Kinetic correlation in the final-state wave function in photo-double-ionization of He

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We evaluate the triply differential cross section (TDCS) for photo-double-ionization of helium. We use a final continuum wave function which correlates the motion of the three particles, through an expansion in products of two-body Coulomb functions. This function satisfies a set of appropriate physical conditions in the coalescence points, in addition to the correct asymptotic behavior condition. We analyze the effect of this correlation in the TDCS and compare our results with experimental data.

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The three-body problem is fundamental in many branches of physics, and many studies have concentrated towards an accurate description of the continuum state Ψ_f of three Coulomb-interacting particles. Photo-double-ionization (PDI) of He is ideally suited to test these models, since correlation effects are notoriously highlighted and play a major role. Two recent reviews describe current experimental and theoretical works on the field [1,2].

The C3 approximation [3,4] entirely considers the electron-electron (e-e) interaction, and writes Ψ_f as the product of three two-body Coulomb wave functions, each one corresponding to a pair of particles, in the two-body energy shell. Using this function, Maulbetsch and Briggs [4] succeeded in calculating angular distributions whose shapes are in very good agreement with the measured data. However, it predicts absolute values of the triply differential cross section (TDCS) which become exponentially small in the threshold region, mainly due to the normalization factor associated with the e-e interaction, instead of the power-law dependence resulting from Wannier theories. Energies of the keV order are required to obtain reliable results [5,6]. The description of the correlated motion of the three particles in the C3 wave can be improved by introducing effective Sommerfeld parameters depending on the coordinates and momenta [7–10]. These models proved to be useful in electron-atom collisions, improving the C3 model results for low-energy projectiles. Lucey *et al.* and Kornberg and Rodriguez have tested these dynamically screened C3 models for PDI of He finding that the C3 magnitude failure in the threshold region is improved and that these models lead to similar angular distributions [10,11].

Another C3-like model was recently introduced by the authors [12], by means of an effective interelectronic distance. This ansatz reduces the electron-electron repulsion enhancing the theoretical cross sections near threshold. Furthermore, a significative correction of the total cross section is achieved in the intermediate energy region, relative to the C3 model.

The recent advance of computing facilities has allowed the implementation of powerful numerical approaches. Nowadays, many numerical and computational intensive methods give cross sections that compare very well with experiments [13–15].

However, an analytical expression for the three charged particles' continuum state remains being an unsolved theoretical problem. With this scope, Miraglia *et al.* [16] recently generalized a formalism used formerly for ion-atom electron emission [17]. Based on physical grounds, they presented a model for Ψ_f, named Φ_A, expressed as a several variable hypergeometric function, which includes potential correlation and an approximated kinetic correlation between the three particles. However, to date this kind of kinetically correlated model has neither been tested in double photoionization of He nor in e-atom ionizing collisions.

In this work, we propose the Φ_A model, for evaluation of PDI of He in the velocity and length gauges in the dipole approximation. Atomic units will be employed throughout this work unless explicitly stated.

The TDCS for absorption of a photon of energy ω and emission of two electrons with momenta $\mathbf{k}_1\mathbf{k}_2$ is given by

$$\frac{d\sigma}{d\Omega_1 d\Omega_2 dE_1} = 4\pi^2 \alpha k_1 k_2 C^{(G)} |T_{fi}^G|^2, \tag{1}$$

where α is the fine-structure constant. The energies of the emitted electrons are $E_1 = k_1^2/2$ and $E_2 = k_2^2/2$, $E_f = E_1 + E_2$ being the total final energy. The T_{fi}^G transition amplitude in the velocity and length gauges is, respectively, given by

$$T_{fi}^V = \langle \Psi_f | \hat{\boldsymbol{\varepsilon}} \cdot (\boldsymbol{\nabla}_a + \boldsymbol{\nabla}_b) | \Psi_i \rangle,$$

$$T_{fi}^L = \langle \Psi_f | \hat{\boldsymbol{\varepsilon}} \cdot (\mathbf{r}_a + \mathbf{r}_b) | \Psi_i \rangle,$$

while the $C^{(G)}$ coefficient reads in each gauge $C^{(V)} = 1/\omega$ and $C^{(L)} = \omega$. The He ground state is given by Ψ_i and the final state Ψ_f represents the two electrons in the continuum sharing the exceeding energy of the annihilated photon. We consider the x axis as the direction of the incident linearly polarized photon, and z corresponding to the polarization vector $\hat{\boldsymbol{\varepsilon}}$. One of the electrons is emitted in the yz plane with angle θ_2 relative to z. The direction of the other is determined by the angles ϕ_1, relative to the yz plane, and θ_1 relative to $\hat{\boldsymbol{\varepsilon}}$.

