Inclusion of the generalized Breit interaction in excitation of highly charged ions by electron impact

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The generalized Breit interaction is included in the scattering matrix elements when determining collision strengths for electron-impact excitation of highly charged ions. We use a relativistic distorted-wave approach that employs a Dirac-Fock-Slater potential to calculate the free-electron wave functions. This same potential is used to calculate the atomic-structure data. Collision strengths are presented for H-like, He-like, and Li-like ions for a range of Z values and impact-electron energies. Good agreement is obtained when comparing to the few existing calculations for hydrogenic ions. The effect of including the interaction is found to be small for ions with $Z \approx 26$, but increases steadily with Z. Changes of nearly 70% are observed for $Z = 92$. Effects for the more complex He-like and Li-like ions are greater than for the hydrogenic analogs for the entire range of Z values considered. The accuracy of some simpler forms of the Breit interaction is also discussed.

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I. INTRODUCTION

Over the past 20 years the Breit interaction, and its relatives, have been applied to atomic structure [1] and processes such as autoionization [2–4] and ionization [5]. As of yet, only a few test cases that include the Breit interaction in calculations for excitation of ions by electron impact have been published [6–8]. These results show significant changes in the collision strengths for ions with high nuclear charge number Z, but are limited to hydrogenic ions with a single bound electron. The purpose of this work is to include the Breit interaction, in various forms, in the scattering matrix elements for electron-impact excitation of various types of highly charged ions and to determine the range of conditions for which the interaction makes a significant contribution. We restrict ourselves to highly charged ions which satisfy $Z > 2N$, where N is the number of bound electrons. This restriction is a direct consequence of the approach put forth by Sampson *et al.* [9] and Zhang, Sampson, and Mohanty [10], and of which the current work is an extension.

The main motivation of this research is to supply the vast amount of atomic data necessary for the modeling and diagnostics of very-high-temperature plasmas. More specifically, in such plasmas with sufficiently low density that the assumption of local thermodynamic equilibrium is not valid a detailed accounting of the atomic processes responsible for populating and depopulating energy levels of the highly charged ions is required. The rates of these processes can then be used to model the plasma to predict and understand its emerging spectra. Examples of such plasmas are those occurring in fusion energy and x-ray laser research [11].

A more fundamental application of this research is the comparison with results for highly charged ions in the recent electron beam ion trap (EBIT) experiments by Marrs *et al.* [12]. Just recently [13], measurements were carried out on He-like ions with atomic numbers as high as 26 and future measurements are planned for Z much beyond this value [14]. For sufficiently high Z, any collision strengths inferred from these latter measurements could exhibit large effects due to the Breit interaction and could be directly compared to the results presented in this paper.

In Sec. II we give an outline of the distorted-wave theory incorporating the Breit interaction in the scattering matrix elements. We also include a brief explanation of the various forms of the Breit interaction used presently and elsewhere in the literature. Section III gives numerical results for H-like, He-like, and Li-like ions. Comparisons are made with other hydrogenic results where appropriate. The final section summarizes the trends observed over the range of Z values and transitions considered. Conclusions are then drawn about the range of conditions for which the Breit interaction makes a significant contribution to the collision strengths.

II. OUTLINE OF THEORY

Since this work is an extension of the distorted-wave approach of Zhang, Sampson, and Mohanty [10], the following outline will closely follow that which is found in Ref. [10] and in the atomic-structure paper of Sampson *et al.* [9]. But before discussing the process of excitation, a brief explanation of the various forms of the Breit interaction is necessary.

A. Breit interaction

Around 1930 Breit published a series of papers [15–17] in an attempt to further explain the fine structure splitting in helium. He suggested the following correction to the Coulomb interaction between two electrons:

$$H_{\mathrm{Br}}=-\frac{1}{r_{12}}[\vec{\alpha}_1\cdot\vec{\alpha}_2+(\vec{\alpha}_1\cdot\vec{n})(\vec{\alpha}_2\cdot\vec{n})] , \tag{1}$$

where r_{12} is the interelectron separation, $\vec{n}$ is a unit vector along $\vec{r}_{12}$, and $\vec{\alpha}_1$ and $\vec{\alpha}_2$ are the usual Dirac matrices. In Eq. (1) and the remainder of this paper distances are in units of Bohr radii and energies are in rydbergs. We shall refer to the above interaction simply as the Breit interaction. It includes both magnetic and retarded corrections to the Coulomb interaction.

We note that the Breit interaction was derived with the intent to explain *bound*-state energy discrepancies. On the other hand, we are primarily interested in scattering phenomena that require the interaction between bound and free electrons. In 1932, Møller [18] derived a relativistic interaction for electron-electron scattering given by

$$M(1,2)=\frac{2}{r_{12}}(1-\vec{\alpha}_1\cdot\vec{\alpha}_2)\exp(i\omega r_{12}) , \tag{2}$$

where ω is the wave number of the photon exchanged between the two electrons. More precisely, Møller scattering was derived for the relativistic interaction between two free electrons, but its form remains the same for bound-free interactions. Note that this interaction already *includes* the Coulomb part of the interaction, while the Breit interaction must be *added* to the usual Coulomb interaction.

The relationship between the Breit and Møller interactions is clarified in the context of QED. We consider the lowest-order Feynman diagram for the exchange of a single virtual photon between two electrons. Using the Coulomb gauge for the photon propagator, the interaction is found to be

$$B(1,2)=-2(\vec{\alpha}_1\cdot\vec{\alpha}_2)\frac{\exp(i\omega r_{12})}{r_{12}} +2(\vec{\alpha}_1\cdot\vec{\nabla}_1)(\vec{\alpha}_2\cdot\vec{\nabla}_2)\frac{\exp(i\omega r_{12})-1}{\omega^2 r_{12}} , \tag{3}$$

where ω is the wave number of the exchanged virtual photon. Following Mann and Johnson [19] we call Eq. (3) the generalized Breit interaction. Once again $B(1,2)$ is *added* to the usual Coulomb interaction as with H_{Br}. One can show that the Breit interaction H_{Br} is the limit of $B(1,2)$ as $\omega\rightarrow 0$ [20]. As the nuclear charge number Z increases we expect ω to also increase and the use of $B(1,2)$ instead of H_{Br} becomes necessary.

If the Lorentz gauge, instead of the Coulomb gauge, is used for the photon propagator, one obtains the Møller interaction given in Eq. (2). Since both the Møller and generalized Breit interactions contain the entire lowest-order Feynman diagram, with retardation included to all orders, they are the most accurate of the interactions and their matrix elements should be identical from gauge invariance. An argument due to Hata and Grant [21] shows that their matrix elements are indeed equal provided that the wave functions used are determined from a local potential such as the Dirac-Fock-Slater potential used in our research. For nonlocal potentials the picture is not so clear and the validity of gauge invariance is questionable. This topic is hotly contested in the literature and a detailed discussion is beyond the scope of this paper. The reader is referred to the literature for an in-depth discussion (e.g., Ref. [22], and the references cited therein). The generalized Breit interaction, Eq. (3), and occasionally its $\omega=0$ limit, the Breit interaction, were chosen for all calculations in this research.

B. Relativistic collision strength theory

The relativistic cross section $Q(i-f)$ for the transition $i\rightarrow f$ is related to the collision strength $\Omega(i-f)$ by

$$Q(i-f)=\frac{\pi a_0^2}{k^2 g_i}\Omega(i-f) , \tag{4}$$

where a_0 is the Bohr radius, g_i is the statistical weight of the initial level of the N-electron target ion, and k is the relativistic wave number. The magnitude of k is related to the relativistic kinetic energy of the free electron by

$$k^2=\varepsilon\left[1+\frac{\alpha^2}{4}\varepsilon\right] , \tag{5}$$

with ε given in rydbergs.

The distorted-wave collision strength is then given by

$$\Omega(i-f)=2\sum_J(2J+1)\times\sum_{\kappa,\kappa'}\left|\left\langle\Psi_i\left|\sum_{\substack{p,q\\p<q}}^{N+1}\left[\frac{2}{r_{pq}}+B(p,q)\right]\right|\Psi_f\right\rangle\right|^2 , \tag{6}$$

which agrees with Eq. (3) of Ref. [10] except that the generalized Breit interaction has been included in the scattering matrix elements. The summations over κ,κ' are the usual partial wave summations over initial and final continuum electron angular momentum quantum numbers, respectively, and the sum over J represents all the possible angular momentum couplings of the free electron with the N-electron target ion states. The initial $(N+1)$-electron system state wave function is

$$\Psi_i=\frac{1}{(N+1)^{1/2}}\sum_{p=1}^{N+1}(-1)^{N+1-p}\times\sum_{M_t,m}C(J_t j M_t m;JM)\Phi_{\alpha J_t}(\mathbf{x}_p^{-1})\times u_{\varepsilon l j m}(\mathbf{x}_p) , \tag{7}$$

where $\mathbf{x}_p^{-1}$ stands for all $(N+1)$-electron coordinates except for those of electron p. The expression for Ψ_f is analogous to the above equation with $\alpha' J_t'$; M_t', ε', l', j', and m' replacing the corresponding unprimed quantities.

