Fully relativistic electron-impact ionization of atomic ions

M. S. Pindzola and M. J. Buie
Department of Physics, Auburn University, Auburn, Alabama 36849
(Received 10 December 1987)

A fully relativistic electron-impact ionization cross section is calculated as a triple partial-wave expansion of the first Born scattering amplitude. The target atomic ion is described by a Dirac-Fock approximation, a *jj* subconfiguration average method is used to calculate the scattering algebra, and the radial partial waves (εlj) are computed in distorted-wave potentials. The resulting general computational scheme is applied to electron-impact ionization of U^{89+}. The fully relativistic cross-section results are compared with those obtained from both nonrelativistic and semirelativistic theories.

I. INTRODUCTION

Although indirect processes in electron-impact ionization of atomic ions have been shown to be quite important,[1] the calculation of the direct ionization process remains an integral part of obtaining a total ionization cross section. One of the most successful methods for calculating direct-ionization cross sections is based on a triple partial-wave expansion of the first Born scattering amplitude.[2] The target atomic ion is described by a Hartree-Fock approximation, while the incident, ejected, and scattered partial waves are calculated as either Coulomb waves[3,4] or frozen-core Hartree-Fock distorted waves.[5] The maximum-interference approximation of Peterkop[2] may be used to account for electron exchange among the ejected and scattered electrons. The resulting nonrelativistic calculational method is commonly called the distorted-wave Born exchange method.

For electron-impact ionization of heavy atomic ions, relativistic effects should play an important role. In this paper the distorted-wave Born exchange method is formulated in terms of a Dirac-Fock approximation for both the target atomic ion and the various partial waves. The resulting fully relativistic distorted-wave Born exchange method is applied to the calculation of the 2*s*-subshell ionization cross section of U^{89+}, in support of recent attempts[6] to measure electron ionization of highly charged uranium using the Bevalac accelerator.

The remainder of this paper is arranged as follows. In Sec. II the fully relativistic distorted-wave Born exchange method for electron-impact direct ionization of atomic ions is formulated. In Sec. III the fully relativistic cross-section results for U^{89+} are compared with those obtained from both nonrelativistic and semirelativistic theories. A brief summary is contained in Sec. IV.

II. THEORY

A nonrelativistic direct-ionization cross section may be calculated in a configuration-average distorted-wave approximation.[7] The most general direct-ionization transition between configurations is of the form

$$e^- + (n_b l_b)^W \rightarrow (n_b l_b)^{W-1} + e^- + e^- , \tag{1}$$

where n is the principal quantum number, l is the angular momentum quantum number, and W is the occupation number of the configuration subshell. The configuration-average direct-ionization cross section (in atomic units) is given by

$$\sigma_{\mathrm{CA}} = \int_0^{E/2} \frac{16W}{k_i^3 k_e k_f} \sum_{l_i,l_e,l_f} \left[\sum_{\lambda} \Omega_d^{\lambda} + \sum_{\lambda'} \Omega_e^{\lambda'} - \sum_{\lambda,\lambda'} | \Omega_{\mathrm{int}}^{\lambda\lambda'} | \right] d(k_e^2/2) , \tag{2}$$

where

$$\Omega_d^{\lambda} = 2(2l_i+1)(2l_e+1)(2l_f+1) A(l_e,l_f,l_b,l_i,\lambda) \times [R^{\lambda}(k_e l_e, k_f l_f; n_b l_b, k_i l_i)]^2 , \tag{3}$$

$$\Omega_e^{\lambda'} = 2(2l_i+1)(2l_e+1)(2l_f+1) B(l_f,l_e,l_b,l_i,\lambda') \times [R^{\lambda'}(k_f l_f, k_e l_e; n_b l_b, k_i l_i)]^2 , \tag{4}$$

$$\Omega_{\mathrm{int}}^{\lambda\lambda'} = 2(2l_i+1)(2l_e+1)(2l_f+1) C(l_e,l_f,l_b,l_i,\lambda,\lambda') \times R^{\lambda}(k_e l_e, k_f l_f; n_b l_b, k_i l_i) \times R^{\lambda'}(k_f l_f, k_e l_e; n_b l_b, k_i l_i) , \tag{5}$$

