Use of the factorized form for the collision strength in exploration of the effect of the generalized Breit interaction

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Expressions are given for the convenient factorized form [Bar-Shalom, Klapisch, and Oreg, Phys. Rev. A **38**, 1773 (1988)] for the collision strength with inclusion of the generalized Breit interaction. This is used to explore further the importance of the inclusion of the generalized Breit interaction in calculating electron-impact excitation cross sections or collision strengths, by considering the inner-shell excitation of Be-like uranium and the $n=2$ to $n=3$ transitions in neonlike xenon and uranium.

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I. INTRODUCTION

In recent years there has been increasing interest in atomic processes involving very highly charged ions, partially due to more interest in very-high-temperature plasmas for purposes such as the development of x-ray lasers. In addition, the development of electron-beam ion traps [1,2] are making it possible to measure various atomic processes for ions in much higher charge states than possible, for example, in crossed-beam experiments. In considering atomic processes in very highly charged ions one would expect that, in addition to using a fully relativistic treatment based on use of the Dirac equation, it might be necessary to include the lowest-order QED correction to the Coulomb interaction, the so-called generalized Breit interaction. This is routinely done in most relativistic atomic structure calculations, which can affect results for excitation cross sections, or equivalently collision strengths, by altering the mixing coefficients, as well as the transition energies. However, inclusion of the generalized Breit interaction in the interaction producing the excitation, or equivalently use of the so-called Møller interaction, has been done in calculations of excitation cross sections or collision strengths only in [3–7].

The calculations in [3–5] were made only for excitation from the $1s$ level to the $n=2$ levels in hydrogenic ions. In addition to these transitions, excitation from the $1s$ to the $n=3$ levels, excitation from the $n=2$ to $n=3$ levels and transitions between the $n=2$ levels in hydrogenic ions were considered in [6] and [7]. There it was found that the effect of the generalized Breit interaction on the latter type of transition is completely negligible for all values for the nuclear charge number Z, but the effect for $n=1-3$ transitions was found to be slightly larger than for $n=1-2$ transitions. The effect for $n=2-3$ transitions was found to be considerably less than excitation from the $1s$ level. Nevertheless, it was found to have up to a 19% effect for hydrogenlike uranium.

More complex ions were also considered in [6] and [7]. In particular, excitation of He-like ions and inner-shell excitation of Li-like ions were considered and the interesting result was found that the effects of inclusion of the generalized Breit interaction is somewhat greater for excitation from the $1s$ subshell in complex ions than for hydrogen ions with the same value for Z.

One of the purposes of the present paper is to do additional test calculations for complex ions in order to indicate more completely the extent of the importance of the generalized Breit interaction on excitation cross sections. This is of considerable practical significance because excitation calculations are generally rather lengthy, especially for complex ions. For example, they are much more lengthy than atomic structure calculations, and inclusion of the Breit interaction tends to further increase the computing time for excitation by somewhat over an order of magnitude. Thus, in order to more completely explore the effect for $1s$ excitation, we consider inner-shell excitation of Be-like uranium. However, we mostly concentrate on the $n=2$ to $n=3$ transitions in highly charged neonlike ions. This is done because these are the simplest complex ions in which that type of transition occurs and because of the well-known importance of neonlike ions for the development of x-ray lasers. We expect the generalized Breit interaction might be of some importance in this case in view of the fact noted previously that it is not completely negligible for the $n=2$ to $n=3$ transitions in hydrogenlike uranium. We also expect the effect to be more important for the analogous transitions in more complex ions as was exhibited in the case of excitation from the $1s$ subshell.

A second objective of the present work is to provide an expression for the collision strength with inclusion of the generalized Breit interaction that is convenient for future large-scale production of atomic data for the conditions in which the Breit interaction is significant. As noted in the preceding paragraph, this is very important because inclusion of the generalized Breit interaction tends to make the calculations over an order of magnitude more lengthy in computing time. For this purpose the appropriate form for the collision strength Ω is the factor-

ized form. In the notation of [8] this expression for the collision strength for excitation from a level U of any ion to a level U' is

$$\Omega(U-U')=8\sum_{\substack{S,S'\\S_1,S_1'}}\sum_{\lambda}B^{\lambda}(U,SS_1;U',S'S_1')Q^{\lambda}(n_al_aj_a,n_a'l_a'j_a';n_{a1}l_{a1}j_{a1},n_{a1}'l_{a1}'j_{a1}') . \quad (1)$$

Here $n_al_aj_a$ and $n_{a1}l_{a1}j_{a1}$ indicate orbitals of the active electron in pure jj coupled states S and S_1 that contribute to initial level U. An analogous statement applies to corresponding primed quantities contributing to the final level U'. This form was first obtained by Bar-Shalom, Klapisch, and Oreg [9] for the purpose of reducing the angular algebra in complex cases where a very large number of transitions involve a relatively small number of orbital transitions. We recognized that this form is very convenient for large-scale calculations of atomic data for a given class of transitions for all members of a large portion of an isoelectronic sequence simultaneously and it was used for that purpose in [10–17].

The reason Eq. (1) is convenient for that purpose is that the B^{λ} coefficients are readily computed quantities that depend only on the target ion properties such as mixing coefficients and ion angular momenta, while the Q^{λ} contain the radial scattering integrals summed over free electron angular momenta and tend to be the lengthy part to calculate. However, the Q^{λ} generally vary smoothly with Z so that detailed calculations need to be made typically for only one Z value in 10. Results for the remaining Z values can be obtained accurately by making fits of the Q^{λ} to power series in Z. We note that Eq. (1) is applicable for ununitarized distorted-wave calculations. However, the accuracy of both the approximation of neglecting unitarization and the distorted-wave approximation improve as Z increases because the scattering matrix elements decrease approximately as $1/Z$. Hence both approximations are at their best and expected to be rather good for the relatively highly charged, high-Z regime for which inclusion of the generalized Breit interaction is important.

In the next section an outline is given for obtaining the detailed expression for the Q^{λ} with inclusion of the generalized Breit interaction. In Sec. III numerical results for collision strengths with inclusion of the generalized Breit interaction are given and discussed. In Sec. IV a brief summary and conclusions are given.