The $\Phi_{\alpha J_t}$ are wave functions representing the N-electron target ion states with total angular momentum J_t and α representing any additional quantum numbers necessary to distinguish the state. These wave functions are built up from jj-coupled, one-electron Dirac spinors, which have the form

$$u_{n\kappa m}=\frac{1}{r}\begin{bmatrix} P_{n\kappa}(r) & \chi_{\kappa m}(\theta,\phi,\sigma) \\ iQ_{n\kappa}(r) & \chi_{-\kappa m}(\theta,\phi,\sigma)\end{bmatrix}, \tag{8}$$

where $P_{n\kappa}$ and $Q_{n\kappa}$ are the large and small components of the radial function, respectively, the $\chi_{\kappa m}$ are the usual spin-orbital angular momentum functions

$$\chi_{\kappa m}=\sum_{m_l,m_S} C(l\tfrac{1}{2}m_l m_S;jm)Y_{lm_l}(\theta,\phi)\delta(m_S|\sigma), \tag{9}$$

and the relativistic quantum number κ takes on the values

$$\kappa=l,\quad j=l-\tfrac{1}{2};\quad \kappa=-(l+1),\quad j=l+\tfrac{1}{2}. \tag{10}$$

The large and small components satisfy the usual coupled differential equations and the reader is referred to Ref. [9] for further details. In addition, several options were added to the structure code of Sampson *et al.* [9]. These were a finite nucleus obtained from a Fermi nuclear charge density, inclusion of the generalized Breit interaction as a perturbation when diagonalizing the Hamiltonian, approximations for the lowest-order vacuum polarization and self-energy QED corrections to the level energies, and inclusion of retardation when calculating electric dipole oscillator strengths.

The $u_{\varepsilon ljm}$ in Eq. (7) are angular momentum representation wave functions for a free electron and are positive energy solutions to the Dirac equation. These continuum wave functions have the same form as the bound spinors of Eq. (8) except that the discrete quantum number n is replaced by the continuous parameter ε. Our choice for the distorted-wave potential used in determining these continuum wave functions is the same Dirac-Fock-Slater potential used in solving for the one-electron spinors of Eq. (8). Thus the continuum wave functions are automatically orthogonal to the bound ones since both are solutions to the Dirac equation with the same central potential.

What remains is to reduce the matrix elements of Eq. (6) to products of angular coefficients and radial integrals. An outline of this reduction for the Coulomb part of the interaction is given in Ref. [10]. Basically, the angular coefficients may be calculated by the angular package in the relativistic atomic structure code of Grant *et al.* [23] and the radial integrals are the Slater integrals appearing in Eqs. (9) and (10) of Ref. [10].

For purposes of comparison there are instances when the above equations must be modified to allow for bound and free orbitals that are not orthogonal. Such is the case when the free and bound radial functions are solutions of the Dirac equation with different central potentials. In particular, Walker [6] uses a central potential equal to the Coulomb potential for the case of hydrogenic ions. When solving for the bound orbitals, the total nuclear charge Z is used. But, when solving for the continuum orbitals, a screened nuclear charge given by $z=Z-1$ is used. This difference results in continuum orbitals that are not orthogonal to the bound ones. Then an extra term must be inserted in the radial integrals. The necessary substitution is

$$\frac{r_<^\lambda}{r_>^{\lambda+1}}\rightarrow\left[\frac{r_<^\lambda}{r_>^{\lambda+1}}-\frac{\delta_{\lambda 0}}{r_1}\right] \tag{11}$$

in the exchange integral of Eq. (10) of Ref. [10]. The choice of r_1 above corresponds to the "prior" approximation, while using r_2 corresponds to the "post" approximation [24]. Like Walker [6], we use the prior approximation when comparing with his data.

The reduction of the generalized Breit interaction can be handled in a similar fashion. The angular coefficients are calculated by using the package of McKenzie, Grant, and Norrington [1]. There are two types of radial integrals that occur in the reduction of the generalized Breit interaction. They are

$$R^\nu(ac,bd)=\int_0^\infty\int_0^\infty \rho_{ac}(r_1)[V_\nu(r_1,r_2;\omega_{ac})+V_\nu(r_1,r_2;\omega_{bd})]\times\rho_{bd}(r_2)dr_1dr_2 \tag{12}$$

and

$$S^k(ac,bd)=\int_0^\infty\int_0^\infty \rho_{ac}(r_1[W_{k-1,k+1,k}(r_1,r_2;\omega_{ac})+W_{k-1,k+1,k}(r_1,r_2;\omega_{bd})]\times\rho_{bd}(r_2)dr_1dr_2, \tag{13}$$

where

$$V_\nu(r_1,r_2;\omega)=[\nu]\omega j_\nu(\omega r_<)n_\nu(\omega r_>) \tag{14}$$

and

$$W_{k-1,k+1,k}(r_1,r_2;\omega) \tag{15}$$

$$=\begin{cases}[k]\omega j_{k-1}(\omega r_1)n_{k+1}(\omega r_2)+\dfrac{[k]^2}{\omega^2}\dfrac{r_1^{k-1}}{r_2^{k+2}}, & r_1<r_2\\ [k]\omega n_{k-1}(\omega r_1)j_{k+1}(\omega r_2), & r_1>r_2.\end{cases}$$

The density $\rho_{ac}(r)$ is given by

$$\rho_{ac}(r)=P_a(r)Q_c(r), \tag{16}$$

with a similar expression for $\rho_{bd}(r)$. For the process of excitation, orbitals a and c represent bound electrons while orbitals b and d represent free electrons. As with the Slater integrals for the Coulomb interaction, there are exchange integrals analogous to the direct integrals above which are obtained by making the exchange $c\leftrightarrow d$ everywhere in Eqs. (12) and (13). In the above equation we also have $[x]\equiv(2x+1)$ and the spherical Bessel functions j_ν and n_ν. The notation used above is that of Grant and Pyper [25] and Grant and McKenzie [26].

Note, however, that these integrals have no imaginary

part, and yet the generalized Breit interaction of Eq. (3) is complex. In fact there is an additional set of integrals which must be calculated that is very similar to R^v and S^k above. One must simply make the replacement $n_v \rightarrow -ij_v$ everywhere in the above equations. The explanation for this replacement becomes obvious when viewing the expansion [27] of

$$\frac{\exp(i\omega r_{12})}{r_{12}} = i\omega \sum_{v=0}^{\infty} (2v+1) j_v(\omega r_<) \times [j_v(\omega r_>) + i n_v(\omega r_>)] \times [\mathbf{C}^v(1)\cdot\mathbf{C}^v(2)] \quad (17)$$

from Eq. (3), where

$$\mathbf{C}^v_q(i) = \left[\frac{\pi}{2v+1}\right]^{1/2} Y_{vq}(i) \quad (18)$$

is a renormalized spherical harmonic. In structure calculations this imaginary part is usually ignored when calculating energies and is attributed to the lifetime of a bound state [20], but we see from Eq. (6) that the scattering matrix elements require the imaginary part of the electron-electron interaction as well as the real part. These imaginary integrals are expected to make a negligible contribution when the energy of the exchanged photon is small (low Z). We will determine from our results presented in the next section whether the contribution is significant for sufficiently high Z values.

There is still one more alteration that must be made to arrive at the actual interaction used in this paper. Instead of using the interaction $B(1,2)$ we replace it by a sum of two similar terms that differ only in their values of ω. The expression for the actual matrix elements, which we will call matrix elements of B_{12}, is

$$\langle A_1 B_2 | B_{12} | C_1 D_2 \rangle = \langle A_1 B_2 | \tfrac{1}{2}\{B_{\omega_{CA}}(1,2) + B_{\omega_{DB}}(1,2)\} | C_1 D_2 \rangle , \quad (19)$$

where $\omega_{CA} = (\varepsilon_C - \varepsilon_A)/2c$ and ε_C, ε_A are the one-electron spinor energies for $|C\rangle$, $|A\rangle$, respectively. The operator $B_\omega(1,2)$ is the same as $B(1,2)$ with the ω dependence stated explicitly.

