Scaling of Coulomb Born cross sections for electron-impact excitation of singly charged ions

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A scaling method applied to plane-wave Born cross sections for electron-impact excitation of neutral atoms is modified and applied to Coulomb Born cross sections for excitations of singly charged ions. The modified scaling for singly charged ions is simpler than the scaling for neutral atoms. Moreover, the former converts Coulomb Born cross sections into accurate results comparable to the convergent close coupling results, as is the case for the scaling for neutral atoms. Comparisons to available theoretical and experimental data on excitations of He^+, Mg^+, and Zn^+ are presented.

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I. INTRODUCTION

In many applications of electron-atom collision cross sections, such as in modeling of fusion plasmas, plasma processing of semiconductors, and planetary atmosphere, there is an acute need for theoretical methods to calculate a large number of excitation cross sections for neutral atoms and lightly charged ions. The scaling methods presented earlier by the present author [1] and the present paper offer simple yet effective tools to calculate such cross sections from wave functions of modest accuracy, e.g., Hartree-Fock wave functions for the target atom.

In an earlier article [1], two simple scaling methods—BE scaling and *f* scaling—for the first-order, plane-wave Born (PWB) cross sections for electron-impact excitation of neutral atoms have been shown to produce cross sections for many neutral atoms with an accuracy comparable to reliable experimental data as well as to more sophisticated theories, such as the *R*-matrix [2], the convergent close coupling (CCC) [3], and the exterior complex scaling [4] methods. The BE scaling corrects the shortcomings of the PWB approximation, while the *f* scaling corrects errors caused by the use of inaccurate wave functions for target atoms. Numerous examples, covering hydrogen through thallium, have been presented in Ref. [1].

In this paper, it is shown that a slightly modified form of the BE scaling can be applied to Coulomb Born (CB) cross sections for electron-impact excitation of singly charged ions in combination with the same *f* scaling discussed in Ref. [1]. The modified scaling, to be referred to as the E scaling, uses only the excitation energy *E*, and achieves similar, remarkable agreement with the CCC results for He^+, and the E- and *f*-scaled CB cross sections for the resonance transitions of Mg^+ and Zn^+ are in good agreement with available experiments.

As is the case for the BE scaling of PWB cross sections [1], the E scaling described in this paper is valid only for dipole- and spin-allowed excitations. The theory is outlined in Sec. II, results are compared to available experimental and theoretical data in Sec. III, and the conclusions are presented in Sec. IV.

II. THEORY

The Coulomb Born approximation is used as the starting point in the present paper because (a) the Coulomb wave is the correct wave function at infinity for an electron colliding with an atomic ion; (b) the CB approximation is the simplest collision theory that exhibits the correct threshold behavior for ion targets [5]; and (c) the CB approximation is valid at high-incident energies. Also, the explicit use of target wave functions in the CB approximation enables the users to distinguish the final state reached, and offers the opportunity to use relativistic wave functions for heavy target ions. In the remainder of this paper, the Coulomb functions used are taken to be for singly charged ions.

In a generic form, first-order CB cross sections σ_{CB} for inelastic collisions are written as

$$\sigma_{\mathrm{CB}}=\frac{4\pi a_0^2 R}{T}F_{\mathrm{CB}}(T), \tag{1}$$

where a_0 is the Bohr radius, R is the Rydberg energy, T is the incident electron energy, and $F_{\mathrm{CB}}(T)$ is the collision strength (multiplied by a constant to be consistent with the standard definition of the collision strength).

Qualitatively, the CB approximation does not account for the exchange effect between the incident and the target electrons, the distortion of the Coulomb waves in the vicinity of the target ion, or the polarization of the target charge cloud due to the presence of the incident electron. The two scaling methods described below correct these deficiencies using simple analytic forms that depend on two atomic properties—the excitation energy *E* and the dipole *f* value for the excitation of interest.

These scalings are valid only for dipole- and spin-allowed, integrated excitation cross sections. The E scaling alters the *T* dependence of integrated cross sections, but does not change the angular shape of the unscaled CB cross sections. As is explained in Ref. [1], these scalings are not effective on dipole- and spin-forbidden excitations because contributions from the first-order Born approximation to such weak excitations are small—e.g., vanishes in spin-forbidden transitions—while contributions from higher-order Born approximation may dominate.

