Scaling laws in double photoionization

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Double-photoionization cross sections are calculated for two-electron targets H^-, He, Li^+, and O^{6+} using a correlated and an uncorrelated two-electron continuum wave function (C3 and C2 models, respectively). As the target nuclear charge Z_T is increased, the double-photoionization cross section is found to scale as Z_T^{-4} and the electron energy distribution as Z_T^{-6}. Conclusions are extracted about the behavior of the cross sections in the high-energy and threshold regions. The ratio of double to single photoionization scales as Z_T^{-2}, as in the case of proton impact.

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INTRODUCTION

In the present work we investigate the influence of the nuclear charge Z_T on the behavior of the cross sections for double photoionization for two-electron atoms in their ground state. Calculations for the systems H^-, He, Li^+, and O^{6+} using two models for the double-continuum wave function are presented and the scaling laws are derived. Special emphasis is devoted to the high-energy and threshold regions.

This work is motivated by the recent interest in double photoionization of He both theoretically [1–4] and experimentally [5,6], and by the challenging problem of double photoionization of atomic negative ions [7], such as H^- here under consideration. For the H^- ion there exists sparse knowledge of the behavior of the cross sections both theoretically [2,8] and experimentally [9]. For other two-electron atoms no available studies exist at present.

The process that we consider is the impact of one linearly polarized photon on two-electron atoms of nuclear charge Z_T in their ground state. The basis observable of the process in the fivefold differential cross section (FDCS) $d^5\sigma^{2+}/d\varepsilon_1 d\Omega_1 d\Omega_2$, where ε_1 is the energy of one of the electrons whose momentum $\mathbf{k}_1$ subtends an element of solid angle $d\Omega_1$. The quantities labeled 2 refer to the other electron. We shall denote $E_f=\varepsilon_1+\varepsilon_2$ as the total final energy and E_γ as the photon energy. From the FDCS, we can perform three integrals in closed form to arrive at a double-differential cross section $d^2\sigma^{2+}/d\varepsilon_1 \sin\theta_{12} d\theta_{12}$ [1], where θ_{12} is the asymptotic angle between $\mathbf{k}_1$ and $\mathbf{k}_2$. The electron energy distribution $d\sigma^{2+}/d\varepsilon_1$ and the total cross section σ^{2+} follow from the usual integrations.

In describing the ground state of a two-electron atom we have employed two types of correlated wave functions, namely, a four-parameter Hylleraas type (labeled BK after the work of Bonham and Kohl [10]), and a multiconfigurational type (labeled SH after the work of Sabelli and Hinze [11]). The correlation energy and the cusp condition at the nucleus of the wave functions employed are displayed in Table I. Notice that the accuracy of the multiconfigurational method decreases as Z_T increases, whereas that of the Hylleraas one does not.

Two models for the double continuum are considered. First, a wave function that is built as a product of three two-body continua (C3 model) [12,13] [see also Eq. (6) of Ref. [1]]. A second model is considered in the independent-electron approximation, C2 in our notation, indicating the product of only two Coulomb waves. This model has been extensively used in double photoionization [1,14]. The C3 and C2 models exactly satisfy the cusp condition at the nucleus.

The method of calculation employing BK C3 states was developed in Ref. [1], whereas employing SH C2 states was reported in Ref. [15]. The numerical calculation using SH-C2 is fairly fast, demanding about 1 h of CPU time per total cross section on a 10-Megaflop computer. The calculation using BK-C3 requires a three-dimensional numerical integral and so it is slow and demands about 20 h per total cross section on the same computer.

As far as total cross sections are concerned there is no point in doing calculations with the C3 final state; the C2 approximation produces reasonable results as compared with the data in a broad range of energies [1]. The positive aspect of the C3 results lies in the singly and multiply differential cross sections, mainly angular distributions, where dramatic disagreements with C2 results are observed. Angular distributions using the C3 were shown to be in good agreement with the *shape* of the experiments even at low energies [16], where the theory is known to fail by orders of magnitude in *absolute* scale. Unfortunately, there are no experiments of differential cross section at large photon energies, say $E_\gamma \geq 1.0$ keV on He, where the C3 state is expected to be applicable.

TABLE I. Correlation energies and cusp ratios for Bonham and Kohl (BK) and Sabelli and Hinze (SH) wave functions for the ground state of two-electron atoms.