II. OUTLINE OF THEORY

To obtain the factorized expression in Eq. (1) we begin by writing down the generalized Breit interaction as

$$B(1,2)=-(\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2)\frac{\exp(i\omega r_{12})}{r_{12}}+(\boldsymbol{\alpha}_1\cdot\boldsymbol{\nabla}_1)(\boldsymbol{\alpha}_1\cdot\boldsymbol{\nabla}_2)\frac{\exp(i\omega r_{12})-1}{\omega^2 r_{12}} , \quad (2)$$

where ω is the wave number of the exchanged virtual photon, $\boldsymbol{\alpha}_1$ and $\boldsymbol{\alpha}_2$ are the usual Dirac matrices, and r_{12} is the interelectron separation. From Grant and Pyper [18] we are actually interested in the matrix elements of the interaction B_{12}, which have the form

$$\langle A_1B_2|B_{12}|C_1D_2\rangle=\langle A_1B_2|\tfrac{1}{2}\{B_{\omega_{CA}}(1,2)+B_{\omega_{DB}}(1,2)\}|C_1D_2\rangle , \quad (3)$$

where $\omega_{CA}=(\varepsilon_C-\varepsilon_A)/2c$ and ε_C and ε_A are the one-electron spinor energies for $|C\rangle$ and $|A\rangle$, respectively. The operator $B_{\omega}(1,2)$ is the same as $B(1,2)$ with the ω dependence stated explicitly and c is the speed of light. Additional information concerning this last modification is given beneath Eq. (19) of [7]. In this paper we shall only give results concerning the interaction in Eq. (2). The extension to Eq. (3) is straightforward and all calculations were actually carried out using this interaction.

For simplicity we first consider the case of excitation in hydrogenic ions. From Eq. (13) of [19] we may write the factorized collision strength in the form

$$\Omega_H(U-U')=8\sum_{\lambda}Q^{\lambda}(n_al_aj_a,n_a'l_a'j_a') , \quad (4)$$

where

$$Q^{\lambda}(n_al_aj_a,n_a'l_a'j_a')=\sum_{\substack{l,l'\\j,j'}}[P^{\lambda}(n_al_aj_a\varepsilon lj;n_a'l_a'j_a'\varepsilon'l'j')]^2 . \quad (5)$$

If one follows the derivation in [19] leading to these last two equations when only the Coulomb interaction is considered, one realizes that the algebraic formalism put forth by Grant and Pyper [18] and Grant and McKenzie [20] allows one to immediately write down the form of P^{λ} with the generalized Breit interaction included. This is possible because their concept of an effective interaction strength preserves the tensor representation of the radial piece of a two-electron operator even though the angular piece may be further manipulated as it is in our case when applying the factorization method. In particular, Eq. (5) of [20] gives the effective interaction strength for the Breit interaction as it is written in Eq. (3). With some rearrangement of factors, and remembering that we are actually writing down expressions relevant for the interaction in Eq. (2), the result is

$$P^{\lambda}(n_al_aj_a\varepsilon lj;n_a'l_a'j_a'\varepsilon'l'j')=(2\lambda+1)^{-1/2}\langle j_a\|C^{\lambda}\|j_a'\rangle\langle j\|C^{\lambda}\|j'\rangle(D^{\lambda}+D_1^{\lambda}+D_2^{\lambda})+\sum_t(-1)^{\lambda+t}(2\lambda+1)^{1/2}\langle j_a\|C^t\|j'\rangle\langle j\|C^t\|j_a'\rangle\begin{Bmatrix}j_a & j' & t\\ j & j_a' & \lambda\end{Bmatrix}(E^t+E_1^t+E_2^t) , \quad (6)$$

where the arguments of the D and E radial integrals have been suppressed for brevity. These integrals, with their respective arguments, have the following form: D^λ is the ordinary direct Coulomb integral

$$D^\lambda(n_a\kappa_a\varepsilon\kappa;n'_a\kappa'_a\varepsilon'\kappa')=\int\int dr_1dr_2r_1^2r_2^2[R_{a,+1}(r_1)R_{a',+1}(r_1)+R_{a,-1}(r_1)R_{a',-1}(r_1)]$$

$$\times\frac{r_<^\lambda}{r_>^{\lambda+1}}[R_{\varepsilon,+1}(r_2)R_{\varepsilon',+1}(r_2)+R_{\varepsilon,-1}(r_2)R_{\varepsilon',-1}(r_2)] \tag{7}$$

while D_1^λ and D_2^λ are the Breit contributions given by

$$D_1^\lambda(n_a\kappa_a\varepsilon\kappa;n'_a\kappa'_a\varepsilon'\kappa')=\sum_{\nu=\lambda-1}^{\lambda+1}v_{\nu\lambda}\sum_{\beta,\beta'=\pm1}(-\beta\beta')E^\nu_{-\beta}(\kappa_a,\kappa'_a;\lambda)\Pi(\kappa_a,\kappa'_a,\nu)E^\nu_{-\beta'}(\kappa,\kappa';\lambda)\Pi(\kappa,\kappa',\nu)$$

$$\times\int\int dr_1dr_2r_1^2r_2^2V_\nu(1,2)R_{a,\beta}(r_1)R_{a',-\beta}(r_1)R_{\varepsilon,\beta'}(r_2)R_{\varepsilon',-\beta}(r_2) \tag{8}$$

and

$$D_2^\lambda(n_a\kappa_a\varepsilon\kappa;n'_a\kappa'_a\varepsilon'\kappa')=\omega_\lambda\Bigg[\sum_{\beta,\beta'=\pm1}(-\beta\beta')E^{\lambda-1}_{-\beta}(\kappa_a,\kappa'_a;\lambda)\Pi(\kappa_a,\kappa'_a,\lambda-1)E^{\lambda+1}_{-\beta'}(\kappa,\kappa';\lambda)\Pi(\kappa,\kappa',\lambda+1)$$

$$\times\int\int dr_1dr_2r_1^2r_2^2W_{\lambda-1,\lambda+1,\lambda}(1,2)R_{a,\beta}(r_1)R_{a',-\beta}(r_1)R_{\varepsilon,\beta'}(r_2)R_{\varepsilon',-\beta'}(r_2)$$

$$+[(\lambda+1)\leftrightarrow(\lambda-1)]\Bigg]. \tag{9}$$

The corresponding exchange integrals are obtained by making the usual exchange of coordinates in the direct integrals, i.e.,

$$E^t\equiv E^t(n_a\kappa_a\varepsilon\kappa;n'_a\kappa'_a\varepsilon'\kappa')=D^t(n_a\kappa_a\varepsilon\kappa;\varepsilon'\kappa'n'_a\kappa'_a)\,, \tag{10}$$

with similar expressions for E_1^t and E_2^t.

