably more accurate because in this regime, where the electron-electron contribution to the potential is more important, use of the MCDF potential in generating the orbitals is expected to be more accurate than use of the DFS potential. However, to use the Grant code it was necessary to transform the results from the logarithmic grid generated by it to a linear grid for the use in the collision program, where a linear grid is needed for accuracy for the very large r contribution. A well-tested subroutine for accomplishing this was provided to us by Moores [19]. Of course, in using the Grant code in treating many members of an isoelectronic sequence simultaneously we calculate things such as the angular algebra that are the same for each ion only once. Also, when using the MCDF atomic-structure data from the Grant code we use a new option for the form for the central potential used in solving the Dirac equation for the impact and scattered electrons, as compared to our earlier work [5–10], where the same DFS potential was used in determining the orbitals for all electrons, bound and free. The potential used for the bound electrons is different from that used for the free electrons anyway when one changes to the MCDF potential for the bound electrons. Hence, it was decided to also use a new form for the potential for the free electrons that would be more precisely appropriate for them. In order to clarify this we repeat with slight change in notation Eqs. (4)–(6) of Ref. [9] giving the Dirac-Fock-Slater potential $V_{DFS}(r)$:

$$V_{DFS}(r) = V'(r) + V_{DFS}^{ex}(r), \quad (20)$$

where

$$V'(r) = -\frac{2Z(r)}{r} + V_c(r), \quad (21)$$

$$V_{DFS}^{ex}(r) = -\left[\frac{24}{\pi}\rho(r)\right]^{1/3}, \quad (22)$$

$$V_c(r) = \sum_{n',\kappa'} w_{n',\kappa'} \int_0^\infty \frac{2}{r_>} [P_{n',\kappa'}^2(r_2) + Q_{n',\kappa'}^2(r_2)] dr_2, \quad (23)$$

and

$$\rho(r) = \frac{1}{4\pi r^2} \sum_{n',\kappa'} w_{n',\kappa'} [P_{n',\kappa'}^2(r) + Q_{n',\kappa'}^2(r)]. \quad (24)$$

Here $w_{n',\kappa'}$ is the occupation number of subshell $n'\kappa' = n'l'j'$, the summation is over all occupied subshells, $r_>$ is the greater of r and r_2 , and $P_{n',\kappa'}$ and $Q_{n',\kappa'}$ are the so-called large and small components of the radial function of an electron in the $n'\kappa'$ subshell. We note that this potential differs slightly from that used in the earlier work of Refs. [5–8] in that the point nuclear charge Z used in those references was replaced in Ref. [9] with a finite nuclear charge $Z(r)$, which differs from Z only for extremely small r , where the Fermi charge distribution (see Chen *et al.* [20]) was used. This is also the option usually used in applications of the Grant code.

In the new option the exchange potential given by Eq. (22) is replaced with a form based on the semiclassical exchange approximation of Riley and Truhlar [21]. In par-

ticular, we use the form of Peek and Mann [22] for the potential. This was used by Mann in the extensive semirelativistic calculations made in Refs. [23–25]. We will hereafter refer to it as the Mann potential $V_M(r)$. It is given by

$$V_M(r) = V'(r) + V_M^{ex}(r), \quad (25)$$

which differs in form from Eq. (20) only in that the exchange contribution given by Eq. (22) is replaced with

$$V_M^{ex}(r) = -\frac{1}{2}[E(\text{Ry}) - V'][(1 + \beta^2)^{1/2} - 1], \quad (26)$$

where

$$\beta^2 = \frac{4\rho}{r^2[E(\text{Ry}) - V']^2} \quad (27)$$

and $E(\text{Ry})$ is the free-electron kinetic energy in rydbergs.

As in our earlier work [5–10], V_c and bound-electron charge density ρ given by Eqs. (23) and (24) are still determined using a mean configuration. In general this can be chosen differently for the impact and scattered electrons, but in the application to $\Delta n = 0$ transitions in Be-like ions discussed in the next section we used the mean configuration

$$1s_{1/2}^2 2s_{1/2}^{0.66} 2p_{1/2}^{0.67} 2p_{3/2}^{0.67} \quad (28)$$

in evaluating Eqs. (23) and (24) for both impact and scattered electrons, so the potential used in calculating their orbitals differed only by the different appropriate free-electron energies used in Eqs. (26) and (27) in the two cases.