and $E = (k_e^2 + k_f^2)/2$. In Eq. (2) k_i, k_e, and k_f are the linear momenta of the incident, ejected, and scattered electrons, respectively; R^{λ} represents the usual Slater radial integral; and the continuum normalization is one times a sine function. The angular coefficients in terms of standard 3-*j* and 6-*j* symbols are given by

$$A(l_e,l_f,l_b,l_i,\lambda) = \begin{pmatrix} l_e & \lambda & l_b \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{pmatrix} l_f & \lambda & l_i \\ 0 & 0 & 0 \end{pmatrix}^2 \Big/ (2\lambda+1) , \tag{6}$$

$$B(l_f,l_e,l_b,l_i,\lambda')=\begin{pmatrix} l_f & \lambda' & l_b \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{pmatrix} l_e & \lambda' & l_i \\ 0 & 0 & 0 \end{pmatrix}^2 \Big/ (2\lambda'+1) , \tag{7}$$

and

$$C(l_e,l_f,l_b,l_i,\lambda,\lambda')=-(-1)^{\lambda+\lambda'} \begin{Bmatrix} l_e & \lambda & l_b \\ 0 & 0 & 0 \end{Bmatrix} \begin{Bmatrix} l_f & \lambda & l_i \\ 0 & 0 & 0 \end{Bmatrix} \begin{Bmatrix} l_f & \lambda' & l_b \\ 0 & 0 & 0 \end{Bmatrix} \begin{Bmatrix} l_e & \lambda' & l_i \\ 0 & 0 & 0 \end{Bmatrix} \begin{Bmatrix} l_e & l_b & \lambda \\ l_f & l_i & \lambda' \end{Bmatrix} . \tag{8}$$

The maximum-interference approximation of Peterkop[2] is imposed by taking the negative of the absolute value of the third term in Eq. (2).

The energies and bound radial orbitals needed to evaluate the cross section of Eq. (2) are calculated in the Hartree-Fock approximation.[8,9] The continuum radial orbitals needed to complete the evaluation of the cross section are obtained by solving the single-channel Schrödinger equation

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{l(l+1)}{2r^2}-\frac{Z}{r}+V_{\rm HF}-\frac{k^2}{2}\right]P_{kl}(r)=0 , \tag{9}$$

where the distorting-potential operator $V_{\rm HF}$ is constructed from previously calculated Hartree-Fock (HF) target orbitals. For rapid evaluation of many continuum orbitals a local distorting potential constructed in a semiclassical exchange approximation[10] has proved quite useful. This exchange term simplifies the solution of the differential equation and generally gives results in close agreement with those obtained from a full nonlocal Hartree-Fock continuum calculation.

A semirelativistic direct-ionization cross section may also be calculated in a configuration-average distorted-wave approximation.[11] The energies and bound radial orbitals needed to evaluate the cross section of Eq. (2) are calculated in the Hartree-Fock approximation with relativistic modifications,[12] which includes the mass-velocity and Darwin corrections within modified differential equations. The continuum radial orbitals are obtained by solving a similarly modified single-channel Schrödinger equation

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{l(l+1)}{2r^2}-\frac{Z}{r}+V_{\rm HFR}+V_{\rm rel}-\frac{k^2}{2}\right]P_{kl}(r) =0 , \tag{10}$$

where the distorting-potential operator $V_{\rm HFR}$ is constructed from previously calculated Hartree-Fock relativistic (HFR) target orbitals. If $V_{\rm HFR}$ is approximated by a local distorting potential $\tilde{V}_{\rm HFR}$, then $V_{\rm rel}$ is given by

$$V_{\rm rel}=-\frac{\alpha^2}{2}\left[\frac{k^2}{2}-\tilde{V}_{\rm HFR}\right]^2 - \delta_{l,0}\frac{\alpha^2}{4}\left[1+\frac{\alpha^2}{2}\left[\frac{k^2}{2}-\tilde{V}_{\rm HFR}\right]\right]^{-1} \times\frac{d\tilde{V}_{\rm HFR}}{dr}\left[\frac{dP_{kl}/dr}{P_{kl}}-\frac{1}{r}\right] , \tag{11}$$

where the first term is the mass-velocity contribution, the second term is the Darwin contribution, and $\alpha=\frac{1}{137}$ is the fine-structure constant. Due to the presence of $P_{kl}(r)$ in the Darwin term, the Schrödinger equation of Eq. (10) must be solved iteratively for $l=0$ continuum orbitals.