In Eqs. (7)–(9) $R_{a,\beta}(r)$ is $1/r$ times the large (small) component of the radial wave function of the bound orbital $a\equiv n_al_aj_a$ if $\beta=+1(-1)$. A similar statement holds for the continuum orbitals labeled $\varepsilon\equiv\varepsilon lj$, where ε is the electron kinetic energy. The expressions for V and W contain the radial pieces of the Breit interaction, while $v_{\nu\lambda}$, ω_λ, $E^\nu_{-\beta}(\kappa_a,\kappa'_a;\lambda)$, and $\Pi(\kappa_a,\kappa'_a,\nu)$ are simple numerical factors, all of which may be found in [18]. The prescription $(\lambda+1)\leftrightarrow(\lambda-1)$ in Eq. (9) implies that the term to the left of the plus sign should be repeated with the λ expressions exchanged.

As it is written, Eq. (6) still does not include the imaginary contributions of the interaction in Eq. (2) because the atomic structure analysis in [18] and [20] was concerned only with the real contribution. This omission is remedied by making the following substitution in Eq. (5):

$$[P^\lambda(n_al_aj_a\varepsilon lj;n'_al'_aj'_a\varepsilon'l'j')]^2$$
$$\rightarrow|P^\lambda(n_al_aj_a\varepsilon lj;n'_al'_aj'_a\varepsilon'l'j')|^2$$
$$=\{\,\mathrm{Re}[P^\lambda(n_al_aj_a\varepsilon lj;n'_al'_aj'_a\varepsilon'l'j')]\}^2$$
$$+\{\,\mathrm{Im}[P^\lambda(n_al_aj_a\varepsilon lj;n'_al'_aj'_a\varepsilon'l'j')]\}^2\,, \tag{11}$$

where Re and Im stand for the real and imaginary parts of their argument. The real part of P^λ is of course given by Eq. (6). The imaginary part is obtained by discarding D^λ and E^t in Eq. (6) and then replacing the remaining Breit integrals with their imaginary counterparts. The imaginary Breit integrals are identical to those given in Eqs. (8) and (9), except that only those terms in V and W which contain n_ν are retained, and then the substitution $n_\nu\rightarrow-ij_\nu$, where n_ν and j_ν are spherical Bessel functions, is made. For the interested reader further details are provided in the discussion in [7] concerning Eq. (17) of that paper.

The generalization to collision strengths of complex ions described by Eq. (1) is straightforward if the method in Sec. II of [8] is followed. In particular Eq. (6) gives the proper form of P^λ provided that the imaginary Breit integrals are included according to the prescription in the preceding paragraph. Then Eq. (4) of [8], modified to allow for a complex interaction,

$$Q^\lambda(n_al_a,n'_al'_aj'_a;n_{a1}l_{a1}j_{a1},n'_{a1}l'_{a1}j'_{a1})=\sum_{\substack{l,l'\\j,j'}}\{\,\mathrm{Re}[P^\lambda(n_al_aj_a\varepsilon lj;n'_al'_aj'_a\varepsilon'l'j')]\,\mathrm{Re}[P^\lambda(n_{a1}l_{a1}j_{a1}\varepsilon lj;n'_{a1}l'_{a1}j'_{a1}\varepsilon'l'j')]$$

$$+\,\mathrm{Im}[P^\lambda(n_al_aj_a\varepsilon lj;n'_al'_aj'_a\varepsilon'l'j')]\,\mathrm{Im}[P^\lambda(n_{a1}l_{a1}j_{a1}\varepsilon lj;n'_{a1}l'_{a1}j'_{a1}\varepsilon'l'j')]\}\,, \tag{12}$$

gives the form of Q^λ for complex ions, which can be used in Eq. (1) of the present paper. The expression for the B^λ coefficients remains unchanged and is given by Eqs. (6), (7), (14), and (19) of [8]. Thus they can be calculated from the level mixing coefficients and angular coefficients provided from a relativistic atomic structure program such as the well-known code of Grant and co-workers [21–23].

III. NUMERICAL RESULTS AND DISCUSSION

Here the expressions given in the preceding section have been applied to Eq. (1) and used to calculate collision strengths for various transitions in highly charged complex ions to further explore the degree and range of importance of the generalized Breit interaction on excitation collision strengths. It should be noted that the relativistic collision strength $\Omega(U-U')$ for a transition $U-U'$ is related to the cross section $Q(U-U')$ for the transition by

$$Q(U-U')=\frac{\pi a_0^2}{g_i k_i^2}\Omega(U-U') , \tag{13}$$

where g_i is the statistical weight of the initial level U, a_0 is the Bohr radius, and k_i is the relativistic wave number of the impact electron. It is related to the relativistic kinetic energy ε_i of the impact electron in rydbergs by

$$k_i^2=\varepsilon_i\left[1+\frac{\alpha^2}{4}\varepsilon_i\right] , \tag{14}$$

where α is the fine-structure constant.

The classes of transitions considered here are (i) inner-shell excitation of Be-like uranium ions and (ii) excitation from the ground level to all 36 $n=3$ levels in neonlike xenon and uranium. In the former case all possible inner-shell transitions involving the orbital transitions $1s$-$2l$ in which the Be-like ion is initially in any of the possible levels involving configurations of the kind $1s^2 2l' 2l''$ were considered. However, in the interest of brevity, numeri-

TABLE I. Labeling of levels by the dominant jj coupled state. For Ne-like ions $(2p\times4)0$ represents the ground state.

