

Single photoionization of highly charged atomic ions including the full electromagnetic-field potential

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A previous fully relativistic time-dependent close-coupling method [Phys. Rev. A **81**, 063431 (2010)], developed to study the photoionization of highly charged atomic ions, is substantially modified to include the full electromagnetic-field potential. Expansion of a one active electron wave function for the time-dependent Dirac equation in spin-orbit eigenfunctions yields close-coupled equations for bispinor radial wave functions. A spherical Bessel function expansion is then used to go beyond the Lorentz gauge dipole approximation to include higher order radiation field operators in both the Lorentz and Coulomb gauges. We test the high-order close-coupling method on the single photoionization of U^{91+} .

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I. INTRODUCTION

Ionization processes involving photon and electron collisions with highly charged atomic ions have been studied for many years using relativistic many-body perturbation theory [1]. Over the last few years a number of nonperturbative close-coupling methods have also been developed to calculate photon and electron collisions with highly charged atomic ions; including the standard relativistic R -matrix method [2,3], the relativistic B -spline R -matrix method [4], the relativistic R -matrix with pseudostates method [5], and the relativistic converged close-coupling method [6]. In recent years the exposure of highly charged atomic ions to intense short radiation field pulses, as produced by the free-electron laser in Hamburg [7], has prompted the development of methods to solve the time-dependent Dirac equation for one active electron atomic ions [8].

Recently, we developed a relativistic time-dependent close-coupling method for the single and double photoionization of highly charged atomic ions [9]. Both the one active electron and two active electron time-dependent close-coupling methods were derived using a lowest order Lorentz gauge for the electromagnetic-field potentials, while the two active electron equations included an electrostatic two-body operator. The difficulty of using many-body perturbation theory to describe the quantal three-body breakup problem makes the relativistic time-dependent close-coupling method for the double photoionization of highly charged atomic ions quite attractive.

In this article, we develop a relativistic time-dependent close-coupling method for the single photoionization of highly charged atomic ions that goes beyond the lowest order dipole approximation to include the full spatial and time dependence of the electromagnetic-field potential. Single photoionization cross sections for U^{91+} are then calculated for various multipole approximations and compared with relativistic lowest order time-independent distorted-wave results. We note that the same all orders radiation field operators derived for the one active electron time-dependent close-coupling equations are identical to those found for each electron in the

two active electron time-dependent close-coupling equations. What then remains for a complete relativistic time-dependent close-coupling method for double photoionization is the inclusion of an electromagnetic and retardation two-body operator.

The rest of the article is organized as follows. In Sec. II A we present the time-dependent Dirac equation in both the Coulomb and Lorentz gauges, in Sec. II B we derive the one active electron time-dependent close-coupled bispinor equations, in Sec. II C we derive the radiation field matrix elements involving the full spatial and time-dependent electromagnetic-field operator, in Sec. II D we present the time-dependent close-coupling (TDCC) cross section, and in Sec. II E we present the time-independent distorted-wave (TIDW) cross section. In Sec. III we calculate single photoionization cross sections for U^{91+} using both the TDCC and TIDW methods. 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. Time-dependent Dirac equation

The time-dependent Dirac equation for a one-electron atomic ion in a time-varying electromagnetic field is given by [10]

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

where

$$H(\vec{r}, t) = \begin{pmatrix} V(r) - U(\vec{r}, t) & c\vec{\sigma} \cdot \vec{p}(\vec{r}) + c\vec{\sigma} \cdot \vec{A}(\vec{r}, t) \\ c\vec{\sigma} \cdot \vec{p}(\vec{r}) + c\vec{\sigma} \cdot \vec{A}(\vec{r}, t) & V(r) - U(\vec{r}, t) - 2c^2 \end{pmatrix}, \quad (2)$$

$$V(r) = -\frac{Z}{r} + V_{\text{HX}}(r), \quad (3)$$

Z is the atomic number, $V_{\text{HX}}(r)$ is a Hartree with local exchange potential, $\vec{\sigma}$ is a Pauli matrix vector, and $\vec{p}(\vec{r}) = -i\vec{\nabla}$. In the Coulomb gauge the electromagnetic-field potentials are given by [11]

$$U(\vec{r}, t) = 0, \quad \vec{A}(\vec{r}, t) = \frac{E}{\omega} \hat{z} \sin(ky - \omega t), \quad (4)$$

while in the Lorentz gauge the electromagnetic-field potentials are given by [11]

