

Electron-impact double ionization of B^+

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Abstract

Time-dependent close-coupling and time-independent distorted-wave methods are used to calculate the electron-impact double-ionization cross section for the $1s^2 2s^2$ ground configuration of the B^+ atomic ion. The direct double-ionization cross section is calculated using the non-perturbative close-coupling method between the direct double-ionization threshold of 63.1 eV and the $1s$ ionization threshold of 218.4 eV. The indirect single ionization–autoionization cross section is calculated using the perturbative distorted-wave method between the $1s$ ionization threshold of 218.4 and 750 eV. The double-ionization cross section calculated using the two methods is compared with a crossed-beam experiment over the entire energy range.

1. Introduction

Electron-impact double ionization of atoms may have contributions from several different collision processes. Two electrons may be directly ionized from the outer subshell resulting in a four-body Coulomb breakup problem. At higher incident energies an electron may be directly ionized from an inner subshell resulting in a three-body Coulomb breakup problem, followed by autoionization. Although the three-body process is generally well described by perturbative distorted-wave calculations, very few *ab initio* calculations have been made for the four-body process.

In recent years, a time-dependent close-coupling (TDCC) method has been used to calculate direct double ionization of the $1s^2$ subshell of He [1, 2], the $2s^2$ outer subshell of Be [3] and the $3s^2$ outer subshell of Mg [4]. A time-independent R -matrix double pseudo-state method has also been used to calculate the direct double ionization of the $2s^2$ outer subshell of Be [3]. The theoretical calculational results were found to be in good agreement with experiment for He [5] and Mg [6, 7].

In this paper, we examine the electron-impact double ionization of B^+ . At low energies we calculate the direct double-ionization cross sections for the outer subshell of the $1s^2 2s^2$ ground configuration using the TDCC method. At higher energies we calculate the indirect double-ionization cross sections coming from the single ionization of the inner subshell of both the $1s^2 2s^2$ ground and $1s^2 2s 2p$ metastable configurations followed by autoionization using a perturbative distorted-wave method. We compare the double-

ionization cross sections for B^+ with experimental crossed-beam measurements [8].

The remainder of this paper is organized as follows. In section 2, we review the TDCC and the configuration-average distorted-wave (CADW) methods. In section 3, we apply the two methods to the calculation of the electron-impact double-ionization cross section of B^+ over a wide energy range to compare with experiment. In section 4, we conclude with a summary and an outlook for future work. Unless otherwise stated, all quantities are given in atomic units.

2. Theory

2.1. Time-dependent close-coupling method

The TDCC method was developed to study atomic and molecular few-body collisions [9]. Formulations of the basic method have been used to solve the problem of two or three continuum electrons in the Coulomb field of an atomic or molecular ion.

The time-dependent Schrodinger equation for electron scattering from two active electrons in an atom is given by

$$i \frac{\partial \Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, t)}{\partial t} = H_{\text{system}} \Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, t), \quad (1)$$

where the non-relativistic Hamiltonian for the scattering system is given by

$$H_{\text{system}} = \sum_{i=1}^3 \left(-\frac{1}{2} \nabla_i^2 - \frac{Z}{r_i} + V_{HX}(r_i) \right) + \sum_{i < j=1}^3 \frac{1}{|\vec{r}_i - \vec{r}_j|}, \quad (2)$$

\vec{r}_i are the electron coordinates, Z is the nuclear charge and $V_{HX}(r)$ is a Hartree with local exchange potential. Expanding the total electronic wavefunction in twice coupled spherical harmonics and substitution into the time-dependent Schrodinger equation yields a set of time-dependent close-coupled partial differential equations for each total $\mathcal{L}\mathcal{S}$ symmetry given by

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

where $P_{l_1 l_2 l_3}^{\mathcal{L}\mathcal{S}}(r_1, r_2, r_3, t)$ is a three-electron radial wavefunction, $T_{l_1 l_2 l_3}(r_1, r_2, r_3)$ is a three-fold sum over one-electron kinetic, nuclear and atomic core operators and $V_{l'_1 l'_2 l'_3, l_1 l_2 l_3}^{\mathcal{L}}(r_i, r_j)$ is a two-electron repulsion operator (see equations (36)–(39) of [9]).