A. E scaling

The BE scaling described in Ref. [1] for excitation of neutral atoms is given by

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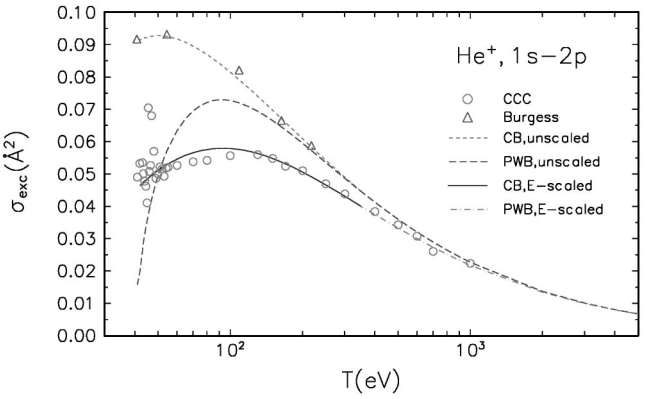

FIG. 1. Comparison of the $1s$-$2p$ excitation cross sections of He^+. Solid curve, E scaled CB cross section; short-dashed curve, unscaled CB cross section; medium-dashed curve, unscaled PWB cross section; dot-dashed curve, E-scaled PWB cross section; circles, CCC cross section [7]; triangles, unscaled CB cross section [8].

$$\sigma_{\mathrm{BE}} = \sigma_{\mathrm{PWB}} T/(T+B+E), \tag{2}$$

where B is the binding energy of the target electron. For singly charged ions, the E scaling below was found to reproduce known accurate results

$$\sigma_{\mathrm{E}} = \sigma_{\mathrm{CB}} T/(T+E). \tag{3}$$

As can be seen in the examples shown in this paper, the E scaling reduces the cross section at low T while keeping the high-T validity of the CB approximation intact. For dipole- and spin-allowed excitations, the peak of the integrated cross section is often at the excitation threshold. Owing to the simple nature of the CB approximation, resonances often observed near the threshold cannot be reproduced. However, as can be seen in comparisons in the next section, E-scaled cross sections go through the rapidly oscillating resonances as a smooth curve, which may be more convenient for modeling applications.

At present, the E scaling cannot be ''derived'' from first principles, as is also the case for the BE scaling for neutral atoms. In the absence of a more fundamental understanding

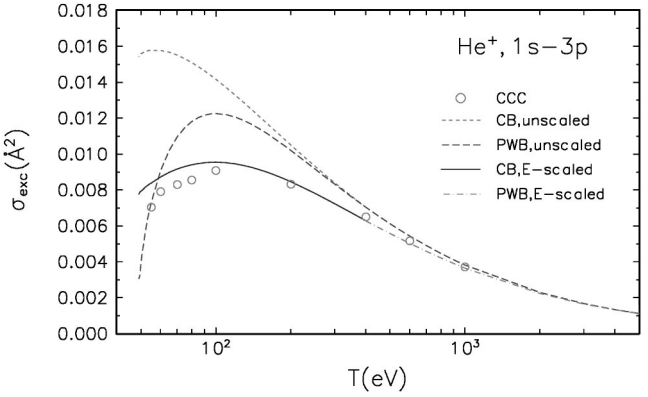

FIG. 2. Comparison of the $1s$-$3p$ excitation cross sections of He^+. See Fig. 1 caption for legend.