Also, since the orbitals of the free electrons are no longer orthogonal to those of the bound electrons it was necessary with the new option to replace the factor $r_{<}^\lambda / r_{>}^{\lambda+1}$ with $r_{<}^\lambda / r_{>}^{\lambda+1} - \delta_{\lambda 0} V_c(r) / 2N$ in the exchange scattering term given by Eq. (10) of Ref. [2]. This is the analog of Mann's [23] Eq. (14), except that a typographical error was made in the latter equation in that $2N$ should replace N , as seen from Mann's [23] Eq. (11).

Of course, in using Eq. (25) the orbitals used in evaluating Eqs. (23) and (24) are those calculated with the Grant code using the MCDF potential rather than the orbitals evaluated using the V_{DFS} potential. However, numerical test cases discussed in the next section indicate this has little effect in most cases as compared with the effect due to use of the different form for the central potential for the free electrons given by Eq. (25) instead of Eq. (20). In fact, even that has an essentially negligible effect except for ions at the very low- Z end of the range given by Eq. (1).

IV. COMPARISONS OF NUMERICAL RESULTS

In Ref. [26] the procedures we have described here were used in calculating collision strengths for all 45 transitions among the 10 levels of the $1s^2 2s^2$, $1s 2s 2p$, and $1s^2 2p^2$ configurations in each of the 85 Be-like ions with Z in the range

$$8 \leq Z \leq 92. \quad (29)$$

Here we discuss numerous test calculations we have

made for Be-like ions to assess the effect of these new modifications in our calculational procedures. A sample of the results is given in Table I for $Z=8$, where the effect of using the MCDF potential for the bound electrons and the Mann form, Eq. (25), for the potential for the free electrons is greatest for ions with Z in the range given by Eq. (29). Although the test calculations were done for all 45 $\Delta n=0$ transitions, in the interests of brevity the results are given only for the transitions from the ground level to the other nine levels. These are quite typical, but the discrepancies between the various sets of calculations, especially the G/M and D/D entries to be discussed in the following paragraphs, tend to be larger than average for these transitions.

In this table three sets of collision strengths are given for three scattered, or final, electron energies E_f in eV for each of the nine transitions. The first set, labeled G/M , are results by the new procedure of using the Grant code for obtaining the atomic-structure data and the Mann form, Eq. (25), for the potential for the free electrons. The second set, labeled D/M , are results by the same

procedure except that DFS bound orbitals were used everywhere in place of MCDF bound orbitals. The third set, labeled D/D , are results by our previous procedure of using the same DFS potential for all electrons, bound and free. We also did test calculations in which the only change made was use of mixing coefficients by our DFS program instead of the Grant program. This was found to have almost no effect. In this connection we note that the mixing included in all cases was all mixing among the states in a complex, that is, having the same set of n values, parity and total ion angular momentum, called J_i or J'_i in Sec. II.

By comparing G/M and D/M entries in Table I one sees that use of the DFS orbitals in place of MCDF orbitals by the Grant code has very little effect in most cases. However, by comparing the D/D entries with the other entries one sees that use of the Mann form for the potential for the free electrons in place of the DFS potential does often have a significant effect for such a low- Z ion. Nevertheless the maximum effect of using the procedures discussed here as represented by the G/M values com-

TABLE I. Comparison of collision strengths for excitation from the ground level of Be-like oxygen by three procedures labeled G/M , D/M , and D/D , which are defined in the text. Numbers in square brackets are powers of 10 by which adjacent entries should be multiplied. Results are given as a function of final, or scattered, electron energy E_f (eV). Upper entries for the transition energies ΔE (eV) are MCDF values by the Grant code, while the lower entries are DFS values by the code of Ref. [1] with modification discussed in the text.

