Photo-double-ionization of the He and Be isoelectronic sequences within an intermediate-energy *R*-matrix framework

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The intermediate-energy R-matrix approach (IERM) has been developed as a first step towards representing a double-electron continua within a general multielectron R-matrix code. Using this method, we study photodouble-ionization of the ground states of the He and Be isoelectronic sequences and show excellent agreement with other theoretical and experimental results. We confirm scaling relations for the photo-double-ionization cross section along the He isoelectronic sequence and suggest a scaling relation, which takes into account the screening effect of the 1s electrons, for the photo-double-ionization cross section for Be-like ions. We also examine trends in the ratio of double to single ionization.

DOI: 10.1103/PhysRevA.88.053413

PACS number(s): 32.80.Fb

I. INTRODUCTION

Experimental advances allowing attosecond photon pulses, reported by Corkum and Krausz [1], in which photons have sufficient energy to excite or cause the emission of one or more electrons, enable multielectron dynamics to be time-resolved. This necessitates accurate theoretical treatment of multielectron dynamics for both a time-independent framework and a time-dependent framework. Recently a time-dependent Rmatrix-based approach has been developed which is capable of studying the interaction of intense short-pulse laser light with many-electron atoms or ions (see Lysaght et al. [2] and Moore et al. [3]). A means of incorporating a double-electron continua in this method and the general time-independent *R*-matrix method is thus sought after. As a first step towards this, the intermediate-energy *R*-matrix (IERM) approach to photoionization has recently been developed by Scott et al. [4]. This approach has been thus far successfully applied to the study of photoionization and photo-double-ionization of He and the study of photodetachment and photo-doubledetachment of H⁻. In this paper we extend this previous work to consider photo-double-ionization of the ground states of He-like and Be-like ions with $Z \leq 10$.

Photo-double-ionization, as an interesting study of electron-electron dynamics, has recently attracted a great deal of attention. The *R* matrix with pseudostates method (RMPS) [5,6] has been used by McLaughlin [7] to study photo-doubleionization of Li⁺ from the ground and excited states and by Griffin et al. [8] to investigate photo-double-ionization of Be and Mg. Kleiman et al. [9] studied photo-double-ionization of Li⁺ using the time-dependent close-coupling approach (TDCC) while Pindzola et al. [10] studied photo-doubleionization of Be and Mg using the same approach. The convergent close coupling (CCC) approach has been used by Kheifets and Bray [11–13] to study photo-double-ionization of various He-like systems. In addition van der Hart and Feng [14] have used a *B*-spline-based *R*-matrix method to investigate photo-double-ionization along the He isoelectronic sequence. Wehlitz et al. measured the photo-double-ionization cross section of Be up to photon energies of 40 eV [15] and of Mg up to 54 eV [16].

The remainder of this paper is organized as follows: in Sec. II we present a summary of the IERM theory of

photoionization of atoms and ions; in Secs. III and IV we describe and present results of calculations for photo-double-ionization of He-like and Be-like ions, respectively. We then draw conclusions and summarize further work in Sec. V.

II. THEORY

A full treatment of the IERM photoionization theory for two-electron atoms and ions has been presented by Scott *et al.* [4]; we therefore present only a summary here, with an extension to allow the study of quasi-two-electron atoms or ions. The total photoionization cross section in the length approximation is

$$\sigma = \frac{8\pi^2 \alpha a_o^2 \omega}{3(2L_i+1)} \sum_{l_f L} |\langle \Psi_f^-||M||\Psi_i\rangle|^2, \tag{1}$$

where α is the fine-structure constant, a_0 is the Bohr radius of hydrogen, ω is the energy of the incident photon in atomic units, and M is the dipole matrix operator. The initial- and finalstate wave functions, Ψ_i and Ψ_f^- , are appropriately normalized solutions of the time-independent Schrödinger equation

$$H\Psi = E\Psi,\tag{2}$$

with the two-electron Hamiltonian given by

$$H = \left(-\frac{1}{2}\nabla_1^2 - \frac{Z}{r_1}\right) + \left(-\frac{1}{2}\nabla_2^2 - \frac{Z}{r_2}\right) + \frac{1}{r_{12}}.$$
 (3)

