Retardation effects and angular coefficients in double photoionization

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(Received 12 December 1994; revised manuscript received 15 June 1995)

Retardation effects on the cross sections for double photoionization of He($^1S_0$) targets are studied at photon energies above 1.0 keV. The dipole asymmetry parameter β is examined first and the importance of correlation in the final and initial states for this quantity is examined. The effects of retardation on the electron angular distributions are studied and the range of validity of a first-order retardation correction is evaluated. Finally, by using a simple model to calculate the total cross section, the contribution of retardation on the double ionization σ^{2+} is calculated and it is found that the ratio of double to single photoionization, including retardation, remains the same as when the dipole velocity approximation is employed.

PACS number(s): 32.80.Fb, 32.30.Rj

I. INTRODUCTION

The double photoionization of helium is one of the simplest processes in atomic physics that requires the solution of the Coulomb three-body problem. In this process, the three-body interaction is manifested in a transparent form because one photon interacts mainly with one electron, while charged particles interact with all the electrons in the atom.

While the three-body continuum problem is still an unresolved problem, great progress has been gained in recent years on the intermediate- and high-energy dynamics of this process. Levin *et al.* [1] have measured the high-energy ratio $R=\sigma^{2+}/\sigma^{+}$ of double to single ionization with the use of synchrotron radiation for photon energies up to 12.0 keV. Many theoretical calculations have been performed for the photoabsorption process, all in accordance with the existence of an asymptotic limit for this quantity with a value of 1.67%. These predictions are based on different methods, namely, (i) in the asymptotic or shake method [2–4], the ratio is obtained as a subtraction from bound-free transitions with only consideration to ground-state correlation and by using a closure relation; (ii) in the many-body perturbation method [5], contributions of the different diagrams of the process, representing a perturbative expansion of the electron-electron interaction, are evaluated in lowest order; and (iii) in the *ab initio* method [6–8], the use of actual approximations for the two-electron continuum wave function are considered. In a previous article [6] we considered the use of the *ab initio* method for helium targets; the application for two-electron atoms was also considered [9].

The high-energy region is characterized by the fact that the ratio $R=\sigma^{2+}/\sigma^{+}$ is nearly constant and a beginning is assigned at about 3.0 keV. Measurements in the intermediate-energy region have also been performed [10]; this region extends far above the threshold and connects with the high-energy region.

Although very different in nature, all three methods outlined above have in common the use of the dipole approximation for the radiation field. It is well known that this approximation is not automatically justified at high photon energies. When considering angular distributions, retardation effects could be maintained even down to threshold [11]. It is the purpose of this work to study in some detail the departures of the calculations done in dipole approximation from those where retardation is considered. Before including retardation, we shall present dipole results of the angular distributions to test the importance of correlation in the final and initial states. Dipole calculations were already performed in our previous work [6], where we have shown that in the dipole velocity approximation the cross section σ^{2+} could be calculated with different models for the double-continuum state, giving similar values for photon energies above 1.0 keV (this feature is also realized when using the acceleration form of the dipole operator [3,7], but not in the length form [6]). It has been shown, however, that Compton scattering dominates ionization above 6.0 keV [4,12,13]. Our study, in consequence, will be restricted to energies between 1.0 and 6.0 keV, where experimental verification is more feasible.

In Sec. II we present a brief description of the theory and the approximations adopted for the wave functions. In Sec. III A the asymmetry parameter β calculated in dipole velocity approximation is presented and compared with other theoretical predictions. In Sec. III B the evaluation of the retardation effects on angular distributions is considered and the first-order retardation correction for the differential cross section $d^3\sigma^{2+}/d\epsilon_1 d\Omega_1$ is examined. Finally, in Sec. III C we use a simple model to evaluate the contribution of retardation on the total cross section σ^{2+}. Conclusions and prospects are outlined in Sec. IV.

II. THEORY

The process that we consider is the impact of one linearly polarized photon on He($^1S_0$) atoms in their ground state. The photon polarization $\hat{\mathbf{e}}$ is assumed to be on the z axis, while the photon momentum $\mathbf{k}_p$ is taken to be directed along the x axis (see Fig. 1).

The photon energy E_γ and the ground-state energy of the helium atom E_0 are related to the ejected electron energies ϵ_1 and ϵ_2 through the conservation law $E_\gamma+E_0=\epsilon_1+\epsilon_2=E_f$, where we have defined E_f as the total final energy of the process. The basic matrix element of the process including retardation (RET) is given by

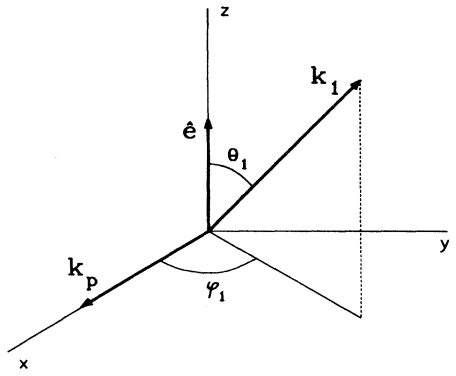

FIG. 1. Coordinate system used in the discussion of retardation effects showing the photon polarization vector $\hat{\mathbf{e}}$, the photon momentum $\mathbf{k}_p$, and the momentum of the observed electron $\mathbf{k}_1$.

$$\mathbf{T}_{\mathrm{RET}}(\mathbf{k}_1,\mathbf{k}_2|\mathbf{k}_p)=\langle\psi_f^-|e^{i\mathbf{k}_p\cdot\mathbf{r}_1}\nabla_1+e^{i\mathbf{k}_p\cdot\mathbf{r}_2}\nabla_2|\psi_i\rangle, \quad (1)$$

where $\psi_f^-(\mathbf{k}_1,\mathbf{k}_2|\mathbf{r}_1,\mathbf{r}_2)$ is the final double-continuum-state wave function and $\psi_i(\mathbf{r}_1,\mathbf{r}_2)$ is the initial ground-state wave function.