$$U(\vec{r}, t) = -Ez \cos(\omega t), \quad (5)$$

$$\vec{A}(\vec{r}, t) = \frac{E}{\omega} \hat{z} \sin(ky - \omega t) + \frac{E}{\omega} \hat{z} \sin(\omega t),$$

where E is the radiation field amplitude, ω is the radiation field frequency, c is the speed of light, and $k = \frac{\omega}{c}$. In lowest order we recover the usual Coulomb gauge potentials:

$$U(\vec{r}, t) = 0, \quad \vec{A}(\vec{r}, t) = -\frac{E}{\omega} \hat{z} \sin(\omega t), \quad (6)$$

and the usual Lorentz gauge potentials:

$$U(\vec{r}, t) = -Ez \cos(\omega t), \quad \vec{A}(\vec{r}, t) = 0. \quad (7)$$

B. Time-dependent close-coupled bispinor equations

The one-electron total wave function is expanded in spin-orbit eigenfunctions given by

$$\vec{\Psi}(\vec{r}, t) = \sum_{\kappa, m} \left(\frac{P_{\kappa m}(r, t)}{r} \Phi_{+\kappa, m}(\theta, \phi) \right), \quad (8)$$

where

$$\Phi_{\kappa, m}(\theta, \phi) = \sum_{m_l, m_s} C_{m_l m_s m}^{l s j} Y_{l m_l}(\theta, \phi) \chi_{m_s}, \quad (9)$$

$\kappa = -(l + 1)$ for $j = l + \frac{1}{2}$, $\kappa = +l$ for $j = l - \frac{1}{2}$, $s = \frac{1}{2}$, $C_{m_l m_s m}^{l s j}$ is a Clebsch-Gordan coefficient, $Y_{l m_l}(\theta, \phi)$ is a spherical harmonic, and χ_{m_s} is a two-component spinor. Upon substitution into the time-dependent Dirac equation, we obtain the following set of time-dependent close-coupled partial differential equations:

$$i \frac{\partial P_{\kappa m}(r, t)}{\partial t} = V(r) P_{\kappa m}(r, t) - \sum_{\kappa', m'} \langle \kappa m | U(\vec{r}, t) | \kappa' m' \rangle P_{\kappa' m'}(r, t) - c \left(\frac{\partial}{\partial r} - \frac{\kappa}{r} \right) Q_{\kappa m}(r, t) + i c \sum_{\kappa', m'} \langle \kappa m | \vec{\sigma} \cdot \vec{A}(\vec{r}, t) | \kappa' m' \rangle Q_{\kappa' m'}(r, t). \quad (10)$$

$$i \frac{\partial Q_{\kappa m}(r, t)}{\partial t} = [V(r) - 2c^2] Q_{\kappa m}(r, t) - \sum_{\kappa', m'} \langle -\kappa m | U(\vec{r}, t) | \kappa' m' \rangle Q_{\kappa' m'}(r, t) + c \left(\frac{\partial}{\partial r} + \frac{\kappa}{r} \right) P_{\kappa m}(r, t) - i c \sum_{\kappa', m'} \langle -\kappa m | \vec{\sigma} \cdot \vec{A}(\vec{r}, t) | \kappa' m' \rangle P_{\kappa' m'}(r, t). \quad (11)$$

In the Coulomb gauge the time-dependent close-coupled equations are given by

$$i \frac{\partial P_{\kappa m}(r, t)}{\partial t} = V(r) P_{\kappa m}(r, t) - c \left(\frac{\partial}{\partial r} - \frac{\kappa}{r} \right) Q_{\kappa m}(r, t) + i c \frac{E}{\omega} \sum_{\kappa', m'} \langle \kappa m | \sigma_z \sin(ky - \omega t) | \kappa' m' \rangle Q_{\kappa' m'}(r, t). \quad (12)$$

$$i \frac{\partial Q_{\kappa m}(r, t)}{\partial t} = (V(r) - 2c^2) Q_{\kappa m}(r, t) + c \left(\frac{\partial}{\partial r} + \frac{\kappa}{r} \right) P_{\kappa m}(r, t) - i c \frac{E}{\omega} \sum_{\kappa', m'} \langle -\kappa m | \sigma_z \sin(ky - \omega t) | \kappa' m' \rangle P_{\kappa' m'}(r, t). \quad (13)$$