The initial two-electron bound state, Ψ_i , is defined by the quantum numbers $L_i S_i \Pi_i$, while the final "ion + electron" continuum state, Ψ_f^- , has the quantum numbers $LS\Pi$. The final state of the residual ion is defined by $L_f S_f \Pi_f$. Both Ψ_i and Ψ_f^- are expanded in terms of appropriate energy-independent *R*-matrix basis states,

$$\Psi_i = \sum_k A_{ki} \Theta_k^{L_i S_i \Pi_i},\tag{4}$$

$$\Psi_f^- = \sum_k A_{ki} \Theta_k^{LS\Pi},\tag{5}$$

where $\Theta_k(\mathbf{r}_1, \mathbf{r}_2)$ are the energy-independent *R*-matrix basis states given by

$$\Theta_{k}^{L_{i}S_{i}\Pi_{i}}(\mathbf{r}_{1},\mathbf{r}_{2}) = \sum_{n_{1}^{\prime}l_{1}^{\prime}n_{2}^{\prime}l_{2}^{\prime}} \chi_{n_{1}^{\prime}l_{1}^{\prime}n_{2}^{\prime}l_{2}^{\prime}}^{L_{i}S_{i}\Pi_{i}}(\mathbf{r}_{1},\mathbf{r}_{2})\beta_{n_{1}^{\prime}l_{1}^{\prime}n_{2}^{\prime}l_{2}^{\prime}}^{L_{i}S_{i}\Pi_{i}}$$
(6)

and

$$\Theta_{k}^{LS\Pi}(\mathbf{r}_{1},\mathbf{r}_{2}) = \sum_{n_{1}l_{1}n_{2}l_{2}} \chi_{n_{1}l_{1}n_{2}l_{2}}^{LS\Pi}(\mathbf{r}_{1},\mathbf{r}_{2})\beta_{n_{1}l_{1}n_{2}l_{2}}^{LS\Pi},$$
(7)

in which the coefficients β are obtained by diagonalizing the relevant two-electron Hamiltonian matrix, and the two-electron functions $\chi_{n_1l_1n_2l_2}^{LS\Pi}(\mathbf{r}_1,\mathbf{r}_2)$ are

$$\chi_{n_{1}l_{1}n_{2}l_{2}}^{LS\Pi}(\mathbf{r}_{1},\mathbf{r}_{2}) = \frac{1}{\sqrt{2}} \{r_{1}^{-1}r_{2}^{-1}u_{n_{1}l_{1}}(r_{1})u_{n_{2}l_{2}}(r_{2})\mathcal{Y}_{l_{1}l_{2}LM_{L}}(\hat{\mathbf{r}}_{1},\hat{\mathbf{r}}_{2}) + (-)^{l_{1}+l_{2}+L+S}r_{1}^{-1}r_{2}^{-1}u_{n_{1}l_{1}}(r_{2})u_{n_{2}l_{2}}(r_{1}) \\ \times \mathcal{Y}_{l_{2}l_{1}LM_{L}}(\hat{\mathbf{r}}_{1},\hat{\mathbf{r}}_{2})\} \quad \text{if} \quad n_{1}l_{1} \neq n_{2}l_{2} \quad (8)$$

and

$$\chi_{nlnl}^{LS\Pi}(\mathbf{r}_{1},\mathbf{r}_{2}) = r_{1}^{-1}r_{2}^{-1}u_{nl}(r_{1})u_{nl}(r_{2})\mathcal{Y}_{llLm_{L}}(\hat{\mathbf{r}}_{1},\hat{\mathbf{r}}_{2}) \quad \text{if} \\ n_{1}l_{1} = n_{2}l_{2}. \tag{9}$$

The radial functions $u_{nl}(r)$ are solutions to the following equation

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2Z}{r} + k_{nl}^2\right)u_{nl}(r) = 0, \quad (10)$$

with the boundary conditions

$$u_{nl}(0) = 0, \quad \left(\frac{a}{u_{nl}}\right)\frac{du_{nl}}{dr}\Big|_{r=a} = 0$$