Be-like uranium		Ne-like xenon		Ne-like uranium	
Level label	jj state	Level label	jj state	Level label	jj state
$A1$	$(1s\ 2\ 2s\ 2)0$	$A1$	$(2p\times4)0$	$A1$	$(2p\times4)0$
$A2$	$(1s\ 2\ 2p^*\ 2)0$	$B1$	$(2p\ 3p)0$	$B1$	$(2p\ 3p)0$
$A3$	$(1s\ 2\ 2p\ 2)0$	$B2$	$(2p^*\ 3p^*)0$	$B2$	$(2p^*\ 3p^*)0$
$G1$	$(1s\ 1\ 2s\ 2\ 2p^*\ 1)0$	$B3$	$(2s\ 3s)0$	$B3$	$(2s\ 3s)0$
$G2$	$[(1s\ 2p^*)0(2p\ 2)0]0$	$C1$	$(2p\ 3p^*)1$	$C1$	$(2p\ 3p^*)1$
$H1$	$(1s\ 1\ 2s\ 2\ 2p^*1)1$	$C2$	$(2p\ 3p)1$	$C2$	$(2p\ 3p)1$
$H2$	$(1s\ 1\ 2s\ 2\ 2p\ 1)1$	$C3$	$(2p^*\ 3p^*)1$	$C3$	$(2p^*\ 3p^*)1$
$H3$	$(1s\ 1\ 2p^*\ 2\ 2p\ 1)1$	$C4$	$(2p^*\ 3p)1$	$C4$	$(2s\ 3s)1$
$H4$	$[(1s\ 2p^*)1(2p\ 2)2]1$	$C5$	$(2s\ 3s)1$	$C5$	$(2p^*\ 3p)1$
$H5$	$[(1s\ 2p^*)1(2p\ 2)0]1$	$C6$	$(2s\ 3d^*)1$	$C6$	$(2s\ 3d^*)1$
$H6$	$(1s\ 1\ 2p\ 3)1$	$D1$	$(2p\ 3p^*)2$	$D1$	$(2p\ 3p^*)2$
$I1$	$(1s\ 1\ 2s\ 2\ 2p\ 1)2$	$D2$	$(2p\ 3p)2$	$D2$	$(2p\ 3p)2$
$I2$	$(1s\ 1\ 2p^*\ 2\ 2p\ 1)2$	$D3$	$(2p^*\ 3p)2$	$D3$	$(2p^*\ 3p)2$
$I3$	$[(1s\ 2p^*)1(2p\ 2)2]2$	$D4$	$(2s\ 3d^*)2$	$D4$	$(2s\ 3d^*)2$
$I4$	$[(1s\ 2p^*)0(2p\ 2)2]2$	$D5$	$(2s\ 3d)2$	$D5$	$(2s\ 3d)2$
$I5$	$(1s\ 1\ 2p\ 3)2$	$E1$	$(2p\ 3p)3$	$E1$	$(2p\ 3p)3$
$K1$	$(1s\ 1\ 2s\ 1\ 2p^*2)0$	$E2$	$(2s\ 3d)3$	$E2$	$(2s\ 3d)3$
$K2$	$\{[(1s\ 2s)1\ 2p^*]3/2\ 2p\}0$	$F1$	$(2p\ 3d^*)0$	$F1$	$(2p\ 3d^*)0$
$K3$	$[(1s\ 2s)0(2p\ 2)0]0$	$F2$	$(2p^*\ 3s)0$	$F2$	$(2p^*\ 3s)0$
$L1$	$(1s\ 1\ 2s\ 1\ 2p^*\ 2)1$	$F3$	$(2s\ 3p^*)0$	$F3$	$(2s\ 3p^*)0$
$L2$	$\{[(1s\ 2s)1\ 2p^*]3/2\ 2p\}1$	$G1$	$(2p\ 3s)1$	$G1$	$(2p\ 3s)1$
$L3$	$\{[(1s\ 2s)1\ 2p^*]1/2\ 2p\}1$	$G2$	$(2p\ 3d^*)1$	$G2$	$(2p\ 3d^*)1$
$L4$	$\{[(1s\ 2s)0\ 2p^*]1/2\ 2p\}1$	$G3$	$(2p^*\ 3s)1$	$G3$	$(2p\ 3d)1$
$L5$	$[(1s\ 2s)1(2p\ 2)0]1$	$G4$	$(2p\ 3d)1$	$G4$	$(2p^*\ 3s)1$
$L6$	$[(1s\ 2s)1(2p\ 2)2]1$	$G5$	$(2p^*\ 3d^*)1$	$G5$	$(2s\ 3p^*)1$
		$G6$	$(2s\ 3p^*)1$	$G6$	$(2p^*\ 3d^*)1$
		$G7$	$(2s\ 3p)1$	$G7$	$(2s\ 3p)1$
		$H1$	$(2p\ 3s)2$	$H1$	$(2p\ 3s)2$
		$H2$	$(2p\ 3d^*)2$	$H2$	$(2p\ 3d^*)2$
		$H3$	$(2p\ 3d)2$	$H3$	$(2p\ 3d)2$
		$H4$	$(2p^*\ 3d^*)2$	$H4$	$(2p^*\ 3d^*)2$
		$H5$	$(2p^*\ 3d)2$	$H5$	$(2p^*\ 3d)2$
		$H6$	$(2s\ 3p)2$	$H6$	$(2s\ 3p)2$
		$I1$	$(2p\ 3d^*)3$	$I1$	$(2p\ 3d^*)3$
		$I2$	$(2p\ 3d)3$	$I2$	$(2p\ 3d)3$
		$I3$	$(2p^*\ 3d)3$	$I3$	$(2p^*\ 3d)3$
		$J1$	$(2p\ 3d)4$	$J1$	$(2p\ 3d)4$

cal results are given here only for those transitions in which the Be-like ion was initially in levels $A1$, $A2$, and $A3$. Results for this subset of transitions are quite typical.