For the ground-state function of helium, we will consider the Bonham and Kohl GS2 correlated state [18] given by

$$\Psi_{GS2} = N_i (e^{-c_1 r_1 - c_2 r_2} + e^{-c_2 r_1 - c_1 r_2})(e^{-z_c r_{12}} + C_0 e^{-\lambda r_{12}}), \tag{2}$$

where the variational parameters have been recalculated in order to avoid the use of a cut-off instead of z_c. Fixing $z_c=0.01$, we obtain for the other coefficients $N_i=1.717\,49$, $c_1=1.4096$, $c_2=2.2058$, $C_0=-0.6244$, and $\lambda=0.244\,712$. This gives a bounding energy $\langle E\rangle=-2.9019$ a.u. compared to the exact $\langle E\rangle_{exact}=-2.903\,724$ a.u. and a cusp condition value at the nucleus of $R_{cusp}=(\partial\Psi_{GS2}/\partial r_{1,2})_{r_{1,2}=0}/(\Psi_{GS2})_{r_{1,2}=0}=-1.807$ instead of the exact value (-2). This simple functional form allows for a calculation of the transition amplitude using Nordsieck-like integrals [6,19].

The function Φ_A satisfies the Schrödinger equation with an approximate nonorthogonal kinetic energy and is given by the following series expansion [16]:

$$\Phi_A=\sum_{j,l,m=0}^{\infty}\frac{(ia_1)_j(ia_2)_l(ia_3)_m(1)_{j+l}}{(1)_{j+l+m}(1)_j(1)_l}\frac{x_1^j}{j!}\frac{x_2^l}{l!}\frac{x_3^m}{m!}, \quad (3)$$

where $a_i=Z_i\mu_i/k_i$ are the Sommerfeld parameters, $x_i=-ik_i\xi_i$, and $\xi_i=r_i+\hat{\mathbf{k}}_i\cdot\mathbf{r}_i$, $i=1,2,3$. Here, Z_i, μ_i, ξ_i, and k_i indicate charges, reduced masses, coordinates, and momentum of each electron relative to nucleus and between the electrons, respectively. The usual notation for the Pochhammer symbol $(a)_r=\Gamma(a+r)/\Gamma(a)$ has been used. Then, the final-state wave function Ψ_{Φ_A} with incoming boundary conditions could be written as

$$\Psi_{\Phi_A}=\frac{N_{\Phi_A}}{(2\pi)^3}e^{i\mathbf{k}_1\cdot\mathbf{r}_1+i\mathbf{k}_2\cdot\mathbf{r}_2}\Phi_A(x_1,x_2,x_3), \quad (4)$$

where N_{Φ_A} is the normalization factor of the Φ_A wave function. Though it is not a rigorous solution, Φ_A satisfies the following physical limits: (a) the regularity properties in the coalescence points, expressed by the Kato conditions at first order; (b) if the nuclear charge Z_T is turned off, this function reduces to the two body electron-electron Coulomb solution; (c) when the interelectronic interaction is set off the C2 model is recovered. Furthermore, when the perturbative ansatz is applied $(x_3\rightarrow 2x_3)$, the united atom limit is recovered, where the far electron almost sees one particle with an effective charge of Z_T-1. This condition could have relevance when describing the extreme asymmetric energy sharing emission, where the process approaches single ionization. We denote the resulting function $\Phi_A^P(x_1,x_2,x_3)=\Phi_A(x_1,x_2,2x_3)$ and note that it does not reduce to a C2 function when the electron-electron interaction is turned off.

The calculation of the transition amplitude is performed expressing the Φ_A function in terms of the "natural base." That is to say, we expand the Φ_A function in terms of Kummer functions,

$$\Phi_A=\sum_{k,l,m=0}^{\infty}A_{k,l,m}\mathcal{F}^k(x_1)\mathcal{F}^l(x_2)\mathcal{F}^m(x_3) \quad (5)$$

with $\mathcal{F}^s(x_j)=x_j^s{}_1F_1[ia_j+s,1+2s,x_j]$. The coefficients are defined in Ref. [16], and the normalization factor N_{Φ_A} is determined from the Redmond asymptotic condition. For comparison purposes, we will also consider the function Φ_A^P.