Following the approach of Burke *et al.* [17], it is possible to rewrite the coefficients A_{ki} and A_{kf} as

$$A_{ki} = G_{ki} \mathbf{W}_{ki}^{T}(a) \mathbf{R}_{i}^{-1} \mathbf{y}_{i}(a), \qquad (11)$$

$$A_{kf} = G_{kf} \mathbf{W}_{kf}^{T}(a) \mathbf{R}_{f}^{-1} \mathbf{y}_{f}^{-}(a), \qquad (12)$$

where matrices y describe the radial motion of the photoelectron, **R** are the *R* matrices, and **W** are surface amplitudes. *i* and *f* represent the initial and final states, respectively. **G** are matrices with diagonal elements, given by

$$G_{ki} = \frac{1}{2a(E_{ki} - E_i)},$$
(13)

$$G_{kf} = \frac{1}{2a(E_{kf} - E_i - \omega)}.$$
 (14)

 E_i is the energy of the initial state, and E_{ki} and E_{kf} are eigenvalues resulting from the diagonalization of the initialand final-state Hamiltonian matrices.

The expression for the cross section can then be written as

$$\sigma = \frac{8\pi^2 \alpha a_0^2 \omega}{3(2L_i+1)} \sum_{l_f L} |\mathbf{y}_f^{-T} \mathbf{R}_f^{-1} \mathbf{W}_f \mathbf{G}_f \mathbf{V}_f^T \mathbf{M} \mathbf{V}_i \mathbf{G}_i \mathbf{W}_i^T \mathbf{R}_i^{-1} \mathbf{y}_i|^2,$$
(15)

where the matrices V_i and V_f have columns composed of the β coefficients. If the chosen *R*-matrix radius is large enough to completely envelope the initial bound state, one of the eigenvalues in Eq. (13) should be extremely close to the energy of the initial state, E_i , and the contribution to the wave function from closed channels in the external region can be neglected. We apply a very small correction to the appropriate element of the Hamiltonian matrix prior to diagonalization, in order to

ensure the eigenvalue is as close as possible. If this particular eigenvalue corresponds to k = k', then

$$A_{ki} = \begin{cases} 1 \text{ for } k = k', \\ 0 \text{ otherwise.} \end{cases}$$
(16)

Equation (11) then simplifies to

$$\sigma = \frac{8\pi^2 \alpha a_0^2 \omega}{3(2L_i+1)} \sum_{l_f L} \left| \mathbf{y}_f^{-T} \mathbf{R}_f^{-1} \mathbf{W}_f \mathbf{G}_f \mathbf{V}_f^T \mathbf{M} \mathbf{V}_{ik'} \right|^2, \quad (17)$$

where $V_{ik'}$ is the eigenvector corresponding to the required eigenvalue.

The photo-double-ionization cross section may be estimated by summing the contributions to the cross section from positive energy pseudostates. A correction is applied to the photo-double-ionization cross section to compensate for any overestimate or underestimate associated with the distribution of pseudostates around the double-ionization threshold.

For the Be-like calculations presented in Sec. IV, the potential $2Zr^{-1}$ in Eq. (10) is replaced by a core potential, V_{core} , given by Bartschat [18], which is made up of three components as follows:

$$V_{\text{core}}^{l}(r) = V_{\text{static}}(r) + V_{\text{exch}} + V_{\text{pol}}^{l}(r), \qquad (18)$$

where the static potential, $V_{\text{static}}(r)$, is the Hartree potential [19] given by

$$V_{\text{static}}(r) = -\frac{Z}{r} + \sum_{n_c, l_c} N_{n_c, l_c} \int_0^\infty dr' \frac{P_{n_c, l_c}^2(r')}{\max(r, r')}, \qquad (19)$$

and N_{n_c,l_c} is the number of electrons in the core orbital P_{n_c,l_c} . V_{exch} is the exchange potential and models the effect of exchange between valence and core electrons: it is of the type first introduced by Furness and McCarthy [20],

$$V_{\text{exch}}(r) = -\frac{1}{2} \{ [V_{\text{static}}(r)^2 + 4\pi\rho(r)]^{\frac{1}{2}} - V_{\text{static}}(r) \}, \quad (20)$$

where the electron density of the core is given by

$$\rho(r) = \sum_{n_c, l_c} N_{n_c, l_c} \frac{P_{n_c, l_c}^2(r)}{4\pi r^2}.$$
(21)

The polarization potential is given by

$$V_{\text{pol}}^{l}(r) = -\frac{\alpha_d(l)}{2r^4} \left[1 - \exp\left\{ -\left(\frac{r}{r_c(l)}\right)^6 \right\} \right], \quad (22)$$

where the dipole polarizability of the core α_d and the cutoff radius r_c are varied, for each orbital angular momentum, l, in order to achieve agreement with ionization potentials from the National Institute of Standards and Technology (NIST) [21].