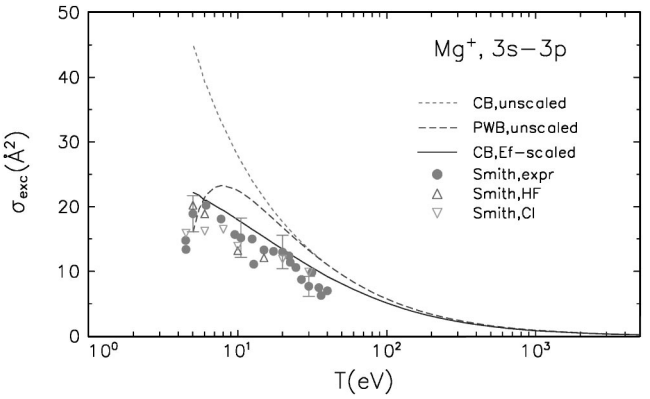

FIG. 3. Comparison of the $3s$-$3p$ excitation cross sections of Mg^+. Solid curve, Ef-scaled CB cross section; short-dashed curve, unscaled CB cross section; medium-dashed curve, unscaled PWB cross section; filled circles, experimental data by Smith *et al.* [9]; triangles, close coupling results by Smith *et al.* [9] using the Hartree-Fock (HF) and configuration interaction (CI) wave functions.

of the origin of the E scaling, the constant E in the E scaling should not be taken literally as a rigid rule, but only as an indicator of the order of magnitude of a constant shift to be added to T. Indeed, as is shown in Ref. [1], heavy, neutral alkaline-earth elements required a constant somewhat larger in magnitude than $B+E$ in BE scaling to reproduce known experimental data at intermediate and low T.

B. *f* Scaling

Coulomb Born cross sections depend on two independent approximations: (a) a first-order perturbation theory using Coulomb waves for the incident and scattered electron, and (b) the use of approximate wave functions for nonhydrogenic targets. The E scaling corrects the deficiency arising from the former approximation. However, if poor target wave functions are used, the results will be unreliable regardless of the E scaling even at high T.

Although computational tools are available to generate wave functions that will produce accurate electric dipole oscillator strengths, or the f values, they are not always easy to use. Besides, the focus of the present paper is the production of accurate excitation cross sections, not wave functions. Often reliable experimental or theoretical f values are available

TABLE I. Excitation energy E in eV and the dipole oscillator strength used for E and f scaling of resonance transitions in He^+, Mg^+, and Zr^+.

Atom	Transition	E	f_{sc}	f_{acc}
He^+	$1s$-$2p$	40.817		0.4162[a]
	$1s$-$3p$	48.376		0.0791[a]
Mg^+	$3s$-$3p$	4.422	0.9840	0.9139[b]
Zn^+	$4s$-$4p$	6.011	1.078	0.8023[b]

[a]Reference [11].
[b]Reference [12].

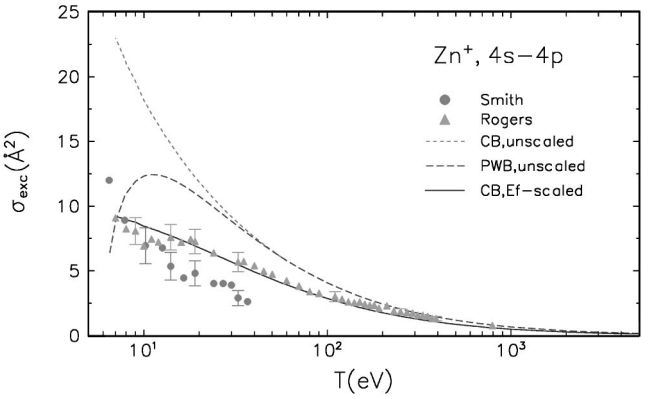

FIG. 4. Comparison of the $4s$-$4p$ excitation cross sections of Zn^+. Solid curve, Ef-scaled CB cross section; short-dashed curve, unscaled CB cross section; medium-dashed curve, unscaled PWB cross section; filled circles, experimental data by Smith *et al.* [9]; filled triangles, experimental data by Rogers *et al.* [10].

for many strong transitions, and it is desirable to take advantage of such results rather than trying to produce very accurate wave functions.

There have been numerous efforts to generate electron-impact excitation cross sections using known f values. For instance, in a popular method known as the Gaunt-factor method [6], the f value for the transition of interest is factored out in front of the collision strength $F_{\mathrm{CB}}(T)$ in Eq. (1), and then $F_{\mathrm{CB}}(T)$ is modified accordingly. Then, the objective of the Gaunt-factor method becomes to find the appropriate collision strengths that will provide reliable cross sections.

