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Sebastian Otranto
Missouri University of Science and Technology, otrantos@mst.edu

C. R. Garibotti

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Kinetic Correlation In Photo-Double-Ionization Processes: The He-Isoelectronic Sequence.

S. Otranto[1†] and C. R. Garibotti[‡]

[†]*Dto. de Física, Universidad Nacional del Sur, 8000 Bahía Blanca, Argentina*
Physics Department, University of Missouri-Rolla, Rolla MO 65401, USA
[‡]*CONICET and Centro Atómico Bariloche, S. C. de Bariloche 8400, Argentina.*

Abstract. Analytical models proposed to represent the two-electron continuum are revisited. Main results obtained with these models are summarized. Recent studies of the photo-double-ionization (PDI) of the He-isoelectronic sequence by means of the recently introduced SC3 model are shown and compared with the results predicted by classical and semi-classical Wannier approaches. By fitting the triply differential cross sections (TDCSs) with the usual dipolar Gaussian form we find that the width has a power dependence on excess energy with exponent 0.25 in the near threshold region and departs from this law with increasing energy.

Keywords: Photo double ionization. Three body Coulomb problem.
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INTRODUCTION

During the last few years, the three body Coulomb problem has been considered in several articles in order to improve the theoretical description of atomic collisions processes [1-7]. The main idea underlying in these articles is to generalize an existing analytical model denoted as C3 [8-9] which fulfills the Redmond asymptotic conditions in the Ω_0 region, where the three particles are far from each other. These generalizations were built requiring a satisfactory description of other possible asymptotic configurations. For many atomic ionization processes, these models lead to a good qualitative description of the cross sections at high and intermediate collision energies, and allow for a partially analytic evaluation of transition amplitudes.

Nowadays, powerful numerical methods have gone beyond the existing analytical models leading to very accurate results for the cross sections for different processes [10-13]. Meanwhile, the description of an approximate continuum wave function for a three Coulomb interacting particles system remains as a challenging theoretical problem.

In a recent paper, we have presented a new analytical model for the two electron continuum, which we have denoted SC3 [14]. This model was formulated as to improve the C3 results for the photo double ionization (PDI) of He in the threshold region. From an approximated analysis in this region we have shown that the scaling

[1] Electronic address: sotranto@uns.edu.ar

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of the interelectronic distance with a multiplicative energy dependent factor leads to a better description of the evaluated cross sections.

In this report, we summarize and discuss the above mentioned generalizations of the C3 model and we show recent results obtained with the SC3 model for the He-isoelectronic sequence. By fitting the TDCS with the usual dipolar Gaussian form [15], we obtain the energy dependence of the widths and compare our results with classical and semi-classical Wannier approaches [16-21].

Atomic units are used unless where explicitly stated.

THE THREE BODY COULOMB PROBLEM

The Schrödinger equation for the two-electron atom is a non-separable differential equation that couples the three possible pairs of particles through the usually denominated non-diagonal kinetic energy W_1 given by

$$W_1 = -\nabla_1 \cdot \nabla_{12} + \nabla_2 \cdot \nabla_{12} \qquad (1)$$

The analytical C3 model [8-9] represents an approximated solution of the Schrödinger equation where only the diagonal terms of the kinetic energy are considered (ie. $W_1 = 0$). Since 1993, several models were developed in order to include the information contained in Eq. (2). C3-type models with coordinates or momenta-dependent charges have been developed by asking the satisfaction of several physical desirable asymptotic limits [1-3,7]. Models based on several variables hypergeometric functions have also been developed with the same aim [4-5]. Most of these models were initially designed and tested in the (e,2e) context. However, they have not been pushed further in the PDI field and up to our knowledge, only a few works have been devoted to their implementation [22-23]. For the screened models, the small number of asymptotic conditions imposed in order to determine the effective charges, leaves considerable freedom to potential models in the reaction region where the particles are close to each other and the information contained in Eq. (2) is supposed to be of vital importance and should be properly accounted.

Very recently, we have introduced another C3-type wave function which boosts the interelectronic distance through the introduction of an energy dependent multiplicative factor [14]. This model, hereafter denoted as SC3 model, was designed in order to correct the well known exponential decreasing behavior given by the C3 model in the threshold region. The latter is well known to be due to an overestimation of the electronic repulsion at low excess energies [24]. In the following section we focus our attention in the PDI process for the He-isoelectronic sequence and we present the results obtained with the SC3 model.