Z_T	$E_{\rm corr}^{\rm BK}(\%)$	$E_{\rm corr}^{\rm SH}(\%)$	$R_{\rm cusp}^{\rm BK}$	$R_{\rm cusp}^{\rm SH}$
1	95.62	99.00	−0.768	−1.049
2	95.72	98.07	−1.807	−2.161
3	95.74	97.24	−2.817	−3.119
8	95.78	96.48	−7.824	−8.073

SCALING LAWS

For a two-electron target with nuclear charge Z_T, the Schrödinger equation can be scaled to give a universal Hamiltonian. We then have to work in the so-called Coulomb units with the only difference that the e-e repulsion $1/r_{12}$ reduces to Z_T^{-1}/r_{12}. So, as $Z_T \to \infty$ the following scaling laws should be observed:

$$\left[\frac{d\sigma^+}{d\Omega},\sigma^+\right](E_f,Z_T)\to\frac{1}{Z_T^2}\left[\frac{d\sigma^+}{d\Omega},\sigma^+\right](E_f/Z_T^2,1)\ , \tag{1}$$

$$\frac{d^5\sigma^{2+}}{d\varepsilon_1 d\Omega_1 d\Omega_2}(E_f,Z_T)\to\frac{1}{Z_T^6}\frac{d^5\sigma^{2+}}{d[\varepsilon_1/Z_T^2]d\Omega_1 d\Omega_2}\times(E_f/Z_T^2,1)\ , \tag{2}$$

$$\frac{d\sigma^{2+}}{d\varepsilon_1}(E_f,Z_T)\to\frac{1}{Z_T^6}\frac{d\sigma^{2+}}{d[\varepsilon_1/Z_T^2]}(E_f/Z_T^2,1)\ , \tag{3}$$

$$\sigma^{2+}(E_f,Z_T)\to\frac{1}{Z_T^4}\sigma^{2+}(E_f/Z_T^2,1)\ . \tag{4}$$

In Fig. 1, C2 and C3 scaled total-cross-section results in the velocity (V) [Fig. 1(a)] and length (L) [Fig. 1(b)] forms are displayed for the double photoionization of

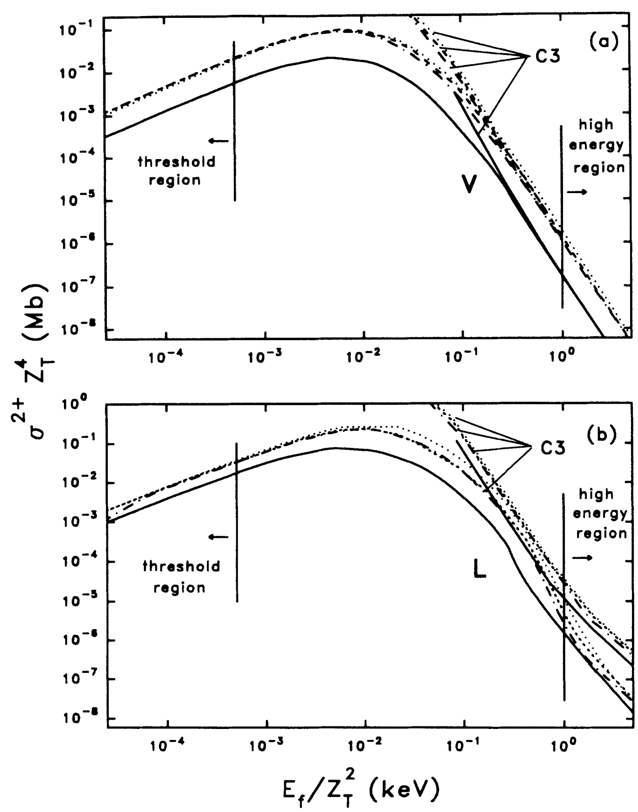

FIG. 1. Scaled total cross section for double photoionization versus the scaled final energy. Calculations are with SH and C2 states and with BK and C3 states (indicated in the figure). Results in (a) velocity gauge and (b) length gauge for H^- (solid line), He (dot-dashed line), Li^+ (dashed line), and O^{6+} (dotted line).

H^-, He, Li^+, and O^{6+} targets in terms of the scaled energy. A good agreement of this scaling is observed for $Z_T \geq 2$; for the worst case $Z_T=1(H^-)$, the results clearly do not follow the general trend. Also, notice that the length-velocity discrepancy in H^- is greater than for the other cases.

We observed that both the C2 and C3 models give just the same value of cross section in the velocity gauge at high energy, falling off as $E_f^{-7/2}$, and for the case of He a good agreement with the data was observed [1]. In the length form the two results disagree, and fall off as $E_f^{-5/2}$. It should be remembered that the C3 model is a high-energy approximation [1], which is why we only plot the results in the falling tail. From the comparison with the experiments on He we expect the C3 approximation to work for energies larger than $E_f/Z_T^2 \simeq 300$ eV.

By theoretical and experimental considerations, the threshold or Wannier region has been considered to extend until $E_f/Z_T^2=0.5$ eV, and the high-energy region to begin at $E_f/Z_T^2=1.0$ keV. They will be discussed separately in the next sections.

