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A Semi-Relativistic Time-Dependent Close-Coupling Method for the Double Photoionization of Ne^{8+}

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ABSTRACT: A semi-relativistic time-dependent close-coupling (TDCC) method is developed that includes the spin-orbit, mass-velocity, and Darwin interactions. The new TDCC method uses a $l_1\ j_1\ l_2\ j_2\ J$ coupling scheme instead of the $l_1\ l_2\ L\ S$ coupling scheme employed in the non-relativistic TDCC method. Calculations are carried out for the double photoionization cross section for the ground state of Ne^{8+}. For the Ne^{8+} atomic ion, the semi-relativistic TDCC results for the $1s^2\ ^1S_0$ level are slightly above the non-relativistic TDCC results for the $1s^2\ ^1S$ term.

1. INTRODUCTION

The double photoionization of atoms has been of long interest due to the difficulty in accurately describing the emission of two electrons at low photon energies. The two continuum electrons are strongly correlated and difficult to describe using many-body perturbation theory.

Good agreement was found early on between experimental measurements[1, 2] for the ratio of double photoionization to single photoionization for He($1s^2$) and non-perturbative theoretical calculations made using the eigenchannel R-matrix method [3], the converged close-coupling method [4], the R-matrix with pseudo-states method [5], the time-dependent close-coupling method [6], and the hyperspherical close-coupling method [7]. Non-perturbative theoretical calculations for the double photoionization of He($1s2s^{1,3}S$) were also made using the eigenchannel R-matrix method [8], the converged close-coupling method [9], and the time-dependent close-coupling method [10].

With the continued development of free electron lasers, the double photoionization of atomic ions has now become of interest. For example, the double photoionization of Li^+ in ground and excited states has been calculated using the converged close-coupling method [11], the B-spline based R-matrix method [12], and the time-dependent close-coupling method [13]. For more highly charged atomic ions, all methods must include semi-relativistic effects, like the spin-orbit interaction.

In this article we develop a semi-relativistic time-dependent close-coupling (TDCC) method for the double photoionization of atoms and their ions. The new TDCC method uses a $l_1\ j_1\ l_2\ j_2\ J$ coupling scheme instead of the $l_1\ l_2\ L\ S$ coupling scheme employed by the non-relativistic TDCC method. Double photoionization cross sections are calculated for the Ne^{8+} atomic ion using the non-relativistic TDCC method for the $1s^2\ ^1S$ term and compared with semi-relativistic TDCC method for the $1s^2\ ^1S_0$ level.

The rest of the paper is organized as follows: in Section 2 we develop a semi-relativistic time-dependent close-coupling method for the double photoionization of atoms and their ions, in Section 3 we calculate double photoionization cross sections for the Ne^{8+} atomic ion, while in Section 4 we conclude with a brief summary and future plans. Unless otherwise stated, we will use atomic units.

2. THEORY

A non-relativistic time-dependent close-coupling method was developed for the double photoionization of atoms using a $l_1\ l_2\ L\ S$ coupling scheme [14]. A semi-relativistic time-dependent close-coupling method will now be developed for the double photoionization of atoms and their ions using a $l_1\ j_1\ l_2\ j_2\ J$ coupling scheme.

The time-dependent Schrodinger equation for a two-electron atom, including spin-orbit, mass-velocity, and Darwin interactions[15], in a time-varying electromagnetic field is given by:

$$
\begin{aligned}
i\frac{\partial\Psi(\vec{r_1},\vec{r_2},t)}{\partial t} &= \sum_{i=1}^{2}\left(-\frac{1}{2}\nabla_i^2 + V(r_i)\right)\Psi(\vec{r_1},\vec{r_2},t) \\
&+\sum_{i=1}^{2}\left(\frac{1}{2c^2}\frac{1}{r_i}\frac{\partial V(r_i)}{\partial r_i}\vec{l_i}\cdot\vec{s_i}\right)\Psi(\vec{r_1},\vec{r_2},t) \\
&+\sum_{i=1}^{2}\left(-\frac{1}{2c^2}(E_i - V(r_i))^2\right)\Psi(\vec{r_1},\vec{r_2},t) \\
&+\sum_{i=1}^{2}\left(-\frac{1}{4c^2}\frac{\partial V(r_i)}{\partial r_i}\frac{\partial}{\partial r_i}\right)\Psi(\vec{r_1},\vec{r_2},t) \\
&+\frac{1}{\left|\vec{r_1}-\vec{r_2}\right|}\Psi(\vec{r_1},\vec{r_2},t) \\
&+E(t)\cos\omega t(r_1\cos\theta_1 + r_2\cos\theta_2)\Psi(\vec{r_1},\vec{r_2},t),
\end{aligned}
\tag{1}
$$

