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Electron angular distributions in double photoionization: Use of effective Sommerfeld parameters

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Abstract. We present calculations of the fivefold differential cross-section (FDCS) for double photoionization of helium at excess energies of 6 and 20 eV above threshold. Our results are obtained using for the final double-continuum state a product of three Coulomb wave functions, with the Sommerfeld parameters modified to describe the strength of interaction of any two particles affected by the third particle. Our calculations are compared with recent absolute measurements by Dörner *et al.* (Phys. Rev. A **57**, 1074 (1998)), both in coplanar and non-coplanar geometries. Very good agreement is obtained for the shape of the angular distributions, and differences in the absolute magnitude exist in comparison with the standard choice of Sommerfeld parameters.

PACS. 32.80.Fb Photoionization of atoms and ions

1 Introduction

In recent years there has been considerable work devoted towards understanding the mechanisms leading to the ejection of two electrons from a charged core [1]. The double photoionization process is of special interest, since the electron-photon interaction is a one-body operator, and therefore double ionization by one photon is a process entirely due to electron correlation. The measurement of the fivefold differential cross-section (FDCS) in double photoionization was first performed by Mazeau *et al.* [2] on Kr in 1991. On helium the first measurement of the FDCS was done by Schwarzkopf *et al.* [3] in 1993. Other measurements of this differential cross-section on He double photoionization have been performed since that moment [4–9], but these experiments provide, in general, only the relative magnitude for the angular distribution of the ionization probability lobes. Only in references [8,9] a first attempt to provide absolute values was performed. Quite recently absolute measurements on He were done by Dörner *et al.* [10] using the COLTRIMS technique [11] for various cases of equal and unequal energy sharing. This experiment is also unique because non-coplanar measurements were performed for the first time.

Theoretical works aiming to describe the experiments mentioned above have been undertaken using different methods: (i) Feagin [12] and Kazanski and Ostrovsky [13] applied a Wannier-type theory valid in the near threshold region; (ii) Pont and Shakeshaft [14] used screened Coulomb waves for each electron and the response function of the atom; and (iii) Maulbetsch and Briggs [15] used a product of three Coulomb waves (usually called C3 model) to describe the double-continuum state.

The Wannier model has been applied up to 20 eV above threshold and good results have been obtained in relative magnitude [10], since this theory does not predict absolute values for the cross-sections. The methods described in (ii) and (iii) have been shown to predict the observed FDCSs in relative magnitude for various coplanar geometries. Nevertheless, the absolute values were not correctly predicted. Large differences in magnitude between these methods have been reported [16].

Our main concern here is to apply a modified version of the C3 approximation. The C3 model predicts incorrect absolute values for the total cross-section near threshold [17,18]. This incorrect behavior of the C3 approach is due to the fact that the normalization of the electron-electron two-body Coulomb wave function decreases exponentially as $k_{12} \to 0$, where k_{12} is the electron-electron relative momentum. Therefore, other alternatives to this approach that could account for the absolute values of the observations are required. Recently, a modification of the C3 wave function has been investigated [19] in the context of electron-atom ionization, introducing effective Sommerfeld parameters that modify the two-body interaction in the presence of the third particle. The results for electron-hydrogen ionization are encouraging [20]. In the present work we apply effective Sommerfeld parameters for calculating FDCSs of He double photoionization.

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We compare our findings with recent measurements by Dörner *et al.* [10]. We recalled that in reference [10] absolute FDCS measurements have been reported.

2 Theory

The most detailed observable of the double photoionization process is the fivefold differential cross-section (FDCS) $d^5\sigma^{2+}/d\epsilon_1 d\Omega_1 d\Omega_2$, 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 with 2 refer to the other electron. The FDCS is given by (atomic units are used throughout)

$$\frac{d^5\sigma^{2+}}{d\epsilon_1 d\Omega_1 d\Omega_2} = \frac{4\pi^2}{c}\frac{k_1 k_2}{\omega}|\hat{\mathbf{e}}\cdot\mathbf{T}_{fi}|^2, \quad (1)$$

where the transition-matrix element here has been chosen within the velocity gauge $\mathbf{T}_{fi} = \langle\Psi_f^-|\nabla_1+\nabla_2|\Psi_i\rangle$, $\hat{\mathbf{e}}$ is the polarization direction, and ω is the photon energy. We also define $E = \epsilon_1 + \epsilon_2$ as the total available energy. In order to calculate accurate $\mathbf{T}_{fi}$ matrix elements we require correlated approximations to describe both the initial- (Ψ_i) and the final-state (Ψ_f^-) of the He target. For the ground state of the helium atom we considered the wave function developed by Bonham and Kohl [21] given by

$$\Psi_i(\mathbf{r}_1,\mathbf{r}_2) = N_i(e^{-ar_1-br_2}+e^{-br_1-ar_2})(1+C_0e^{-\lambda_0 r_{12}}). \quad (2)$$

