Fully relativistic time-dependent close-coupling method for electron-impact ionization of atomic ions

M. S. Pindzola, J. A. Ludlow, and F. Robicheaux
Department of Physics, Auburn University, Auburn, Alabama, 36849 USA

J. Colgan and C. J. Fontes
Los Alamos National Laboratory, Los Alamos, New Mexico, 87545 USA
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A fully relativistic time-dependent close-coupling method is developed based on Dirac's covariant formulation of quantum mechanics. The expansion of a one-electron wave function in spin-orbit eigenfunctions yields the well-known coupled Dirac equations in two radial wave functions, while the expansion of a two-electron wave function in coupled spin-orbit eigenfunctions yields close-coupled Dirac equations in four radial wave functions. The time-dependent Dirac equations are solved directly using numerical methods that avoid the Fermi doubling pathology. Test calculations are carried out using the one-electron coupled equations for $j=\frac{1}{2}$ elastic potential scattering from Ne^{9+} at 2.00 keV and using the two-electron close-coupled equations for $J=0,1$ ionization of Ne^{9+} at 4.15 keV.

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I. INTRODUCTION

The electron-impact direct ionization of an atom or atomic ion yields two continuum electrons moving in the Coulomb field of the residual ion: the quantal three-body breakup problem. For neutral atoms and low-charged atomic ions, a low-order perturbative treatment of the problem is not very accurate. The perturbative distorted-wave method can be up to 40% high for total peak cross sections, while for certain energies and angles the differential cross sections can be off by a factor of 2 or more. Over the last two decades the converged close-coupling, R matrix with pseudostates, and time-dependent close-coupling methods [1–3] have generated accurate total and differential ionization cross sections for a number of atoms and low-charged ions using a nonperturbative solution of the nonrelativistic Schrödinger equation.

For highly charged atomic ions, a low-order perturbative solution of the fully relativistic Dirac equation [4,5] is reasonably accurate for total ionization cross sections. In the next few years, experiments at new ion-beam facilities [6] may be able to begin observations of differential ionization cross sections for highly charged ions. Recently, convergent close-coupling [7] and R matrix with pseudostates [8] methods have been developed based on a nonperturbative solution of the fully relativistic Dirac equation. Although only model problems were tested with the new methods, total and differential ionization cross sections of highly charged atomic ions will appear soon.

In this paper, a time-dependent close-coupling method is developed for the direct solution of the Dirac equation. Using spherical polar coordinates, a one-electron wave function is expanded in spin-orbit eigenfunctions to derive the well-known coupled Dirac equations in two radial wave functions [9,10]. An expansion of a two-electron wave function in coupled spin-orbit eigenfunctions yields close-coupled Dirac equations in four radial wave functions [11]. The one- and two-electron time-dependent Dirac equations are solved directly using numerical methods developed previously for the one- and two-electron time-dependent Schrödinger equations [12]. Care is taken to choose discretization methods that avoid the Fermi doubling pathology [13]. The one-electron time-dependent coupled equations are solved for $j=\frac{1}{2}$ elastic scattering off the Hartree potential for Ne^{9+} by 2.00 keV incident electrons. The two-electron time-dependent close-coupled equations are solved for $J=0,1$ ionization of Ne^{9+} by 4.15 keV incident electrons. In both test calculations, comparisons are made with cross-section results obtained by solving the time-dependent Schrödinger equation.

The rest of the paper is organized as follows. In Sec. II we develop a fully relativistic time-dependent close-coupling method for the electron-impact ionization of atomic ions. In Sec. III we apply fully relativistic time-dependent methods to calculate electron-impact elastic and inelastic cross sections for Ne^{9+}. In Sec. IV, we conclude with a summary and an outlook for future work. Unless otherwise stated, all quantities are given in atomic units.