where $V(r_i) = -\frac{Z}{r_i}$, $\vec{l_i}$ is the orbital angular momentum, $\vec{s_i}$ is the spin angular momentum, and c is the speed of light. We choose a linearly polarized radiation field in the "length" gauge where $E(t)$ is the electric field amplitude and ω is the radiation field frequency.

2.1. TDCC Equations

Expanding the total wave function, $\psi(\vec{r}_1,\vec{r}_2,t)$, in coupled spin-orbit eigenfunctions for each symmetry and substitution into Eq. (1), including the spin-orbit, mass-velocity, and Darwin interactions, yields the following time-dependent close-coupled partial differential equations:

$$
\begin{aligned}
i\frac{\partial P^J_{l_1 j_1 l_2 j_2}(r_1,r_2,t)}{\partial t} &= \sum_{i=1}^{2} T_{l_i j_i}(r_i) P^J_{l_1 j_1 l_2 j_2}(r_1,r_2,t) \\
&+\sum_{l_1' j_1' l_2' j_2'} V^J_{l_1 j_1 l_2 j_2, l_1' j_1' l_2' j_2'}(r_1,r_2) P^J_{l_1' j_1' l_2' j_2'}(r_1,r_2,t) \\
&+\sum_{l_1' j_1' l_2' j_2' J'} W^{JJ'}_{l_1 j_1 l_2 j_2, l_1' j_1' l_2' j_2'}(r_1,t) P^{J'}_{l_1' j_1' l_2' j_2'}(r_1,r_2,t) \\
&+\sum_{l_1' j_1' l_2' j_2' J'} W^{JJ'}_{l_1 j_1 l_2 j_2, l_1' j_1' l_2' j_2'}(r_2,t) P^{J'}_{l_1' j_1' l_2' j_2'}(r_1,r_2,t).
\end{aligned}
\tag{2}
$$

The kinetic, nuclear, spin-orbit, mass-velocity, and Darwin operator is given by:

$$T_{l_i j_i}(r_i) = -\frac{1}{2}\frac{\partial^2}{\partial r_i^2} + \frac{l_i(l_i+1)}{2r_i^2} + V(r_i)$$

$$+\frac{1}{4c^2}\frac{[j_i(j_i+1) - l_i(l_i+1) - \frac{3}{4}]}{r_i}\frac{\partial V(r_i)}{\partial r_i}$$

$$-\frac{1}{2c^2}[\varepsilon_i - V(r_i)]^2 - \frac{1}{4c^2}\frac{\partial V(r_i)}{\partial r_i}[\frac{\partial}{\partial r_i} + \frac{\kappa_i}{r_i}], \tag{3}$$

where $\kappa_i = -(l_i + 1)$ for $j_i = l_i + \frac{1}{2}$ and $\kappa_i = + l_i$ for $j_i = l_i - {}^1/_2$. The electron-electron interaction energy operator, derived using expressions for the scalar product of two tensor operators and uncoupling formulae for reduced matrix elements [15], is given by:

$$V^J_{l_1 j_1 l_2 j_2, l_1' j_1' l_2' j_2'}(r_1, r_2) = (-1)^{2j_1' + j_2 + j_2' + J + 1}$$

$$\times\sqrt{(2l_1+1)(2l_2+1)(2l_1'+1)(2l_2'+1)}$$

$$\times\sqrt{(2j_1+1)(2j_2+1)(2j_1'+1)(2j_2'+1)}$$

$$\times\sum_\lambda \frac{(r_1, r_2)^\lambda_<}{(r_1, r_2)^{\lambda+1}_>}\begin{pmatrix} l_1 & \lambda & l_1' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & \lambda & l_2' \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times\begin{Bmatrix} l_1 & \frac{1}{2} & j_1 \\ j_1' & \lambda & l_1' \end{Bmatrix}\begin{Bmatrix} l_2 & \frac{1}{2} & j_2 \\ j_2' & \lambda & l_2' \end{Bmatrix}$$

$$\times\begin{Bmatrix} j_1 & j_2 & J \\ j_2' & j_1' & \lambda \end{Bmatrix}. \tag{4}$$