The parameters of this wave function are given in reference [21]. The energy for the He ground state obtained with this correlated wave function is -2.901923 a.u., close to the well-known exact value -2.903724 a.u. For the final-state wave function we consider a product of three Coulomb waves (C3 model) [22,23]

$$\Psi_f^-(\mathbf{k}_1,\mathbf{k}_2|\mathbf{r}_1,\mathbf{r}_2) = \mathcal{P}_{12}\frac{1}{(2\pi)^3}e^{i\mathbf{k}_1\cdot\mathbf{r}_1+i\mathbf{k}_2\cdot\mathbf{r}_2} \times N(\xi_1)N(\xi_2)N(\xi_{12})F_1F_2F_{12}, \quad (3)$$

where $F_j = {}_1F_1(i\xi_j,1,-ik_jr_j-i\mathbf{k}_j\cdot\mathbf{r}_j)$ $(j=1,2,12)$ is the confluent hypergeometric function, $N(\xi_j) = \exp(-\pi\xi_j/2)\,\Gamma(1-i\xi_j)$ is the Coulomb factor, and ξ_j is the Sommerfeld parameter. In equation (3) $\mathcal{P}_{12} = (1+P_{12})/\sqrt{2}$, where P_{12} is the exchange operator. As usual we denote $\mathbf{r}_{12} = \mathbf{r}_1-\mathbf{r}_2$ and $\mathbf{k}_{12} = (\mathbf{k}_1-\mathbf{k}_2)/2$ for the interelectronic coordinate and relative momentum, respectively. In the standard C3 approximation the Sommerfeld parameters are given by

$$\xi_j = -\frac{Z}{k_j}\ (j=1,2) \quad \text{and} \quad \xi_{12} = \frac{1}{2k_{12}}, \quad (4)$$

with $Z = 2$ being the He nuclear charge. A modification of this approach has been proposed [19,20], introducing effective Sommerfeld parameters depending on the momentum vectors of the emitted electrons. One choice of these parameters is given by

$$\xi_j' = -\frac{Z-(k_j/4k_{12})\sin^2\theta A}{k_j} \quad (j=1,2) \quad (5)$$

and

$$\xi_{12}' = \frac{1-\sin^2\theta A}{2k_{12}}\,. \quad (6)$$

The term A in the preceding equations reads

$$A(k_1,k_2,k_{12}) = 1-\frac{|k_1-k_2|}{4k_{12}}, \quad (7)$$

and $\theta = 0.5\cos^{-1}(\hat{\mathbf{k}}_1\cdot\hat{\mathbf{k}}_2)$.

These modified Sommerfeld parameters satisfy the condition

$$\sum\xi_j = \sum\xi_j'. \quad (8)$$

This is a generalization of the Peterkop condition [24], which was formulated initially for two Coulomb wave functions. Equation (8) therefore guarantees the proper asymptotic condition of the wave function when all three particles are far away of each other. The effective charge (Z_{eff}) of the ion seen by the two outgoing electrons is in the range: $Z-1 < Z_{eff} < Z$, and $Z^i_{eff} \to Z$ as $k_j \to \infty$ $(i \neq j)$, as may be expected.

The calculation of the transition-matrix $\mathbf{T}_{fi}$ was done using the numerical code developed in reference [17]. The inclusion of effective Sommerfeld parameters (Eqs. (5, 6)) into the code is straightforward.

3 Results and discussion

We present in this section results for the fivefold differential cross-section using effective Sommerfeld parameters (Eqs. (5, 6)) into the C3 model (Eq. (3)), and using the standard version of this approach (Eqs. (3, 4)). Our results are confronted with recent absolute measurements reported in the work by Dörner *et al.* [10].

In Figure 1 we show the He FDCS in coplanar geometry at the photon energy $\omega = 99$ eV. One electron is detected at an angle of 30° with respect to the polarization axis ($\hat{\mathbf{e}}$). Results are displayed for three different energies of this electron: 2 eV, 10 eV and 18 eV, in Figures 1a–1c, respectively. The solid lines are the calculations using the effective Sommerfeld parameters, the dashed lines are those using the standard C3 model, and the dot-dashed lines are the ones using the fourth-order Wannier theory of Feagin (as appear in Ref. [10]). This particular set of data has been chosen for two reasons: first, our calculations are expected to work better at higher energies, and 99 eV is the highest energy presented in the data of reference [10]; and second, the Wannier-model calculations do not work very well in these cases, because 20 eV above threshold is far off the Wannier saddle. We observe that our results give similar angular patterns to those of the Wannier calculations, although for some angles the agreement with the experiments is better using our approach. C3 calculations using both choices of Sommerfeld parameters give nearly the same angular patterns, although differences appear at the level of the absolute magnitude. Both C3 calculations