The initial condition for the solution of the TDCC(3e) equations is a product of a two-electron radial wavefunction, obtained by the solution of a set of TDCC(2e) equations for the relaxation of a two-active-electron atom in imaginary time, and a one-electron Gaussian wavepacket with propagation energy $\frac{k_0^2}{2}$. Following time propagation of the TDCC(3e) equations, the total double-ionization cross section is given by

$$\begin{aligned} \sigma_{\text{double}} &= \frac{\pi}{2k_0^2} \int_0^\infty dk_1 \int_0^\infty dk_2 \int_0^\infty dk_3 \sum_{\mathcal{L}, \mathcal{S}} (2\mathcal{L} + 1)(2\mathcal{S} + 1) \\ &\times \sum_{L, S} \sum_{l_1, l_2, l_3} |P_{l_1 l_2 l_3, L S}^{\mathcal{L}\mathcal{S}}(k_1 l_1, k_2 l_2, k_3 l_3)|^2, \end{aligned} \quad (4)$$

where $P_{l_1 l_2 l_3, L S}^{\mathcal{L}\mathcal{S}}(k_1 l_1, k_2 l_2, k_3 l_3)$ is a three-electron momentum space wavefunction found by the projection of the time-evolved coordinate space wavefunctions onto fully anti-symmetric products of three box-normalized continuum orbitals (see equations (48)–(49) of [9]).

2.2. Configuration-average distorted-wave method

The CADW method was first applied to calculate total cross sections for electron-impact excitation, ionization and recombination of atoms and their ions [10]. A general transition for direct ionization has the form

$$(nl)^w k_i l_i \rightarrow (nl)^{w-1} k_e l_e k_f l_f, \quad (5)$$

where w is a subshell occupation number, nl are quantum numbers of the bound electron and $k_i l_i$, $k_e l_e$ and $k_f l_f$ are quantum numbers of the initial, ejected and final continuum electrons, respectively. The ionization cross section is given by

$$\sigma_{\text{single}} = \int_0^{E/2} d\epsilon_e \frac{32w}{k_i^3 k_e k_f} \sum_{l_i, l_e, l_f} (M_d + M_e - M_x), \quad (6)$$

where the linear momentum $k = \sqrt{2\epsilon}$, the total energy $E = \epsilon_{nl} + \epsilon_i = \epsilon_e + \epsilon_f$ and the continuum normalization is chosen as 1 times a sine function. The direct, exchange and interference scattering terms, M , are products of standard

algebraic n_j symbols and radial integrals which include static electrodynamic interactions [10]. The energies and bound orbitals needed to evaluate the cross section are calculated using Cowan's atomic structure package [11]. The continuum radial orbitals are obtained by solving a single-channel Schrodinger equation for various choices of scattering potentials [12, 13].

3. Results

We divide the calculation of the electron-impact double ionization of B^+ into two parts. For incident energies below the 1s ionization threshold, the direct double-ionization cross section is calculated using the non-perturbative TDCC method. Only a small number of incident energies are needed to determine the shape and magnitude of the smoothly varying cross section. For incident energies above the 1s ionization threshold, the indirect double-ionization cross section is calculated using the perturbative CADW method. Since an experiment for energies above the 1s ionization threshold contains both direct and indirect double-ionization contributions, we check the indirect CADW calculations by adding to them an experimental extrapolation of the direct double-ionization cross section from below the 1s ionization threshold.

In past calculations for the electron-impact direct double ionization of He, Be and Mg, we employed a $(192)^3$ point lattice with a uniform mesh spacing of $\Delta r = 0.20$. TDCC(3e) calculations for He [1], with a direct double-ionization potential of 79.0 eV, were made up to 2.5 times threshold and found to be in good agreement with experiment. TDCC(3e) calculations for Be [3], with a direct double-ionization threshold of 27.5 eV, were made up to 3.5 times threshold and found to be in good agreement with R -matrix calculations near threshold. TDCC(3e) calculations for Mg [4], with a direct double-ionization threshold of 22.7 eV, were made up to 2.5 times threshold and found to be in good agreement with experiment. Additional TDCC(3e) calculations for He [2] were made using a $(384)^3$ point lattice with a uniform mesh spacing of $\Delta r = 0.10$. On average, the propagation time for the Schrodinger equation increases by a factor of 4 for each factor of 2 decrease in the mesh spacing. The $\Delta r = 0.10$ calculations for He were made up to 5.0 times threshold and found to agree with the earlier $\Delta r = 0.20$ calculations up to 2.5 times threshold. Direct double-ionization cross sections at ever higher incident energies require an ever larger number of lattice points and an ever longer propagation time to describe the faster probability flows, resulting in an increasingly difficult computational task.