In the Lorentz gauge the time-dependent close-coupled equations are given by

$$i \frac{\partial P_{\kappa m}(r, t)}{\partial t} = V(r) P_{\kappa m}(r, t) + E \sum_{\kappa', m'} \langle \kappa m | z \cos(\omega t) | \kappa' m' \rangle P_{\kappa' m'}(r, t) - c \left(\frac{\partial}{\partial r} - \frac{\kappa}{r} \right) Q_{\kappa m}(r, t) + i c \frac{E}{\omega} \sum_{\kappa', m'} \langle \kappa m | \sigma_z (\sin(ky - \omega t) + \sin(\omega t)) | \kappa' m' \rangle Q_{\kappa' m'}(r, t). \quad (14)$$

$$i \frac{\partial Q_{\kappa m}(r, t)}{\partial t} = (V(r) - 2c^2) Q_{\kappa m}(r, t) + E \sum_{\kappa', m'} \langle -\kappa m | z \cos(\omega t) | \kappa' m' \rangle Q_{\kappa' m'}(r, t) + c \left(\frac{\partial}{\partial r} + \frac{\kappa}{r} \right) P_{\kappa m}(r, t) - i c \frac{E}{\omega} \sum_{\kappa', m'} \langle -\kappa m | \sigma_z (\sin(ky - \omega t) + \sin(\omega t)) | \kappa' m' \rangle P_{\kappa' m'}(r, t). \quad (15)$$

C. Radiation field matrix elements

In the Coulomb gauge the lowest order radiation field matrix element is given by

$$\begin{aligned} & \langle \kappa m | \sigma_z \sin(\omega t) | \kappa' m' \rangle \\ &= \delta_{l,l'} \sin(\omega t) 2\sqrt{3/2} (-1)^{l+2j-m+\frac{3}{2}} \sqrt{(2j+1)(2j'+1)} \begin{pmatrix} l & 1 & l' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} j & 1 & j' \\ -m & 0 & m' \end{pmatrix} \left\{ \begin{matrix} l & \frac{1}{2} & j \\ 1 & j' & \frac{1}{2} \end{matrix} \right\}. \end{aligned} \quad (16)$$

In the Lorentz gauge the lowest order radiation field matrix element is given by

$$\begin{aligned} & \langle \kappa m | z \cos(\omega t) | \kappa' m' \rangle \\ &= r \cos(\omega t) (-1)^{j+j'-m+\frac{3}{2}} \sqrt{(2l+1)(2l'+1)(2j+1)(2j'+1)} \begin{pmatrix} l & 1 & l' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} j & 1 & j' \\ -m & 0 & m' \end{pmatrix} \left\{ \begin{matrix} l & \frac{1}{2} & j \\ j' & 1 & l' \end{matrix} \right\}. \end{aligned} \quad (17)$$

Reduction of the matrix elements to standard 3j and 6j symbols is made by using the Wigner-Eckart theorem and uncoupling formulas to reduced matrix elements [12].

In both the Coulomb and Lorentz gauges, higher order radiation field matrix elements are obtained by first using the spherical Bessel function expansion [13]:

$$\sin(ky - \omega t) = \text{Im} \left(\sum_{K,Q} i^K (2K+1) C_{KQ}^*(\hat{y}) j_K(kr) C_{KQ}(\hat{r}) e^{-i\omega t} \right), \quad (18)$$

where $C_{KQ}(\hat{r})$ is a spherical tensor and $j_K(kr)$ is a spherical Bessel function. For example, in the Coulomb gauge the time-dependent close-coupled equations for $K \leq 1$ are given by

$$\begin{aligned} i \frac{\partial P_{\kappa m}(r,t)}{\partial t} &= V(r) P_{\kappa m}(r,t) - c \left(\frac{\partial}{\partial r} - \frac{\kappa}{r} \right) Q_{\kappa m}(r,t) - ic \frac{E}{\omega} j_0(kr) \sin(\omega t) \sum_{\kappa',m'} \langle \kappa m | \sigma_z C_{00}(\hat{r}) | -\kappa' m' \rangle Q_{\kappa' m'}(r,t) \\ &\quad - 3ic \frac{E}{\omega} j_1(kr) \sin(\omega t) \sum_{\kappa',m'} \langle \kappa m | \sqrt{\frac{1}{2}} \sigma_z C_{1+1}(\hat{r}) + \sqrt{\frac{1}{2}} \sigma_z C_{1-1}(\hat{r}) | -\kappa' m' \rangle Q_{\kappa' m'}(r,t). \end{aligned} \quad (19)$$