The advantage in using B_{12} is that it is valid for off-diagonal matrix elements as well as diagonal ones. On the other hand, $B(1,2)$ is valid only for diagonal ones and is equivalent to B_{12} when $\omega_{CA} = \omega_{BD}$. Mittleman [28–30] derived this operator by using a succession of contact transformations to decouple the electron and radiation fields and it is claimed to be correct to order $O(\alpha^2)$ [25]. Use of B_{12} will also take into account part of the fourth-order effects (two-photon exchange) [21]. In this paper, however, only single-photon exchange is included in its entirety.

Finally, in addition to Eq. (3), we are also interested in the interaction originally formulated by Breit, Eq. (1). The radial integrals for the Breit interaction can be found by taking the $\omega = 0$ limit of Eqs. (14) and (15). The results are

$$V_v(r_1, r_2; \omega) \rightarrow r_<^v / r_>^{v+1} \quad (20)$$

and

$$W_{v-1,v+1,v}(r_1, r_2; \omega) \rightarrow -\tfrac{1}{2}[v][\bar{U}_{v-1}(r_1, r_2) - \bar{U}_{v+1}(r_1, r_2)] , \quad (21)$$

where

$$\bar{U}_v(r_1, r_2) = \begin{cases} r_1^v / r_2^{v+1} & \text{if } r_1 < r_2 \\ 0 & \text{if } r_1 > r_2 . \end{cases} \quad (22)$$

The application of Eq. (19) is not necessary in this case because the interaction is independent of ω. As stated earlier we expect this interaction to break down for sufficiently high Z ions as will be evident from the data displayed in the next section.

III. NUMERICAL RESULTS AND DISCUSSION

A. Test cases

The first collision strengths we calculated that included the generalized Breit interaction were for comparison with the test cases evaluated by Walker [6] in the middle 1970s. He calculated collision strengths for transitions from the $1s_{1/2}$ ground state to the $2s_{1/2}$, $2p_{1/2}$, and $2p_{3/2}$ states in H-like ions with atomic numbers $Z = 25$, 50, and 100. We compare results for the latter two Z values, where he found the effect of the Breit interaction to be significant. As mentioned in Sec. II, for the test cases considered by Walker, we use the modification in Eq. (11) in the exchange Coulomb integrals in conjunction with a screened nuclear potential to obtain the continuum wave functions. All other data presented in this section were found using the same potential for determining both bound and free electrons. This was the unscreened nuclear potential for hydrogenic ions and the Dirac-Fock-Slater potential for He-like and Li-like ions. For the hydrogenic ions considered here, the difference in results from the screened and unscreened procedures was almost undetectable.

Also we note that Walker's data were calculated using the Møller interaction given in Eq. (2). Since the required wave functions were calculated from a local potential, we can expect, by gauge invariance arguments [21], that the collision strengths obtained with the Møller interaction will be equal to those obtained with the generalized Breit interaction. Therefore Walker's results can be used as a valid test for our excitation collision code before moving on to more complex cases such as He-like and Li-like ions.

In Table I we present our results (rows labeled O) for the scaled cross sections Z^4Q in units of πa_0^2, along with Walker's results (rows labeled W), for hydrogenic ions with $Z = 50$ and 100. The transitions listed are for those between the $n = 1$ and 2 levels. The impact-electron energies are $E = 0.8E_I$, E_I, and $4E_I$, where E_I is the ionization energy of the $1s_{1/2}$ level (approximately 35 keV for $Z = 50$ and 162 keV for $Z = 100$), calculated with the Dirac-Fock-Slater structure code using the pure Coulomb potential due to the unscreened nuclear charge

Z. Unfortunately, our Dirac-Fock-Slater structure code was not able to provide a converged wave function for the $2p_{1/2}$ level for such a high Z value as 100. Therefore the values of the $1s_{1/2}$-$2p_{1/2}$ cross sections are listed as zeros in the table.

We did, however, use bound wave functions generated from the more elaborate code of Grant and co-workers [1,23] to calculate the same $n=1$-2 cross sections with the same physical approximations made as in the present case. For $Z=100$, Grant's code did obtain a converged wave function for the $2p_{1/2}$ level along with the other $n=1$ and 2 levels. Therefore cross sections calculated with Grant's bound wave functions (rows labeled G) are also given in Table I for the usual impact-electron energies.

The method for labeling transitions in this table and all subsequent ones is

$$nl^*=nlj,\quad j=l-\tfrac{1}{2}\ , \tag{23}$$

$$nl=nlj,\quad j=l+\tfrac{1}{2}\ . \tag{24}$$

For example,

$$2s=2s_{1/2},\quad 2p^*=2p_{1/2},\quad 2p=2p_{3/2}\ ,$$

$$3d^*=3d_{3/2},\quad 3d=3d_{5/2},\ \text{etc.} \tag{25}$$

There are actually four cross sections listed for each transition in Table I and all subsequent tables. The column labeled C lists results that use only the Coulomb interaction when calculating the scattering matrix elements for the cross sections. The results in column B were calculated with inclusion of the matrix elements of the Breit interaction, Eq. (1). The columns labeled GB and GBI list cross sections that were calculated with the generalized Breit interaction. The GB calculations, however, use only the real part of the expansion given in Eq. (17) for the generalized Breit interaction. Even though Walker did not include analogous GB and B calculations for all three energies, we list our results for comparative purposes to be discussed in the next subsection.

For each of the three impact energies we see that our data agree with Walker's to within 0.5% for all transitions and both Z values. This agreement gives us confidence that our method is in fact correct and that there are no errors in our computer code. We reserve our

TABLE I. Comparison of scaled cross sections (Z^4Q) in units of πa_0^2 for hydrogenic ions with $Z=50$ and 100 at impact electron energies of $0.8E_I$, E_I, and $4E_I$.

		$Z=50$						$Z=100$			
Transition		C	B	GB	GBI	Transition		C	B	GB	GBI
		$E=0.8E_I$						$E=0.8E_I$			
1s-2s	O	0.5331	0.6123	0.6140	0.6145	1s-2s	O	0.9914	1.5863	1.6129	1.6322
	W	0.534			0.616		W	0.996			1.641
							G	0.9932	1.5879	1.6146	1.6339
1s-2p*	O	0.6262	0.6153	0.6219	0.6224	1s-2p*	O	0.0000	0.0000	0.0000	0.0000
	W	0.626			0.624		W	0.649			1.035
							G	0.6491	0.9019	0.9994	1.0244
1s-2p	O	1.1214	1.0989	1.1063	1.1072	1s-2p	O	0.6550	0.7161	0.8008	0.8343
	W	1.122			1.109		W	0.658			0.842
							G	0.6585	0.7199	0.8044	0.8379
		$E=E_I$						$E=E_I$			
1s-2s	O	0.4438	0.5064	0.5082	0.5085	1s-2s	O	0.8269	1.2514	1.2816	1.2928
	W	0.4445	0.5072		0.5095		W	0.8304	1.2566		1.2994
							G	0.8283	1.2526	1.2829	1.2941
1s-2p*	O	0.5536	0.5428	0.5466	0.5470	1s-2p*	O	0.0000	0.0000	0.0000	0.0000
	W	0.5536	0.5414		0.5474		W	0.5228	0.7154		0.8296
							G	0.5227	0.7173	0.8040	0.8241
1s-2p	O	1.0127	0.9829	0.9934	0.9941	1s-2p	O	0.5940	0.6241	0.7068	0.7346
	W	1.0133	0.9855		0.9958		W	0.5974	0.6292		0.7402
							G	0.5973	0.6283	0.7102	0.7382
		$E=4E_I$						$E=4E_I$			
1s-2s	O	0.1577	0.1689	0.1701	0.1701	1s-2s	O	0.3479	0.4026	0.4167	0.4169
	W	0.158			0.170		W	0.349			0.418
							G	0.3485	0.4032	0.4173	0.4176
1s-2p*	O	0.3741	0.3658	0.3757	0.3759	1s-2p*	O	0.0000	0.0000	0.0000	0.0000
	W	0.372			0.374		W	0.346			0.576
							G	0.3481	0.4247	0.5660	0.5745
1s-2p	O	0.7253	0.7028	0.7154	0.7157	1s-2p	O	0.5647	0.5595	0.6989	0.7113
	W	0.720			0.710		W	0.565			0.714
							G	0.5672	0.5631	0.7017	0.7141

analysis of the data itself until the next section where we introduce new data and systematically explore the range of conditions for which the generalized Breit interaction can make a significant contribution to the excitation collision strengths.