A fully relativistic direct-ionization cross section may be calculated in a subconfiguration-average distorted-wave approximation. The most general direct-ionization transition between subconfigurations is of the form

$$e^-+(n_bl_bj_b)^W\rightarrow(n_bl_bj_b)^{W-1}+e^-+e^- , \tag{12}$$

where $j=l\pm\frac{1}{2}$ $(l\neq 0)$ is the total angular momentum quantum number. The subconfiguration-average direct-ionization cross section is given by

$$\sigma_{\rm SCA}=\int_0^{E/2}\frac{16W_1}{p_i^3p_ep_f}\sum_{l_i,l_e,l_f}\left[\sum_{\lambda}\bar{\Omega}_d^{\lambda}+\sum_{\lambda'}\bar{\Omega}_e^{\lambda'}-\sum_{\lambda,\lambda'}|\bar{\Omega}_{\rm int}^{\lambda\lambda'}|\right]d\varepsilon_e , \tag{13}$$

where

$$\bar{\Omega}_d^{\lambda}=\sum_{j_i,j_e,j_f}(2j_i+1)(2j_e+1)(2j_f+1)\bar{A}(l_e,j_e,l_f,j_f,l_b,j_b,l_i,j_i,\lambda)[R^{\lambda}(\varepsilon_el_ej_e,\varepsilon_fl_fj_f;n_bl_bj_b,\varepsilon_il_ij_i)]^2 , \tag{14}$$

$$\bar{\Omega}_e^{\lambda'}=\sum_{j_i,j_e,j_f}(2j_i+1)(2j_e+1)(2j_f+1)\bar{B}(l_f,j_f,l_e,j_e,l_b,j_b,l_i,j_i,\lambda')[R^{\lambda'}(\varepsilon_fl_fj_f,\varepsilon_el_ej_e;n_bl_bj_b,\varepsilon_il_ij_i)]^2 , \tag{15}$$

$$\bar{\Omega}_{\rm int}^{\lambda\lambda'}=\sum_{j_i,j_e,j_f}(2j_i+1)(2j_e+1)(2j_f+1)\bar{C}(l_e,j_e,l_f,j_f,l_b,j_b,l_i,j_i,\lambda,\lambda') \times R^{\lambda}(\varepsilon_el_ej_e,\varepsilon_fl_fj_f;n_bl_bj_b,\varepsilon_il_ij_i)R^{\lambda'}(\varepsilon_fl_fj_f,\varepsilon_el_ej_e;n_bl_bj_b,\varepsilon_il_ij_i) , \tag{16}$$

and $E=\varepsilon_e+\varepsilon_f$. For relativistic calculations the energy ε is the total energy of the electron minus its rest energy, $p=(2\varepsilon+\alpha^2\varepsilon^2)^{1/2}$ is the linear momentum, R^λ represents a Slater radial integral containing both large and small components, and the continuum normalization is $(1+\alpha^2\varepsilon/2)^{1/2}$ times a sine function. The angular coefficients are given by

$$\bar{A}(l_e,j_e,l_f,j_f,l_b,j_b,l_i,j_i,\lambda)=\begin{pmatrix} j_e & \lambda & j_b \\ \frac{1}{2} & 0 & -\frac{1}{2}\end{pmatrix}^2\begin{pmatrix} j_f & \lambda & j_i \\ \frac{1}{2} & 0 & -\frac{1}{2}\end{pmatrix}^2\Big/(2\lambda+1)\,, \tag{17}$$

provided $(l_e+l_b+\lambda)$ and $(l_f+l_i+\lambda)$ are both even, otherwise $\bar{A}=0$;

$$\bar{B}(l_f,j_f,l_e,j_e,l_b,j_b,l_i,j_i,\lambda')=\begin{pmatrix} j_f & \lambda' & j_b \\ \frac{1}{2} & 0 & -\frac{1}{2}\end{pmatrix}^2\begin{pmatrix} j_e & \lambda' & j_i \\ \frac{1}{2} & 0 & -\frac{1}{2}\end{pmatrix}^2\Big/(2\lambda'+1)\,, \tag{18}$$

provided $(l_f+l_b+\lambda')$ and $(l_e+l_i+\lambda')$ are both even, otherwise $\bar{B}=0$; and