HIGH-ENERGY REGION

For He it has been shown both experimentally and theoretically that there exists a high-energy region, also called asymptotic, for which the ratio $R=\sigma^{2+}/\sigma^+$ is nearly constant, and this value was determined to be 1.67% [2,3]. For the ions H^- and Li^+, this ratio has been determined to be [2] 1.50% and 0.87%, respectively. From scaling considerations R scales as Z_T^{-2}, and extrapolating the Li^+ value one obtains $R \simeq 0.87(3/Z_T)^2$ %. In this region the cross section σ^{2+} falls off as $E_f^{-7/2}$, and the formula

$$\sigma^{2+}(E_f,Z_T)=\sigma_\infty(Z_T)E_f^{-7/2} \tag{5}$$

holds for a Z_T target. For the He case we can identify this region for the energies $E_f > 4.0$ keV, which has an experimental [6] as well as a theoretical [1] justification. From the scaling, we can infer that the high-energy region for a two-electron target should begin at about $E_f \simeq 1.0$ keV $\times Z_T^2$.

From our velocity results of total cross sections the following constants were extracted: $\sigma_\infty(1) = 1.89\times10^{-7}, \sigma_\infty(2)=9.26\times10^{-6}, \sigma_\infty(3)=4.48\times 10^{-5}$, and $\sigma_\infty(8)=2.34\times10^{-3}$ in Mb keV$^{7/2}$. From Eq. (5) and using the scaling equation (4) the following value is obtained: $\sigma_\infty(Z_T)\simeq 2.34(Z_T/80)^3$ in Mb keV$^{7/2}$.

THRESHOLD REGION

The Wannier [17] theory for double photoionization of a two-electron target predicts that the total cross section varies with E_f as

$$\sigma^{2+}(E_f,Z_T)=\sigma_0(Z_T)E_f^m\ , \tag{6}$$

where $\sigma_0(Z_T)$ is a constant depending only on the nuclear charge and $m=\frac{1}{4}[(100Z_T-9)/(4Z_T-1)]^{1/2}-\frac{1}{4}$; m takes the values 1.127, 1.056, 1.036, and 1.012 for

$Z_T = 1,2,3$, and 8, respectively, and $m \to 1$ as $Z_T \to \infty$.

For the case of He numerous studies in the threshold region exist [18-20], whereas for H^- only scarce data have been collected. It has been experimentally verified [18,19] that the validity of the power law $\sigma^{2+}(E_f,2)=\sigma_0(2)E_f^{1.056}$ in He ranges up to about 2 eV above threshold, and an experimental value for the constant $\sigma_0(2)$ was found to be 1.02×10^{-3} Mb [18] (when E_f is in eV). No theoretical estimate for this quantity has been done. For the H^- ion there exists an experimental verification of the power law $\sigma^{2+}(E_f,1)\propto E_f^{1.127}$ [9]; a theoretical calculation of the constant $\sigma_0(1)$ [8] gives a value of 3.14×10^{-2} Mb.

Results using the C2 model are presented in Fig. 2 in the length and velocity forms and compared with the Wannier formula Eq. (6) drawn as a solid line. The experimental results of Kossmann *et al.* [18] for He are included, and show that the length form presents a good behavior at threshold. The constants $\sigma_0(1)=0.0314$ Mb and $\sigma_0(2)=0.001\,02$ Mb were used, and for $Z_T \geq 3$ the experimental He value $\sigma_0(2)$ was extrapolated from Eq. (6) (considering $m=1$) and the scaling equation (4) as $\sigma_0(Z_T)=0.001\,02(2/Z_T)^6$ Mb. Notice that the theoretical value $\sigma_0(1)=3.14\times10^{-2}$ Mb obtained in Ref. [8] using a semiclassical approximation appears to be of the correct order of magnitude.