$$\begin{aligned} i \frac{\partial Q_{\kappa m}(r,t)}{\partial t} &= (V(r) - 2c^2) Q_{\kappa m}(r,t) + c \left(\frac{\partial}{\partial r} + \frac{\kappa}{r} \right) P_{\kappa m}(r,t) + ic \frac{E}{\omega} j_0(kr) \sin(\omega t) \sum_{\kappa',m'} \langle -\kappa m | \sigma_z C_{00}(\hat{r}) | \kappa' m' \rangle P_{\kappa' m'}(r,t) \\ &\quad + 3ic \frac{E}{\omega} j_1(kr) \sin(\omega t) \sum_{\kappa',m'} \langle -\kappa m | \sqrt{\frac{1}{2}} \sigma_z C_{1+1}(\hat{r}) + \sqrt{\frac{1}{2}} \sigma_z C_{1-1}(\hat{r}) | \kappa' m' \rangle P_{\kappa' m'}(r,t). \end{aligned} \quad (20)$$

The matrix elements involving the $\sigma_z C_{KQ}(\hat{r})$ operators may be evaluated by the introduction of a complete set of $|\kappa'' m''\rangle$ states:

$$\langle \kappa m | \sigma_z C_{KQ}(\hat{r}) | \kappa' m' \rangle = 2 \sum_{\kappa'', m''} \langle \kappa m | S_{10} | \kappa'' m'' \rangle \langle \kappa'' m'' | C_{KQ}(\hat{r}) | \kappa' m' \rangle. \quad (21)$$

For the $|\kappa m\rangle = |lsjm\rangle$ coupled state, S_{10} operates only on $|sm_s\rangle$ and $C_{KQ}(\hat{r})$ operates only on $|lm_l\rangle$, leading to the higher order matrix element given by

$$\begin{aligned} \langle \kappa m | \sigma_z C_{KQ}(\hat{r}) | \kappa' m' \rangle &= 2\sqrt{\frac{3}{2}} \begin{pmatrix} l & K & l' \\ 0 & 0 & 0 \end{pmatrix} (-1)^{l+2j-m+j'+K} \sqrt{(2l+1)(2l'+1)(2j+1)(2j'+1)} \\ &\quad \times \sum_{j'', m''} (-1)^{j''-m''} (2j''+1) \begin{pmatrix} j & 1 & j'' \\ -m & 0 & m'' \end{pmatrix} \begin{pmatrix} j'' & K & j' \\ -m'' & Q & m' \end{pmatrix} \left\{ \begin{matrix} l & \frac{1}{2} & j \\ 1 & j'' & \frac{1}{2} \end{matrix} \right\} \left\{ \begin{matrix} l & \frac{1}{2} & j'' \\ j' & K & l' \end{matrix} \right\}. \end{aligned} \quad (22)$$

D. Time-dependent close-coupling (TDCC) cross section

A complete set of single-particle radial orbitals may be obtained by diagonalization of the time-independent radial Dirac equation given by

$$\begin{pmatrix} V(r) - 2c^2 & c \left(\frac{\partial}{\partial r} + \frac{\kappa}{r} \right) \\ -c \left(\frac{\partial}{\partial r} - \frac{\kappa}{r} \right) & V(r) \end{pmatrix} \begin{pmatrix} Q_{\epsilon\kappa}(r) \\ P_{\epsilon\kappa}(r) \end{pmatrix} = \epsilon \begin{pmatrix} Q_{\epsilon\kappa}(r) \\ P_{\epsilon\kappa}(r) \end{pmatrix}, \quad (23)$$

where the total energy $E = \epsilon + c^2$. The initial condition of the solution of the time-dependent close-coupled equations for photoionization of the $n_i \kappa_i$ ground state is given by

$$\begin{aligned} P_{\kappa m}(r, t=0) &= P_{n_i \kappa_i}(r) \delta_{\kappa, \kappa_i} \delta_{m, m_i}, \\ Q_{\kappa m}(r, t=0) &= Q_{n_i \kappa_i}(r) \delta_{\kappa, \kappa_i} \delta_{m, m_i}. \end{aligned} \quad (24)$$

Following time propagation of the time-dependent close-coupled equations, the single photoionization cross section is given by [9]

$$\sigma = \frac{\omega}{IT} \sum_{\kappa m} \sum_{\epsilon \kappa > 0} \left| \int_0^\infty dr P_{\epsilon \kappa}(r) P_{\kappa m}(r, t \rightarrow \infty) + \int_0^\infty dr Q_{\epsilon \kappa}(r) Q_{\kappa m}(r, t \rightarrow \infty) \right|^2, \quad (25)$$

where I is the field intensity and T is the field pulse length.