A word should be said about how the levels are labeled. All states in a complex, that is, having the same set of n values, parity, and J value, are considered to form a group, which we label by a capital letter. Each of the levels in a group is indicated by a number following the group label. For example, the ground level in both Be-like and Ne-like ions is labeled $A1$. The levels involved in the transitions we considered and the jj coupled states making the dominant contribution to each level are given in Table I for both the Be-like and Ne-like ions considered. In doing this we used the notation

$$n_a l_a^* = n_a l_a j_a, \quad j_a = l_a - \tfrac{1}{2} \tag{15}$$

and

$$n_a l_a = n_a l_a j_a, \quad j_a = l_a + \tfrac{1}{2} . \tag{16}$$

Thus, for example,

$$2s = 2s_{1/2}, \quad 2p^* = 2p_{1/2}, \quad 3d = 3d_{5/2} . \tag{17}$$

In addition, when giving the states in neonlike ions we used the abbreviations

$$(2p\,3l'_a j'_a)J'_t = (1s^2_{1/2}\,2s^2_{1/2}\,2p^2_{1/2}\,2p^3_{3/2}\,3l'_a j'_a)J'_t , \tag{18}$$

$$(2s\,3l'_a j'_a)J'_t = (1s^2_{1/2}\,2s_{1/2}\,2p^2_{1/2}\,2p^4_{3/2}\,3l'_a j'_a)J'_t , \tag{19}$$

etc. because a hole in a subshell behaves like a single electron in the subshell when determining the angular momentum state of the ion, while filled subshells contribute nothing.

The near-threshold collision strengths for the subset of inner-shell excitation transitions corresponding to excitation from the levels of group A in Be-like uranium are given in Table II. The transition energies in rydbergs ΔE are also included. As in [6] and [7], the headings, C, GB, and GBI indicate results obtained using the pure Coulomb interaction, the Coulomb interaction plus the real part of the generalized Breit interaction, and the Coulomb interaction plus the full generalized Breit interaction, respectively. By comparing GB and GBI entries one sees that the contribution of the imaginary part of the generalized Breit interaction is not very important,

TABLE II. Near-threshold collision strengths for innershell ($n = 1$–2) excitation of selected transitions in Be-like uranium. The final electron energy is 1000 eV in all cases. $x[y] = x10^y$.

Transition	ΔE (Ry)	C	GB	GBI	Transition	ΔE (Ry)	C	GB	GBI
$A1$-$G1$	7051	3.371[−5]	1.229[−5]	1.254[−5]	$A2$-$I5$	7969	2.669[−12]	4.113[−12]	4.130[−12]
$A1$-$G2$	7719	1.268[−11]	4.700[−12]	4.791[−12]	$A3$-$I1$	6694	3.131[−9]	4.597[−9]	4.618[−9]
$A2$-$G1$	6997	3.841[−7]	1.399[−7]	1.427[−7]	$A3$-$I2$	6732	1.853[−9]	2.725[−9]	2.737[−9]
$A2$-$G2$	7666	2.036[−9]	7.536[−10]	7.683[−10]	$A3$-$I3$	7041	2.894[−9]	4.306[−9]	4.325[−9]
$A3$-$G1$	6388	1.736[−12]	6.229[−13]	6.357[−13]	$A3$-$I4$	7051	2.207[−11]	3.285[−11]	3.299[−11]
$A3$-$G2$	7056	3.406[−5]	1.243[−5]	1.267[−5]	$A3$-$I5$	7359	3.280[−5]	4.940[−5]	4.962[−5]
$A1$-$H1$	7043	1.170[−4]	1.911[−4]	1.942[−4]	$A1$-$K1$	7076	1.626[−6]	2.516[−6]	2.522[−6]
$A1$-$H2$	7362	1.127[−4]	1.011[−4]	1.059[−4]	$A1$-$K2$	7375	7.562[−10]	1.175[−9]	1.177[−9]
$A1$-$H3$	7400	1.572[−7]	1.414[−7]	1.481[−7]	$A1$-$K3$	7708	2.776[−8]	4.330[−8]	4.340[−8]
$A1$-$H4$	7707	1.209[−11]	1.088[−11]	1.140[−11]	$A2$-$K1$	7023	1.448[−4]	2.239[−4]	2.244[−4]
$A1$-$H5$	7711	3.850[−11]	6.394[−11]	6.459[−11]	$A2$-$K2$	7322	5.706[−8]	8.859[−8]	8.878[−8]
$A1$-$H6$	8027	7.396[−14]	6.603[−14]	6.915[−14]	$A2$-$K3$	7655	5.812[−10]	9.061[−10]	9.082[−10]
$A2$-$H1$	6990	1.337[−6]	2.182[−6]	2.217[−6]	$A3$-$K1$	6414	1.269[−11]	1.948[−11]	1.952[−11]
$A2$-$H2$	7309	1.589[−7]	1.420[−7]	1.488[−7]	$A3$-$K2$	6713	2.431[−8]	3.745[−8]	3.753[−8]
$A2$-$H3$	7347	1.128[−4]	1.011[−4]	1.059[−4]	$A3$-$K3$	7045	1.460[−4]	2.259[−4]	2.264[−4]
$A2$-$H4$	7654	1.768[−9]	1.589[−9]	1.665[−9]	$A1$-$L1$	7057	6.128[−7]	9.691[−7]	9.842[−7]
$A2$-$H5$	7658	6.175[−9]	1.023[−8]	1.033[−8]	$A1$-$L2$	7370	2.081[−10]	3.273[−10]	3.324[−10]
$A2$-$H6$	7974	3.225[−12]	3.004[−12]	3.152[−12]	$A1$-$L3$	7376	8.713[−11]	1.370[−10]	1.391[−10]
$A3$-$H1$	6380	5.871[−12]	9.525[−12]	9.656[−12]	$A1$-$L4$	7389	1.232[−10]	1.937[−10]	1.967[−10]
$A3$-$H2$	6699	5.760[−9]	5.229[−9]	5.478[−9]	$A1$-$L5$	7689	1.112[−8]	1.741[−8]	1.768[−8]
$A3$-$H3$	6738	2.918[−9]	2.553[−9]	2.632[−9]	$A1$-$L6$	7693	3.398[−13]	5.320[−13]	5.402[−13]
$A3$-$H4$	7045	8.275[−10]	7.629[−10]	7.815[−10]	$A2$-$L1$	7004	5.427[−5]	8.591[−5]	8.725[−5]
$A3$-$H5$	7048	1.183[−4]	1.933[−4]	1.964[−4]	$A2$-$L2$	7317	1.540[−8]	2.425[−8]	2.463[−8]
$A3$-$H6$	7365	5.640[−5]	5.061[−5]	5.302[−5]	$A2$-$L3$	7323	6.402[−9]	1.008[−8]	1.023[−8]
$A1$-$I1$	7356	6.553[−5]	9.869[−5]	9.911[−5]	$A2$-$L4$	7336	8.922[−9]	1.404[−8]	1.426[−8]
$A1$-$I2$	7395	9.159[−8]	1.381[−7]	1.387[−7]	$A2$-$L5$	7636	2.512[−10]	3.935[−10]	3.996[−10]
$A1$-$I3$	7703	3.487[−11]	5.320[−11]	5.342[−11]	$A2$-$L6$	7640	2.388[−13]	3.741[−13]	3.799[−13]
$A1$-$I4$	7714	2.772[−13]	4.231[−13]	4.249[−13]	$A3$-$L1$	6395	2.642[−12]	4.241[−12]	4.308[−12]
$A1$-$I5$	8022	3.560[−14]	5.496[−14]	5.519[−14]	$A3$-$L2$	6707	7.306[−9]	1.164[−8]	1.182[−8]
$A2$-$I1$	7303	9.302[−8]	1.398[−7]	1.404[−7]	$A3$-$L3$	6714	3.305[−9]	5.265[−9]	5.347[−9]
$A2$-$I2$	7342	6.566[−5]	9.882[−5]	9.925[−5]	$A3$-$L4$	6726	5.383[−9]	8.571[−9]	8.705[−9]
$A2$-$I3$	7650	5.666[−9]	8.628[−9]	8.664[−9]	$A3$-$L5$	7027	5.486[−5]	8.681[−5]	8.817[−5]
$A2$-$I4$	7661	3.789[−11]	5.771[−11]	5.796[−11]	$A3$-$L6$	7031	1.926[−9]	3.048[−9]	3.095[−9]