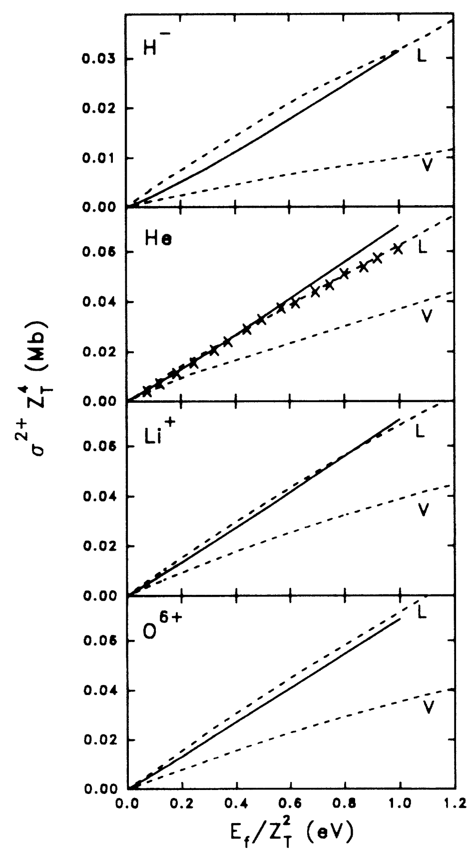

FIG. 2. Scaled total cross section in the threshold region calculated with SH and C2 states (dashed line) versus the scaled final energy. The solid line represents the power law $\sigma^{2+}(E_f,Z_T)=\sigma_0(Z_T)E_f^m$. H^- with $\sigma_0(1)=3.14\times10^{-2}$ Mb and $m=1.127$; He with $\sigma_0(2)=1.02\times10^{-3}$ Mb and $m=1.056$ together with the experimental points ($\times$) of Ref. [18]; Li^+ with $\sigma_0(3)=8.95\times10^{-5}$ Mb and $m=1.036$; and O^{6+} with $\sigma_0(8)=2.49\times10^{-7}$ Mb and $m=1.012$.

DIFFERENTIAL CROSS SECTIONS

The electron energy distributions using the C2 and C3 models are displayed in Figs. 3(a) and 3(b), respectively. The scale energy was chosen to be $E_f/Z_T^2 \simeq 730$ eV, which corresponds to a photon energy of $E_\gamma \simeq 744, 3000, 6770$, and 48 345 eV for $Z_T=1,2,3$, and 8, respectively. One sees a general good agreement of the scaling for $Z_T=2,3$, and 8, whereas the H^- result as expected departs from this limiting behavior. Inspecting the C3 model one observes a flat top peak at the very center of the distribution (the so called W form) differing from the U form given by the C2 model. Experiments would be very welcome to determine the real form.

SUMMARY

In this Brief Report calculations of double-photoionization cross sections have been presented for two-electron targets H^-, He, Li^+, and O^{6+} using the C2 and C3 approximations for the double continuum. A simple scaling relation has been derived, which estab-

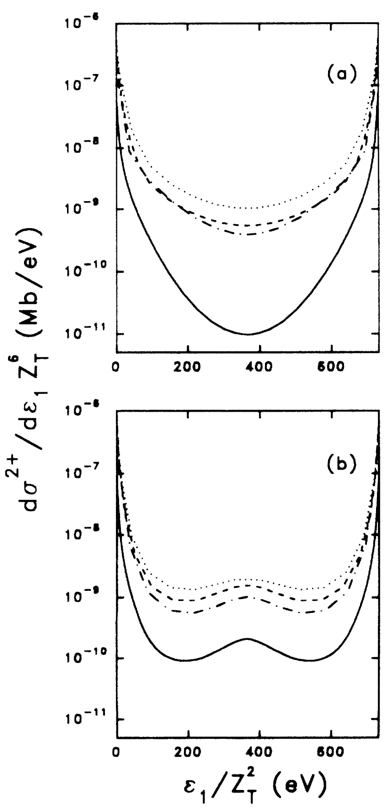

FIG. 3. Scaled electron energy distribution (velocity formulation) as a function of the scaled energy of an electron for $E_f/Z_T^2 \simeq 730$ eV (a) employing SH and C2 states, and (b) employing BK and C3 states. The curves are labeled as in Fig. 1.

lishes that the total cross section σ^{2+} scales with Z_T^{-4}, and the electron energy distribution $d\sigma^{2+}/d\varepsilon_1$ and the FDCS scale with Z_T^{-6}. The fit of the H^- results to this scaling is not very good, because the Z_T dependence of the cross section rises for large Z_T.

The high-energy region has been determined to begin at about $E_f \simeq (1.0 \text{ keV}) \times Z_T^2$, while the threshold region extends to $E_f \simeq (0.5 \text{ eV}) \times Z_T^2$. In this context, the asymptotic ratio of double to single photoionization could be given by $R \simeq 7.4/Z_T^2$ % for $Z_T \geq 3$, and the constant σ_0 appearing in the Wannier power law could be estimated to be $\sigma_0 \simeq (6.5\times 10^{-2}\text{Mb})/Z_T^6$ for $Z_T \geq 3$.

We point out that in the process of double ionization of a two-electron target by proton impact the cross section $\sigma^{2+}_{\text{proton}}$ scales as Z_T^{-6} [21]. For single photoionization $\sigma^{+}_{\text{photon}} \sim Z_T^{-2}$, whereas for proton impact $\sigma^{+}_{\text{proton}} \sim Z_T^{-4}$, and the ratio $R = \sigma^{2+}/\sigma^{+} \sim Z_T^{-2}$ for both processes. This scaling should serve as a tool for investigating the e-e correlation in two-electron targets, which with recent progress in ion sources will become readily feasible.

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