The radiation field energy operators, derived using the Wigner-Eckart theorem and uncoupling formulae for reduced matrix elements [15], are given by:

$$W^{JJ'}_{l_1 j_1 l_2 j_2, l_1' j_1' l_2' j_2'}(r_1, t) = E(t)\cos\omega t \cdot r_1 \delta_{l_2, l_2'}\delta_{j_2, j_2'}$$

$$\times(-1)^{j_1 + j_1' + j_2 + J + J' - M + \frac{1}{2}}\sqrt{(2J+1)(2J'+1)}$$

$$\times\sqrt{(2l_1+1)(2l_1'+1)(2j_1+1)(2j_1'+1)}$$

$$\times\begin{pmatrix} l_1 & 1 & l_1' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} J & 1 & J' \\ -M & 0 & M' \end{pmatrix}$$

$$\times \begin{Bmatrix} j_1 & j_2 & J \\ J' & 1 & j_1' \end{Bmatrix} \begin{Bmatrix} l_1 & \frac{1}{2} & j_1 \\ j_1' & 1 & l_1' \end{Bmatrix} \tag{5}$$

and

$$W^{JJ'}_{l_1 j_1 l_2 j_2, l_1' j_1' l_2' j_2'}(r_2,t) = E(t)\cos\omega t \cdot r_2 \delta_{l_1,l_1'} \delta_{j_1,j_1'}$$

$$\times (-1)^{j_1+2j_2'+2J-M+\frac{1}{2}} \sqrt{(2J+1)(2J'+1)}$$

$$\times \sqrt{(2l_2+1)(2l_2'+1)(2j_2+1)(2j_2'+1)}$$

$$\times \begin{pmatrix} l_2 & 1 & l_2' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} J & 1 & J' \\ -M & 0 & M' \end{pmatrix}$$

$$\times \begin{Bmatrix} j_1 & j_2 & J \\ 1 & J' & j_2' \end{Bmatrix} \begin{Bmatrix} l_2 & \frac{1}{2} & j_2 \\ j_2' & 1 & l_2' \end{Bmatrix}. \tag{6}$$

We assume $M = M' = 0$ in Eqs.(5) and (6). We also note that the semi-relativistic TDCC equations in imaginary time (τ) for a two-electron atom with no electromagnetic field present are given by:

$$-\frac{\partial \overline{P}^{J_0}_{l_1 j_1 l_2 j_2}(r_1,r_2,\tau)}{\partial \tau} = \sum_{i=1}^{2} T_{l_i j_i}(r_i) \overline{P}^{J_0}_{l_1 j_1 l_2 j_2}(r_1,r_2,\tau)$$

$$+ \sum_{l_1' j_1' l_2' j_2'} V^{J_0}_{l_1 j_1 l_2 j_2, l_1' j_1' l_2' j_2'}(r_1,r_2) \overline{P}^{J_0}_{l_1' j_1' l_2' j_2'}(r_1,r_2,\tau). \tag{7}$$

2.2. Bound and Continuum Radial Wavefunctions

Single particle radial wave functions, needed for the relaxation in imaginary time and the propagation in real time of the semi-relativistic TDCC equations, are obtained using matrix diagonalization and lowest order perturbation theory. We first repeatedly diagonalize a Hamiltonian given by:

$$H(r) = -\frac{1}{2}\frac{\partial^2}{\partial r^2} + \frac{l(l+1)}{2r^2} + V(r) + V_{SO}(r), \tag{8}$$

where

$$V_{SO}(r) = \frac{1}{4c^2} \frac{[j(j+1) - l(l+1) - \frac{3}{4}]}{r} \frac{\partial V(r)}{\partial r} \tag{9}$$

is the spin-orbit interaction [15]. All the bound and continuum energies and wavefunctions are then corrected in first order perturbation theory using:

$$V_{mv}(r) = -\frac{1}{2c^2}(\varepsilon - V(r))^2 \tag{10}$$

for the mass-velocity interaction [15] and

$$V_D(r) = -\frac{1}{4c^2}\frac{\partial V(r)}{\partial r}\left(\frac{\partial}{\partial r} + \frac{\kappa}{r}\right)\delta_{\kappa,-1} \tag{11}$$

for the Darwin interaction [15].