THE PDI PROCESS

The PDI process has proven to be one of the more stringent tests for any theory posed to describe the two-electron continuum. Due to the mono-electronic character of the operators conforming the dipole Hamiltonian, this process only can be achieved

through electronic correlation and in general, results turn to be extremely sensitive on the modeling performed in both initial and final states [25]. Maulbetsch and Briggs studied the PDI of He using the C3 model to represent the two-electron continuum. The C3 model, even showing nice angular distributions given its simplicity, evidenced the necessity of new models mainly at low energies at which experimental data started to be available.

As has been shown by Lucey *et al.* [22] the use of approximations for both the initial and final states which do not correspond to the same Hamiltonian, leads to gauge discrepancies due to the lack of satisfaction of the Heisenberg equation of motion. In their work, a C3 model with coordinate and momentum-dependent charges proposed by Berakdar in 1996 [2] was used and disagreement between gauges was obtained for a whole set of initial state wave functions of different accuracy.

However, for the equal energy sharing regime where both electrons leave the reaction region with the same velocity, angular shapes obtained in velocity and length gauge are in good agreement with each other even when magnitude differences are obtained. Huetz *et al.* [15] pointed out that in this regime the TDCS can be rewritten as the product of a correlation factor times an angular factor:

$$\frac{d\sigma}{d\Omega_1 d\Omega_2 dE_1} = C(\theta_{12}, E_f, Z)(\cos\theta_1 + \cos\theta_2)^2. \quad (2)$$

During the last few years, the Gaussian shape for the correlation factor has become of standard use with its full width at half maximum considered as an empirical parameter over a wide range of excess energies [26-27]:

$$C(\theta_{12}, E_f, Z) = A(E_f, Z)\exp\left[-\frac{4\ln 2\left(\theta_{12} - 180°\right)^2}{\Gamma\left(E_f, Z\right)^2}\right]. \quad (3)$$

Semi-classical Wannier approaches have generally assumed the following energy dependence for the width Γ, even when they obtain somewhat different values for Γ_0.

$$\Gamma(E_f, Z) = \Gamma_0(Z)E_f^{1/4}. \quad (4)$$

In order to show the contrast between models we can point out that Altick model leads to the Z-independent value $\Gamma_0 = 66.7$eV [20] while Rau predicts a constant value for Γ for Z≥3, indicating the complete absence of correlation footprints [16].

The PDI of the He-isoelectronic sequence was initially considered by Kornberg and Miraglia who proposed scalings for the TDCS, singly differential cross sections (SDCS) and total cross sections (TCS) [28]. The validity of the TCS scaling was also confirmed with the CCC method [10]. The validity of the TDCS scaling was recently shown by Otranto and Garibotti [14] with the SC3 model. According to Kornberg and Miraglia, the TDCS should verify the following scaling,

$$\frac{d\sigma}{d\Omega_1 d\Omega_2 dE_1}(E_f, Z) = \frac{1}{Z^6}\frac{d\sigma}{d\Omega_1 d\Omega_2 d(E_1/Z^2)}(E_f/Z^2, 1) \quad (5)$$

In Fig. 1 we present the TDCS in the SC3 model [14] for different ions and $E_f/Z^2=5eV$. For increasing nuclear charge, the angular distributions tend to the uncorrelated distribution $(1+\cos\theta_2)^2$. The maximum of the two lobes goes to $\theta_1=0$ and the distributions approach the envelope. It can be seen that convergence predicted by the scaling is achieved in the infinite nuclear charge limit.

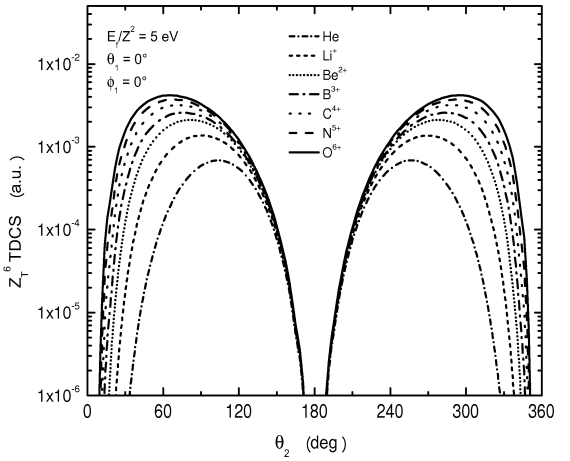

FIGURE 1. Scaled TDCS for $E_f/Z^2=5eV$ and Z=2,..,8.