In contrast, the E scaling and the f scaling leave the collision strength from the Coulomb Born approximation intact, while the factors multiplying the collision strength are altered. The f scaling is based on the ratio of an accurate f value to a less reliable f value produced by the target wave functions actually used to generate σ_{CB}

$$\sigma_{\mathrm{CBmc}}=(f_{\mathrm{mc}}/f_{\mathrm{sc}})\sigma_{\mathrm{CBsc}}, \tag{4}$$

where σ_{CBmc} stands for the CB cross section using accurate, or multiconfiguration wave functions with the corresponding f value denoted by f_{mc} while σ_{CBsc} stands for the CB cross section using uncorrelated, or single configuration wave functions with the corresponding f value denoted by f_{sc}.

The E scaling and the f scaling can be applied consecutively if needed. For later use, we introduce a short-hand notation

$$\sigma_{\mathrm{E}f}=\sigma_{\mathrm{E}}(f_{\mathrm{mc}}/f_{\mathrm{sc}}). \tag{5}$$

III. COMPARISON TO EXPERIMENTS AND OTHER THEORIES

A. Heliun ion

Unscaled CB cross sections are compared in Figs. 1 and 2 to E-scaled CB cross sections and the excitation cross sections from the CCC method for the $1s-2p$ and $3p$ excitations of He^+ [7]. Note the high accuracy of the CB cross section for the $2p$ excitation by Burgess [8] considering the limited computing capability available in early 1960s.

Although E-scaled CB cross sections cannot account for the resonances near the threshold, the overall agreement with the CCC results is remarkable. Figures 1 and 2 also demonstrate that unscaled CB cross sections agree with unscaled PWB cross sections at $T\sim 300$ eV and higher, while the E-scaled and CCC results agree with the unscaled PWB cross sections only at $T\sim 1$ keV or higher. For nonhydrogenic ions, it is common to calculate the CB cross sections using partial-wave expansion, which becomes impractical for high T because very large number of partial waves are required. For the intermediate and high values of T where the unscaled CB and PWB cross sections agree, one can substitute E-scaled PWB cross sections, i.e., σ_{CB} in Eq. (3) replaced by σ_{PWB}, for E-scaled CB cross sections, resulting in considerable savings in computing time. The values of E and f to generate the scaled CB cross sections in Figs. 1 and 2 are presented in Table I, and the scaled CB cross sections are listed in Table II.

B. Magnesium and zinc ions

The BE- and f-scaled PWB cross sections agree well with reliable experimental data for the resonance transitions of neutral alkali metals, as has been shown in Ref. [1]. Hence, it is not surprising that the E-scaled CB cross sections agree well with experiments on the resonance transitions of Mg^+ and Zn^+ as is shown in Figs. 3 and 4.

For ion targets, available experimental data are sparse and not as reliable as the data for neutral atoms. For instance, the data by Smith *et al.* for Mg^+ [9] and for Zn^+ [9] have been measured by the energy loss method, i.e., the angular distribution of the scattered electron with a given energy loss that corresponds to the excitation energy E was measured. Such an experiment has difficulty in measuring cross sections at very small scattering angles in the forward direction where the cross section rises rapidly. The angular extrapolation necessary to obtain the integrated cross section introduces a large uncertainty. Part of the scatter in the experimental data by Smith *et al.* shown in Figs. 3 and 4 may have been caused by this type of difficulty. Note that the resonances in the $2p$ excitation of He^+ (Fig. 1) are limited to very near the threshold, while the scatter in the Smith data in Figs. 3 and 4 persists to the highest incident energy used. Figure 3 also includes theoretical results from the close-coupling method calculated using Hartree-Fock (marked Smith, HF) and correlated (marked Smith, CI) target wave functions [9]. The close-coupling results converge toward the E-scaled CB cross section for $T\sim 20$ eV, indicating that the scatter in the experimental data beyond $T\sim 20$ eV is likely to have come from experimental uncertainties.

For Zn^+ in Fig. 4, older experimental data by Rogers *et al.* [10] are also presented. Rogers *et al.* detected light emitted by the excited ion, hence their data are likely to be more reliable for the integrated cross section being compared in Fig. 4. The data by Rogers *et al.* clearly demonstrate that resonances are limited to $T\sim 20$ eV or lower, providing another clue that the data by Smith *et al.* may have much

TABLE II. Scaled Coulomb Born cross sections in A^2 for He^+, Mg^+, and Zn^+. T = incident electron energy in eV; σ_E = E scaled, Eq. (3); σ_{Ef} = E and f scaled, Eq. (5).