II. THEORY

A. General time-dependent equations

The time-dependent Dirac equation for one electron moving in the Coulomb field of the nucleus is given by [9,10]

$$i\frac{\partial\vec{\Psi}(\vec{r},t)}{\partial t}=H(\vec{r})\vec{\Psi}(\vec{r},t), \tag{1}$$

where

$$H(\vec{r})=\begin{pmatrix} V(r) & c\vec{\sigma}\cdot\vec{p}(\vec{r}) \\ c\vec{\sigma}\cdot\vec{p}(\vec{r}) & V(r)-2c^2 \end{pmatrix}, \tag{2}$$

$V(r)=-\frac{Z}{r}$, Z is the nuclear charge, $\vec{\sigma}$ are the Pauli matrices, and $\vec{p}(\vec{r})=-i\nabla$. The one-electron wave function may be expanded in spin-orbit eigenfunctions,

$$\vec{\Psi}(\vec{r},t) = \begin{pmatrix} \dfrac{P_\kappa(r,t)}{r}\Phi_{+\kappa,m}(\theta,\phi) \\ i\dfrac{Q_\kappa(r,t)}{r}\Phi_{-\kappa,m}(\theta,\phi) \end{pmatrix}, \tag{3}$$

where

$$\Phi_{\kappa,m}(\theta,\phi) = \sum_{m_l,m_s} C^{lsj}_{m_l m_s m} Y_{lm_l}(\theta,\phi)\chi_{m_s}, \tag{4}$$

$\kappa=-(l+1)$ for $j=l+\frac{1}{2}$, $\kappa=+l$ for $j=l-\frac{1}{2}$, $s=\frac{1}{2}$, $C^{lsj}_{m_l m_s m}$ is a Clebsch-Gordan coefficient, $Y_{lm}(\theta,\phi)$ is a spherical harmonic, and χ_{m_s} is a two-component spinor. Substitution of Eq. (3) into Eq. (1) and projection onto the spin-orbit eigenfunctions yields the time-dependent coupled equations,

$$i\frac{\partial P_\kappa(r,t)}{\partial t} = V(r)P_\kappa(r,t) - c\left(\frac{\partial}{\partial r} - \frac{\kappa}{r}\right)Q_\kappa(r,t), \tag{5}$$

$$i\frac{\partial Q_\kappa(r,t)}{\partial t} = [V(r) - 2c^2]Q_\kappa(r,t) + c\left(\frac{\partial}{\partial r} + \frac{\kappa}{r}\right)P_\kappa(r,t). \tag{6}$$

The time-dependent Dirac equation for two electrons moving in the Coulomb field of the nucleus is given by [11]

$$i\frac{\partial \vec{\Psi}(\vec{r}_1,\vec{r}_2,t)}{\partial t} = H(\vec{r}_1,\vec{r}_2)\vec{\Psi}(\vec{r}_1,\vec{r}_2,t), \tag{7}$$

where

$$H(\vec{r}_1,\vec{r}_2) = \begin{pmatrix} V(\vec{r}_1,\vec{r}_2) & c\vec{\sigma}\cdot\vec{p}_1 & c\vec{\sigma}\cdot\vec{p}_2 & 0 \\ c\vec{\sigma}\cdot\vec{p}_1 & V(\vec{r}_1,\vec{r}_2) - 2c^2 & 0 & c\vec{\sigma}\cdot\vec{p}_2 \\ c\vec{\sigma}\cdot\vec{p}_2 & 0 & V(\vec{r}_1,\vec{r}_2) - 2c^2 & c\vec{\sigma}\cdot\vec{p}_1 \\ 0 & c\vec{\sigma}\cdot\vec{p}_2 & c\vec{\sigma}\cdot\vec{p}_1 & V(\vec{r}_1,\vec{r}_2) - 4c^2 \end{pmatrix}, \tag{8}$$