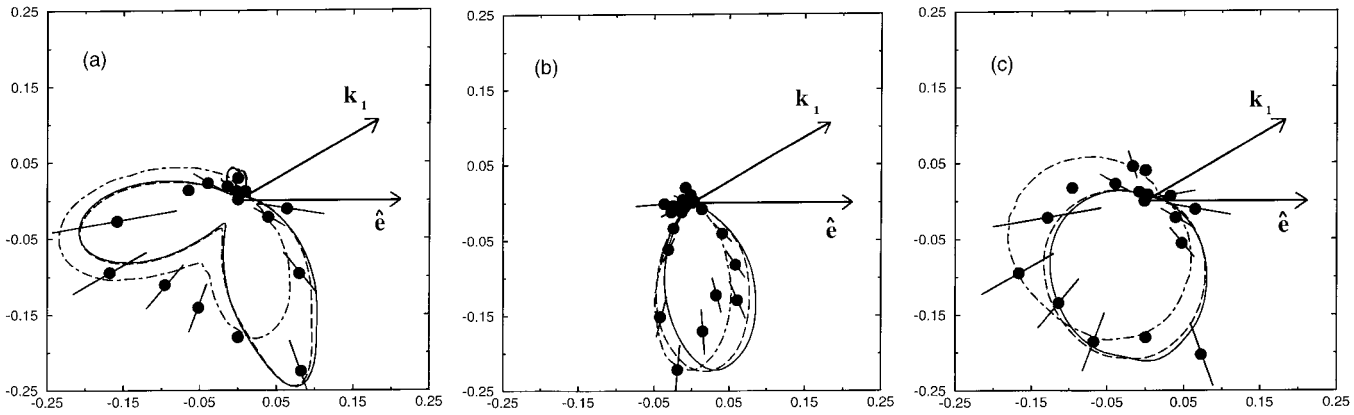

Fig. 1. The FDCS in coplanar geometry for a photon energy of 99 eV. The first electron is ejected at an angle $\theta_1 = 30^\circ$ with respect to the polarization axis ($\hat{\mathbf{e}}$). (a) $\epsilon_1 = 2$ eV, (b) $\epsilon_1 = 10$ eV, and (c) $\epsilon_1 = 18$ eV. Solid line: C3 model with effective Sommerfeld parameters (Eqs. (5, 6)) and initial state of reference [21]. Dashed line: standard C3 model with the same initial state. Dot-dashed line: fourth-order Wannier calculation of Feagin (Ref. [10]). Heavy dots: experimental results of reference [10] for $\theta_1 = 20{-}40^\circ$, $\varphi_1 = 0{-}20^\circ$, and $\epsilon_1/E = 0{-}0.2$, 0.5, 0.8$-$1 for (a), (b), and (c), respectively. The data are on absolute scale in 10^{-4} a.u.; the lines are scaled to the figure. Note that, although the Wannier calculations are not absolute, our results have been adjusted at one point to the data. The true maxima are in each case: (a) 1.16×10^{-5} a.u., (b) 1.65×10^{-5} a.u., and (c) 1.10×10^{-5} a.u. for C3*, and (a) 1.02×10^{-5} a.u., (b) 1.39×10^{-5} a.u., and (c) 9.22×10^{-6} a.u. for C3 calculations. Here C3* refers to the C3 model with the effective Sommerfeld parameters, and C3 to the standard approach.

