

Electron-impact double ionization of helium at high energies

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Electron-impact double-ionization cross sections for the helium atom are calculated by direct solution of a nine-dimensional Schrödinger equation using a time-dependent close-coupling method. Previous calculations are extended to higher incident electron energies using a simple factor-of-2 reduction in the mesh spacing for the three-dimensional radial lattice. The recent calculations, computationally more than an order of magnitude more difficult, are found to be in good agreement with experiment from threshold to beyond the peak of the cross section at 275 eV.

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Recently a nonperturbative theoretical method was developed to treat three continuum electrons moving in the field of a charged atomic core—that is, a solution of the quantal Coulomb four-body problem. The method is based on the reduction of the time-dependent Schrödinger equation in nine spatial dimensions to a set of time-dependent close-coupled equations on a three-dimensional radial lattice. The three-dimensional (3D) time-dependent close-coupling (TDCC) method has been applied to the electron-impact double ionization of He [1] and H^- [2], as well as the double autoionization of hollow atom states of Li [3] and He^- [4].

In this Brief Report, we extend our previous TDCC calculations for the electron-impact double ionization of He [1] to higher incident electron energies. Unless otherwise stated, all quantities are given in atomic units. With a double-ionization potential of 79 eV, the experimental peak of the He double-ionization cross section is around 275 eV [5]. Our previous TDCC calculations for He, employing a $\Delta r=0.20$ radial lattice spacing, only reported cross sections for incident electron energies from threshold to 200 eV. Our most recent TDCC calculations for He, employing a $\Delta r=0.10$ radial lattice spacing, now report cross sections for incident electron energies from threshold to 400 eV. By reducing the radial lattice spacing, we should be able to better treat the continuum electrons at the higher energies. With the same cube size, the new 3D radial lattice has 8 times as many points, requires a smaller time step, and thus computationally is more than an order of magnitude more challenging.

Our motivation for this study is to gauge the computational resources needed to successfully apply the nonperturbative 3D TDCC method to the electron-impact double ionization of various atoms and their ions. For example, with a double-ionization potential of 14.4 eV the experimental peak of the H^- double-ionization cross section is around 60 eV [6], and thus the $\Delta r=0.20$ radial lattice spacing employed in our previous TDCC calculations for H^- [2] appears adequate. However, with a double-ionization potential of 200 eV, the experimental peak of the Li^+ double-ionization cross section is around 700 eV [7], possibly requiring a quite small radial lattice for the standard TDCC method.

For electron-impact ionization of an atom with two active electrons, the angular reduction of the time-dependent

Schrödinger equation in nine spatial dimensions yields a set of time-dependent coupled partial differential equations given by [1]

$$i \frac{\partial P_{l_1 l_2 l_3}^{\mathcal{L}\mathcal{S}}(r_1, r_2, r_3, t)}{\partial t} = T_{l_1 l_2 l_3}(r_1, r_2, r_3) P_{l_1 l_2 l_3}^{\mathcal{L}\mathcal{S}}(r_1, r_2, r_3, t) + \sum_{l'_1, l'_2, l'_3} \sum_{i < j=1}^3 V_{l_1 l_2 l_3, l'_1 l'_2 l'_3}^{\mathcal{L}}(r_i, r_j) \times P_{l'_1 l'_2 l'_3}^{\mathcal{L}\mathcal{S}}(r_1, r_2, r_3, t) \quad (1)$$

for each $\mathcal{L}\mathcal{S}$ symmetry, where $T_{l_1 l_2 l_3}(r_1, r_2, r_3)$ contains kinetic energy, nuclear potential, and core Hartree local-exchange potentials, while $V_{l_1 l_2 l_3, l'_1 l'_2 l'_3}^{\mathcal{L}}(r_i, r_j)$ contains the full Coulomb repulsion operators between the three active electrons. We note that core potentials are not needed for helium. Standard numerical methods are used to obtain a discrete representation of the radial wave functions and all operators on a three-dimensional lattice. The r_1 , r_2 , and r_3 coordinates are partitioned over the many processors on a massively parallel computer.