B. H-like ions

We now discuss our excitation collision strengths, beginning with hydrogenic ions, for a range of Z values, transitions, and impact-electron energies. In this paper we focused on three Z values encompassing a range that will demonstrate the extent to which the generalized Breit interaction is important in calculating excitation collision strengths. We chose ions with $Z=26$ (iron), 54 (xenon), and 92 (uranium).

For hydrogenic ions we considered transitions from the $n=1$ ground state to the $n=2$ and 3 levels, from the $n=2$ to the $n=3$ levels, and among the $n=2$ levels. We also varied the impact-electron energy from near threshold to about six threshold units for some of the $Z=92$ calculations. Unless otherwise stated, the near-threshold energies were chosen so that the energy of the scattered electron is about 1% of the corresponding transition energy, except for the $n=2$-2 transitions for which the lowest scattered electron energies are equal to those for the $n=1$-2 transitions.

We begin by listing in Table II our near-threshold, hydrogenic collision strengths for the $n=1$-2 and 2-2 transitions with $Z=26$, 54, and 92. As expected, the $Z=26$ collision strengths are relatively insensitive to inclusion of any form of the Breit interaction. Except for a small 3.5% increase in the collision strength of the $1s_{1/2}$-$2s_{1/2}$ transition, the results show practically no effect when any form of the Breit interaction is used in the calculations.

On the other hand, the $Z=54$ data show an appreciable increase of 18% in the $1s_{1/2}$-$2s_{1/2}$ collision strength. We see similar increases in the $Z=50$ data from Table I. Because this transition involves two s electrons we expect that it would exhibit the largest effect of all the $n=1$-2 and 2-2 transitions. In fact, the other five transitions show effects hardly rising above 1% even for this fairly large Z value.

Another observation is that, for these Z values of 50 and 54, there is practically no difference ($<0.2\%$) in whether or not one includes the imaginary part of the generalized Breit interaction when calculating the scattering matrix elements. This behavior can be explained in the following way. The imaginary piece contains the product of two j-type spherical Bessel functions, as can be seen from Eq. (17), while the real piece contains a product of the form jn. The greatest contribution of the generalized Breit interaction to the radial integrals in Eqs. (12) and (13) occurs for arguments of the Bessel functions, (ωr), that are relatively small. For small arguments, the n-type Bessel functions approach negative infinity, while the j-type functions are finite and on the order of one. So, a product of the form jn will be much larger than a product of the form jj, at least for small arguments.

TABLE II. Collision strengths for $n=1$ to $n=2$ and $n=2$ to $n=2$ transitions in hydrogenic ions with $Z=26$, 54, 92. The final scattered energies are 70 and 300 eV for ions with $Z=26$ and 54, respectively. For ions with $Z=92$ the final scattered energy is 2000 eV for the $n=1$-2 transitions and 900 eV for the $n=2$-2 transitions. $x[y]=x\times10^{y}$.

Transition	C	B	GB	GBI
		$Z=26$		
1s-2s	1.139[−3]	1.179[−3]	1.179[−3]	1.179[−3]
1s-2p*	1.488[−3]	1.470[−3]	1.471[−3]	1.471[−3]
1s-2p	2.893[−3]	2.866[−3]	2.868[−3]	2.868[−3]
2s-2p*	4.919[−1]	4.919[−1]	4.919[−1]	4.919[−1]
2s-2p	3.056[−1]	3.057[−1]	3.057[−1]	3.057[−1]
2p*-2p	2.594[−2]	2.593[−2]	2.593[−2]	2.593[−2]
		$Z=54$		
1s-2s	3.271[−4]	3.849[−4]	3.862[−4]	3.867[−4]
1s-2p*	3.667[−4]	3.640[−4]	3.676[−4]	3.680[−4]
1s-2p	6.412[−4]	6.265[−4]	6.346[−4]	6.354[−4]
2s-2p*	8.567[−2]	8.574[−2]	8.574[−2]	8.574[−2]
2s-2p	5.638[−2]	5.637[−2]	5.637[−2]	5.637[−2]
2p*-2p	5.658[−3]	5.642[−3]	5.646[−3]	5.646[−3]
		$Z=92$		
1s-2s	2.074[−4]	3.189[−4]	3.233[−4]	3.265[−4]
1s-2p*	1.543[−4]	1.944[−4]	2.107[−4]	2.145[−4]
1s-2p	1.821[−4]	1.894[−4]	2.075[−4]	2.130[−4]
2s-2p*	1.384[−2]	1.396[−2]	1.395[−2]	1.396[−2]
2s-2p	1.366[−2]	1.350[−2]	1.352[−2]	1.352[−2]
2p*-2p	1.613[−3]	1.593[−3]	1.605[−3]	1.607[−3]

As for the collision strengths calculated with only the Breit interaction (column B), they too differ by less than a percent from the generalized Breit interaction calculations for most of the listed transitions. However, this behavior changes as we go to higher Z values, which we discuss next.

The near-threshold collision strengths for $Z=92$ in Table II exhibit much greater effects than the previous data for $Z=26$ and 54. First we mention that the $n=1$-2 collision strengths in this table were calculated with a final electron energy of $E_f=2000$ eV, which roughly equals 2% of the transition energy in question. This differs from the usual 1% because we wanted to compare with the recent results of Moores and Pindzola and coworkers [7,8]. The $n=2$-2 transitions were calculated with $E_f=900$ eV.

Looking at the $Z=92$ data we immediately see effects for all three of the $n=1$-2 transitions, not just the $1s_{1/2}$-$2s_{1/2}$ transition. The percentage increases due to inclusion of the generalized Breit interaction are 57%, 39%, and 17% for the three transitions and are in good agreement with the results of Moores and Pindzola [8]. We saw similar large percentage increases, as high as 65%, among the near-threshold $n=1$-2 collision strengths for $Z=100$ when viewing Table I. The effects were slightly greater than the $Z=92$ data in all cases, which is to be expected since the Z value is slightly greater. As with the $Z=50$ and 54 data, the transition involving two s electrons is most greatly affected for high Z. But, unlike the lower Z results, the transitions involving the $2p$ electrons are significantly affected in the very high Z regime.

By comparing the GB and GBI entries in the tables one sees that neglecting the imaginary piece of the generalized Breit interaction results in a maximum discrepancy of 2.7% for $Z=92$ and 4% for $Z=100$ for the $n=1$-2, near-threshold collision strengths. From our discussion in Sec. II, it follows that including the imaginary piece doubles the number of radial integrals that must be evaluated for the generalized Breit interaction part of the calculations. Since the effects of the imaginary piece change the collision strengths by only a few percent, which is acceptable for most plasma applications, we can cut the total computing time approximately in half by ignoring this term because the generalized Breit interaction part of the calculations is responsible for the bulk of the total computing time. On the other hand, we now find that simply using the Breit interaction given by Eq. (1) is not a valid approximation if the cross sections are to be obtained within a few percent. Specifically, using the more approximate Breit interaction data listed in column B can result in a discrepancy as high as 12% for $Z=92$ and 17% for $Z=100$ for near-threshold energies. As for the $n=2$-2 collision strengths, they are seemingly unaffected by any form of the Breit interaction, even for Z values as high as 92, thus confirming that the $1s$ electron is all important for the generalized Breit interaction to have a large effect on the collision strengths.

To see the effects of higher impact energies on high Z collision strengths, we present Table III, which contains additional collision strengths for the $n=1$-2 transitions with $E_f=100$, 300, and 500 keV for $Z=92$. Another pattern is uncovered here by noticing the steady decrease in the effect of the Breit interaction on the $1s_{1/2}$-$2s_{1/2}$ collision strengths with increasing impact energy. The effect decreases from 57% at threshold to 17% for a scattered energy of 500 keV. The effect on the $2p_{1/2}$ and $2p_{3/2}$ transitions declines slightly and then increases with energy. Similar trends were duplicated by the $Z=100$ data in Table I. Of course, the actual percentage changes are greater for $Z=100$ than for $Z=92$. In examining the relative effects of the three forms of the Breit interaction that we considered for these high impact energy calculations, we observe that ignoring the imaginary piece is even less important for the high impact energy results given in Tables I and III than it is for near-threshold energies. The GB column gives collision strengths accurate to within 2% of the GBI values calculated with the full interaction for high impact energies. However, as with the near-threshold data, the $\omega=0$ limit results differ significantly from the full interaction collision strengths.

