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Electron-impact-ionization cross sections for highly ionized heliumlike atoms

S. M. Younger
National Bureau of Standards, Washington, D.C. 20234
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Cross sections for electron-impact ionization from the ground states of four ions in the helium isoelectronic sequence have been calculated in the distorted-wave Born-exchange approximation. The results are in good agreement with available experimental data. Exchange in the scattering matrix element was found to be important in the determination of accurate cross sections. An isoelectronic plot of the scaled cross section permits ready interpolation of the nonrelativistic ionization cross section for any ion in the helium sequence in the incident electron energy range 1–5 times threshold.

I. INTRODUCTION

There is an urgent need within the fusion plasma effort for accurate information on the electron-impact ionization of highly ionized atoms. Such data are required to model the ionization balance in high-temperature plasmas and are also components in some diagnostic techniques. Until recently the only sources of data for the electron-impact-ionization cross sections of highly ionized atoms were simple semi-empirical formulas such as that of Lotz,[1] or semiclassical collision models such as the binary-encounter approximation[2] or the exchange classical impact parameter (ECIP) method.[3] While these simple procedures can sometimes yield data within a factor of two of experiment, they remain untested in the region of high ionic charge states where the most critical data need exists.

Attempts to apply quantum approximations to ionization have been made most notably by Golden and Sampson[4] and by Moores.[5] Their methods have been based primarily on a Coulomb-Born approximation with various approximations for exchange in the transition matrix element. Golden and Sampson have applied the scaled hydrogenic approximation to ionization from the states $1s$–$4f$,[6] and anticipate reasonable accuracy when $Z/N>3$, where Z is the nuclear charge and N the total number of target electrons. Jakubowicz and Moores[7] and co-workers have applied the Coulomb-Born exchange approximation of Rudge and Seaton.[8] Recently, the author has applied a distorted-wave version of the Born-exchange approximation (DBe) to the ionization of hydrogenlike and lithiumlike atoms, and has compared the results to those obtained with Coulomb and plane-wave scattering states.[9]

The present work describes the *ab initio* calculation of electron-impact-ionization cross sections of highly ionized heliumlike ions, where a significant amount of experimental data is available for comparison. Section II gives a brief review of the theory of the DBe technique for ionization cross-section calculations. Section III presents the results and compares them to existing theoretical and experimental data.

II. METHOD

Ignoring knockout processes, where the incident electron changes places with a bound electron which, along with a spectator, leaves the atom, the Born-exchange scattering cross section has been shown to be of the same form as for ionization from a one-electron atom times a statistical factor of 2.[10]

The distorted-wave Born-exchange approximation has been described in detail in a previous publication.[9] Partial-wave expansions are employed to describe the three continuum electrons (one incident, two final state) and the Hartree-Fock ground-state wave functions of Clementi and Roetti[11] were used for the target. The initial continuum state was computed in the potential

$$V_{1s^2} = -Z/r + 2J_{1s}(r)\,, \tag{1}$$

where

$$J_{1s}(r) = \frac{1}{r}\int_0^r [P_{1s}(\rho)]^2 d\rho + \int_r^\infty \frac{[P_{1s}(r)]^2}{\rho}\, d\rho \tag{2}$$

is the direct electrostatic potential of a $1s$ heliumlike Hartree-Fock orbital whose radial part is denoted $P_{1s}(r)$. In the direct matrix element, the ejected (lower energy) electron was computed in the potential

$$V_{1s} = -Z/r + J_{1s}(r) \tag{3}$$

and the scattered (higher-energy) electron in V_{1s^2}. In the exchange matrix element this pairing is reversed—the ejected electron is computed in V_{1s^2} and the scattered electron in V_{1s}. This somewhat nonphysical choice for the exchange matrix element partial waves is tolerated in order to obtain orthogonal overlapping orbitals in the matrix element and has been found to yield cross sections in good agreement with available experimental data.[7,9] We follow our previous convention in choosing the phase of the matrix element to maximize the exchange contribution.

III. RESULTS

Electron-impact-ionization cross sections computed in the distorted-wave Born-exchange approximation for ionization from the ground states of Li II, B IV, N VI, and Na X are given in Table I. To demonstrate the effect of electron exchange in the transition matrix element we also list "distorted-wave truncated"[8] cross sections which neglect exchange and interference effects entirely. The no-exchange cross sections are given in parentheses.

Figure 1 shows an isoelectronic plot of the scaled cross section

$$\overline{Q} = uI^2Q\,, \tag{4}$$

where u is the incident electron energy in ionization threshold units, I is the ionization energy in eV, and Q is the total cross section in cm^2. Such a plot is of particular interest in that it allows ready interpolation of the nonrelativistic ionization cross section of any ion in the helium isoelectronic sequence over the energy region considered.