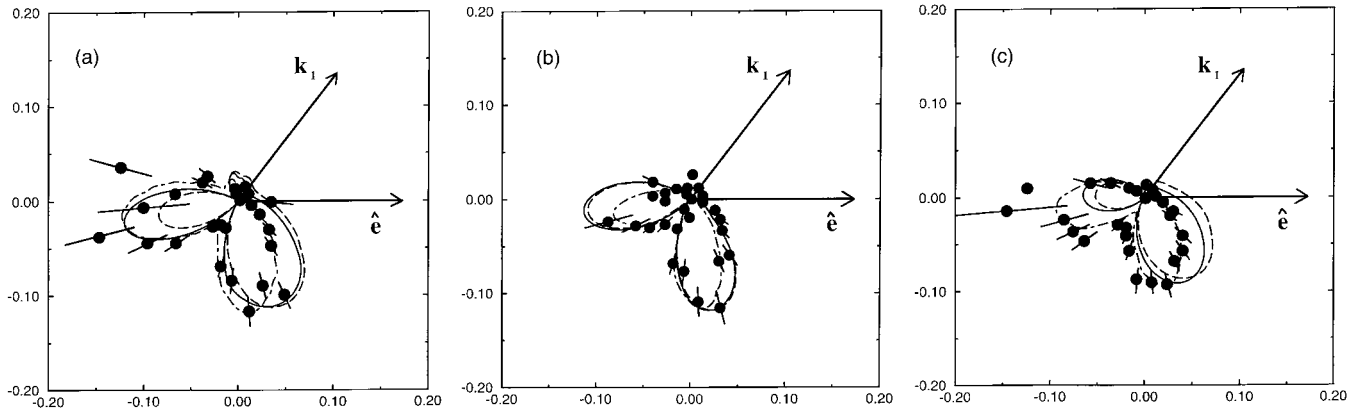

Fig. 2. The FDCS in non-coplanar geometry for a photon energy of 85 eV. The first electron is ejected at an angle $\theta_1 = 52.5^\circ$, and with an azimuthal angle (with respect to the plane defined by $\hat{\mathbf{e}}$ and $\mathbf{k}_2$) $\varphi_1 = 67.5^\circ$. (a) $\epsilon_1 = 0.6$ eV, (b) $\epsilon_1 = 3.0$ eV, and (c) $\epsilon_1 = 5.4$ eV. The curves are labeled as in Figure 1. Heavy dots: experimental results of reference [10] for $\theta_1 = 40{-}65^\circ$, $\varphi_1 = 45{-}90^\circ$, and $\epsilon_1/E = 0{-}0.2$, 0.5, 0.8$-$1 for (a), (b), and (c), respectively. The data are on absolute scale in 10^{-4} a.u.; the lines are scaled to the figure. The true maxima are in each case: (a) 1.70×10^{-7} a.u., (b) 3.71×10^{-7} a.u., and (c) 1.60×10^{-7} a.u. for C3*, and (a) 8.77×10^{-8} a.u., (b) 1.28×10^{-7} a.u., and (c) 8.10×10^{-8} a.u. for C3 calculations.

are smaller than the data at 99 eV; however, we note that the use of effective Sommerfeld parameters gives results closer in magnitude to the observed FDCSs.

In Figure 2 we show results at a lower photon energy ($\omega = 85$ eV). In this case the calculations have been performed for a non-coplanar geometry. The structures of the predicted lobes obtained using our approach are now also similar to the measured data. The Wannier-model calculations reproduce very well these data because we are in an energy region where this approach is accurate. We found that the use of effective Sommerfeld parameters is able to describe better some features, for example the lobe at $\theta_2 \simeq 190^\circ$ in Figure 2a. The striking fact is that the use of effective Sommerfeld parameters gives now a factor of two with respect to the standard C3 calculations. This would indicate that the exponential decrease in the absolute value of the cross-section for $E \to 0$ is attenuated, at least partially, by the use of effective Sommerfeld parameters.

We point out that in the experimental data the one-electron values $(\epsilon_1, \theta_1, \varphi_1)$ were recorded within specific ranges. In our calculations we used for ϵ_1, θ_1, and φ_1 the midpoint of the corresponding data intervals, as was also done for the Wannier calculations in reference [10]. We remark that for a complete comparison with the experiment

the calculations should be done in the form

$$\frac{1}{\Delta\epsilon_1}\frac{1}{\Delta\theta_1}\frac{1}{\Delta\varphi_1}\int d\epsilon_1 \int \sin\theta_1 d\theta_1 \int d\varphi_1 \frac{d^5\sigma^{2+}}{d\epsilon_1 d\Omega_1 d\Omega_2}\,. \quad (9)$$

However, calculations using acceptance ranges as in equation (9) would demand in our case important computational work. Some differences may arise if the calculations are performed using equation (9), but the changes are expected to be minor ones.

In conclusion, we have presented results for fivefold differential cross-sections in double-photoionization using effective Sommerfeld parameters into the C3 model. We have compared these calculations with recent absolute measurements performed by Dörner *et al.* [10]. The use of this method give angular distributions similar to those predicted by the standard C3 model, although there are differences in the absolute magnitude given by both approaches. Our calculations and those using the Wannier-type theory of Feagin [12] give similar results for the shape of the distributions. Regarding the measurements [10], our calculations provide a better agreement at the level of absolute values at excess energies of 20 eV. The final-state descriptions used in the present work improve when the photon energy increases; we expect that for excess energies much larger than 20 eV a closer agreement with experimental data at the level of absolute values will be obtained. Finally, we would like to mention the recent work of Kheifets and Bray [25] using the convergent close-coupling (CCC) technique applied to the calculations of FDCSs. In that work, the CCC method's results were shown to agree with the absolute measurements of references [8,9].

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