Upper level	ΔE (eV)	E_f (eV)	G/M	D/M	D/D
$2s2p \ ^3P_0$	10.29	10	2.743[-2]	2.795[-2]	2.610[-2]
	10.27	75	1.514[-2]	1.511[-2]	1.362[-2]
		100	1.689[-3]	1.662[-3]	1.568[-3]
$2s2p \ ^3P_1$	10.31	10	8.227[-2]	8.385[-2]	7.830[-2]
	10.29	75	4.541[-2]	4.534[-2]	4.089[-2]
		500	5.075[-3]	5.008[-3]	4.736[-3]
$2s2p \ ^3P_2$	10.36	10	1.370[-1]	1.397[-1]	1.305[-1]
	10.33	75	7.558[-2]	7.550[-2]	6.810[-2]
		500	8.414[-3]	8.298[-3]	7.833[-3]
$2s2p \ ^1P_1$	21.28	10	3.028[0]	3.017[0]	3.093[0]
	21.10	75	4.066[0]	4.079[0]	4.120[0]
		500	6.504[0]	6.454[0]	6.506[0]
$2p^2 \ ^3P_0$	26.77	10	1.631[-3]	1.615[-3]	1.369[-3]
	26.88	75	6.393[-4]	6.259[-4]	5.209[-4]
		500	3.178[-5]	2.972[-5]	2.681[-5]
$2p^2 \ ^3P_1$	26.79	10	4.873[-3]	4.833[-3]	4.098[-3]
	26.70	75	1.904[-3]	1.872[-3]	1.559[-3]
		500	8.857[-5]	8.785[-5]	7.919[-5]
$2p^2 \ ^3P_2$	26.83	10	8.084[-3]	8.023[-3]	6.809[-3]
	26.74	75	3.152[-3]	3.108[-3]	2.590[-3]
		500	1.486[-4]	1.483[-4]	1.340[-4]
$2p^2 \ ^1D_2$	30.09	10	1.626[-2]	1.641[-2]	1.667[-2]
	29.97	75	2.288[-2]	2.312[-2]	2.342[-2]
		500	3.342[-2]	3.371[-2]	3.336[-2]
$2p^2 \ ^1S_0$	37.57	10	2.535[-3]	2.862[-3]	2.878[-3]
	37.36	75	2.468[-3]	2.778[-3]	2.785[-3]
		500	2.410[-3]	2.706[-3]	2.681[-3]

pared to the previous procedures represented by the D/D values is that the latter are 16% lower than the former for the weak transitions to the $2p^2\ ^3P$ levels. These correspond to double electron jumps and occur only through configuration mixing.

In Table II the present G/M and D/D results are also compared with the relativistic distorted-wave results of Qian, Kim, and Desclaux [11] (labeled QKD) for the $2s^2\ ^1S_0-2s2p\ ^1,^3P_1$ transitions in Be-like ions with $Z=10, 26$, and 54. The atomic-structure data used in the calculations in Ref. [11] were obtained with an improved version of the MCDF code of Desclaux [27], which is similar to the Grant code. As expected, the agreement between G/M and QKD collision strengths is seen to be very good, usually within 1–2% with the exception of the results for the highest energies. Specifically, for the $2s^2\ ^1S_0-2s2p\ ^3P_1$ transition in Be-like neon the QKD result exceeds the G/M value by 18% for an impact-electron energy E_i of 10^4 eV (the highest energy QKD considered). However, the collision strength is extremely small and unimportant for this energy and the agreement is very good (within 1%) for $E_i \leq 1000$ eV. For the other high-energy cases the QKD results are typically 4% or 5% lower than the G/M values. This is largely a consequence of the fact that in Ref. [11] the collision strength appears to be defined differently than we do. In particular, in the usual relation between cross section and collision strength,

$$Q = \frac{\pi a_0^2}{k_i^2 g_i} \Omega, \quad (30)$$

they appear to use for k_i^2 [see Eq. (4) of Ref. [11]] the

nonrelativistic expression for the kinetic energy of the incident electron $\frac{1}{2}mv_i^2$ (Ry), while we use the relativistic relation

$$k_i^2 = [E_i(\text{Ry})] \left[1 + \frac{\alpha^2}{4} [E_i(\text{Ry})] \right], \quad (31)$$

where α is the fine-structure constant and $E_i(\text{Ry})$ is the relativistic kinetic energy of the incident electron in rydbergs.

Also as expected from the discussion of Table I, one sees that the D/D values in Table II are close to the G/M values except for the weak spin change transition $2s^2\ ^1S_0-2s2p\ ^3P_1$ when $Z=10$, which is dominated by the exchange contribution and where the D/D values are about 7% below the G/M values for low energy.

V. SUMMARY AND CONCLUSIONS

There are essentially two parts to the paper. In the first part we have shown how a relativistic distorted-wave program that uses the factorization method of Bar-Shalom, Klapisch, and Oreg [12] can be very easily made completely general by identifying a key parameter we call $f^\lambda(S, S')$ with the $d_{aa}^\lambda(S, S')$ coefficients evaluated in general in the MCT module of the well-known relativistic atomic-structure program of Grant and co-workers [13–15]. These coefficients, or their LS -coupling analogs, enter in the general calculation of matrix elements of one-particle operators, such as occurs in determining radiative oscillator strengths, and should be present in most general atomic-structure programs. Thus the analogous procedure could be used as well to put a nonrelativistic or

TABLE II. Comparison of collision strengths for excitation from the ground level in Be-like neon, iron, and xenon by various procedures and workers. Notation is as in Table I except that the QKD entries are those of Qian, Kim, and Desclaux [11]; results are given as a function of incident electron energy E_i (eV); and the third entries for the transition energies ΔE (eV) are the QKD values.