$V(\vec{r}_1,\vec{r}_2) = V(r_1) + V(r_2) + \frac{1}{|\vec{r}_1-\vec{r}_2|}$, and one neglects magnetic and retardation effects. The two-electron wave function may be expanded in coupled spin-orbit eigenfunctions for each total angular-momentum symmetry J,

$$\vec{\Psi}(\vec{r}_1,\vec{r}_2,t) = \begin{pmatrix} \displaystyle\sum_{j_1,j_2} \frac{PP^J_{\kappa_1\kappa_2}(r_1,r_2,t)}{r_1 r_2} \sum_{m_1,m_2} C^{j_1 j_2 J}_{m_1 m_2 M}\Phi_{+\kappa_1,m_1}(\theta_1,\phi_1)\Phi_{+\kappa_2,m_2}(\theta_2,\phi_2) \\ i\displaystyle\sum_{j_1,j_2} \frac{QP^J_{\kappa_1\kappa_2}(r_1,r_2,t)}{r_1 r_2} \sum_{m_1,m_2} C^{j_1 j_2 J}_{m_1 m_2 M}\Phi_{-\kappa_1,m_1}(\theta_1,\phi_1)\Phi_{+\kappa_2,m_2}(\theta_2,\phi_2) \\ i\displaystyle\sum_{j_1,j_2} \frac{PQ^J_{\kappa_1\kappa_2}(r_1,r_2,t)}{r_1 r_2} \sum_{m_1,m_2} C^{j_1 j_2 J}_{m_1 m_2 M}\Phi_{+\kappa_1,m_1}(\theta_1,\phi_1)\Phi_{-\kappa_2,m_2}(\theta_2,\phi_2) \\ \displaystyle\sum_{j_1,j_2} \frac{QQ^J_{\kappa_1\kappa_2}(r_1,r_2,t)}{r_1 r_2} \sum_{m_1,m_2} C^{j_1 j_2 J}_{m_1 m_2 M}\Phi_{-\kappa_1,m_1}(\theta_1,\phi_1)\Phi_{-\kappa_2,m_2}(\theta_2,\phi_2) \end{pmatrix}, \tag{9}$$

where $C^{j_1 j_2 j_3}_{m_1 m_2 m_3}$ are Clebsch-Gordan coefficients. Substitution of Eq. (9) into Eq. (7) and projection onto the coupled spin-orbit eigenfunctions yields the time-dependent close-coupled equations,

$$\begin{aligned} i\frac{\partial PP^J_{\kappa_1\kappa_2}(r_1,r_2,t)}{\partial t} &= [V(r_1) + V(r_2)]PP^J_{\kappa_1\kappa_2}(r_1,r_2,t) + \sum_{\kappa_1',\kappa_2'} W^J_{+\kappa_1,+\kappa_2,+\kappa_1',+\kappa_2'}(r_1,r_2)PP^J_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\ &\quad - c\left(\frac{\partial}{\partial r_1} - \frac{\kappa_1}{r_1}\right)QP^J_{\kappa_1\kappa_2}(r_1,r_2,t) - c\left(\frac{\partial}{\partial r_2} - \frac{\kappa_2}{r_2}\right)PQ^J_{\kappa_1\kappa_2}(r_1,r_2,t), \end{aligned} \tag{10}$$

$$\begin{aligned} i\frac{\partial QP^J_{\kappa_1\kappa_2}(r_1,r_2,t)}{\partial t} &= [V(r_1) + V(r_2) - 2c^2]QP^J_{\kappa_1\kappa_2}(r_1,r_2,t) + \sum_{\kappa_1',\kappa_2'} W^J_{-\kappa_1,+\kappa_2,-\kappa_1',+\kappa_2'}(r_1,r_2)QP^J_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\ &\quad + c\left(\frac{\partial}{\partial r_1} + \frac{\kappa_1}{r_1}\right)PP^J_{\kappa_1\kappa_2}(r_1,r_2,t) + c\left(\frac{\partial}{\partial r_2} - \frac{\kappa_2}{r_2}\right)QQ^J_{\kappa_1\kappa_2}(r_1,r_2,t), \end{aligned} \tag{11}$$