Figure 2 compares the present DBe results for Li^+ with the experimental crossed-beam data of Lineberger *et al.*[12] and Peart and Dolder,[13] as well as the Coulomb-Born no-exchange calculation of Moores and Nussbaumer.[14] Excellent agreement is obtained between the DBe results and both experiments. Of particular interest is the importance of exchange in determining an accurate cross section. Figures 3–5 show similar comparisons between DBe results and the crossed-beam data of Crandall *et al.*[15] for B IV, C V, and N VI. Explicit calculations were not performed for C V—rather the isoelectronic plot in Fig. 1 was used to interpolate between results for neighboring B IV and N VI. Only fair agreement is obtained between theory and experiment for N VI. No experimental data is available for Na X.

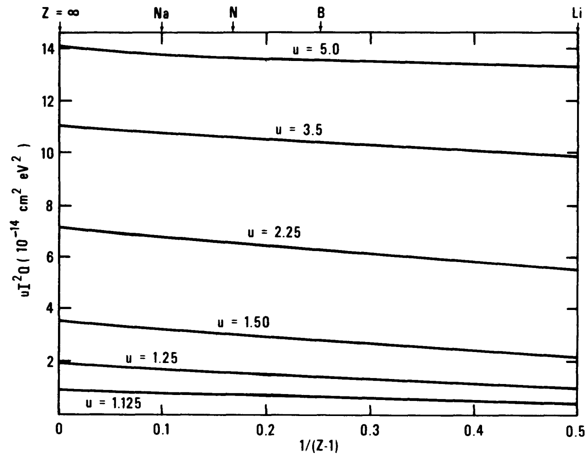

FIG. 1. Isoelectronic plot of the nonrelativistic scaled electron-impact-ionization cross sections uI^2Q for heliumlike ions in units of $cm^2\,eV^2$. Each curve corresponds to a fixed incident electron energy measured in ionization threshold units $u = E_i/I$.

TABLE I. Electron-impact-ionization cross section for highly ionized heliumlike atoms computed in the distorted-wave Born-exchange approximation.[a]

$u = E_i/I$	Li II $Q(10^{-18}\ cm^2)$ $I = 75.638$ eV	B IV $Q(10^{-19}\ cm^2)$ $I = 259.37$ eV	N VI $Q(10^{-19}\ cm^2)$ $I = 552.06$ eV	Na X $Q(10^{-20}\ cm^2)$ $I = 1465.1$ eV
1.125	0.771	0.988	0.244	0.375
	(0.845)	(1.03)	(0.249)	(0.374)
1.25	1.45	1.73	0.421	0.643
	(1.67)	(1.89)	(0.447)	(0.667)
1.50	2.55	2.77	0.660	0.991
	(3.04)	(3.16)	(0.734)	(1.08)
2.25	4.31	4.14	0.949	1.39
	(5.20)	(4.87)	(1.10)	(1.59)
3.5	4.94	4.43	0.990	1.43
	(5.81)	(5.16)	(1.15)	(1.64)
5.0	4.65	4.03	0.890	1.28
	(5.34)	(4.61)	(1.01)	(1.45)

[a] Distorted-wave results neglecting exhange are given in parentheses.

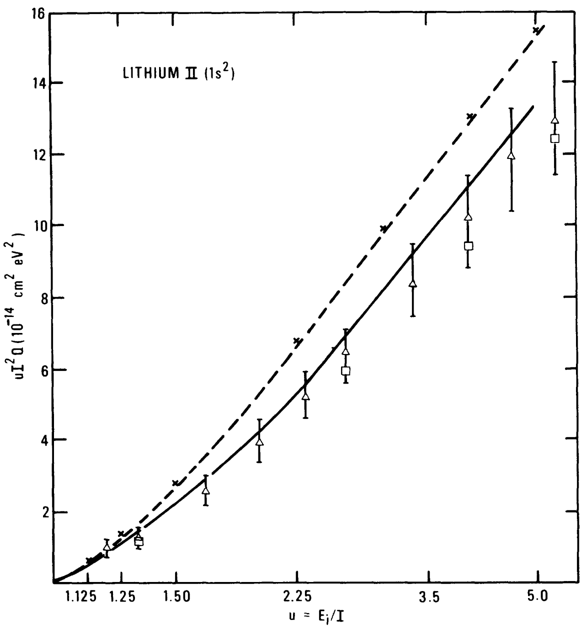

FIG. 2. Comparison of the present distorted-wave results for Li II with crossed-beam measurements and the Coulomb-Born no-exchange calculation of Moores and Nussbaumer. —— distorted wave with exchange; --- distorted wave without exchange; × Coulomb-Born, Ref. 14; △ crossed-beam, Ref. 12; □ crossed-beam, Ref. 13.