Non-perturbative TDCC(3e) calculations were carried out for electron-impact double ionization of the outer subshell of the $1s^2 2s^2$ ground configuration of B^+ . Using a $(192)^2$ point lattice with a uniform mesh spacing of $\Delta r = 0.20$ and a core pseudo-potential, relaxation of the TDCC(2e) equations in imaginary time yielded two-electron radial wavefunctions with a double-ionization potential of 63.3 eV, compared to the experimental value of 63.1 eV [14]. In keeping with previous calculations for He, Be and Mg, we used a $(192)^3$ point lattice

with a uniform mesh spacing of $\Delta r = 0.20$ to propagate the TDCC(3e) equations in real time for $\mathcal{L} = 0 - 5$ $S = \frac{1}{2}$ total symmetries and for incident energies of 100 eV, 150 eV and 200 eV. As used in previous TDCC(3e) calculations for Be [3] and Mg [4], the number of coupled channels, $(l_1 l_2 l_3)$, ranged from 11 for $\mathcal{L} = 0$ to 81 for $\mathcal{L} = 5$, while the partial cross sections were extrapolated to higher \mathcal{L} using a nonlinear angular momentum fitting expression given by

$$\sigma(\mathcal{L}) = c_1 \mathcal{L}^{c_2} e^{-c_3 \mathcal{L}}, \quad (7)$$

where c_i are fitting coefficients.

Perturbative CADW calculations were carried out for electron-impact single ionization of the inner subshell of both the $1s^2 2s^2$ ground and $1s^2 2s 2p$ metastable configurations of B^+ . For ionization of a tightly bound inner subshell, the CADW method should be reasonably accurate. Our Hartree–Fock calculations [11] yield an inner subshell ionization potential of 218.4 eV for the $1s^2 2s^2$ ground configuration and 216.9 eV for the $1s^2 2s 2p$ metastable configuration. The background direct double-ionization cross section for energies greater than the inner subshell ionization potential is given by an experimental fitting formula [8]

$$\sigma_{\text{double}} = (1.8 \times 10^8) (1 - e^{-3(1-u)}) \frac{(u-1)}{I_d^3 (u+0.5)^2}, \quad (8)$$

where the cross section is in Kb ($1.0 \times 10^{-21} \text{ cm}^2$), $I_d = 63.1 \text{ eV}$, $u = E/I_d$ and E is the incident energy in eV. The total double-ionization cross section for energies greater than the inner subshell ionization potential is given by

$$\sigma_{\text{total}} = \sigma_{\text{double}} + \sigma_{\text{single}} B_{\text{auto}}. \quad (9)$$

For low charged atomic ions, the autoionization rates are much stronger than the radiative rates, so setting the autoionization branching ratios for the $1s 2s^2$ and $1s 2s 2p$ configurations of B^{2+} to 1 is an excellent approximation.

The electron-impact double-ionization cross section results using the TDCC and CADW methods are compared with experimental crossed-beam measurements [8] in figure 1. The B^+ ion beam in the experiment contains a mixture of ground and metastables, the exact fraction of each unknown, but usually dominated by the ground state. The cross section peaks at close to 700 eV.

At incident energies less than the $1s$ ionization threshold, the TDCC cross sections for the double ionization of the outer subshell of the $1s^2 2s^2$ ground configuration are found to be just below the error bars of the crossed-beam experiment [8]. We reserve the computationally intensive TDCC calculations for the direct double ionization of the outer subshells of the $1s^2 2s 2p$ metastable configuration until the precise value is known for the fraction of metastables in the experiment.