E. Time-independent distorted-wave (TIDW) cross section

In the lowest order Lorentz gauge for the radiation field, the perturbative distorted-wave cross section for the transition $n_i \kappa_i \rightarrow \epsilon_f \kappa_f$ is given by [9]

$$\sigma = \frac{8\pi\omega}{p_f c} \left(1 + \frac{\epsilon_f}{2c^2}\right) \sum_{l_f, j_f} \frac{(2j_f + 1)}{3} \begin{pmatrix} j_i & 1 & j_f \\ \frac{1}{2} & 0 & -\frac{1}{2} \end{pmatrix} \times \left(\int_0^\infty r dr [P_{\epsilon_f \kappa_f}(r) P_{n_i \kappa_i}(r) + Q_{\epsilon_f \kappa_f}(r) Q_{n_i \kappa_i}(r)] \right)^2, \quad (26)$$

where $\epsilon_f = (\omega - I_p)$, I_p is the ionization potential, and $p_f = \sqrt{2\epsilon_f + \frac{\epsilon_f^2}{c^2}}$. The sum over l_f in Eq. (26) includes only terms for which $l_i + l_f + 1$ is an even number. The bound radial orbitals, $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$, are calculated using a Dirac-Fock atomic structure code [1], while the continuum radial orbitals, $P_{\epsilon\kappa}(r)$ and $Q_{\epsilon\kappa}(r)$, are calculated by numerical integration of the radial Dirac equation for specific energy values. The continuum normalization for all the distorted waves is one times a sine function.

III. RESULTS

We first diagonalized the Hamiltonian of Eq. (23) for U^{91+} on a 512-point uniform radial mesh with $\Delta r = 0.001$ using a fifth-order finite differencing scheme for the $\frac{\partial}{\partial r}$ operator and $V(r) = -\frac{92}{r}$. For $\kappa = -1$, we find six bound positive-energy sea eigenfunctions and 506 continuum positive-energy sea eigenfunctions. The ground state for $\kappa = -1$ has an energy of -126 keV, while the highest energy continuum state has an energy of 9432 keV. Increasing the number of lattice points will drop the ground-state energy towards the experimental value of -132 keV [14]. We also find 512 ‘‘filled’’ negative-energy sea eigenfunctions. Six additional diagonalizations were made for $\kappa = +1, -2, +2, -3, +3, -4$. The $\kappa = -1$ ground-state eigenfunctions are used in the initial conditions of Eq. (24), while the seven κ sets of continuum positive-energy sea eigenfunctions are used in the cross-section projections found in Eq. (25).

Using an intensity of 10^{18} W/cm² and a photon energy of 200 keV, we propagated the TDCC equations for 10 radiation field periods on a uniform time mesh with $\Delta t = 2.0 \times 10^{-5}$. We list 32 possible coupled channels in Table I. In lowest order for both the Coulomb gauge of Eq. (16) and the Lorentz gauge of Eq. (17), the $3j$ symbols involving l, l' and j, j' greatly restrict the possible coupled channels. Thus, the ground-state channel 1 ($1s \frac{1}{2} \frac{1}{2}$) couples only to continuum channel 3 ($\epsilon p \frac{1}{2} \frac{1}{2}$)

TABLE I. Coupled channels for the photoionization of U^{91+} .

Channel	κ	j	m	l
1	-1	0.5	+0.5	0
2	-1	0.5	-0.5	0
3	+1	0.5	+0.5	1
4	+1	0.5	-0.5	1
5	-2	1.5	+1.5	1
6	-2	1.5	+0.5	1
7	-2	1.5	-0.5	1
8	-2	1.5	-1.5	1
9	+2	1.5	+1.5	2
10	+2	1.5	+0.5	2
11	+2	1.5	-0.5	2
12	+2	1.5	-1.5	2
13	-3	2.5	+2.5	2
14	-3	2.5	+1.5	2
15	-3	2.5	+0.5	2
16	-3	2.5	-0.5	2
17	-3	2.5	-1.5	2
18	-3	2.5	-2.5	2
19	+3	2.5	+2.5	3
20	+3	2.5	+1.5	3
21	+3	2.5	+0.5	3
22	+3	2.5	-0.5	3
23	+3	2.5	-1.5	3
24	+3	2.5	-2.5	3
25	-4	3.5	+3.5	3
26	-4	3.5	+2.5	3
27	-4	3.5	+1.5	3
28	-4	3.5	+0.5	3
29	-4	3.5	-0.5	3
30	-4	3.5	-1.5	3
31	-4	3.5	-2.5	3
32	-4	3.5	-3.5	3

and to continuum channel 6 ($\epsilon p \frac{3}{2} \frac{1}{2}$). The lowest order Coulomb gauge cross section is found to be 139 b, while the lowest order Lorentz gauge cross section is found to be 142 b.