TABLE III. Collision strengths for $n=1$ to $n=2$ transitions in hydrogenic ions with $Z=92$. The final scattered energies are 100, 300, and 500 keV.

Transition	C	B	GB	GBI
		Final energy is 100 keV		
$1s$-$2s$	2.641[−4]	3.548[−4]	3.648[−4]	3.660[−4]
$1s$-$2p^*$	2.106[−4]	2.457[−4]	2.758[−4]	2.805[−4]
$1s$-$2p$	3.270[−4]	3.150[−4]	3.508[−4]	3.582[−4]
		Final energy is 300 keV		
$1s$-$2s$	4.047[−4]	4.830[−4]	4.981[−4]	4.985[−4]
$1s$-$2p^*$	4.299[−4]	4.996[−4]	5.940[−4]	6.014[−4]
$1s$-$2p$	7.361[−4]	7.189[−4]	8.280[−4]	8.396[−4]
		Final energy is 500 keV		
$1s$-$2s$	5.714[−4]	6.475[−4]	6.677[−4]	6.678[−4]
$1s$-$2p^*$	7.062[−4]	8.127[−4]	1.073[−3]	1.083[−3]
$1s$-$2p$	1.226[−3]	1.217[−3]	1.495[−3]	1.511[−3]

The maximum differences are 34% for $Z=92$ and 35% for $Z=100$.

We next consider transitions involving excitation to the five $n=3$ levels: $3s_{1/2}$, $3p_{1/2}$, $3p_{3/2}$, $3d_{3/2}$, and $3d_{5/2}$. The near-threshold collision strengths for these transitions are presented in Table IV for $Z=26$, 54, and 92. For $Z=26$ and 54 we see very similar results to those for the $n=1$-2 transitions. The three forms of the Breit interaction yield results that differ by at most 1.5% for both Z values. The effect of including the interaction for ions with $Z=26$ is small, but can become appreciable for ions with $Z=54$. In fact, the effect of the generalized Breit interaction on these $n=1$-3 transitions for $Z=54$ are slightly larger than those observed for the $n=1$-2 transitions, which is most likely due to the larger transition energies involved in the $n=1$-3 transitions.

The $Z=92$ data in Table IV again show very significant increases in collision strengths due to the presence of the generalized Breit interaction in the scattering matrix elements. In this case the increases range from 24% to 68% for the five transitions. Higher impact energies are expected to result in similar significant increases, analogous to the $n=1$-2 collision strengths. For this large Z value we again see the trend that collision strengths calculated with only the real part of the generalized Breit interaction agree with calculations using the full interaction to within a few percent ($\leq 2.5\%$). Using the more approximate Breit interaction results in differences of over 9% for four out of the five transitions, once more suggesting that the $\omega=0$ limit is not adequate for high Z calculations.

We could continue by listing results for the 15 $n=2$-3 transitions for ions with $Z=26$, 54, and 92. However, the effects are not as significant as the previous results, so we present only a representative data set for the most strongly affected results for ions with $Z=92$. The remainder of the $n=2$-3 results will only be summarized here. The interested reader may contact one of us (C.J.F.) or consult the thesis in Ref. [31] for greater detail.

As in all previous transitions the near-threshold data for the 15 $n=2$-3 transitions for $Z=26$ exhibited very little effect due to including any form of the Breit interaction in the scattering matrix elements as compared with only using the Coulomb interaction. From the data presented thus far, it appears that, at least for hydrogenic ions, there is little need to include the generalized Breit interaction in calculating excitation cross sections for Z values in the vicinity of 26 for any of the usual transitions of interest. In the next subsection we see that this is less true for He-like and Li-like ions.

Also for $Z=54$ there are only small changes in the near-threshold collision strengths for the $n=2$-3 transitions due to any form of the Breit interaction. In general, the changes were a couple of percent, becoming as high as 4.5%. The form of the Breit interaction chosen to do the calculations did not appear to matter at all. Something to note is that the effect of the generalized Breit interaction has been, for the most part, to increase collision strength values. However, for the $n=2$-3 transitions with $Z=54$, decreases occur about as frequently as increases.

For $Z=92$ we first calculated the near-threshold collision strengths for the $n=2$-3 collision strengths, which are presented in Table V. From the table it appears that the effect of the generalized Breit interaction on these transitions is quantitatively somewhere in between its effect on the $n=1$-2 and 2-2 transitions. On average, the effect of the generalized Breit interaction is a change of $\pm 5\%$ in the collision strengths with an occasional change

TABLE IV. Collision strengths for $n=1$ to $n=3$ transitions in hydrogenic ions with $Z=26$, 54, and 92. The final scattered energies are 83, 300, and 2000 eV, respectively.

Transition	C	B	GB	GBI
		$Z=26$		
1*s*-3*s*	2.408[−4]	2.500[−4]	2.501[−4]	2.501[−4]
1*s*-3*d**	6.279[−5]	6.323[−5]	6.326[−5]	6.326[−5]
1*s*-3*d*	9.026[−5]	9.168[−5]	9.173[−5]	9.173[−5]
1*s*-3*p**	3.176[−4]	3.156[−4]	3.160[−4]	3.160[−4]
1*s*-3*p*	6.230[−4]	6.199[−4]	6.200[−4]	6.200[−4]
		$Z=54$		
1*s*-3*s*	6.894[−5]	8.267[−5]	8.307[−5]	8.320[−5]
1*s*-3*d**	1.475[−5]	1.541[−5]	1.555[−5]	1.556[−5]
1*s*-3*d*	1.832[−5]	1.975[−5]	1.999[−5]	2.000[−5]
1*s*-3*p**	7.960[−5]	8.118[−5]	8.235[−5]	8.244[−5]
1*s*-3*p*	1.444[−4]	1.441[−4]	1.457[−4]	1.458[−4]
		$Z=92$		
1*s*-3*s*	4.312[−5]	7.008[−5]	7.141[−5]	7.231[−5]
1*s*-3*d**	4.768[−6]	5.844[−6]	6.343[−6]	6.372[−6]
1*s*-3*d*	4.008[−6]	5.208[−6]	5.832[−6]	5.860[−6]
1*s*-3*p**	3.519[−5]	4.573[−5]	4.981[−5]	5.061[−5]
1*s*-3*p*	4.598[−5]	5.046[−5]	5.540[−5]	5.680[−5]

TABLE V. Collision strengths for $n=2$ to $n=3$ transitions in hydrogenic ions with $Z=92$. The final scattered energy is 200 eV.

Transition	C	B	GB	GBI
2*s*-3*s*	1.131[−3]	1.217[−3]	1.217[−3]	1.217[−3]
2*s*-3*d**	5.436[−4]	5.888[−4]	5.886[−4]	5.887[−4]
2*s*-3*d*	7.826[−4]	8.102[−4]	8.090[−4]	8.092[−4]
2*s*-3*p**	3.282[−4]	3.064[−4]	3.097[−4]	3.106[−4]
2*s*-3*p*	1.864[−4]	1.940[−4]	1.942[−4]	1.952[−4]
2*p**-3*s*	7.849[−5]	9.367[−5]	9.309[−5]	9.351[−5]
2*p**-3*d**	1.989[−3]	1.825[−3]	1.838[−3]	1.842[−3]
2*p**-3*d*	3.780[−4]	3.807[−4]	3.832[−4]	3.834[−4]
2*p**-3*p**	1.184[−3]	1.264[−3]	1.265[−3]	1.265[−3]
2*p**-3*p*	2.655[−4]	2.501[−4]	2.524[−4]	2.529[−4]
2*p*-3*s*	2.956[−4]	3.071[−4]	3.071[−4]	3.079[−4]
2*p*-3*d**	1.573[−3]	1.518[−3]	1.524[−3]	1.525[−3]
2*p*-3*d*	6.928[−3]	6.536[−3]	6.579[−3]	6.585[−3]
2*p*-3*p**	4.413[−4]	4.387[−4]	4.408[−4]	4.414[−4]
2*p*-3*p*	3.096[−3]	3.294[−3]	3.300[−3]	3.301[−3]

getting as high as 8% and a maximum change of 19%. In an attempt to see if these changes would become more significant at higher scattered energies, we calculated the same 15 collision strengths for $Z=92$ with impact-electron energies of about two, four and six times threshold. For the most part we observed similar changes with an occasional 10% effect, but no results approached the large 50% plus effects seen in the $n=1$-2 and 1-3 cases.