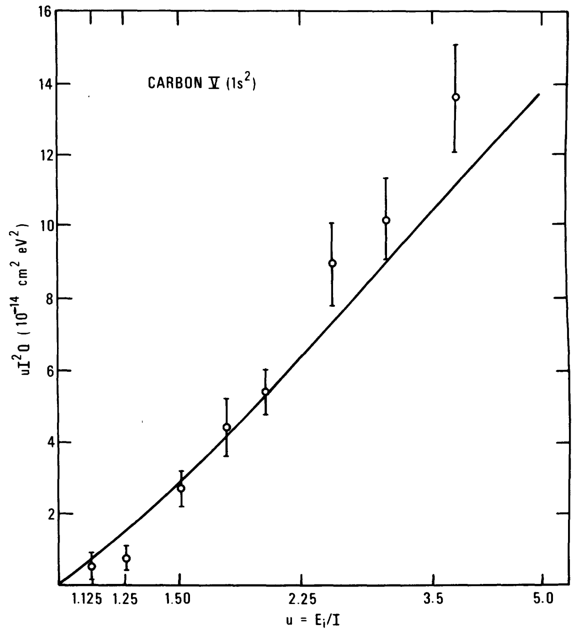

FIG. 4. Comparison of the present distorted-wave results for C V with crossed-beam measurements. The distorted-wave cross sections were interpolated from isoelectronic data for the neighboring ions B IV and N VI. —— distorted-wave Born exchange; ○ crossed-beam, Ref. 15.

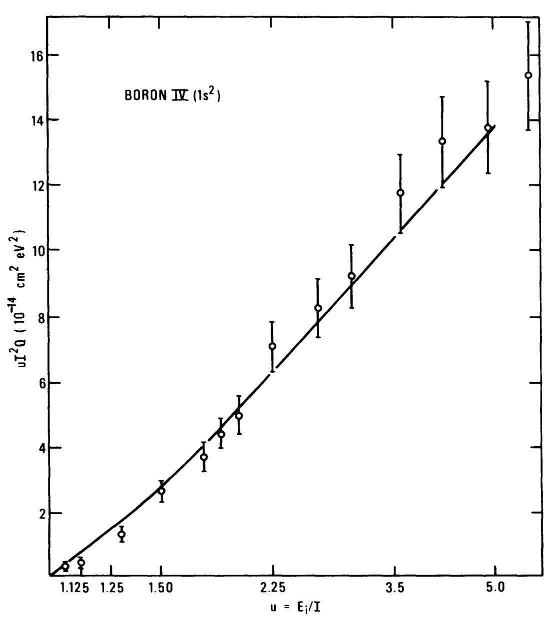

FIG. 3. Comparison of the present distorted-wave results for B IV with crossed-beam measurements. —— distorted-wave Born exchange; ○ crossed-beam, Ref. 15.

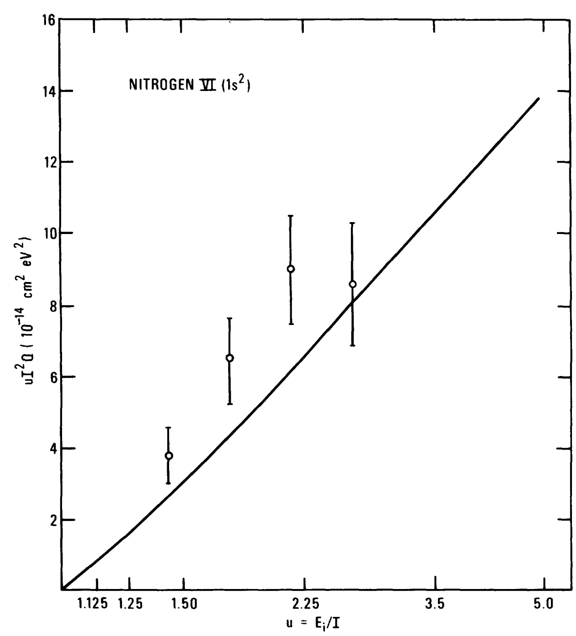

FIG. 5. Comparison of the present distorted-wave results for N VI with crossed-beam measurements. —— distorted-wave Born exchange; ○ crossed-beam, Ref. 15.

IV. CONCLUSION

Electron-impact-ionization cross sections have been calculated in the distorted-wave Born-exchange approximation using Hartree-Fock target wave functions. Good agreement between theory and experimental crossed-beam data was found for Li II, B IV, and C V. Exchange in the scattering matrix element was found to be important in the determination of an accurate cross section, reducing the no-exchange value by ~10–15% at five times threshold. Target configuration interaction effects are expected to be negligible for highly ionized heliumlike ions. No consideration of resonances was given, however, the close agreement between theory and experiment indicates that such an omission may not be serious. The regular behavior of the isoelectronic plot shown in Fig. 1 indicates that scaling of the ionization cross section by the square of the ionization energy (Thomson scaling) is an efficient manner of presenting cross-section data along an isoelectronic sequence.

ACKNOWLEDGMENT

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