2.3. Initial and Final States

The initial conditions for the solution of the semi-relativistic TDCC equations of Eq. (7) are given by:

$$\overline{P}^{J_0}_{s\frac{1}{2}s\frac{1}{2}}(r_1, r_2, \tau = 0) = P_{1s\frac{1}{2}}(r_1)P_{1s\frac{1}{2}}(r_2) \tag{12}$$

for the $1s^2\ ^1S_0$ ($J_0 = 0$) level. The bound radial wavefunction, $P_{1s\frac{1}{2}}(r)$, is obtained by diagonalization of $H(r)$ of Eq. (8) and the application of lowest order perturbation theory using Eqs. (10) and (11). Upon relaxation in imaginary time on a numerical lattice the resulting ground state wavefunction obtained by summing over the $l_1\ j_1\ l_2\ j_2$ partial waves for $\overline{P}^{J_0}_{l_1 j_1 l_2 j_2}\left(r_1, r_2, \tau \to \infty\right)$ is fully correlated.

The initial condition for the solution of the semi-relativistic TDCC equations of Eq. (2) is given by:

$$P^J_{l_1 j_1 l_2 j_2}(r_1, r_2, t = 0) = \overline{P}^{J_0}_{l_1 j_1 l_2 j_2}(r_1, r_2, \tau \to \infty)\delta_{J,J_0}. \tag{13}$$

Upon propagation in real time on a numerical lattice the resulting electromagnetically perturbed wavefunction obtained by summing over the $l_1\ j_1\ l_2\ j_2$ partial waves for $P^J_{l_1 j_1 l_2 j_2}\left(r_1, r_2, t \to \infty\right)$ is fully correlated.

Momentum space amplitudes are given by:

$$A^J_{l_1 j_1 l_2 j_2}(k_1, k_2) = \int_0^\infty dr_1 \int_0^\infty dr_2 P_{k_1 l_1 j_1}(r_1)P_{k_2 l_2 j_2}(r_2)$$
$$\times P^J_{l_1 j_1 l_2 j_2}(r_1, r_2, t \to \infty), \tag{14}$$

where the continuum radial wavefunctions, $P_{klj}(r)$, are obtained by diagonalization of $H(r)$ of Eq. (8) and the application of lowest order perturbation theory using Eqs. (10) and (11). The total double photoionization cross section is then given by:

$$\sigma = \frac{\omega}{IT}\int_0^\infty dk_1 \int_0^\infty dk_2 \sum_{l_1 j_1 l_2 j_2 J} \left|A^J_{l_1 j_1 l_2 j_2}(k_1, k_2)\right|^2, \tag{15}$$

where I is the radiation field intensity and T is the total time for propagation.

3. RESULTS

Double photoionization cross sections for the ground state of Ne^{8+} are calculated using the non-relativistic and semi-relativistic TDCC methods. A lattice of 720×720 points is used with a uniform grid spacing of $\Delta r_1 = \Delta r_2 = 0.01$ and including up to $l \le 5$ or $lj \le 5\frac{11}{2}$ coupled channel angular momenta.

Double photoionization cross sections for the $1s^2\ ^1S$ term of Ne^{8+} are calculated using the non-relativistic TDCC method. Relaxation on the lattice with the 6 $L = 0$ coupled channels found in Table 1 yields a ground state of Ne^{8+}

with an energy of $E = -2549$ eV. Propagation on the lattice with the 16 $L = 0$, 1 coupled channels presented in Table 1 yields the total double photoionization cross sections presented in Fig. 1. At the photon energy of 3500 eV the cross section is found to peak at a value of 12.4 b.