C. He-like ions

Since our survey of H-like collision strengths was rather in depth and the transitions of interest for He-like ions have very similar radial matrix elements to those of H-like ions, we give collision strengths for only one set of transitions for He-like ions. These are the six transitions of the form

$$1s^2+e_i^- \rightarrow 1s2l+e_f^- \tag{26}$$

for which near-threshold results are given for the usual Z values of 26, 54, and 92 in Table VI.

As far as the relative effects of using the different forms of the Breit interaction are concerned, one sees that they follow the same pattern as for hydrogenic ions. That is,

TABLE VI. Collision strengths for the six $n=1$ to $n=2$ transitions in He-like ions with $Z=26$, 54, 92. The final scattered energies are 70, 300, and 1000 eV, respectively.

Transition	C	B	GB	GBI
		$Z=26$		
1*s*2-(1*s*2*s*)0	7.687[−4]	8.102[−4]	8.101[−4]	8.101[−4]
1*s*2-(1*s*2*s*)1	3.626[−4]	3.600[−4]	3.604[−4]	3.604[−4]
1*s*2-(1*s*2*p**)0	2.267[−4]	2.108[−4]	2.108[−4]	2.108[−4]
1*s*2-(1*s*2*p**)1	8.079[−4]	8.140[−4]	8.143[−4]	8.143[−4]
1*s*2-(1*s*2*p*)1	2.122[−3]	2.077[−3]	2.077[−3]	2.077[−3]
1*s*2-(1*s*2*p*)2	1.065[−3]	1.082[−3]	1.083[−3]	1.083[−3]
		$Z=54$		
1*s*2-(1*s*2*s*)0	2.260[−4]	2.777[−4]	2.772[−4]	2.773[−4]
1*s*2-(1*s*2*s*)1	9.931[−5]	1.046[−4]	1.062[−4]	1.066[−4]
1*s*2-(1*s*2*p**)0	6.211[−5]	4.468[−5]	4.474[−5]	4.477[−5]
1*s*2-(1*s*2*p**)1	2.854[−4]	3.016[−4]	3.055[−4]	3.058[−4]
1*s*2-(1*s*2*p*)1	4.113[−4]	3.769[−4]	3.798[−4]	3.804[−4]
1*s*2-(1*s*2*p*)2	2.332[−4]	2.548[−4]	2.579[−4]	2.580[−4]
		$Z=92$		
1*s*2-(1*s*2*s*)0	1.503[−4]	2.321[−4]	2.311[−4]	2.319[−4]
1*s*2-(1*s*2*s*)1	5.531[−5]	8.456[−5]	8.961[−5]	9.198[−5]
1*s*2-(1*s*2*p**)0	3.383[−5]	1.198[−5]	1.246[−5]	1.289[−5]
1*s*2-(1*s*2*p**)1	1.194[−4]	1.815[−4]	1.965[−4]	1.997[−4]
1*s*2-(1*s*2*p*)1	1.156[−4]	9.763[−5]	1.041[−4]	1.087[−4]
1*s*2-(1*s*2*p*)2	6.474[−5]	9.128[−5]	1.009[−4]	1.016[−4]

all three forms give almost the same results for $Z=26$ and 54 while use of the $\omega=0$ limit, Eq. (1), leads to appreciable error for $Z=92$ and neglect of the imaginary part has little effect, even for $Z=92$ ($\leq 4.5\%$). On the other hand, the effect of the generalized Breit interaction on the collision strengths for He-like ions is appreciably increased as compared with H-like ions for the same Z value. The maximum effect for each Z value is only a few percent more, but a much larger fraction of transitions are appreciably affected. For example, there is a decrease of 7% in the collision strength for the $1s^2$-$(1s2p^*)0$ transition in ions with $Z=26$, while there was essentially no effect for the $1s$-$2p^*$ transition in H-like ions with this value of Z. More remarkably, the collision strength for the $1s^2$-$(1s2p^*)0$ transition in He-like ions with $Z=54$ is decreased by 28% upon inclusion of the generalized Breit interaction. In addition, the other transitions involving excitation to a $2p^*$ or $2p$ state are changed by $\pm 7\%$ and 11%, while for H-like ions with $Z=54$ the results for the $1s$-$2p^*$ and $1s$-$2p$ transitions at the same scattered electron energy were changed by less than 1%. Of course, results summed over final target J values are similar to the corresponding results for hydrogenic ions.

D. Li-like ions

The final data we present are for Li-like ions, those ions with three bound electrons. Here we consider all possible transitions of the form

$$1s^2 2l + e_i^- \rightarrow 1s2l'2l'' + e_f^- \ . \tag{27}$$

These inner-shell excitation transitions produce satellites to the He-like $n=1$-2 lines that are important for plasma diagnostic purposes [32–34]. There are 42 transitions in all, 11 from the ground level and 15 and 16 for $2l$ in Eq. (27) equalling $2p^*$ and $2p$, respectively. Table VII lists the 19 relevant levels ordered according to energy among the levels in each complex. In general a complex consists of all states with the same parity, total angular momentum J, and principle quantum numbers n. Next to each level in the table is a number that is used to represent the level in the tables to follow. The levels are labeled by their dominant jj-coupled state in the relevant complex with the total J value and intermediate J listed when necessary. Hence, for example, level 12 predominantly consists of a jj-coupled state with a total J value of $\frac{5}{2}$ which was obtained by coupling the $1s_{1/2}$ electron to the $2p^2$ subshell with a J value of 2.

The number of radial integrals required for even this simple Li-like case was large enough to warrant an energy interpolation scheme that would yield accurate integrals with a much reduced computing time. The method used in this paper is identical to the Lagrangian scheme used in Ref. [10] expect that, in addition to the Slater integrals, the Breit integrals in Eqs. (12) and (13) were also interpolated. We ran several detailed test cases to compare with the interpolated collision strengths. In all cases, the calculated results agreed with the interpolated values to within less than a percent.

Near-threshold results for the collision strengths for the inner-shell transitions of Eq. (27) are given for $Z=26$, 54, and 92 in Table VIII. One sees that the results follow a similar pattern to those for He-like ions. That is, the relative effects of using the three different forms for the Breit interaction are again similar to those observed for H-like ions with corresponding values of Z. However, as with He-like ions, the importance of including the generalized Breit interaction is somewhat greater for Li-like than H-like ions. The maximum effect for a given Z value is increased by quite a small amount as compared with H-like ions, but the effects on individual transitions become significant for lower Z and for a larger fraction of these transitions, even though results summed over J values are quite similar to those for H-like ions.

TABLE VII. Labeling of levels by dominant jj state for the 19 levels involved in inner-shell excitation of a $1s$ electron to an $n=2$ subshell in Li-like ions.

jj state	Level labels as a function of Z		
	$Z=26$	$Z=54$	$Z=92$
$[(1s\times 2)0\,2s]1/2$	1	1	1
$[(1s\times 2)0\,2p^*]1/2$	2	2	2
$[(1s\times 2)0\,2p]3/2$	3	3	3
$[1s(2s\times 2)0]1/2$	4	4	4
$[1s(2p^*\times 2)0]1/2$	5	5	5
$[(1s2p^*)1\,2p]1/2$	6	6	6
$[1s(2p\times 2)0]1/2$	7	7	7
$[(1s2p^*)0\,2p]3/2$	8	9	9
$[(1s2p^*)1\,2p]3/2$	9	8	8
$[1s(2p\times 2)2]3/2$	10	10	10
$[(1s2p^*)1\,2p]5/2$	11	11	11
$[1s(2p\times 2)2]5/2$	12	12	12
$[(1s2s)1\,2p^*]1/2$	13	13	13
$[(1s2s)0\,2p^*]1/2$	14	14	14
$[(1s2s)1\,2p]1/2$	15	15	15
$[(1s2s)1\,2p^*]3/2$	16	16	16
$[(1s2s)1\,2p]3/2$	17	17	17
$[(1s2s)0\,2p]3/2$	18	18	18
$[(1s2s)1\,2p]5/2$	19	19	19

IV. SUMMARY AND CONCLUSIONS

In this work we have presented the framework necessary to include the generalized Breit interaction in the scattering matrix elements for electron-impact excitation of highly charged ions. This framework consisted of a fully relativistic Dirac-Fock-Slater approach to the atomic structure and a fully relativistic distorted-wave method for calculating excitation collision strengths. The relativistic structure code of Sampson *et al.* [9] was altered to include options for a finite nuclear potential with a Fermi nuclear charge distribution, inclusion of the generalized Breit interaction perturbatively, approximations for the lowest-order vacuum polarization, and self-energy QED corrections to the level energies and retarded oscillator strengths.