$$\bar{C}(l_e,j_e,l_f,j_f,l_b,j_b,l_i,j_i,\lambda,\lambda')$$
$$=+2(-1)^{\lambda+\lambda'}\begin{pmatrix} j_e & \lambda & j_b \\ \frac{1}{2} & 0 & -\frac{1}{2}\end{pmatrix}\begin{pmatrix} j_f & \lambda & j_i \\ \frac{1}{2} & 0 & -\frac{1}{2}\end{pmatrix}\begin{pmatrix} j_f & \lambda' & j_b \\ \frac{1}{2} & 0 & -\frac{1}{2}\end{pmatrix}\begin{pmatrix} j_e & \lambda' & j_i \\ \frac{1}{2} & 0 & -\frac{1}{2}\end{pmatrix}\begin{Bmatrix} j_e & j_b & \lambda \\ j_f & j_i & \lambda'\end{Bmatrix}, \tag{19}$$

provided $(l_e+l_b+\lambda)$, $(l_f+l_i+\lambda)$, $(l_f+l_b+\lambda')$, and $(l_e+l_i+\lambda')$ are all even, otherwise $\bar{C}=0$. The interference approximation imposed in Eq. (13) is not the maximum interference, but it does correspond in the nonrelativistic limit to the direct-exchange phase choice of Eq. (2). The maximum interference is obtained by moving the absolute value found in the third term of Eq. (13) inside the triple j sum for $\bar{\Omega}_{\rm int}^{\lambda\lambda'}$.

The energies and bound radial orbitals needed to evaluate the cross section of Eq. (13) are calculated in the Dirac-Fock approximation.[13,14] The continuum radial orbitals needed to complete the evaluation of the cross section are obtained by solving the single-channel Dirac equation

$$\left[\frac{d}{dr}+\frac{\kappa}{r}\right]P_{\varepsilon lj}(r)+\alpha[V_n(r)-\varepsilon-2/\alpha^2+V_{\rm DF}]Q_{\varepsilon lj}(r)=0\,,$$
$$\left[\frac{d}{dr}-\frac{\kappa}{r}\right]Q_{\varepsilon lj}(r)-\alpha[V_n(r)-\varepsilon+V_{\rm DF}]P_{\varepsilon lj}(r)=0\,, \tag{20}$$

where the distorting-potential operator $V_{\rm DF}$ is constructed from previously calculated Dirac-Fock (DF) target orbitals. In Eq. (20) $\kappa=\pm(j+\frac{1}{2})$ and $V_n(r)$ is the nuclear potential. A relativistic generalization of the semiclassical exchange approximation is used to construct a local distorting potential for calculation of the hundreds of continuum orbitals needed to evaluate the cross section of Eq. (13).

III. RESULTS

General purpose computer codes have been written based on the configuration-average cross section of Eq. (2) and the subconfiguration-average cross section of Eq. (13). The configuration-average ionization code (CAION) has been used for many years to generate direct-ionization cross sections for atomic ions of interest to controlled fusion research. In fact, the generally favorable agreement found between the CAION code results and a wide variety of crossed-beam experiments forms an empirical justification for the maximum-interference approximation employed in the cross section of Eq. (2). The new subconfiguration-average ionization code (SCAION) was first tested by calculating the $3s$-subshell ionization cross section for Al^{2+}. At the cross-section peak the numerical cross-section results from the CAION and SCAION codes agree to three significant figures; this should be expected since relativistic effects in Al^{2+} are quite small. In purely scalar operational terms the SCAION code is intrinsically a factor of 2^4 or 2^5 times slower than the CAION code due to the increase in both the number of partial waves (l versus lj) and the number of radial orbital components (1 versus 2).

To explore the validity of semirelativistic theories of ionization and to support channeling experiments using the Belavac accelerator, we used the CAION and SCAION codes to calculate the $2s$-subshell ionization cross section for U^{89+}. Various atomic parameters for U^{89+} are given in Table I based on a $1s^22s$ single-configuration approxi-

TABLE I. Atomic parameters for U^{89+}.