III. PHOTO-DOUBLE-IONIZATION OF THE HE ISOELECTRONIC SEQUENCE

A. Calculation

Details of the calculation of photo-double-ionization cross sections for He-like ions, in the $1s^2$ ${}^{1}S^{e}$ ground state, with atomic number Z = 2, ..., 10 are presented in this section. Dipole selection rules allow only one final state of the system, ${}^{1}P^{o}$. For each ion, physical orbitals 1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, 4f of the relevant H-like

TABLE I. *R*-matrix radii in atomic units selected for the low- and high-energy calculations for each He-like ion.

Ion	Low-energy radius	High-energy radius
H ^{-a}	110.00	60.00
He ^a	70.00	40.00
Li ⁺	47.00	26.50
Be ²⁺	35.00	20.00
B^{3+}	28.00	16.00
C^{4+}	23.30	13.35
N ⁵⁺	22.00	11.45
O^{6+}	19.00	10.00
F^{7+}	18.00	8.90
Ne ⁸⁺	16.00	8.00

^aScott et al. [4].

ion are included and augmented with pseudo-orbitals n = 5, ..., 38 and orbital angular momentum l = 0, ..., 3. The photoionized electron, in both its initial "bound" and final ejected state, is represented using the same one-electron basis except that a total of 70 radial functions were included per orbital angular momentum. The inclusion of pseudo-orbitals gives rise to pseudostates, which allow the photo-double-ionization cross section to be approximated by summing the cross section to the positive-energy pseudostates lying above the double-ionization threshold. Since the two-electron wave function of the He-like ground state is represented in terms of products of H-like orbitals [see Eqs. (4)–(10) the inclusion of the initial ground state.

As in the evaluation detailed by Scott *et al.* [4], the photo-double-ionization cross sections presented in this section consist of two calculations. At energies close to the double-ionization threshold, where the cross section is rapidly increasing, it is important to have a dense pseudostate basis, and therefore a larger radius is selected. For the second calculation this radius is reduced, allowing the same number of pseudostates to span a larger energy region in which the cross section is not varying so rapidly. The radii used in these calculations are shown in Table I. The *R*-matrix radius for each ion was chosen so that the cross section was fully converged. There are a total of 146 H-like residual ion target states in each calculation, with at least 104 of these lying above the double-ionization threshold for the low-energy calculations and at least 108 for the high-energy calculations.

As noted in Sec. II a small correction is applied to the appropriate element of the two-electron Hamiltonian matrix prior to diagonalization in order to bring the energy of the ground state into agreement with NIST values; the correction and energies are detailed in Table II.

B. Results

To compare in more detail with recent work, we present, in Fig. 1 the photo-double-ionization cross section for the Li⁺ ion and compare with data from the RMPS calculation of McLaughlin [7], TDCC calculation of Pindzola *et al.* [24], and CCC data from Kheifets and Bray [11–13]. The present results lie just below the RMPS data and just above the TDCC calculation across the energy region. Agreement with the CCC

TABLE II. Calculated ground-state ionization potentials in atomic units for each He-like ion along with the correction added to the Hamiltonian matrix prior to diagonalization to improve agreement with NIST values.

Atom, ion	Calculated	Correction	NIST
H-	-0.5231^{a}	-0.0081^{a}	-0.5278 ^b
He	-2.8997^{a}	-0.0042^{a}	-2.9037 ^c
Li ⁺	-7.2755	-0.0061	-7.2798^{d}
Be ²⁺	-13.6540	-0.0170	-13.6566^{d}
B ³⁺	-22.0139	-0.0208	-22.0348^{d}
C^{4+}	-32.3883	-0.0276	-32.4160^{d}
N ⁵⁺	-44.7572	-0.0443	-44.8016^{d}
O^{6+}	-59.1322	-0.0612	-59.1935 ^d
F ⁷⁺	-75.5045	-0.0893	-75.5939 ^d
Ne ⁸⁺	-93.8796	-0.1253	-94.0050^{d}

^aScott *et al*. [4].



^cPekeris [23].