The distorted-wave, excitation collision code of Zhang, Sampson, and Mohanty [10] was extended to include the generalized Breit interaction in the scattering matrix ele-

TABLE VIII. Collision strengths for inner-shell excitation in Li-like ions with $Z=26$, 54, and 92. The final scattered energies are 70, 300, and 1000 eV, respectively.

Transition	C	B	GB	GBI
		$Z=26$		
1-4	1.032[−3]	1.067[−3]	1.068[−3]	1.068[−3]
1-5	1.257[−5]	1.300[−5]	1.300[−5]	1.300[−5]
1-6	5.331[−6]	5.513[−6]	5.514[−6]	5.514[−6]
1-7	6.718[−5]	6.947[−5]	6.949[−5]	6.949[−5]
1-13	4.628[−4]	4.425[−4]	4.426[−4]	4.426[−4]
1-14	1.088[−3]	1.074[−3]	1.074[−3]	1.074[−3]
1-15	7.858[−4]	7.644[−4]	7.647[−4]	7.647[−4]
1-16	9.560[−4]	9.638[−4]	9.642[−4]	9.642[−4]
1-17	2.802[−3]	2.745[−3]	2.747[−3]	2.747[−3]
1-18	8.610[−4]	8.737[−3]	8.742[−4]	8.742[−4]
1-19	1.282[−3]	1.302[−3]	1.303[−3]	1.030[−3]
2-4	5.638[−5]	5.581[−5]	5.586[−5]	5.586[−5]
2-5	7.290[−4]	7.228[−4]	7.230[−4]	7.230[−4]
2-6	1.607[−3]	1.575[−3]	1.576[−3]	1.576[−3]
2-7	1.120[−4]	1.111[−4]	1.111[−4]	1.111[−4]
2-8	8.183[−4]	8.311[−4]	8.316[−4]	8.316[−4]
2-9	2.161[−3]	2.110[−3]	2.112[−3]	2.112[−3]
2-10	8.374[−5]	8.315[−5]	8.320[−5]	8.320[−5]
2-11	8.994[−4]	9.136[−4]	9.141[−4]	9.141[−4]
2-12	3.802[−4]	3.862[−4]	3.864[−4]	3.865[−4]
2-13	2.290[−4]	2.274[−4]	2.276[−4]	2.276[−4]
2-14	1.269[−3]	1.337[−3]	1.337[−3]	1.337[−3]
2-15	2.546[−4]	2.676[−4]	2.676[−4]	2.676[−4]
2-16	3.553[−4]	3.525[−4]	3.529[−4]	3.529[−4]
2-17	8.150[−5]	8.087[−5]	8.095[−5]	8.095[−5]
2-18	4.621[−5]	4.585[−5]	4.590[−5]	4.590[−5]
3-4	5.136[−5]	5.089[−5]	5.094[−5]	5.095[−5]
3-5	1.976[−4]	1.990[−4]	1.991[−4]	1.991[−4]
3-6	6.905[−4]	6.901[−4]	6.904[−4]	6.904[−4]
3-7	1.201[−3]	1.190[−3]	1.191[−3]	1.191[−3]
3-8	9.831[−4]	9.494[−4]	9.496[−4]	9.496[−4]
3-9	1.090[−3]	1.069[−3]	1.070[−3]	1.070[−3]
3-10	4.136[−3]	4.059[−3]	4.062[−3]	4.062[−3]
3-11	1.919[−3]	1.939[−3]	1.940[−3]	1.940[−3]
3-12	3.502[−3]	3.502[−3]	3.504[−3]	3.504[−3]
3-13	1.387[−5]	1.377[−5]	1.378[−5]	1.378[−5]
3-14	3.790[−5]	3.761[−5]	3.765[−5]	3.765[−5]
3-15	1.897[−4]	1.882[−4]	1.884[−4]	1.884[−4]
3-16	1.306[−4]	1.298[−4]	1.299[−4]	1.299[−4]
3-17	1.188[−3]	1.237[−3]	1.237[−3]	1.237[−3]
3-18	2.185[−3]	2.297[−3]	2.296[−3]	2.296[−3]
3-19	7.246[−4]	7.190[−4]	7.197[−4]	7.197[−4]
		$Z=54$		
1-4	3.077[−4]	3.614[−4]	3.625[−4]	3.629[−4]
1-5	1.423[−5]	1.672[−5]	1.677[−5]	1.679[−5]
1-6	1.945[−8]	2.285[−8]	2.292[−8]	2.295[−8]
1-7	1.434[−6]	1.684[−6]	1.690[−6]	1.692[−6]
1-13	1.439[−4]	1.261[−4]	1.270[−4]	1.271[−4]
1-14	1.826[−4]	1.759[−4]	1.776[−4]	1.779[−4]
1-15	2.542[−4]	2.321[−4]	2.340[−4]	2.344[−4]
1-16	3.622[−4]	3.842[−4]	3.889[−4]	3.893[−4]
1-17	5.034[−4]	4.676[−4]	4.717[−4]	4.725[−4]
1-18	2.341[−4]	2.411[−4]	2.437[−4]	2.439[−4]
1-19	2.804[−4]	3.059[−4]	3.095[−4]	3.097[−4]

Table VIII (*Continued*).

Transition	C	B	GB	GBI
2-4	1.608[−5]	1.600[−5]	1.619[−5]	1.620[−5]
2-5	3.251[−4]	3.241[−4]	3.276[−4]	3.280[−4]
2-6	2.757[−4]	2.527[−4]	2.548[−4]	2.553[−4]
2-7	6.442[−7]	6.399[−7]	6.457[−7]	6.460[−7]
2-8	1.923[−4]	2.083[−4]	2.107[−4]	2.108[−4]
2-9	5.146[−4]	4.710[−4]	4.749[−4]	4.757[−4]
2-10	2.708[−7]	2.938[−7]	2.973[−7]	2.974[−7]
2-11	2.791[−4]	3.046[−4]	3.082[−4]	3.084[−4]
2-12	1.026[−6]	1.121[−6]	1.134[−6]	1.134[−6]
2-13	7.223[−5]	7.727[−5]	7.832[−5]	7.854[−5]
2-14	4.403[−4]	5.410[−4]	5.401[−4]	5.403[−4]
2-15	1.908[−6]	2.298[−6]	2.299[−6]	2.301[−6]
2-16	1.306[−4]	1.374[−4]	1.395[−4]	1.400[−4]
2-17	1.334[−6]	1.402[−6]	1.424[−6]	1.428[−6]
2-18	3.814[−7]	4.010[−7]	4.073[−7]	4.085[−7]
3-4	1.073[−6]	1.046[−6]	1.059[−6]	1.060[−6]
3-5	1.183[−6]	1.223[−6]	1.235[−6]	1.235[−6]
3-6	1.908[−4]	2.014[−4]	2.038[−4]	2.041[−4]
3-7	3.149[−4]	3.086[−4]	3.117[−4]	3.121[−4]
3-8	3.082[−4]	2.850[−4]	2.876[−4]	2.878[−4]
3-9	3.202[−4]	2.954[−4]	2.980[−4]	2.983[−4]
3-10	8.866[−4]	8.275[−4]	8.348[−4]	8.361[−4]
3-11	5.710[−4]	6.031[−4]	6.105[−4]	6.112[−4]
3-12	7.051[−4]	7.320[−4]	7.401[−4]	7.407[−4]
3-13	2.111[−7]	2.221[−7]	2.256[−7]	2.263[−7]
3-14	3.090[−7]	3.251[−7]	3.301[−7]	3.312[−7]
3-15	6.564[−5]	6.903[−5]	7.011[−5]	7.033[−5]
3-16	2.368[−6]	2.625[−6]	2.650[−6]	2.655[−6]
3-17	1.727[−4]	1.903[−4]	1.922[−4]	1.926[−4]
3-18	8.533[−4]	1.048[−3]	1.046[−3]	1.046[−3]
3-19	1.985[−4]	2.088[−4]	2.120[−4]	2.127[−4]
		$Z=92$		
1-4	1.998[−4]	3.078[−4]	3.117[−4]	3.148[−4]
1-5	4.989[−6]	7.688[−6]	7.785[−6]	7.863[−6]
1-6	4.174[−12]	6.438[−12]	6.528[−12]	6.593[−12]
1-7	3.945[−8]	6.090[−8]	6.184[−8]	6.246[−8]
1-13	7.320[−5]	7.176[−5]	7.747[−5]	7.894[−5]
1-14	7.390[−5]	7.243[−5]	7.822[−5]	7.975[−5]
1-15	7.552[−5]	6.306[−5]	6.776[−5]	7.079[−5]
1-16	1.577[−4]	2.387[−4]	2.596[−4]	2.638[−4]
1-17	1.266[−4]	1.143[−4]	1.235[−4]	1.282[−4]
1-18	7.768[−5]	8.641[−5]	9.449[−5]	9.648[−5]
1-19	7.770[−5]	1.093[−4]	1.208[−4]	1.216[−4]
2-4	3.751[−6]	4.711[−6]	5.108[−6]	5.197[−6]
2-5	1.487[−4]	1.868[−4]	2.026[−4]	2.061[−4]
2-6	7.628[−5]	6.391[−5]	6.870[−5]	7.177[−5]
2-7	7.515[−9]	9.432[−9]	1.020[−8]	1.033[−8]
2-8	7.851[−5]	8.734[−5]	9.551[−5]	9.754[−5]
2-9	1.252[−4]	1.126[−4]	1.217[−4]	1.263[−4]
2-10	2.457[−9]	2.474[−9]	2.686[−9]	2.764[−9]
2-11	7.771[−5]	1.093[−4]	1.208[−4]	1.216[−4]
2-12	4.578[−9]	6.513[−9]	7.201[−9]	7.249[−9]
2-13	5.463[−5]	8.382[−5]	8.677[−5]	8.836[−5]
2-14	2.812[−4]	4.348[−4]	4.330[−4]	4.346[−4]
2-15	6.074[−8]	9.412[−8]	9.414[−8]	9.464[−8]