Approximation	Total energy (keV)	Ionization potential (keV)	$\langle r_{2s}\rangle$ (a.u.)
Hartree-Fock	−256.6	27.80	0.066
Hartree-Fock relativistic	−293.4	32.81	0.055
Dirac-Fock	−295.2	32.92	0.054
Dirac-Fock with Breit and QED	−294.2	32.84	

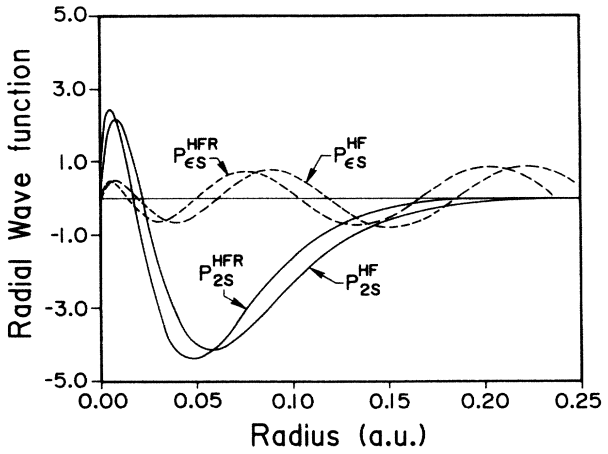

FIG. 1. Hartree-Fock (HF) and Hartree-Fock with relativistic modifications (HFR) bound and continuum orbitals for U^{89+}. The solid curves are different approximations for the $2s$ orbital; the dashed curves are s-wave continuum orbitals calculated at an energy of 500 a.u.

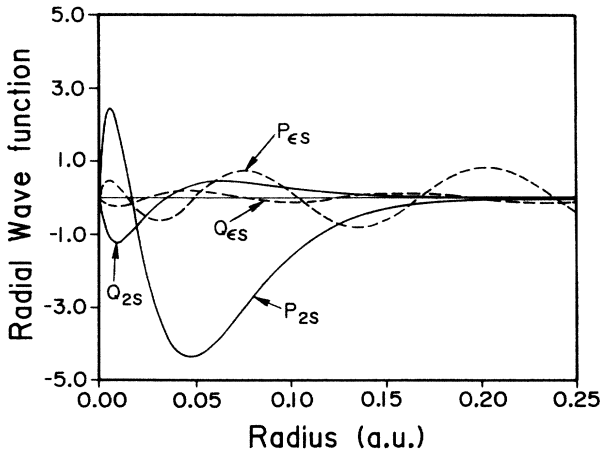

FIG. 2. Dirac-Fock bound and continuum orbitals for U^{89+}. The solid curves are the large P and small Q components of the $2s$ orbitals; the dashed curves are components of an s-wave continuum orbital calculated at an energy of 500 a.u.

mation for the ground state. The HF and HFR results are obtained using Cowan's bound-state wave-function computer code,[9] while the DF results are obtained from Grant's code.[14] The HFR method accounts for 95% of the 38.6-keV difference in the HF and DF total energies. The HFR method also does quite well in comparison with the DF results for both the ionization potential and the $2s$-subshell mean radius. Many previous research papers, the latest by Kobus and Jaskolski,[15] have shown that the HFR method is able to produce orbital energies and transition probabilities in very good agreement with the DF method for a wide variety of heavy atoms and ions.

For near-threshold electron scattering from U^{89+}, relativistic corrections to the Coulomb electron-electron interaction, $e^2/|\mathbf{r}_i-\mathbf{r}_j|$, should be small. As shown in Table I, transverse Breit and QED perturbation theory corrections, obtained from McKensie's code,[16] are found to raise the DF total energy by only 0.3% for the $1s^22s$ configuration. The cross-section correction due to the exchange of a virtual transverse photon, which is the analog of the atomic structure Breit interaction, has generally been found[17] to be small for incident electron energies much less than the electron rest mass, which is the case here.

Bound and continuum radial orbitals for U^{89+} in various approximations are presented in Figs. 1 and 2. The s-wave continuum orbitals are calculated with an energy of 500 a.u. (13.6 keV). We find several items of interest in examining these wave-function plots. The first item is that the substantial phase difference in the HF and HFR continuum orbitals shown in Fig. 1 is mainly caused by the V_{Rel} potential operator of Eq. (11). The mass-velocity term is quite attractive while the Darwin term is mildly repulsive. The second item is that both the bound and continuum HFR orbitals of Fig. 1 are in very good agreement with the large component DF orbitals of Fig. 2. In fact, the agreement is within the width of the lines used to draw the curves. The third item is that the small-component DF orbitals of Fig. 2 are quite appreciable at small distances from the nucleus.