^dNIST [21].

calculation is excellent for all energies. We note that Scott *et al.* [4] also achieved excellent agreement with experiment with a IERM calculation for He, again confirming that the IERM method performs well. Also shown in Fig. 1 is a fit of the shape function of Pattard [25] to the current data. Pattard showed that the cross section for multiple photoionization processes in which all electrons are ionized can be parametrized as follows:

$$\sigma(\epsilon) = \sigma_M x^{\alpha} \left(\frac{\alpha + 7/2}{\alpha x + 7/2} \right)^{(\alpha + 7/2)},$$
(23)

where σ_M is the maximum value of the cross section, and the Wannier threshold exponent [26], α , depends on the charge of



FIG. 1. (Color online) Photo-double-ionization cross section for Li⁺ for photon energies in the range 200 to 650 eV. Black solid line, present calculation; brown dashed line, shape function of Pattard [25] [Eq. (23)] fit to the current data; purple diamonds, RMPS McLaughlin [7]; green squares, TDCC Pindzola *et al.* [24]; red triangles, CCC Kheifets [13].



FIG. 2. Photo-double-ionization cross sections along the He isoelectronic sequence. Note that cross sections have been smoothed with an 8th-degree polynomial fit.

the residual ion, Z_r , and is given by

$$\alpha = \frac{1}{4} \left[\left(\frac{100Z_r - 9}{4Z_r - 1} \right)^{1/2} - 1 \right].$$
 (24)

 $x = \epsilon/\epsilon_M$, where ϵ is the excess energy above the doubleionization threshold and ϵ_M is the energy value of the maximum in the photo-double-ionization cross section. σ_M and ϵ_M were set as adjustable parameters when fitting the shape function to the current data and the shape function is shown to fit the current data very well in Fig. 1, with only a slight difference around the peak in the cross section. The photodouble-ionization cross sections for He-like ions with Z = $3, \ldots, 10$ are presented in Fig. 2; note that all cross sections increase rapidly to a maximum after the double-ionization threshold, after which they decrease smoothly. Very small oscillations in the cross sections have been smoothed using an 8th-degree polynomial fit to the data. These oscillations arise as a result of the many pseudostate thresholds and may be eliminated by a number of methods, of which some examples are given by Scott et al. [4]. Figure 3 shows the photo-doubleionization cross sections along the He isoelectronic sequence: the cross section is scaled by Z^4 and plotted against the photon energy, ϵ , relative to the double-ionization threshold scaled by Z^{-2} . We note that, while the scaled cross sections for all the systems except H⁻ are in good agreement with each other, the



FIG. 3. (Color online) Z-scaled photo-double-ionization cross sections plotted against the photon energy, ϵ , relative to the double-ionization threshold. Note that cross sections have been smoothed with an 8th-degree polynomial fit. The He calculation is from Scott *et al.* [4].

maximum in the cross section for He lies highest, with the maximum decreasing with Z; excellent agreement is achieved for the highest Z values. This is in agreement with the scaling laws proposed by Kronberg and Miraglia [27], who also noted that the data for H⁻ did not follow the general trend.

IV. PHOTO-DOUBLE-IONIZATION OF THE BE ISOELECTRONIC SEQUENCE

A. Calculation

In this section details of the calculation of photo-doubleionization cross sections for Be-like ions in the ground $1s^22s^2$ ${}^{1}S^{e}$ state, with atomic number $Z = 4, \ldots, 10$, are presented. Again, ${}^{1}P^{o}$ is the only permitted final state of the system. For each ion, physical orbitals 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, 4fof the relevant Li-like ion are included in the expansion of the wave function and augmented by pseudo-orbitals n =5, ..., 35 with orbital angular momentum l = 0, ..., 5. It is worth noting that the He-like calculations of Sec. III had fully converged by l = 3 while terms up to l = 5 were required for full convergence of the cross sections here. However the effect of including higher angular momentum terms became less as Z increased. The $1s^2$ core is treated as "frozen" and is represented for each ion using the core potential detailed in Sec. II. As in Sec. III, the calculations for each ion are split into low- and high-energy evaluations. Again, a relatively large radius is used in order to achieve a denser pseudostate basis at energies just above the double-ionization threshold, while a smaller radius is used for the higher energy calculation. The radii used are presented in Table III. There are a total of 258 Li-like target states in each calculation with 115 lying above the double-ionization threshold for the low-energy calculations and between 122 and 130 for the high-energy calculations. We again apply a small correction to the appropriate element of the Hamiltonian matrix prior to diagonalization in order to bring our calculated ground-state energy into agreement with NIST values. The original calculated energies, along with the

TABLE III. *R*-matrix radii in atomic units selected for low- and high-energy calculations for each Be-like ion.