generally under a 5% effect. However, comparison of either the GB or GBI entries with the C entries indicates that inclusion of the generalized Breit interaction has more than a 50% effect for the vast majority of transitions, while the effect on the near-threshold collision strengths for the analogous $1s\text{-}2l_aj_a$ excitation transitions in H-like uranium ions was found in [6,7] (see Table II of [7]) to exceed 50% for only the $1s\text{-}2s$ transition. This is another extreme example of the fact noted in [7] that when the collision strength for a given orbital transition in an H-like ion is effectively divided among many transitions in a more complex ion of the same nuclear charge the effect of the generalized Breit interaction on the individual transitions is often much larger for the complex ion.

In Tables III and IV collision strengths are given for the 36 $n=2$ to $n=3$ transitions in neonlike xenon and uranium ions, respectively. In each case results are given for two final electron energies E_f, which correspond to near threshold and roughly 3 times threshold for the impact electron energy. The column headings have the same meanings as in Table II. One sees that in all cases GB and GBI entries differ by much less than 1% and hence one can omit the imaginary part of the generalized Breit interaction for the $n=2$ to $n=3$ transitions, which saves nearly a factor of 2 in computing time. In fact it appears from the results in Table II and in [6] and [7] that this can be done for all types of transitions in obtaining results accurate to about the 5% level.

In comparing the GB or GBI entries with the C entries in Tables III and IV one sees that the generalized Breit interaction can have quite a large effect for the $n=2$ to $n=3$ transitions in neonlike ions. For example, it enhances the collision strengths by 79% and 53% for the $A1\text{-}C2$ and $A1\text{-}H3$ transitions at $E_f=30\,000$ eV (about 3 times threshold) in neonlike uranium, and it has more than a 10% effect for nearly half of all transitions. For neonlike xenon the effect is much less, but it does enhance the collision strength by 18% for the $A1\text{-}C2$ transition at $E_f=9000$ eV. However, even for neonlike uranium the effect is large ($>25\%$) only for transitions in which the collision strength is down by more than a fac-

TABLE III. Collision strengths for $n=2$ to $n=3$ transitions in Ne-like xenon.