Table VIII (*Continued*).

Transition	C	B	GB	GBI
2-16	7.366[−5]	1.125[−4]	1.192[−4]	1.224[−4]
2-17	1.723[−8]	2.613[−8]	2.775[−8]	2.848[−8]
2-18	8.373[−9]	1.269[−8]	1.348[−8]	1.383[−8]
3-4	1.710[−8]	1.763[−8]	1.915[−8]	1.967[−8]
3-5	8.801[−9]	9.171[−9]	9.945[−9]	1.013[−8]
3-6	7.903[−5]	1.196[−4]	1.301[−4]	1.322[−4]
3-7	8.922[−5]	9.311[−5]	1.015[−4]	1.041[−4]
3-8	1.552[−4]	2.143[−4]	2.328[−4]	2.367[−4]
3-9	1.384[−4]	7.328[−5]	7.771[−5]	7.977[−5]
3-10	2.533[−4]	2.267[−4]	2.447[−4]	2.541[−4]
3-11	2.369[−4]	3.586[−4]	3.900[−4]	3.963[−4]
3-12	1.934[−4]	2.394[−4]	2.632[−4]	2.670[−4]
3-13	1.609[−9]	2.478[−9]	2.617[−9]	2.688[−9]
3-14	9.813[−9]	1.510[−8]	1.595[−8]	1.639[−8]
3-15	3.682[−5]	5.622[−5]	5.956[−5]	6.114[−5]
3-16	6.856[−8]	1.056[−7]	1.069[−7]	1.081[−7]
3-17	8.076[−5]	1.235[−4]	1.300[−4]	1.332[−4]
3-18	5.901[−4]	9.126[−4]	9.085[−4]	9.119[−4]
3-19	1.105[−4]	1.688[−4]	1.788[−4]	1.836[−4]

ments. The code is completely general in that collision strengths for any ion with any number of bound electrons may be calculated. Of course, due to the approximations associated with the Dirac-Fock-Slater and distorted-wave approaches, the values obtained are expected to be highly accurate only when the relationship $Z > 2N$ exists between the ionic atomic number and the number of bound electrons.

Collision strengths using three different forms of the Breit interaction were calculated with this code and presented in this work. These three forms were the interaction originally formulated by Breit, given in Eq. (1); the generalized Breit interaction, given by Eq. (3), which represents the lowest-order Feynman diagram for exchange of a single virtual photon between two electrons; and the real part of the generalized Breit interaction. Results obtained from these three forms are labeled B, GBI, and GB, respectively, in the tables.

Numerical results were reported for H-like, He-like, and Li-like ions with Z values of 26, 54, and 92. These Z values were chosen to explore the effective range of the generalized Breit interaction when calculating excitation collision strengths. The three ion types were chosen primarily for their importance in high-temperature plasma modeling and diagnostics and for their likelihood of undergoing transitions involving tightly bound electrons that are sensitive to the effects of the Breit interaction. A number of transitions were also considered to ascertain the scope of the interaction's effect. Four different sets of transitions were examined for hydrogenic ions, while the $1s^2$-$1s2l$ transitions were considered for He-like ions, and the $1s^2 2l$-$1s2l'2l''$ transitions were considered for Li-like ions.

For low Z values ($Z \lesssim 26$) there appears to be not much need to include any form of the Breit interaction in excitation collision strength calculations, although the generalized Breit interaction does produce effects as large as 7% and 5% for He-like and Li-like ions with $Z = 26$. For larger Z values ($Z \approx 54$) the effect of the generalized Breit interaction on collision strengths becomes appreciable ($\sim 20\%$) for certain transitions among tightly bound electrons. Also, the other two forms of the interaction are almost as good (within a couple of percent) at predicting these collision strengths. For high Z values ($Z \approx 92$) there are significant effects in all collision strengths involving transitions between $1s$ and higher electrons. Many of these changes are in the range of 30–60 %. Even the $n = 2$-3 collision strengths involving less tightly bound electrons mostly exhibit 5–10 % changes for $Z = 92$. Collision strengths for $n = 2$-2 transitions were not appreciably affected by the generalized Breit interaction for any Z value considered, at least for H-like ions. The energy of the exchanged photon is apparently too small for these transitions to make a significant contribution, even for high Z ions.

The real part of the generalized Breit interaction yields collision strengths that are very close to those values obtained with the full interaction for all transitions, Z values, electron energies, and number of bound electrons considered in this work. A maximum deviation of about 4.5% between the two calculations is observed for high Z ions in a few transitions. Usually, these deviations are less than 2%. This last result is of some practical importance since most of the computing time for calculating the collision strengths is required for the evaluation of the Breit radial integrals. Excluding the imaginary integrals amounts to a reduction in computing time by almost a factor of 2. Using the $\omega = 0$ limit of the generalized Breit interaction, however, resulted in greater than 10% discrepancies for some transitions in very high Z ions.

Finally we mention the important and perhaps surprising conclusion that the inclusion of the generalized Breit interaction in the scattering matrix elements appears to

have a somewhat larger effect on collision strengths for complex ions than for hydrogenic ions. For example, the near-threshold results for the $1s$-$2p^*$ and $1s$-$2p$ transitions in H-like ions with $Z=54$ were found to be affected by less than 1%. On the other hand, the collision strengths for one of the four analogous transitions in He-like ions with this Z value was decreased by 28% and those for the remaining transitions were changed by $\pm 7\%$ and 11%. Of course, as one would expect must be true, results summed over final target ion J values are very similar to the corresponding results for hydrogenic ions. The explanation is that the Breit interaction does affect some individual matrix elements appreciably, even for quite low Z, but the effect is largely cancelled upon summation over a significant number of quantum numbers. Along this same line we note that even for $Z=92$ it was found by Pindzola *et al.* [5] that for ionization, which is analogous to excitation summed over many final nlj values, the generalized Breit interaction has little effect on the cross sections until very high impact-electron energies are considered.

In view of this fact that inclusion of the generalized Breit interaction is more important for complex ions, and also that even for H-like ions it was found to be of some significance for the $n=2$-3 transitions, one would expect that its inclusion might be important for excitation of complex ions such as Ne-like and F-like ions for a fairly wide range of high Z values. We expect to investigate this possibility in future work.

Due to the lack of experimental data for excitation collision strengths of H-like, He-like, and Li-like ions with $28 \leq Z \leq 92$ it is impossible to check our calculated results with physical measurements for the regime in which the Breit interaction has an appreciable effect. The best comparison we can offer is with the few theoretical test cases provided by Walker [6] and Moores and Pindzola [8] for hydrogenic ions. The agreement with these results is very good. In the future, the most likely source of high Z collision strength measurements would appear to be the EBIT experiments of Beiersdorfer *et al.* While no excitation measurements have yet been reported for the transitions in H-like, He-like, and Li-like ions for the higher Z values explored in this work, it is expected that such measurements by EBIT will be made in future work [14].

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