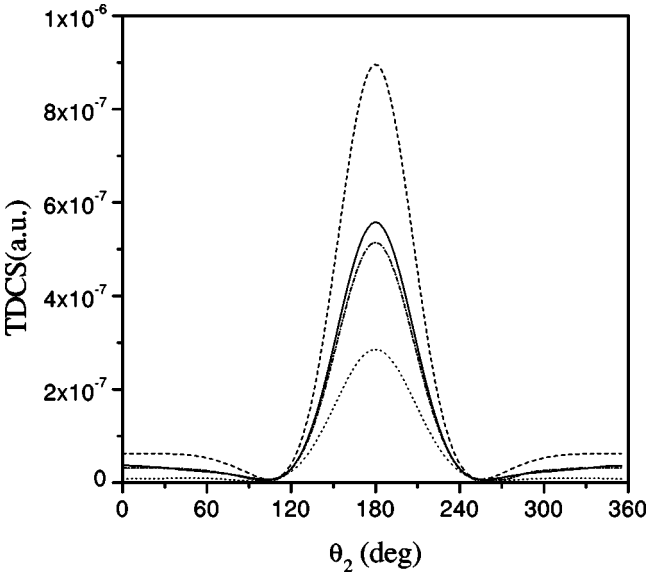

FIG. 1. TDCS for $E_1=1$ eV, $E_2=449$ eV, $\theta_1=0°$ and $\phi_1=0°$ using the different orders of the expansion of the Φ_A model in the natural base. Theories: dotted line, order 0; dashed line, order 2; dot-dashed line, order 3; solid line, order 4.

The transition amplitude could be expressed as a linear combination of amplitudelike terms, corresponding to different orders of the expansion of Φ_A. The integrals are calculated following Colavecchia *et al.* [19]. This methodology traduces in a fast convergence, just a few terms of the linear combination being necessary to obtain an stable value for the whole transition amplitude.

To analyze the convergence of the expansion given by Eq. (5), we show in Fig. 1 the TDCS for $E_1=1$ eV, $E_2=449$ eV and $\theta_1=0°$, $\phi_1=0°$ resulting from the Φ_A model expansion up to different orders is equal to (order is equal to $k+l+m$), in the velocity gauge. Here we show up to order 4, since the next two orders do not introduce noticeable differences. The order zero corresponds to the C3 model as noted above.

We compare our theoretical results with the experimental data obtained by Dörner *et al.* [20] using COLTRIMS technique [21]. Due to the energy and angular resolutions involved at the experimental method, a plain comparison between theory and data could not be performed. The theoretical values must be averaged inside the detection volume. We have found that an angular five-point average at the mean detection energy is enough to obtain a stable description of the TDCS.

We compare the results given by the Φ_A model in both gauges, and the C3 model in velocity gauge with the experimental TDCS for $E_1=E_2=3$ eV. In Fig. 2, one of these electrons is detected in the angular ranges $\theta_1\in(40°,65°)$, $\phi_1\in(0°,20°)$. It can be seen that the C3 model gives a good angular description of the electron distribution but fails by two orders of magnitude to the experimental data. The other terms in Eq. (5) add coherently in the amplitude and the Φ_A model predicts a TDCS that differs from the C3 model by a factor between 2 and 3. It could be seen that the angular shapes of the distributions in both gauges are in good agree-

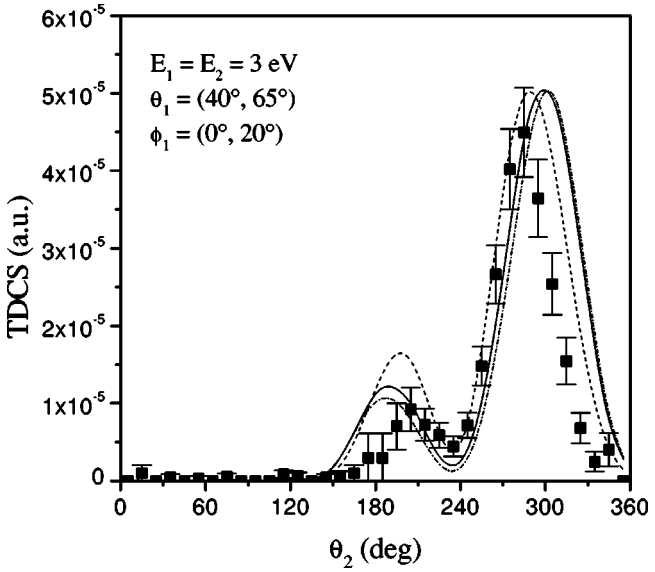

FIG. 2. TDCS for $E_\gamma = 85$ eV and equal energy sharing of the exceeding energy between electrons. solid line, Φ_A model velocity gauge; dot-dashed line, Φ_A model length gauge; dashed line, C3 velocity gauge. The scaling factors associated with the theories to reach the data are respectively: 280, 7.27, and 104.5.