At incident energies greater than the $1s$ ionization threshold, the CADW cross sections for the single ionization of the inner subshell of the $1s^2 2s^2$ ground configuration using all $N - 1$ scattering potentials [13], added to the experimental background fit of equation (8), are found to be within the error bars of the crossed-beam experiment [8]. The CADW cross sections for the single ionization of the inner subshell of the $1s^2 2s 2p$ metastable configuration using all $N - 1$ scattering potentials [13], added to the experimental background fit

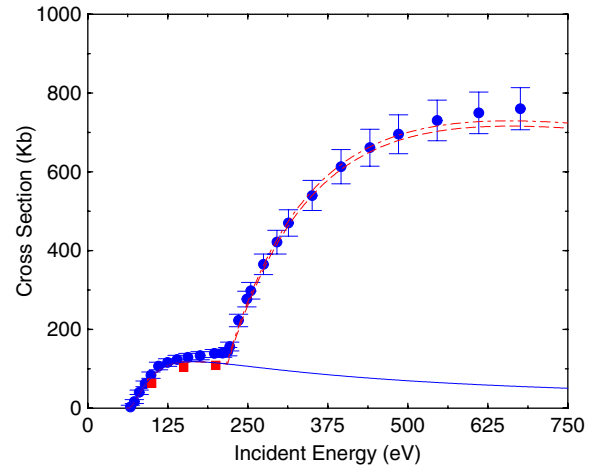


Figure 1. Electron-impact double ionization of B^+ . Solid squares: TDCC calculations for the double ionization of the outer subshell of the $1s^2 2s^2$ ground configuration, dashed line: CADW calculations for the single ionization of the inner subshell of the $1s^2 2s^2$ ground configuration added to a background double ionization fit, dot-dashed line: CADW calculations for the single ionization of the inner subshell of the $1s^2 2s 2p$ metastable configuration added to a background double ionization fit, solid circles: experiment [8], solid line: double ionization fit to experiment [8] ($1.0 \text{ Kb} = 1.0 \times 10^{-21} \text{ cm}^2$).

(This figure is in colour only in the electronic version)

of equation (8), are found to be slightly higher than the ground configuration results, but still within the error bars of the crossed-beam experiment [8]. We note that CADW cross sections using a mixture of N and $N - 1$ scattering potentials [12], added to the experimental background fit of equation (8), are just below the error bars of the crossed-beam experiment [8].

4. Summary

In conclusion, we have carried out non-perturbative TDCC and perturbative CADW calculations for the electron-impact double ionization of B^+ . The direct double-ionization cross sections between the direct double-ionization threshold at 63.1 eV and the $1s$ ionization threshold at 218.4 eV, and the indirect double-ionization cross sections between the $1s$ ionization threshold at 218.4 eV and 750 eV, are compared with a crossed-beam experiment [8]. In the future, we plan to apply the TDCC and CADW methods to calculate double-ionization cross sections for other singly charged atomic ions, for example Li^+ and Al^+ .

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References

- [1] Pindzola M S, Robicheaux F, Colgan J, Witthoef M C and Ludlow J A 2004 *Phys. Rev. A* **70** 032705
- [2] Pindzola M S, Robicheaux F and Colgan J 2007 *Phys. Rev. A* **76** 024704
- [3] Pindzola M S, Ballance C P, Robicheaux F and Colgan J 2010 *J. Phys. B: At. Mol. Opt. Phys.* **43** 105204
- [4] Pindzola M S, Ludlow J A, Robicheaux F, Colgan J and Griffin D C 2009 *J. Phys. B: At. Mol. Opt. Phys.* **42** 215204
- [5] Shah M B, Elliott D S, McCallion P and Gilbody H B 1988 *J. Phys. B: At. Mol. Opt. Phys.* **21** 2751
- [6] McCallion P, Shah M B and Gilbody H B 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** 1051
- [7] Boivin R F and Srivastava S K 1998 *J. Phys. B: At. Mol. Opt. Phys.* **31** 2381
- [8] Shevelko V P, Tawara H, Scheuermann F, Fabian B, Muller A and Salzborn E 2005 *J. Phys. B: At. Mol. Opt. Phys.* **38** 525
- [9] Pindzola M S *et al* 2007 *J. Phys. B: At. Mol. Opt. Phys.* **40** R39
- [10] Pindzola M S, Griffin D C and Bottcher C 1986 *Atomic Processes in Electron–Ion and Ion–Ion Collisions (NATO ASI B 145)* (New York: Plenum) p 75
- [11] Cowan R D 1981 *The Theory of Atomic Structure and Spectra* (Berkeley, CA: University of California Press)
- [12] Younger S M 1981 *Phys. Rev. A* **24** 1278
- [13] Botero J and Macek J H 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** L405
- [14] <http://physics.nist.gov/PhysRefData>