In Fig. 2 we present the ratio of the theoretical TDCS to the angular factor. That is the SC3 correlation factor. Four different ions are considered at the excess energy of 20eV. As can be inferred from the figure, Gaussian fits properly reproduce the angular behavior of the correlation factor [14].

In Fig. 3 a) and b) we represent the $\Gamma(E_f,Z)$ as a function of E_f and $E_f^{1/4}$ respectively. It can be seen that for low excess energies, the widths behave like predicted by Eq. (5) and that departure from this law is obtained as energy increases. However this departure is charge dependent. As the nuclear charge increases, a wide window of the Wannier region is obtained. From Fig. 3a) we can see that the SC3 tends to agree with the predictions of the Z-independent model of Altick [20]. By the other side, from Figs. 2 and 3 we see that for charge values higher than 3 a clear dependence of the correlation factor with the interelectronic angle is obtained in contrast with the flat prediction of Rau [16]. A mean linear fitting of the present results leads $\Gamma(E_f,Z)=63.6\ E_f^{1/4}$ which is valid up to 40eV excess energy for the larger charges here considered.

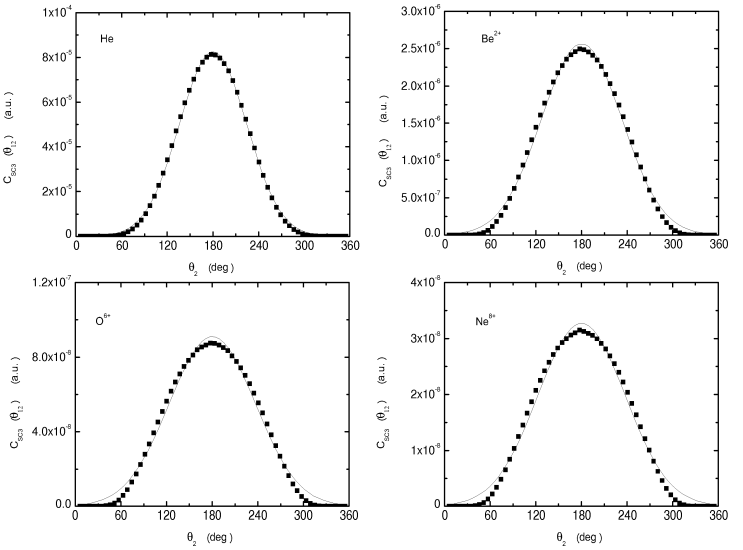

FIGURE 2. SC3 Correlation coefficients for ions with charge Z=2,4,8,10. The excess energy is 20eV. The Gaussian fit (solid line) has been included for comparison.

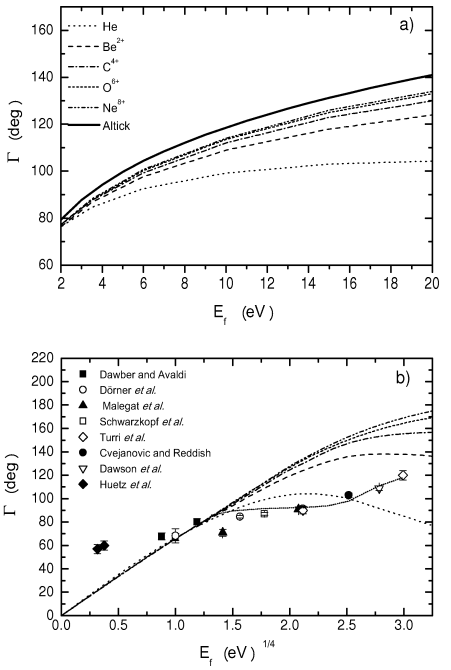

FIGURE 3. $\Gamma(E_f, Z)$ as a function of E_f a) and $E_f^{1/4}$ b). The short-dotted-line corresponds to the CCC theory. The experimental points included for the He target are those shown in Ref. [29].

CONCLUSIONS

We presented results given by the SC3 method for the PDI of the He-isoelectronic sequence ions and in the equal energy sharing regime. We showed that the SC3 results are well described by a Gaussian parametrization up to relatively high energies and nuclear charges. The resulting widths converge to the prediction of Altick's model, indicating that the electron-electron correlation keeps relevant for increasing nuclear charges. This contradicts other Wannier-type models like those developed by Rau [16] and Gailitis and Peterkop [17]. Even when the SC3 model is a perturbative model, the width behavior it displays is in concordance with the Wannier theory at low energies. Furthermore, we find that the threshold region extends up to higher energies as the nuclear charge increases, indicating an energy widening of the Wannier region.

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