		$E_f=50$ eV			$E_f=9000$ eV		
Transition	ΔE (Ry)	C	GB	GBI	C	GB	GBI
$A1\text{-}B1$	325.6	5.477[−3]	5.579[−3]	5.579[−3]	6.459[−3]	6.531[−3]	6.531[−3]
$A1\text{-}B2$	342.8	4.123[−3]	4.196[−3]	4.196[−3]	4.836[−3]	4.892[−3]	4.892[−3]
$A1\text{-}B3$	358.1	3.414[−3]	3.483[−3]	3.483[−3]	4.263[−3]	4.315[−3]	4.315[−3]
$A1\text{-}C1$	315.9	4.940[−4]	4.652[−4]	4.652[−4]	1.273[−4]	1.227[−4]	1.227[−4]
$A1\text{-}C2$	322.4	4.972[−4]	5.186[−4]	5.186[−4]	1.250[−4]	1.474[−4]	1.474[−4]
$A1\text{-}C3$	340.4	3.762[−4]	3.809[−4]	3.809[−4]	9.244[−5]	9.801[−5]	9.801[−5]
$A1\text{-}C4$	347.0	4.800[−4]	4.458[−4]	4.458[−4]	1.255[−4]	1.181[−4]	1.181[−4]
$A1\text{-}C5$	356.7	2.151[−4]	2.219[−4]	2.219[−4]	4.953[−5]	5.259[−5]	5.259[−5]
$A1\text{-}C6$	378.2	3.806[−4]	3.744[−4]	3.744[−4]	9.029[−5]	9.083[−5]	9.083[−5]
$A1\text{-}D1$	316.1	8.012[−4]	8.111[−4]	8.111[−4]	7.580[−4]	7.700[−4]	7.700[−4]
$A1\text{-}D2$	323.0	5.907[−4]	5.736[−4]	5.736[−4]	5.996[−4]	6.018[−4]	6.018[−4]
$A1\text{-}D3$	347.2	6.271[−4]	6.369[−4]	6.370[−4]	5.231[−4]	5.344[−4]	5.344[−4]
$A1\text{-}D4$	378.5	1.054[−3]	1.087[−3]	1.087[−3]	1.174[−3]	1.211[−3]	1.211[−3]
$A1\text{-}D5$	380.6	2.858[−3]	2.875[−3]	2.875[−3]	5.604[−3]	5.648[−3]	5.648[−3]
$A1\text{-}E1$	322.4	8.947[−4]	9.244[−4]	9.244[−4]	2.048[−4]	2.208[−4]	2.208[−4]
$A1\text{-}E2$	379.7	8.687[−4]	8.884[−4]	8.884[−4]	2.014[−4]	2.142[−4]	2.142[−4]
$A1\text{-}F1$	330.2	4.457[−4]	4.138[−4]	4.138[−4]	9.398[−5]	8.555[−5]	8.555[−5]
$A1\text{-}F2$	333.6	5.911[−5]	5.786[−5]	5.786[−5]	1.859[−5]	1.794[−5]	1.794[−5]
$A1\text{-}F3$	363.5	6.394[−5]	6.095[−5]	6.095[−5]	1.696[−5]	1.576[−5]	1.576[−5]
$A1\text{-}G1$	309.5	3.182[−4]	3.227[−4]	3.227[−4]	1.199[−3]	1.198[−3]	1.198[−3]
$A1\text{-}G2$	330.7	1.087[−3]	1.074[−3]	1.074[−3]	2.755[−4]	2.802[−4]	2.802[−4]
$A1\text{-}G3$	333.6	2.972[−3]	2.869[−3]	2.869[−3]	7.433[−3]	7.263[−3]	7.263[−3]
$A1\text{-}G4$	334.8	1.461[−2]	1.428[−2]	1.428[−2]	2.926[−2]	2.870[−2]	2.870[−2]
$A1\text{-}G5$	356.7	9.969[−3]	9.679[−3]	9.679[−3]	2.072[−2]	2.021[−2]	2.021[−2]
$A1\text{-}G6$	363.7	3.238[−4]	3.208[−4]	3.208[−4]	8.630[−4]	8.455[−4]	8.455[−4]
$A1\text{-}G7$	370.3	5.454[−4]	5.278[−4]	5.278[−4]	2.099[−3]	2.051[−3]	2.051[−3]
$A1\text{-}H1$	309.1	3.203[−4]	3.290[−4]	3.290[−4]	9.096[−5]	9.566[−5]	9.566[−5]
$A1\text{-}H2$	331.2	7.829[−4]	7.570[−4]	7.570[−4]	1.341[−4]	1.314[−4]	1.314[−4]
$A1\text{-}H3$	332.5	1.092[−3]	1.119[−3]	1.119[−3]	2.055[−4]	2.297[−4]	2.297[−4]
$A1\text{-}H4$	355.4	6.855[−4]	6.911[−4]	6.911[−4]	1.274[−4]	1.342[−4]	1.342[−4]
$A1\text{-}H5$	356.9	1.069[−3]	1.058[−3]	1.058[−3]	2.143[−4]	2.189[−4]	2.189[−4]
$A1\text{-}H6$	370.0	2.781[−4]	2.811[−4]	2.811[−4]	7.752[−5]	7.985[−5]	7.985[−5]
$A1\text{-}I1$	330.9	1.020[−3]	1.072[−3]	1.072[−3]	7.205[−4]	7.430[−4]	7.430[−4]
$A1\text{-}I2$	333.0	6.991[−4]	6.926[−4]	6.926[−4]	5.013[−4]	5.051[−4]	5.051[−4]
$A1\text{-}I3$	357.1	8.046[−4]	8.103[−4]	8.103[−4]	5.534[−4]	5.640[−4]	5.640[−4]
$A1\text{-}J1$	332.2	1.445[−3]	1.487[−3]	1.487[−3]	2.618[−4]	2.806[−4]	2.806[−4]

TABLE IV. Collision strengths for $n=2$ to $n=3$ transitions in Ne-like uranium.