ment but they clearly differ in magnitude. In Fig. 3, we display the TDCS for the same energies, and $\theta_1 \in (40°,65°)$, $\phi_1 \in (20°,45°)$. In this case, the strict noncoplanar geometry is explored. Good agreement between theoretical and experimental angular distributions is obtained with both models. Recently Knapp *et al.* [22] obtained relative TDCS for $E_1 = 1$ eV, $E_2 = 449$ eV and $\theta_1 \in (-10°,10°)$, $\phi_1 \in (-25°,25°)$. In Fig. 4, we compare experimental and theoretical results, where data have been normalized for comparison with the theories. We show the Φ_A model and the Φ_A^P model in velocity and length gauges, and the C3 model in velocity gauge. The Φ_A^P model was included here due to the asymmetric distribution of energy between the electrons considered. It could be seen that both Φ_A and C3 models in the velocity gauge fail to predict the $\cos^2\theta_2$-like distribution inferred from the experimental data. On the other side, the Φ_A^P

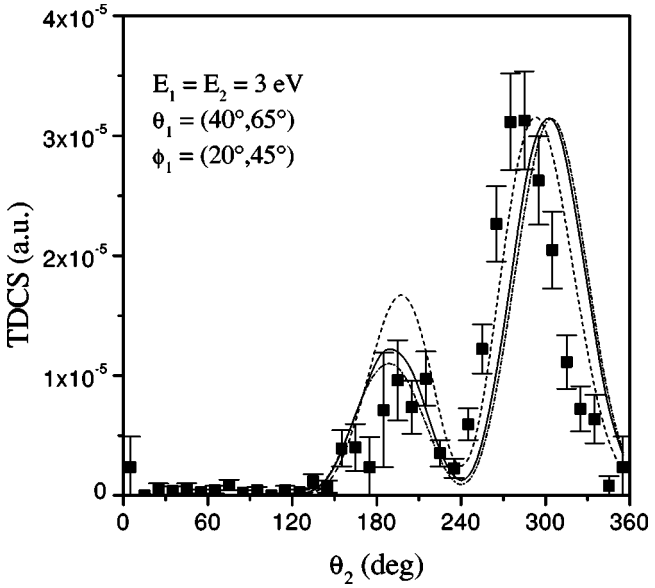

FIG. 3. TDCS for $E_\gamma = 85$ eV in equal energy sharing regime and noncoplanar geometry. Theories as in Fig. 2. The scaling factors associated with the theories to reach the data are, respectively: 220, 5.7, and 95.

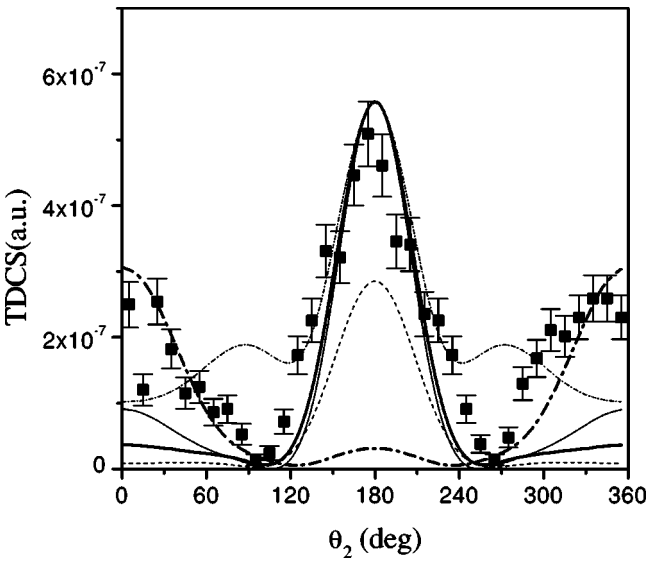

FIG. 4. TDCS for $E_1 = 1$ eV and $E_2 = 449$ eV. The angular range is given by $\theta_1 \in (-10°,10°)$ and $\phi_1 \in (-25°,25°)$. Theories and scaling factors are given by the following: solid line, Φ_A^P velocity gauge (*1.48); heavy-solid line, Φ_A velocity gauge; dot-dashed line, Φ_A^P length gauge (*0.31); heavy-dot-dashed line, Φ_A length gauge (*0.025); dashed line, C3 velocity gauge.