$$i\frac{\partial PQ^J_{\kappa_1\kappa_2}(r_1,r_2,t)}{\partial t} = [V(r_1)+V(r_2)-2c^2]PQ^J_{\kappa_1\kappa_2}(r_1,r_2,t) + \sum_{\kappa_1',\kappa_2'} W^J_{+\kappa_1,-\kappa_2,+\kappa_1',-\kappa_2'}(r_1,r_2)PQ^J_{\kappa_1'\kappa_2'}(r_1,r_2,t)$$
$$+ c\left(\frac{\partial}{\partial r_1}-\frac{\kappa_1}{r_1}\right)QQ^J_{\kappa_1\kappa_2}(r_1,r_2,t) + c\left(\frac{\partial}{\partial r_2}+\frac{\kappa_2}{r_2}\right)PP^J_{\kappa_1\kappa_2}(r_1,r_2,t), \tag{12}$$

$$i\frac{\partial QQ^J_{\kappa_1\kappa_2}(r_1,r_2,t)}{\partial t} = [V(r_1)+V(r_2)-4c^2]QQ^J_{\kappa_1\kappa_2}(r_1,r_2,t) + \sum_{\kappa_1',\kappa_2'} W^J_{-\kappa_1,-\kappa_2,-\kappa_1',-\kappa_2'}(r_1,r_2)QQ^J_{\kappa_1'\kappa_2'}(r_1,r_2,t)$$
$$- c\left(\frac{\partial}{\partial r_1}+\frac{\kappa_1}{r_1}\right)PQ^J_{\kappa_1\kappa_2}(r_1,r_2,t) - c\left(\frac{\partial}{\partial r_2}+\frac{\kappa_2}{r_2}\right)QP^J_{\kappa_1\kappa_2}(r_1,r_2,t). \tag{13}$$

The electron-electron coupling operator is given by

$$W^J_{\kappa_1,\kappa_2,\kappa_1',\kappa_2'}(r_1,r_2) = (-1)^{2j_1'+j_2+j_2'+J+1}\sqrt{(2l_1+1)(2l_1'+1)(2l_2+1)(2l_2'+1)}\sqrt{(2j_1+1)(2j_1'+1)(2j_2+1)(2j_2'+1)}$$
$$\times\sum_{\lambda}\frac{r_<^\lambda}{r_>^{\lambda+1}}\begin{pmatrix} l_1 & \lambda & l_1' \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_2 & \lambda & l_2' \\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l_1 & \frac{1}{2} & j_1 \\ j_1' & \lambda & l_1'\end{Bmatrix}\begin{Bmatrix} l_2 & \frac{1}{2} & j_2 \\ j_2' & \lambda & l_2'\end{Bmatrix}\begin{Bmatrix} j_1 & j_2 & J \\ j_2' & j_1' & \lambda\end{Bmatrix}, \tag{14}$$

where $r_<=\min(r_1,r_2)$, $r_>=\max(r_1,r_2)$, and standard $3j$ and $6j$ symbol notation is used.

A complete set of single-particle radial orbitals, $P_{\epsilon\kappa}(r)$ and $Q_{\epsilon\kappa}(r)$, may be obtained by Hamiltonian diagonalization of the one-electron radial Dirac equation given by

$$\begin{pmatrix} V(r)-2c^2 & c\left(\frac{\partial}{\partial r}+\frac{\kappa}{r}\right) \\ -c\left(\frac{\partial}{\partial r}-\frac{\kappa}{r}\right) & V(r)\end{pmatrix}\begin{pmatrix} Q_{\epsilon\kappa}(r) \\ P_{\epsilon\kappa}(r)\end{pmatrix} = \epsilon\begin{pmatrix} Q_{\epsilon\kappa}(r) \\ P_{\epsilon\kappa}(r)\end{pmatrix}, \tag{15}$$

where the total energy $E=\epsilon+c^2$. For electron scattering from highly charged ions, the incoming large component radial wave packet is given by