Ion	Low-energy radius	High-energy radius
Be	79.82	39.88
B^+	52.43	24.94
C^{2+}	40.03	21.55
N ³⁺	30.91	17.47
O^{4+}	26.25	16.99
F ⁵⁺	21.42	12.98
Ne ⁶⁺	18.96	11.48

corrections applied, and the NIST energies are presented in Table IV.

B. Results

In this section we present photo-double-ionization cross sections for Be-like ions. In Fig. 4 we give results for the photodouble-ionization cross section for Be and compare them with the experimental data of Wehlitz et al. [15]. Good agreement is obtained throughout the energy range, except that our results lie slightly higher at the peak occurring just below 40 eV. We also compare our results, in Fig. 4, with data from several theoretical calculations: the CCC data of Kheifets and Bray [28] lies slightly above the present results at energies beneath 35 eV and slightly below at higher energies; data from the TDCC calculation of Colgan and Pindzola [29] predicts the peak in the cross section at around 37 eV to be slightly higher than the IERM results. The RMPS calculation of Griffin et al. [8] agrees well with the present results across the energy range. A fit of the shape function of Pattard [25] [given by Eq. (23)] to the current data is included in Fig. 4. Similarly to Fig. 1, the shape function fits the present data excellently apart from a slight deviation around the maximum in the cross section, this agreement is typical for the other atoms and ions studied in this paper.

The percentage ratio of double ionization to single ionization in photoionization of Be is compared with experiment and other theories in Fig. 5. We achieve excellent agreement with the experimental results of Wehlitz *et al.* [15] and the TDCC results of Pindzola *et al.* [10] across the energy range, while the CCC data of Kheifets and Bray [30] lie above the present results across the energy range. The RMPS data of Pindzola

TABLE IV. Calculated ground-state ionization potentials in atomic units for each Be-like ion along with the correction added to the appropriate Hamiltonian matrix element prior to diagonalization to improve agreement with NIST values.

Atom, ion	Calculated	Correction	NIST
Be	-1.0190	-0.0082	-1.0119 ^a
B^+	-2.3047	-0.0152	-2.3184^{a}
C^{2+}	-4.1394	-0.0104	-4.1299^{a}
N ³⁺	-6.4492	0.0047	-6.4445^{a}
O^{4+}	-9.3853	-0.1678	-9.2315ª
F ⁵⁺	-12.5857	0.0046	-12.5811^{a}
Ne ⁶⁺	-16.4099	0.0062	-16.4037^{a}

^aNIST [21].





FIG. 4. (Color online) Photo-double-ionization cross sections for neutral Be. Black solid line, present results; brown dashed line, a fit of the shape function of Pattard [25] [Eq. (23)] to the current data; blue circles, experimental results of Wehlitz *et al.* [15]; red triangles, CCC results of Kheifets and Bray [28]; green squares, TDCC results of Colgan and Pindzola [29]; purple diamonds, RMPS data of Griffin *et al.* [8].

et al. [10] is very slightly lower than the present data at around 30 eV and higher at 40 eV, but agrees well elsewhere. The excellent agreement with experimental and other theoretical data, shown in Figs. 4 and 5, shows that the core potential used in the calculations in this section is functioning correctly and further indicates the validity of the IERM approach.

Individual cross sections for Be-like ions with Z = 4, ..., 10 are presented in Fig. 6, where we again note the common shape of the photo-double-ionization cross section. At low Z the scaling of Z^4 in the cross section and Z^{-2} in the excess energy above the double-ionization threshold is not appropriate for the photo-double-ionization cross section for Be-like ions. We suggest that this is due to the screening effect of the 1*s* electrons and show in Fig. 7 that, by replacing



FIG. 5. (Color online) Percentage ratio of double ionization to single ionization in the photoionization of Be. Black solid line, present results; blue circles, experimental results of Wehlitz *et al* [15]; red triangles, CCC results of Kheifets and Bray [30]; green squares, TDCC results of Pindzola *et al*. [24]; purple diamonds, RMPS results of Griffin *et al*. [8].



FIG. 6. Photo-double-ionization cross sections along the Be isoelectronic sequence. Note that cross sections have been smoothed with an 8th-degree polynomial fit.