The initial condition for the TDCC solution is given by

$$P_{l_1 l_2 l_3}^{\mathcal{L}\mathcal{S}}(r_1, r_2, r_3, t=0) = \delta_{l_1, l} \delta_{l_2, l} \delta_{L, L'} P_{ll}^{L' S'}(r_1, r_2) \delta_{l_3, \mathcal{L}} G_{k_0 \mathcal{L}}(r_3), \quad (2)$$

where $P_{ll}^{L' S'}(r_1, r_2)$ is a correlated radial wave function for the two target electrons of the ground state with $L'=S'=0$, $G_{k_0 \mathcal{L}}(r)$ is a Gaussian radial wave packet, $\frac{k_0}{2}$ is the incident electron energy, and $S=\frac{1}{2}$. For example, $P_{1105}^{5(1/2)}(r_1, r_2, r_3, t=0) = P_{11}^{00}(r_1, r_2) G_{k_0 5}(r_3)$.

Collision probabilities are obtained from the fully evolved radial wave functions $P_{l_1 l_2 l_3}^{\mathcal{L}\mathcal{S}}(r_1, r_2, r_3, t \rightarrow \infty)$ by projection onto fully antisymmetric products of spatial and spin wave functions. The TDCC double-ionization cross section is given by

$$\sigma_{dion} = \frac{\pi}{2k_0^2} \sum_{l_1, l_2, l_3} \sum_{L, S} \sum_{\mathcal{L}, S} \sum_{k_1, k_2, k_3} (2\mathcal{L} + 1)(2S + 1) \times \mathcal{P}_{l_1 l_2 L_3 \mathcal{L}, \frac{1}{2} \frac{1}{2} S_2 S_3 S}(k_1, k_2, k_3), \quad (3)$$

where $\mathcal{P}_{l_1 l_2 L_3 \mathcal{L}, \frac{1}{2} \frac{1}{2} S_2 S_3 S}(k_1, k_2, k_3)$ are momentum-space collision probabilities. The sums over the momenta are restricted so that the overall energy

$$E = E_{atom} + \frac{k_0^2}{2} = E_{ion} + \frac{k_1^2}{2} + \frac{k_2^2}{2} + \frac{k_3^2}{3} \quad (4)$$

is approximately conserved.

The distorted-wave (DW) electron-impact double-ionization cross section for ground-state helium is given by [1]

$$\sigma_{dion} = \frac{16}{\pi k_0^3} \int_0^E d\left(\frac{k_1^2}{2}\right) \int_0^{E-k_1^2/2} d\left(\frac{k_2^2}{2}\right) \times \sum_{l_1, l_2, l_3, l_n} \sum_S \sum_{\mathcal{L}} \frac{2(2\mathcal{L} + 1)}{k_1 k_2 k_3} |V_{fi}|^2. \quad (5)$$

The second-order perturbation theory matrix element V_{fi} involves a sum over n bound states and an integral over k_n continuum states. The singularity in the denominator of the matrix element is handled by standard evaluation of a principal value integration and an imaginary term.

Previous TDCC calculations for the electron-impact double ionization of He [1] employed a $(192)^3$ -point lattice with a $\Delta r = 0.20$ radial lattice spacing. The present TDCC calculations employ a $(384)^3$ -point lattice with a $\Delta r = 0.10$ radial lattice spacing. In both TDCC calculations the number of $l_1 l_2 L_3$ coupled channels varied from 11 for the $\mathcal{L} = 0$ partial cross sections to 63 for the $\mathcal{L} = 4$ partial cross sections. To obtain total cross sections, second-order perturbative DW calculations were carried out for the $\mathcal{L} = 0$ to $\mathcal{L} = 9$ partial cross sections. The DW calculations were then scaled to agree with the TDCC calculations at $\mathcal{L} = 4$ and then fit to an extrapolation function of the form $f(\mathcal{L}) = A\mathcal{L}^B e^{-C\mathcal{L}}$ to obtain the relatively small partial-wave cross sections for $\mathcal{L} \geq 10$ [1]. Thus, the final total cross sections are sums of TDCC results for $\mathcal{L} = 0-4$, scaled DW results for $\mathcal{L} = 5-9$, and extrapolated scaled DW results for $\mathcal{L} \geq 10$. We note that additional TDCC calculations using 87 channels on a $(192)^3$ -point lattice with a $\Delta r = 0.20$ radial lattice spacing were made for the $\mathcal{L} = 5$ partial cross sections. Scaling the DW calculations to agree with the TDCC calculations at $\mathcal{L} = 5$ had only a small effect on the final total cross sections. We note that the scaled DW cross sections for $\mathcal{L} \geq 5$ represent 13% of the total cross section at 100 eV incident energy, steadily increasing to 47% of the total cross section at 400 eV incident energy. We also note that summing the unscaled DW results over all $\mathcal{L}$ yields final total cross sections almost an order of magnitude larger than our TDCC results.