$$F_\kappa(r) = Ne^{-(r-a)^2/2w^2}e^{-i(pr+\tilde{q}/p\,\ln(2pr)-\tilde{l}\pi/2+\delta_{\tilde{l}})}, \tag{16}$$

where N is a normalization constant, a is the localization radius of the wave packet, w is the width of the wave packet, $p=\sqrt{\epsilon^2+2c^2\epsilon}/c$ is the relativistic momentum, $\tilde{q}=q(1+\frac{\epsilon}{c^2})$, q is the asymptotic charge, $\tilde{l}(\tilde{l}+1)=\kappa(\kappa+1)-(q^2/c^2)$, and $\delta_{\tilde{l}}$ is the Coulomb phase shift. From Eq. (15) the incoming small component radial wave packet is given by

$$G_\kappa(r) = \frac{c}{\epsilon+2c^2+\frac{q}{r}}\left[\frac{a}{w^2}-\frac{r}{w^2}-i\left(p+\frac{\tilde{q}}{pr}\right)+\frac{\kappa}{r}\right]F_\kappa(r). \tag{17}$$

B. One-electron elastic scattering

The one-electron time-dependent coupled (TDC) equations of Eqs. (5) and (6) may be used to investigate electron-impact elastic potential scattering from hydrogenic ions. The initial radial wave functions are given by

$$P_\kappa(r,t=0) = F_\kappa(r), \tag{18}$$

$$Q_\kappa(r,t=0) = G_\kappa(r). \tag{19}$$

For scattering off ions in the ground state, the TDC equations are propagated in the potentials

$$V_a(r) = -\frac{Z}{r}+\int_0^\infty\frac{1}{r_>}([P_{1s(1/2)}(r')]^2+[Q_{1s(1/2)}(r')]^2)dr' \tag{20}$$

and

$$V_b(r) = -\frac{(Z-1)}{r}, \tag{21}$$

where $P_{1s(1/2)}(r)$ and $Q_{1s(1/2)}(r)$ are obtained by diagonalization of the Hamiltonian with $V(r)=-\frac{Z}{r}$. Following time propagation of the TDC equations, the elastic potential scattering probability is given by

$$\mathcal{P}(\kappa) = \sum_{\epsilon>0}\left|\int_0^\infty drP_{\epsilon\kappa}(r)[P^a_\kappa(r,t\to\infty)-P^b_\kappa(r,t\to\infty)]\right.$$
$$\left.+\int_0^\infty drQ_{\epsilon\kappa}(r)[Q^a_\kappa(r,t\to\infty)-Q^b_\kappa(r,t\to\infty)]\right|^2, \tag{22}$$

where $P_{\epsilon\kappa}(r)$ and $Q_{\epsilon\kappa}(r)$ are obtained by diagonalization of the Hamiltonian with $V(r)=-\frac{(Z-1)}{r}$. The total elastic potential scattering cross section is given by

$$\sigma_{pot} = \frac{\pi}{4\epsilon_0} \sum_{\kappa} (2j+1)\mathcal{P}(\kappa), \tag{23}$$

where ϵ_0 is the incident energy.

C. Two-electron inelastic scattering

The two-electron time-dependent close-coupled (TDCC) equations of Eqs. (10)–(13) may be used to investigate electron-impact ionization of hydrogenic ions. The initial radial wave functions are constructed as symmetric or antisymmetric products of the bound radial orbital of one electron and the incoming radial wave packet of the other electron. For example, for $1s\frac{1}{2}\epsilon s\frac{1}{2}$ $J=0,1$ even-parity scattering, the initial radial wave functions are given by

$$PP^{J}_{\kappa_1=-1\kappa_2=-1}(r_1,r_2,t=0) = \sqrt{\frac{1}{2}}[P_{1s(1/2)}(r_1)F_{\epsilon s(1/2)}(r_2) + (-1)^J F_{\epsilon s(1/2)}(r_1) \times P_{1s(1/2)}(r_2)], \tag{24}$$