	σ_E			σ_{Ef}	
T	$He^+(1s\text{-}2p)$	$He^+(1s\text{-}3p)$	T	$Mg^+(3s\text{-}3p)$	$Zn^+(4s\text{-}4p)$
42	0.046 45		5	22.205	
43	0.046 97		6	20.964	
44	0.047 85		7	20.192	9.206
45	0.048 83		8	19.421	8.940
46	0.049 03		10	17.966	8.445
47	0.049 54		12	16.787	8.081
48	0.050 13		15	15.321	7.542
49	0.050 59	0.007 760	20	13.435	6.788
50	0.051 11	0.007 928	25	12.012	6.189
51	0.051 55	0.008 032	30	10.892	5.694
52	0.051 97	0.008 155	35	9.980	5.281
53	0.052 35	0.008 230	40	9.214	4.930
54	0.052 73	0.008 320	45	8.621	4.625
55	0.053 10	0.008 390	50	8.096	4.358
60	0.054 61	0.008 729	60	7.229	3.927
70	0.056 57	0.009 169	70	6.541	3.589
80	0.057 56	0.009 404	80	5.982	3.307
90	0.057 92	0.009 515	90	5.519	3.070
100	0.057 87	0.009 543	100	5.128	2.867
150	0.054 79	0.009 124	150	3.824	2.175
200	0.050 58	0.008 453	200	3.080	1.768
250	0.046 60	0.007 804	250	2.593	1.498
300	0.043 09	0.007 226	300	2.249	1.305
350	0.040 01	0.006 720	350	1.990	1.159
400	0.037 45	0.006 277	400	1.789	1.045
450	0.035 23	0.005 904	450	1.627	0.953
500	0.033 27	0.005 577	500	1.494	0.877
600	0.029 98	0.005 024	600	1.288	0.758
700	0.027 32	0.004 578	700	1.135	0.670
800	0.025 13	0.004 210	800	1.017	0.601
900	0.023 30	0.003 901	900	0.922	0.546
1000	0.021 74	0.003 639	1000	0.845	0.501

higher experimental uncertainties for $T > 20$ eV than the authors have indicated.

Accurate f values for the resonance transitions of Mg^+ and Zn^+ were obtained from Johnson, Liu, and Sapirstein [12] who used the relativistic random-phase approximation, and excitation energies from the National Institute of Standards and Technology atomic databases [13]. The values of E and f to generate the scaled CB cross sections in Figs. 3 and 4 are presented in Table I, and the scaled CB cross sections are listed in Table II. The excitation energies listed in Table I are for the excitations to the $np_{1/2}$ levels.

IV. CONCLUSIONS

The results presented in this paper and those in Ref. [1] for neutral atoms clearly demonstrate the utility of scaling the incident electron energy T in the denominator of Eq. (1) to obtain reliable electron-impact cross sections for dipole- and spin-allowed excitations of singly charged ions and neutral atoms. The E scaling corrects the shortcomings of the Born approximation, while the f scaling emulates accurate wave functions. Judging from the examples presented in this paper, the E scaling is expected to be effective for both light and heavy singly charged ions. At present, there is no ''derivation'' of the E scaling from first principles. Applications to more singly charged ions may eventually provide clues to the reason for the success of the E scaling as well as the BE scaling for neutral atoms. In this respect, it is desirable to have more experiments of the type Rogers *et al.* [10] have performed to obtain reliable integrated cross sections for comparison.

The trend between the E scaling for singly charged ions and the BE scaling for neutral atoms suggests that the required shifting of T in the denominators of Eqs. (2) and (3) for multiply charged ions may be smaller. Work to adapt the E scaling further for multiply charged ions is in progress, but drawing definitive conclusions becomes difficult as reliable

experimental data are scarce for such ions. Since the E scaling and *f* scaling do not distinguish between atomic and molecular ions, these scalings are expected to work as well to electronic excitations of molecular ions, after suitable averaging of vibrational and rotational excitations.

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