Transition	ΔE (Ry)	$E_f=150$ eV C	$E_f=150$ eV GB	$E_f=150$ eV GBI	$E_f=30\,000$ eV C	$E_f=30\,000$ eV GB	$E_f=30\,000$ eV GBI
$A1$-$B1$	1047.8	2.568[−3]	2.705[−3]	2.705[−3]	2.196[−3]	3.295[−3]	3.295[−3]
$A1$-$B2$	1252.1	1.087[−3]	1.151[−3]	1.151[−3]	1.324[−3]	1.377[−3]	1.377[−3]
$A1$-$B3$	1286.5	1.184[−3]	1.264[−3]	1.264[−3]	1.539[−3]	1.603[−3]	1.603[−3]
$A1$-$C1$	960.5	1.435[−4]	1.205[−4]	1.206[−4]	3.815[−5]	3.439[−5]	3.439[−5]
$A1$-$C2$	1040.7	1.708[−4]	2.013[−4]	2.014[−4]	4.359[−5]	7.814[−5]	7.814[−5]
$A1$-$C3$	1246.7	1.301[−4]	1.413[−4]	1.413[−4]	3.842[−5]	4.719[−5]	4.720[−5]
$A1$-$C4$	1282.6	1.033[−4]	1.121[−4]	1.122[−4]	2.890[−5]	3.672[−5]	3.673[−5]
$A1$-$C5$	1328.1	1.377[−4]	1.099[−4]	1.100[−4]	4.153[−5]	3.526[−5]	3.527[−5]
$A1$-$C6$	1395.3	1.025[−4]	9.760[−5]	9.761[−5]	2.687[−5]	2.803[−5]	2.803[−5]
$A1$-$D1$	960.5	3.500[−4]	3.690[−4]	3.690[−4]	3.902[−4]	4.131[−4]	4.131[−4]
$A1$-$D2$	1041.9	1.986[−4]	1.841[−4]	1.842[−4]	2.109[−4]	2.152[−4]	2.152[−4]
$A1$-$D3$	1328.0	1.566[−4]	1.682[−4]	1.682[−4]	1.030[−4]	1.140[−4]	1.140[−4]
$A1$-$D4$	1395.6	3.975[−4]	4.406[−4]	4.406[−4]	6.450[−4]	6.985[−4]	6.985[−4]
$A1$-$D5$	1413.9	5.757[−4]	5.797[−4]	5.797[−4]	1.129[−3]	1.150[−3]	1.150[−3]
$A1$-$E1$	1040.6	2.831[−4]	3.175[−4]	3.175[−4]	6.575[−5]	8.430[−5]	8.431[−5]
$A1$-$E2$	1412.5	2.201[−4]	2.406[−4]	2.407[−4]	5.372[−5]	6.821[−5]	6.821[−5]
$A1$-$F1$	1056.2	1.540[−4]	1.214[−4]	1.214[−4]	3.398[−5]	2.542[−5]	2.542[−5]
$A1$-$F2$	1231.6	2.169[−5]	2.152[−5]	2.154[−5]	6.991[−6]	6.355[−6]	6.358[−6]
$A1$-$F3$	1298.7	2.714[−5]	2.411[−5]	2.413[−5]	7.605[−6]	6.067[−6]	6.070[−6]
$A1$-$G1$	945.5	2.481[−4]	2.418[−4]	2.422[−4]	8.034[−4]	7.814[−4]	7.819[−4]
$A1$-$G2$	1057.1	6.699[−4]	6.401[−4]	6.404[−4]	8.399[−4]	8.078[−4]	8.083[−4]
$A1$-$G3$	1078.3	6.175[−3]	5.777[−3]	5.782[−3]	1.326[−2]	1.261[−2]	1.261[−2]
$A1$-$G4$	1231.9	6.625[−5]	8.194[−5]	8.207[−5]	8.365[−5]	9.395[−5]	9.404[−5]
$A1$-$G5$	1298.6	3.007[−4]	2.890[−4]	2.896[−4]	7.558[−4]	7.199[−4]	7.208[−4]
$A1$-$G6$	1346.1	1.818[−3]	1.682[−3]	1.684[−3]	3.796[−3]	3.573[−3]	3.576[−3]
$A1$-$G7$	1379.8	7.075[−5]	7.986[−5]	8.029[−5]	2.893[−4]	2.907[−4]	2.914[−4]
$A1$-$H1$	944.6	1.318[−4]	1.457[−4]	1.458[−4]	3.579[−5]	4.285[−5]	4.286[−5]
$A1$-$H2$	1057.9	2.350[−4]	2.097[−4]	2.097[−4]	3.921[−5]	3.605[−5]	3.605[−5]
$A1$-$H3$	1074.7	3.540[−4]	3.893[−4]	3.893[−4]	6.722[−5]	1.027[−4]	1.027[−4]
$A1$-$H4$	1344.1	1.708[−4]	1.768[−4]	1.768[−4]	3.707[−5]	4.464[−5]	4.464[−5]
$A1$-$H5$	1361.8	2.428[−4]	2.380[−4]	2.380[−4]	5.447[−5]	5.996[−5]	5.996[−5]
$A1$-$H6$	1379.2	8.746[−5]	9.309[−5]	9.316[−5]	2.730[−5]	3.154[−5]	3.155[−5]
$A1$-$I1$	1056.9	3.493[−4]	4.101[−4]	4.101[−4]	2.709[−4]	3.014[−4]	3.014[−4]
$A1$-$I2$	1075.7	2.211[−4]	2.171[−4]	2.171[−4]	1.778[−4]	1.830[−4]	1.830[−4]
$A1$-$I3$	1362.0	1.828[−4]	1.890[−4]	1.890[−4]	1.359[−4]	1.457[−4]	1.457[−4]
$A1$-$J1$	1073.9	4.499[−4]	4.972[−4]	4.972[−4]	8.006[−5]	1.018[−4]	1.018[−4]

tor of 100 from that of the strongest transition. Thus, for purposes such as plasma modeling, it appears that including the generalized Breit interaction in determining the scattering matrix elements for $n=2$ to $n=3$ excitation is probably not of great importance, but preferably should be done for very high Z. On the other hand, the work here and in [6] and [7] indicates that the interaction must be included for excitation from the $1s$ subshell for all but low Z.

In carrying out the present calculations we used atomic structure data generated by the Grant computer code [21–23] and an upgraded version of the relativistic distorted-wave program of [24] modified to include the generalized Breit interaction as described in Sec. II. Thus, except for the latter modification, the procedures used were the same as those described in detail in [8]. As a check that no coding errors were made in including the Breit interaction we did test calculations for several cases using the alternative angular formulation used in [6] and [7] and obtained agreement with the present results.

IV. SUMMARY AND CONCLUSIONS

An outline for obtaining the convenient factorized form [9] for the collision strength has been given for the case that includes the generalized Breit interaction in determining the scattering matrix elements for excitation. This result was then used to further explore the degree of importance of including the generalized Breit interaction in calculating excitation cross sections, or collision strengths, for complex ions. Near-threshold collision strengths for inner-shell excitation of Be-like uranium were calculated and it was found that for the vast majority of these transition the generalized Breit interaction has more than a 50% effect. Also for transitions involving $1s$-$2p_{1/2}$ and $1s$-$2p_{3/2}$ the effect is considerably greater than for the analogous transitions in hydrogenlike ions of the same nuclear charge.

In addition, the 36 possible $n=2$ to $n=3$ transitions in neonlike xenon and uranium were considered for near threshold and about three times threshold for the impact

electron energy. These results further confirm the fact found here for Be-like ions and found earlier [7] for He-like and Li-like ions that the effect of including the generalized Breit interaction on collision strengths is usually considerably more important for complex ions than for the corresponding transitions in H-like ions with the same nuclear charge.

Although effects up to 18% and 79% were found for the $n=2$ to $n=3$ transitions in neonlike xenon and uranium, respectively, the very large effects occur only for weak transitions, in contrast to the case of excitation from the $1s$ subshell. Hence, although the generalized Breit interaction should probably be included in calculating collision strengths for $n=2$ to $n=3$ transitions in complex ions with very high Z, it appears that at least for applications to plasma modeling, its effect is probably of great importance only in treating excitation from the $1s$ subshell.

In future work we expect to use the factorized form for the collision strength with inclusion of the generalized Breit interaction in large scale calculations for excitation from the $1s$ subshell in all He-like, Li-like, and Be-like ions with Z in the range $25 \lesssim Z \leq 92$.

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