$$QP^{J}_{\kappa_1=-1\kappa_2=-1}(r_1,r_2,t=0) = \sqrt{\frac{1}{2}}[Q_{1s(1/2)}(r_1)F_{\epsilon s(1/2)}(r_2) + (-1)^J G_{\epsilon s(1/2)}(r_1) \times P_{1s(1/2)}(r_2)], \tag{25}$$

$$PQ^{J}_{\kappa_1=-1\kappa_2=-1}(r_1,r_2,t=0) = \sqrt{\frac{1}{2}}[P_{1s(1/2)}(r_1)G_{\epsilon s(1/2)}(r_2) + (-1)^J F_{\epsilon s(1/2)}(r_1) \times Q_{1s(1/2)}(r_2)], \tag{26}$$

$$QQ^{J}_{\kappa_1=-1\kappa_2=-1}(r_1,r_2,t=0) = \sqrt{\frac{1}{2}}[Q_{1s(1/2)}(r_1)G_{\epsilon s(1/2)}(r_2) + (-1)^J G_{\epsilon s(1/2)}(r_1) \times Q_{1s(1/2)}(r_2)], \tag{27}$$

with all other $PP^{J}_{\kappa_1\kappa_2}(r_1,r_2,t=0)$, $QP^{J}_{\kappa_1\kappa_2}(r_1,r_2,t=0)$, $PQ^{J}_{\kappa_1\kappa_2}(r_1,r_2,t=0)$, and $QQ^{J}_{\kappa_1\kappa_2}(r_1,r_2,t=0)$ radial wave functions for $\kappa_1 \neq -1$ and $\kappa_2 \neq -1$ set to zero. Following time propagation of the TDCC equations, the total ionization probability is given by

$$\begin{aligned}\mathcal{P}(J) = 2 \sum_{\kappa_1,\kappa_2} \sum_{\epsilon_1>\epsilon_2} \sum_{\epsilon_2>0} \Bigg| & \int_0^\infty dr_1 \int_0^\infty dr_2 P_{\epsilon_1\kappa_1}(r_1) P_{\epsilon_2\kappa_2}(r_2) PP^{J}_{\kappa_1\kappa_2}(r_1,r_2,t\to\infty) \\ & + \int_0^\infty dr_1 \int_0^\infty dr_2 Q_{\epsilon_1\kappa_1}(r_1) P_{\epsilon_2\kappa_2}(r_2) QP^{J}_{\kappa_1\kappa_2}(r_1,r_2,t\to\infty) \\ & + \int_0^\infty dr_1 \int_0^\infty dr_2 P_{\epsilon_1\kappa_1}(r_1) Q_{\epsilon_2\kappa_2}(r_2) PQ^{J}_{\kappa_1\kappa_2}(r_1,r_2,t\to\infty) \\ & + \int_0^\infty dr_1 \int_0^\infty dr_2 Q_{\epsilon_1\kappa_1}(r_1) Q_{\epsilon_2\kappa_2}(r_2) QQ^{J}_{\kappa_1\kappa_2}(r_1,r_2,t\to\infty) \Bigg|^2 .\end{aligned} \tag{28}$$

The total ionization cross section is given by

$$\sigma_{ion} = \frac{\pi}{8\epsilon_0} \sum_{parity} \sum_{J} (2J+1)\mathcal{P}(J), \tag{29}$$

where ϵ_0 is the incident energy.

III. RESULTS

A. One-electron elastic scattering

To construct the Hartree potential of Eq. (20) for Ne^{9+}, we begin by a diagonalization of the Hamiltonian of Eq. (15) with $\kappa=-1$ and $V(r)=-\frac{10}{r}$. We choose a 500 point mesh with a uniform mesh spacing of $\Delta r=0.01$. For the discretization choice

$$\frac{\partial P(r)}{\partial r} = \frac{P(r_{i+1}) - P(r_{i-1})}{2\Delta r}, \tag{30}$$

$$\frac{\partial Q(r)}{\partial r} = \frac{Q(r_{i+1}) - Q(r_{i-1})}{2\Delta r}, \tag{31}$$