Using the spherical Bessel function expansion of Eq. (18) for $K \leq 1$, we solved the TDCC equations as found in Eqs. (19) and (20) at the same photon energy of 200 keV. Since the $C_{KQ}(\hat{r})$ spherical tensor operator removes restrictions on m, m' coupling, we carry out calculations involving the first 18 coupled channels of Table I, that is, ($s \frac{1}{2} m$), ($p \frac{1}{2} m$), ($p \frac{3}{2} m$), ($d \frac{3}{2} m$), and ($d \frac{5}{2} m$). The Coulomb gauge cross section is now found to be 179 b, an almost 30% increase over the lowest order result.

Using the spherical Bessel function expansion of Eq. (18) for $K \leq 2$, we then solved the TDCC equations as found in Eqs. (19) and (20) with the addition of terms involving $j_2(kr)$ and $\sigma_z C_{2Q}(\hat{r})$ at again the same photon energy of 200 keV. Using all 32 coupled channels of Table I, the Coulomb gauge cross section is now found to be 172 b, indicating convergence of the spherical Bessel function expansion.

Finally, we solved the TDCC equations for both $K = 0$ and $K \leq 2$ in the Coulomb gauge at photon energies of 150, 175, 200, and 250 keV. In Fig. 1, the TDCC cross sections are compared with TIDW cross sections, obtained in lowest order

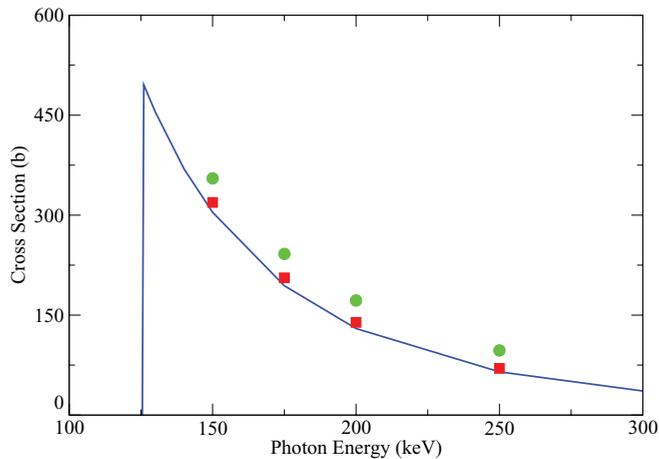


FIG. 1. (Color online) Single photoionization of U^{91+} . Solid (blue) curve, TIDW calculations; squares (red), TDCC ($K = 0$) calculations; circles (green), TDCC ($K \leq 2$) calculations ($1.0 \text{ b} = 1.0 \times 10^{-24} \text{ cm}^2$).

Lorentz gauge using Eq. (26) with $I_p = 126 \text{ keV}$. The TDCC $K = 0$ cross sections are found to be in good agreement with the TIDW cross sections at all energies. The TDCC $K \leq 2$ cross sections are found to be consistently above the low-order TDCC $K = 0$ and TIDW results.

IV. SUMMARY

Using the Dirac equation with a full electromagnetic-field potential in both the Coulomb and Lorentz gauges, relativistic

time-dependent close-coupled equations were derived for the single photoionization of one active electron highly charged atomic ions. Key steps were the introduction of a spherical Bessel function expansion and the reduction of matrix elements involving $\sigma_z C_{KQ}(\hat{r})$ tensor operators using a complete sum over $|\kappa'' m''\rangle = |l'' s'' j'' m''\rangle$ coupled states. As a test case, the single photoionization cross section for U^{91+} is found to be converged using $K \leq 2$ spherical Bessel functions. At photon energies ranging from 150 to 250 keV, the $K \leq 2$ time-dependent close-coupling cross sections are found to be approximately 30% higher than low-order time-independent distorted-wave cross sections.

In the future, we plan to derive relativistic time-dependent close-coupling equations for two active electron highly charged atomic ions which will include a full electromagnetic-field potential and an electromagnetic and retardation two-body operator. Total and differential cross sections will then be calculated for single- and double-ionization processes observed in x-ray-laser interactions with highly charged atomic ions.

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