Double photoionization cross sections for the $1s^2\ ^1S_0$ level of Ne^{8+} are calculated using the semi-relativistic TDCC method. Relaxation on the lattice with the 11 $J = 0$ coupled channels found in Table 2 yields a ground state of Ne^{8+} with an energy of $E = -2559$ eV, in good agreement with the NIST recommended value of $E = -2558$ eV[16]. Propagation on the lattice with the 39 $J = 0$, 1 coupled channels presented in Table 2 yields the total double photoionization cross sections presented in Fig. 1. The cross sections at the 6 photon energies are slightly above the non-relativistic TDCC results.

Table 1
TDCC $l_1\ l_2\ L$ coupled channels for the $1s^2\ ^1S$ term

channel	(l_1, l_2)	L	channel	(l_1, l_2)	L
1	*s, s*	0	1	*s, p*	1
2	*p, p*	0	2	*p, s*	1
3	*d, d*	0	3	*p, d*	1
4	*f, f*	0	4	*d, p*	1
5	*g, g*	0	5	*d, f*	1
6	*h, h*	0	6	*f, d*	1
			7	*f, g*	1
			8	*g, f*	1
			9	*g, h*	1
			10	*h, g*	1

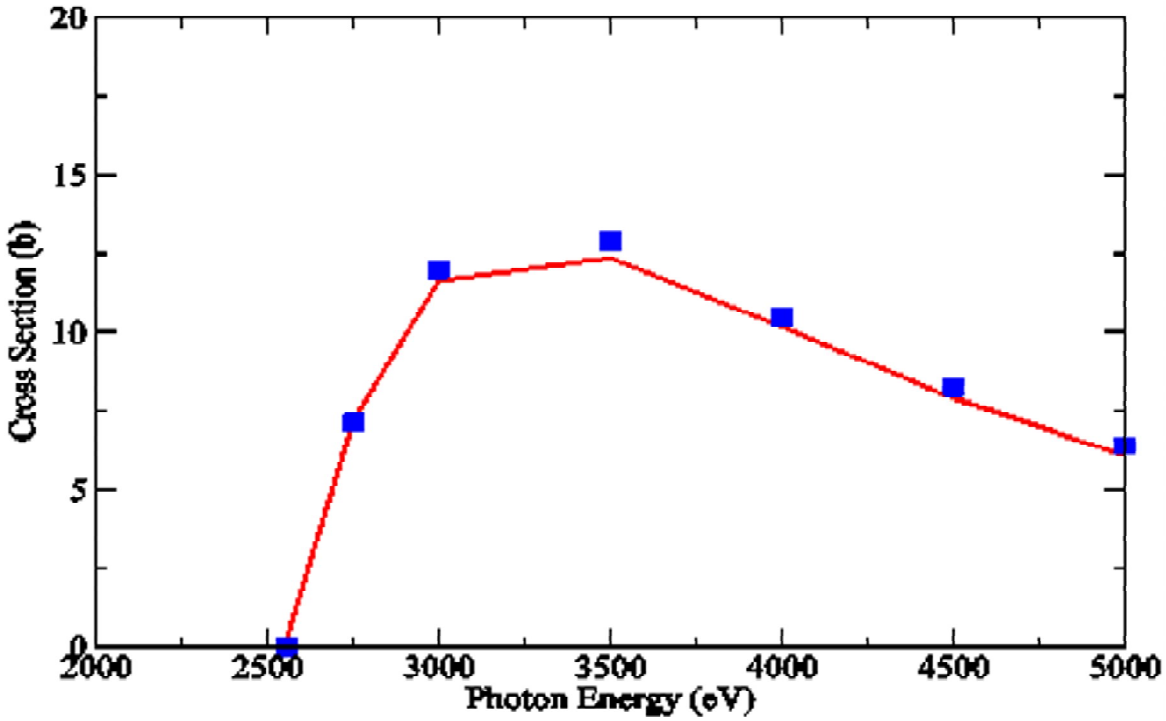

Figure 1: Double photoionization of the $1s^2$ ground configuration of Ne^{8+}. Solid line (red): non-relativistic TDCC for the ^1S term, squares (blue): semi-relativistic TDCC for the $^1S_0$ level (1.0 b = 1.0 $\times 10^{-24}$ cm^2).