Electron-ionization cross sections for the $2s$ subshell of U^{89+} are presented in Table II and Fig. 3. The HF and HFR results, which differ by almost a factor of 2 at the peak of the cross section, are both calculated using the CAION code. The semirelativistic theory prediction of a decrease in the cross section is based, in part, on the relativistic contraction of the $2s$ target orbital. Based on the DF results calculated using the new SCAION code, however, the semirelativistic HFR theory has substantially overestimated the cross-section reduction. The source of the difference between the DF and HFR results can be traced to the neglect of the small-component wave function inherent in the HFR method. If one repeats the DF calculation using a modified version of the SCAION code which ignores small-component contributions, the DF modified and HFR results agree to within 12%. The

TABLE II. Cross sections for U^{89+}.

Energy (threshold units)	Hartree-Fock (10^{-24} cm^2)	Hartree-Fock relativistic (10^{-24} cm^2)	Dirac-Fock (10^{-24} cm^2)
1.10	5.44	3.13	4.09
1.50	15.77	9.03	12.07
2.00	19.22	10.98	15.11

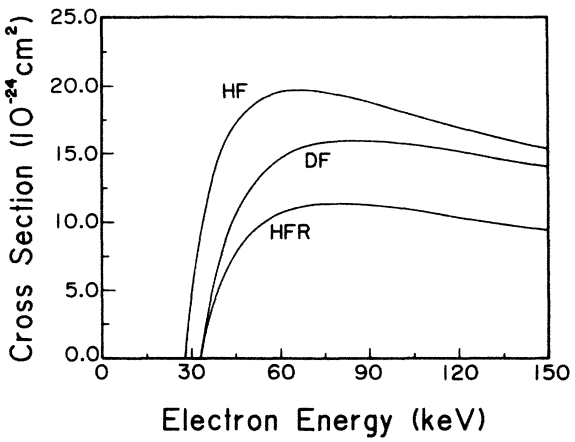

FIG. 3. Electron-impact ionization cross section for U^{89+}. The three solid curves are different approximations: Hartree-Fock (HF), Hartree-Fock with relativistic modifications (HFR), and Dirac-Fock (DF).

remaining discrepancy is probably due to the omission of the spin-orbit interaction in the semirelativistic theory.

We speculate that the poor performance of the HFR method in predicting the electron-ionization cross section for U^{89+} is due to a combination of three factors. The first factor is that the $1s^22s$ configuration is quite sensitive to relativistic effects since the configuration contains only $l=0$ penetrating orbitals. The second factor is that the small-component effect on continuum normalization cannot be ignored in a problem involving three partial waves. The third factor is that the Coulomb matrix elements involved in the electron-ionization calculation are more sensitive to the small components than the dipole matrix elements involved in transition probability calculations. They may simply weight regions near the nucleus more heavily where the small components are largest, as, for instance, in the calculation of $\langle 1/r \rangle$ as opposed to $\langle r \rangle$.

Before closing this section we make a comment on the choice of continuum phase in the SCAION code. The cross-section results for U^{89+} presented in Table II and Fig. 3 were all obtained using the approximation of maximum interference between the direct and exchange terms for each l partial cross section. If one repeats the DF calculation using a modified version of the SCAION code which employs the maximum interference between the direct and exchange terms for each lj partial cross section, the original DF results are lowered by an additional 4%. Unfortunately, the difference between the l and lj interference approximations for other atomic ions may be larger than found here for U^{89+}. The proper choice of continuum phase in electron-ionization theory remains a long-standing problem.

IV. SUMMARY

In this paper we first derived a fully relativistic theory for electron-impact ionization of atomic ions and then applied the calculational method to the electron ionization of U^{89+}. The fully relativistic cross-section results for U^{89+} were found to be much larger than the cross-section predictions of semirelativistic theory. The difference was attributed, in large measure, to the fact that the Dirac small-component wave function is ignored in semirelativistic theory. To better understand the range of validity of the semirelativistic theory of electron-impact ionization, we plan to extend our studies in the future to other atomic ions in the uranium isonuclear sequence.

ACKNOWLEDGMENTS

We wish to thank R. D. Cowan for making his atomic structure programs available to us. We would also like to thank D. C. Griffin, C. Bottcher, and C. E. Bemis, Jr. for useful discussions. This work was supported by the Office of Fusion Energy, U.S. Department of Energy, under Contract No. DE-FG05-86ER53217 with Auburn University.

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