we obtain a complete set of 500 "negative-energy sea" solutions, spanning $\epsilon_1=-190,687$ eV to $\epsilon_{500}=-69.1$ eV, and a complete set of 500 "positive-energy sea" solutions, spanning $\epsilon_1=-1362.4$ eV to $\epsilon_{500}=+143,275$ eV. The symmetric discretization of Eqs. (30) and (31) results in a doubling of some of the positive-energy sea eigenvalues, that is, $\epsilon_2=\epsilon_3=-341.1$ eV and $\epsilon_4=\epsilon_5=-151.6$ eV. For the discretization choice

$$\frac{\partial P(r)}{\partial r} = \frac{3P(r_{i+1}) + 10P(r_i) - 18P(r_{i-1}) + 6P(r_{i-2}) - P(r_{i-3})}{12\Delta r}, \tag{32}$$

$$\frac{\partial Q(r)}{\partial r} = \frac{Q(r_{i+3}) - 6Q(r_{i+2}) + 18Q(r_{i+1}) - 10Q(r_i) - 3Q(r_{i+1})}{12\Delta r}, \tag{33}$$

the Fermi doubling problem [13] is removed. In other words, central differences lead to a bivalued relativistic energy dispersion relation, while backward-forward differences lead to a single valued relativistic energy dispersion relation (see Fig. 1 of Ref. [14]). The lowest-energy positive-energy sea eigenfunctions, $P_{1s(1/2)}(r)$ and $Q_{1s(1/2)}(r)$, are then used to construct the ground-state Hartree potential for Ne^{9+}.

The TDC equations of Eqs. (5) and (6) with $\kappa=-1$ are propagated for 25 000 time steps with a uniform time step of $\Delta t=0.000\,02$ using both potentials $V_a(r)$ of Eq. (20) and $V_b(r)$ of Eq. (21) with $Z=10$. Radial derivatives make use of the nonsymmetric discretization choice of Eqs. (32) and (33). The initial conditions of Eqs. (18) and (19) use radial wave packets with an incident energy of 2.00 keV, a localization radius of $a=2.50$, and a width of $w=0.625$. Following time propagation of the TDC equations, the elastic potential scattering probability is extracted using Eq. (22) with the 494 $\epsilon>0$ positive-energy sea eigenfunctions found from diagonalization of the Hamiltonian with $V(r)=-\frac{9}{r}$. The $j=\frac{1}{2}$ elastic Hartree potential scattering cross section for Ne^{9+} at 2.00 keV from Eq. (23) is found to be 15.5 kb, where 1.0 kb $=1.0\times10^{-21}$ cm^2. A similar calculation using the time-dependent Schrödinger equation [12] yields an $l=0$ cross section of 16.3 kb. Additional calculations obtained by integrating the time-independent radial Schrödinger and Dirac equations for Hartree potential phase shifts yield similar s-wave elastic potential cross sections.

B. Two-electron inelastic scattering

To calculate the $J=0,1$ ionization cross section for Ne^{9+}, we begin by diagonalization of the Hamiltonian of Eq. (15) with $\kappa=\pm1,\pm2,\pm3$ and $V(r)=-\frac{10}{r}$. We choose a 512 point mesh with a uniform mesh spacing of $\Delta r=0.01$ and the nonsymmetric radial discretization of Eqs. (32) and (33). The initial conditions of Eqs. (24)–(27), on a 512×512 point lattice with $\Delta r_1=\Delta r_2=0.01$, use the lowest-energy positive-energy sea eigenfunctions $P_{1s(1/2)}(r)$ and $Q_{1s(1/2)}(r)$ from the $\kappa=-1$ diagonalization and radial wave packets with an initial energy of 4.15 keV, a localization radius of $a=2.50$, and a width of $w=0.625$.