Table 2
TDCC $l_1 j_1 l_2 j_2 J$ coupled channels for the $1s^2\ ^1S_0$ level

channel	$(l_1 j_1, l_2 j_2)$	*J*	*channel*	$(l_1 j_1, l_2 j_2)$	*J*
1	$s\frac{1}{2}, s\frac{1}{2}$	0	1	$s\frac{1}{2}, p\frac{1}{2}$	1
2	$p\frac{1}{2}, p\frac{1}{2}$	0	2	$p\frac{1}{2}, s\frac{1}{2}$	1
3	$p\frac{3}{2}, p\frac{3}{2}$	0	3	$s\frac{1}{2}, p\frac{3}{2}$	1
4	$d\frac{3}{2}, d\frac{3}{2}$	0	4	$p\frac{3}{2}, s\frac{1}{2}$	1
5	$d\frac{5}{2}, d\frac{5}{2}$	0	5	$p\frac{1}{2}, d\frac{3}{2}$	1
6	$f\frac{5}{2}, f\frac{5}{2}$	0	6	$d\frac{3}{2}, p\frac{1}{2}$	1
7	$f\frac{7}{2}, f\frac{7}{2}$	0	7	$p\frac{3}{2}, d\frac{3}{2}$	1
8	$g\frac{7}{2}, g\frac{7}{2}$	0	8	$d\frac{3}{2}, p\frac{3}{2}$	1
9	$g\frac{9}{2}, g\frac{9}{2}$	0	9	$p\frac{3}{2}, d\frac{5}{2}$	1
10	$h\frac{9}{2}, h\frac{9}{2}$	0	10	$d\frac{5}{2}, p\frac{3}{2}$	1
11	$h\frac{11}{2}, h\frac{11}{2}$	0	11	$d\frac{3}{2}, f\frac{5}{2}$	1
			12	$f\frac{5}{2}, d\frac{3}{2}$	1
			13	$d\frac{5}{2}, f\frac{5}{2}$	1
			14	$f\frac{5}{2}, d\frac{5}{2}$	1
			15	$d\frac{5}{2}, f\frac{7}{2}$	1
			16	$f\frac{7}{2}, d\frac{5}{2}$	1

(*contd...*)

(*Table 2 contd...*)

channel	$(l_1 j_1, l_2 j_2)$	*J*	*channel*	$(l_1 j_1, l_2 j_2)$	*J*
			17	$f\frac{5}{2}, g\frac{7}{2}$	1
			18	$g\frac{7}{2}, f\frac{5}{2}$	1
			19	$f\frac{7}{2}, g\frac{7}{2}$	1
			20	$g\frac{7}{2}, f\frac{7}{2}$	1
			21	$f\frac{7}{2}, g\frac{9}{2}$	1
			22	$g\frac{9}{2}, f\frac{7}{2}$	1
			23	$g\frac{7}{2}, h\frac{9}{2}$	1
			24	$h\frac{9}{2}, g\frac{7}{2}$	1
			25	$g\frac{9}{2}, h\frac{9}{2}$	1
			26	$h\frac{9}{2}, g\frac{9}{2}$	1
			27	$g\frac{9}{2}, h\frac{11}{2}$	1
			28	$h\frac{11}{2}, g\frac{9}{2}$	1

4. SUMMARY

A semi-relativistic time-dependent close-coupling method was developed that includes the spin-orbit, mass-velocity, and Darwin interations through the use of a $l_1\, j_1\, l_2\, j_2\, J$ coupling scheme. Double photoionization cross sections for the Ne^{8+} atomic ion were calculated for the $1s^2\ {}^1S_0$ level. A lattice with 720 × 720 points, a uniform grid spacing of $\Delta r_i = 0.01$, and $lj \le 5\frac{11}{2}$ coupled channel angular momenta was used. The semi-relativistic TDCC calculations for the $1s^2\ {}^1S_0$ level were found to be slightly above the non-relativistic TDCC calculations for the $1s^2\ {}^1S$ term.

In the future, we plan to continue the application of the semi-relativistic time-dependent close-coupling method based on a $l_1 j_1 l_2 j_2 J$ coupling scheme to atoms and their ions. We note that for more highly charged atomic ions, like Kr^{34+}, that the semi-relativistic TDCC method fails and one must use a fully-relativistic TDCC method [17]. Thus, we plan to apply the semi-relativistic TDCC method to the outer subshells of alkaline atoms and their low charged ions in the calculation of total and differential cross sections for single photon and two-photon double ionization to compare with new experimental measurements.

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