Electron-impact double-ionization cross sections for He are shown in Fig. 1. The TDCC results for a $\Delta r = 0.20$ radial lattice spacing are shown as the diamonds at 50-eV intervals from 100 eV to 300 eV incident electron energy. As reported

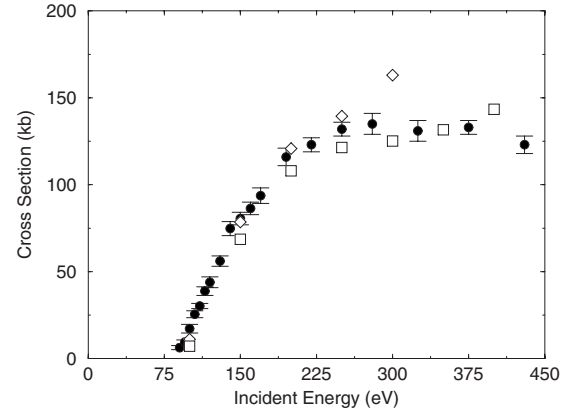


FIG. 1. Electron-impact double-ionization cross section for the helium atom. Diamonds: time-dependent close-coupling calculations with a $\Delta r = 0.20$ radial lattice spacing. Squares: time-dependent close-coupling calculations with a $\Delta r = 0.10$ radial lattice spacing. Solid circles with error bars: experiment [5] (1 kb = 10^{-21} cm²).

previously [1], the TDCC results are in good agreement with experiment [5] from threshold to 200 eV. However, previously unreported $\Delta r = 0.20$ TDCC results begin to rise above the general trend of the experimental results above 200 eV. The TDCC results for a $\Delta r = 0.10$ radial lattice spacing are shown as the squares at 50-eV intervals from 100 eV to 400 eV incident electron energy. The new $\Delta r = 0.10$ TDCC results are lower than the $\Delta r = 0.20$ TDCC results, but are in good agreement with experiment from threshold to 400 eV, beyond the peak of the cross section at 275 eV. We note that the slight upturn of the $\Delta r = 0.10$ TDCC results at 400 eV indicates that a further reduction in the radial lattice spacing is needed for even higher incident electron energies.

In summary, we have extended previous TDCC calculations [1] for electron-impact double ionization of the helium atom to higher incident electron energies by a factor-of-2 reduction in the mesh spacing for the 3D radial lattice. The most recent TDCC calculations, computationally more than an order of magnitude more difficult, are found to be in good agreement with experiment [5] from threshold to beyond the peak of the cross section at 275 eV. As illustrated by these TDCC calculations, the radial lattice spacing must give an adequate representation of the bound electrons near the nucleus and the continuum electrons at high momentum. Another variable in the scattering problem is the overall cube size, which needs to be fairly large at threshold to treat long-range correlation effects of relatively slow-moving free electrons, but might be reduced in step with a decreasing radial lattice spacing at higher incident electron energies. In the future, we plan to apply the 3D TDCC method to study electron-impact double ionization of two-electron valence subshell atoms with relatively small double-ionization potentials, like Be at 27.5 eV and Mg at 22.7 eV. We also plan to continue our studies of the double ionization of He by calculating energy and angle differential cross sections at incident energies around 100 eV in support of recent reaction microscope experiments [8].

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