The TDCC equations of Eqs. (10)–(13) for the six coupled channels listed in Table I are propagated for 36 000 time steps with a uniform time step of $\Delta t=0.000\,01$. Radial derivatives make use of the nonsymmetric discretization choice, that is, Eq. (32) for $\frac{\partial}{\partial r_1}$ and $\frac{\partial}{\partial r_2}$ on $PP^J_{\kappa_1\kappa_2}(r_1,r_2,t)$, Eq. (33) for $\frac{\partial}{\partial r_1}$ and $\frac{\partial}{\partial r_2}$ on $QQ^J_{\kappa_1\kappa_2}(r_1,r_2,t)$, and appropriate mixtures for $QP^J_{\kappa_1\kappa_2}(r_1,r_2,t)$ and $PQ^J_{\kappa_1\kappa_2}(r_1,r_2,t)$. To make use of massively parallel computers, the 512×512 point lattice is partitioned over processors in the r_2 coordinate. Following time propagation of the TDCC equations, the ionization probabilities are extracted using Eq. (28) with the appropriate simple products of $P_{\epsilon_1\kappa_1}(r_1)P_{\epsilon_2\kappa_2}(r_2)$ positive-energy sea eigenfunctions and $\epsilon_1>\epsilon_2>0$. The $J=0$ ionization cross section for Ne^{9+} at 4.15 keV from Eq. (29) is found to be 0.291 kb, while the $J=1$ cross section is 0.045 kb. A similar four coupled channels calculation using the time-dependent Schrödinger equation yields an $L=0$, $S=0$ cross section of 0.295 kb and an $L=0$, $S=1$ cross section of 0.057 kb. Additional calculations obtained using perturbative distorted-wave methods for the time-independent Schrödinger and Dirac equations yield similar total s-wave ionization cross sections. We note that while the number of coupled channels needed for s-wave cross sections is relatively small, the number of coupled channels needed for higher l-wave cross sections can become quite sizeable.

TABLE I. Fully relativistic coupled channels for $J=0$ and 1 and even parity.

Channel	l_1	j_1	κ_1	l_2	j_2	κ_2
1	0	$\frac{1}{2}$	−1	0	$\frac{1}{2}$	−1
2	1	$\frac{1}{2}$	+1	1	$\frac{1}{2}$	+1
3	1	$\frac{3}{2}$	−2	1	$\frac{3}{2}$	−2
4	2	$\frac{3}{2}$	+2	2	$\frac{3}{2}$	+2
5	2	$\frac{5}{2}$	−3	2	$\frac{5}{2}$	−3
6	3	$\frac{5}{2}$	+3	3	$\frac{5}{2}$	+3

IV. SUMMARY

In analogy with the derivation of the time-dependent coupled Dirac equations for one electron in a central field, the time-dependent close-coupled Dirac equations have been derived for two electrons moving in a central field and interacting through an electrostatic repulsion. Each coupled channel is described by four radial wave functions, while the interaction between coupled channels is expressed in terms of a standard multipole expansion of the electrostatic operator. Standard numerical methods that avoid the Fermi doubling problem are used to formulate initial value conditions, propagate the time-dependent equations, and extract scattering probabilities and cross sections. Test calculations using the one-electron coupled equations are found to give a reasonable $j=\frac{1}{2}$ elastic Hartree potential scattering cross section for Ne^{9+} at 2.00 keV incident energy. Further test calculations using the two-electron close-coupled equations are found to give reasonable $J=0,1$ ionization cross sections for Ne^{9+} at 4.15 keV incident energy.

In the future, the application of the fully relativistic time-dependent close-coupling method to the electron-impact ionization of highly charged atomic ions will be quite challenging. The small radial mesh spacings and time propagation steps needed will necessitate a partition of the 2D radial lattice over computing processors in both the r_1 and r_2 coordinates. As has been shown in perturbative distorted-wave calculations for highly charged ions [4,5], additional magnetic

and retardation effects must be included in the electron-electron interaction. Finally, the calculation of experimentally observable nonperturbative effects in the electron ionization of highly charged ions will probably require the calculation of detailed energy and angle differential cross sections.

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