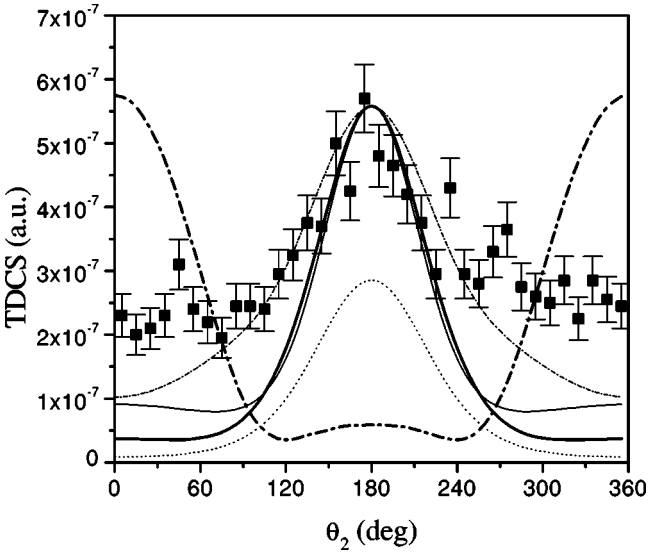

FIG. 5. TDCS for $E_1 = 449$ eV and $E_2 = 1$ eV. The angular range is as in Fig. 4. Theories and scaling factors are the following given by: solid line, Φ_A^P velocity gauge (*1.48); heavy-solid line, Φ_A velocity gauge; dot-dashed line, Φ_A^P length gauge (*0.31); heavy-dot-dashed line, Φ_A length gauge (* 0.047); dashed line, C3 velocity gauge.

model in velocity gauge tends to correct this failure, enhancing the distribution in the polarization direction. The strong peak for $\theta_2 = 180°$ shows that the final-state correlation introduced by these models overestimates the repulsion effects between the two emitted electrons. Furthermore, the length gauge calculations do predict an enhancement in the polarization direction but now the repulsion between the electrons is underestimated in the Φ_A model. This feature is partially corrected by the Φ_A^P model in the length gauge. In Fig. 5, we show the TDCS for $E_1 = 449$ eV, $E_2 = 1$ eV and $\theta_1 \in (-10°, 10°)$, $\phi_1 \in (-25°, 25°)$. The experimental data predict a quasi-isotropic distribution while the C3 and Φ_A models in velocity gauge overestimate again the electron-electron repulsion. It could be seen that the Φ_A^P model in velocity gauge slightly corrects this failure. The length gauge description of the Φ_A model predicts erroneously a maximum in the distribution corresponding to both electrons leaving in the same direction. The Φ_A^P model in length gauge, however, corrects this feature leaving a description that is in agreement with the velocity gauge one.

In summary, we have tested a correlated wave function that has been recently proposed to tackle with the two-electron continuum. The final wave function used here is the more general available proposal up to date, to express the three-body continuum as a superposition of separable products of two-body waves. The expansion coefficients were determined from mathematical and physical conditions. For PDI of He atoms, we found that the usual magnitude failure of the C3 model in the threshold region is not corrected by the present model. Due to the initial bound state for the two electrons, Lucey *et al.* [11] have found that the TDCS for PDI is mainly determined by the final-state wave function when the three Coulomb-interacting particles are near (i.e., $r_1, r_2 < 20$ a.u.). Usual approximate analytical solutions have been generated by extension to short distances of the correct asymptotic condition in the region Ω_0 of the configuration space, in which all three interparticle distances are large. This gives an inaccurate description in the coalescence points, where two or three particles are near. This would leave a clear indication that a more precise description of the nonorthogonal kinetic energy should be included, besides asking to the wave function the satisfaction of some desirable physical limits. The present results suggest that improvements for functions based on the natural base must be carefully analyzed to search for an appropriate analytical expression of the three-body continuum state.

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