Z	Upper level	ΔE (eV)	E_i (eV)	G/M	D/D	QKD	
10	$2s2p\ ^3P_1$	13.99	100	2.910[−2]	2.714[−2]	2.886[−2]	
		13.95	500	6.502[−3]	6.077[−3]	6.500[−3]	
		14.07	5000	2.834[−4]	2.989[−4]	3.200[−4]	
	$2s2p\ ^1P_1$	28.31	100	2.388[0]	2.411[0]	2.344[0]	
		28.12	500	3.558[0]	3.590[0]	3.504[0]	
		28.29	5000	5.536[0]	5.597[0]	5.430[0]	
	26	$2s2p\ ^3P_1$	47.18	500	1.152[−2]	1.144[−2]	1.172[−2]
			47.15	1000	1.212[−2]	1.199[−2]	1.225[−2]
				10000	1.548[−2]	1.522[−2]	1.519[−2]
$2s2p\ ^1P_1$		95.06	500	3.626[−1]	3.619[−1]	3.585[−1]	
		94.88	1000	4.106[−1]	4.105[−1]	4.097[−1]	
			10000	6.670[−1]	6.690[−1]	6.395[−1]	
54		$2s2p\ ^3P_1$	128.03	1000	2.010[−2]	1.961[−2]	1.953[−2]
			128.67	5000	2.643[−2]	2.673[−2]	2.586[−2]
			128.11	10000	3.045[−2]	3.071[−2]	2.919[−2]
	$2s2p\ ^1P_1$	534.38	1000	5.964[−2]	5.920[−2]	5.884[−2]	
		534.94	5000	7.668[−2]	7.707[−2]	7.484[−2]	
		533.70	10000	9.044[−2]	9.067[−2]	8.583[−2]	

semirelativistic distorted-wave program into the factorized form. This form is the most convenient and efficient form for a distorted-wave program for excitation of ions and can be very easily coded following the outline provided here. This form was designed originally by Bar-Shalom, Klapisch, and Oreg [12] to reduce the angular part of the calculation and the number of radial integrals in treating complex transitions in a single ion, but was recognized in Refs. [1,2] to be very convenient for large-scale calculations for a given class of transitions for a very large portion of an isoelectronic sequence simultaneously and has been used for that purpose in Refs. [5–10,26].

In the second part of the paper, expected improved accuracy in our relativistic distorted-wave approach has been obtained by replacement of the atomic-structure data by the Dirac-Fock-Slater code in Ref. [1] with that of the well-known multiconfiguration Dirac-Fock program of Grant and co-workers [13–15] and by replacing the form for the potential for the free electrons by a more appropriate form given by Eqs. (25)–(27). Results obtained with these modifications are compared with relativistic distorted-wave results of Qian, Kim, and Desclaux [11]. When account is taken of the fact that the collision strength is defined slightly differently in the latter, very good agreement is obtained. The difference in results by the current and earlier procedures is also very slight except for the low- Z end of the range given by Eq. (1). With the current procedure the range of validity is probably extended to about $Z \geq 1.5N$ in most cases. Actually, in saying this we mean that for this range of Z the

results are probably quite accurate, within a few percent, for the “direct” or nonresonance part of the collision strength. The resonance contribution, which is expected to be important for some of the fairly weak transitions, especially for the lower- Z values, can later be calculated by the relativistic version of the method used by Cowan [28], in which the resonance or indirect contribution is treated as a two-step process of electron capture followed by autoionization. This can then be added to the results by the present method to obtain the total contribution. We expect to do this in future work.

It should also be pointed out that test calculations for H-like, He-like, and Li-like ions made in Refs. [18,29] indicate that the generalized Breit interaction should be included in calculating the scattering matrix elements for excitation from the $1s$ shell in ions with $Z \geq 30$. Hence, we expect to modify our codes to include an option to efficiently do this in future work.

ACKNOWLEDGMENTS

This work was partially supported by the U.S. Department of Energy through a Lawrence Livermore National Laboratory Subcontract. One of us (D.H.S.) wishes to thank the Mathematical Institute, University of Oxford, for use of their facilities and the U. K. Science and Engineering Research Council for partial support during the later stages of this work. In addition, we express our thanks to Dr. David L. Moores for providing us with a copy of his convenient procedure for transforming a logarithmic grid to a linear grid.

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