Z with an effective nuclear charge Z_{eff} and applying the He scaling laws to the Be isoelectronic sequence, this screening effect can be accounted for. The effective charge is given by $Z_{\text{eff}} = Z - \delta$, where we determined δ to be 1.65 by matching the height of the peaks in the cross section for each ion. Bluett



FIG. 7. (Color online) Scaled photo-double-ionization cross sections along the Be isoelectronic sequence plotted against the photon energy, ϵ , relative to the double-ionization threshold.

TABLE V. Calculated maximum in the ratio of double ionization to single ionization compared to the value predicted by Eq. (26). Values used for the ionization thresholds in Eq. (26) were obtained from the NIST database [21].

	Atom, ion	Calculated	Predicted
He-like	H^-	9.07	13.60
	He	3.89	3.93
	Li ⁺	1.89	1.60
	Be^{2+}	1.11	0.87
	B^{3+}	0.71	0.55
	C^{4+}	0.50	0.39
	N ⁵⁺	0.37	0.30
	O^{6+}	0.29	0.23
	F^{7+}	0.23	0.19
	Ne ⁸⁺	0.18	0.16
Be-like	Be	2.58	2.19
	\mathbf{B}^+	1.37	1.05
	C^{3+}	0.81	0.62
	N^{4+}	0.54	0.42
	O^{5+}	0.39	0.31
	F ⁶⁺	0.29	0.24
	Ne ⁷⁺	0.22	0.20

et al. [31] and Wehlitz [32] observed that the maximum in the ratio of double to single photoionization of various atoms and molecules can be predicted using a simple formula involving the single- and double-ionization thresholds of the system in question. They show that the maximum in the ratio may be predicted as a percentage by

$$R_{\rm max} = E_2^{1/2} - E_1^{1/2}, \qquad (25)$$

where E_1 and E_2 are the appropriate single- and doubleionization thresholds in eV. In line with this, we find that for most of the atoms and ions studied here that the maximum ratio follows the trend

$$R_{\rm max} = E_2^{1/Z_r} - E_1^{1/Z_r}, \qquad (26)$$



FIG. 8. (Color online) Maximum values of the ratio of double to single ionization for He-like and Be-like atoms and ions. Black squares, present calculation; red circles, predicted by Eq. (26).

where Z_r is the charge of the residual ion. The values for the maximum value of the ratio of double to single ionization predicted by the model and the calculated values are presented in Table V and Fig. 8. Apart from those of H⁻ the calculated and model values agree reasonably well and can be seen to follow a similar trend with Z.

V. CONCLUSIONS

We have, further to Scott *et al.* [4], demonstrated the usefulness of the IERM approach to photoionization in the calculation of photo-double-ionization cross sections for twoelectron atoms and ions, which we have presented for He-like and Be-like ions with $Z \leq 10$. We found that angular momenta terms up to l = 5 were required for the convergence of Be-like photo-double-ionization calculations while l = 3 sufficed for He-like photo-double-ionization calculations. Excellent agreement has been shown with other theoretical methods, including the RMPS data of McLaughlin [7] and Griffin *et al.* [8], the TDCC calculation of Pindzola *et al.* [24], and the CCC data of Kheifets and Bray [11]. We have also demonstrated excellent agreement with the experimental results of Wehlitz et al. [15] and confirmed the scaling laws put forward by Kornberg and Miraglia [27] for the photo-double-ionization cross section along the He isoelectronic sequence. We suggest a scaling relation along the Be isoelectronic sequence with an effective nuclear charge that takes the screening effect of the core electrons into account. We find that the maximum in the ratio of double to single ionization for the majority of the atoms and ions studied can be predicted with reasonable accuracy using a relationship between the single- and double-ionization thresholds, similarly to Bluett et al. [31] and Wehlitz [32]. This work adds weight to the suggestion that this approach could be successfully incorporated into a many-electron *R*-matrix approach as part of a multipurpose R-matrix code capable of representing multiple electron ejection. The IERM codes are currently being used to carry out photoionization calculations on He-like and Be-like ions in excited initial states.

ACKNOWLEDGMENTS

The authors would like to thank Professor Ralf Wehlitz for providing his data in numerical form. A.J.K. and M.W.M. were supported by Northern Ireland DEL postgraduate studentships.

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