The basic observable of the double-photoionization process is the fivefold differential cross section (5DCS)

$$\frac{d^5\sigma_{\mathrm{RET}}^{2+}}{d\epsilon_1 d\Omega_1 d\Omega_2}=\left(\frac{4\pi^2}{c}\right)\frac{k_1k_2}{E_\gamma}|\hat{\mathbf{e}}\cdot\mathbf{T}_{\mathrm{RET}}(\mathbf{k}_1,\mathbf{k}_2|\mathbf{k}_p)|^2, \quad (2)$$

where ϵ_1 is the energy of one of the electrons whose momentum $\mathbf{k}_1$ subtends an element of solid angle $d\Omega_1$ and the quantities labeled with 2 refer to the other electron. In Eq. (2) the final-state wave function is assumed to be normalized to the δ function in the momentum space. Atomic units are used ($\hbar=m_e=a_0=1$).

Integrating the 5DCS over the angles of electron 2 leads to the triple differential cross section (3DCS)

$$\frac{d^3\sigma_{\mathrm{RET}}^{2+}}{d\epsilon_1 d\Omega_1}=\int d\Omega_2\frac{d^5\sigma_{\mathrm{RET}}^{2+}}{d\epsilon_1 d\Omega_1 d\Omega_2}. \quad (3)$$

In the dipole (DIP) approximation the 3DCS does not depend on the angle φ_1, so it is usually referred to as a double differential cross section (2DCS) $d^2\sigma_{\mathrm{DIP}}^{2+}/d\epsilon_1\sin\theta_1 d\theta_1$ [14]; alternatively, another approach uses the 2DCS given by $d^2\sigma_{\mathrm{DIP}}^{2+}/d\epsilon_1\sin\theta_{12}d\theta_{12}$, where θ_{12} is the asymptotic angle between vectors $\mathbf{k}_1$ and $\mathbf{k}_2$, which have a closed-form expression [6], thereby reducing the number of integrations of the 5DCS if the total cross section is calculated. When retardation is considered the former simplifications do *not* hold and a total cross section σ^{2+} demands five integrations, which is a formidable task if complex wave functions are employed. Formulas in the dipole approximation have been given in Ref. [6]; however, the dipole velocity formulation is simply obtained from the previous equations by setting $\mathbf{k}_p=\mathbf{0}$ and thus

$$\mathbf{T}_{\mathrm{DIP}}(\mathbf{k}_1,\mathbf{k}_2)=\mathbf{T}_{\mathrm{RET}}(\mathbf{k}_1,\mathbf{k}_2|\mathbf{k}_p=\mathbf{0}). \quad (4)$$

In this article we will restrict our dipole calculations to the velocity form of the T matrix.

The bound state wave functions employed are of the Hylleraas type [15] and of the multiconfigurational type [16] and shall be denoted as GS1, Hylleraas type, $E_{\mathrm{corr}}=33\%$; GS2, Hylleraas type, $E_{\mathrm{corr}}=96\%$; and SH, Multiconfigurational type, $E_{\mathrm{corr}}=98\%$. The double-continuum wave functions are approximated by the product of three Coulomb waves (C3 model) and by the product of two Coulomb waves (C2 model). The C3 model satisfies the correct asymptotic boundary condition [17]; it is given by

$$\psi_{\mathrm{C3}}^-(\mathbf{k}_1,\mathbf{k}_2|\mathbf{r}_1,\mathbf{r}_2)=\mathscr{P}_{12}\psi_{\mathbf{k}_1}^-(Z_T;\mathbf{r}_1)\psi_{\mathbf{k}_2}^-(Z_T;\mathbf{r}_2)\times D^-(\xi_{12},\mathbf{k}_{12};\mathbf{r}_{12}), \quad (5)$$

where $\psi_{\mathbf{k}}^-(Z;\mathbf{r})=\psi_{\mathbf{k}}^0(\mathbf{r})D^-(\xi,\mathbf{k};\mathbf{r})$ is the Coulomb continuum wave function, $\psi_{\mathbf{k}}^0(\mathbf{r})=\exp(i\mathbf{k}\cdot\mathbf{r})/(2\pi)^{(3/2)}$ is the free plane wave,

$$D^-(\xi,\mathbf{k};\mathbf{r})=N(\xi)_1F_1(i\xi,1,-ikr-i\mathbf{k}\cdot\mathbf{r}) \quad (6)$$

is the Coulomb distortion, $N(\xi)=\exp(-\pi\xi/2)\Gamma(1-i\xi)$ is the Coulomb factor, $\xi=-\mu Z/k$ is the Sommerfeld parameter, and μ is the reduced mass. As usual, we denote $\mathbf{r}_{12}=\mathbf{r}_1-\mathbf{r}_2$, $\mathbf{k}_{12}=(\mathbf{k}_1-\mathbf{k}_2)/2$, $\xi_1=-Z_T/k_1$, $\xi_2=-Z_T/k_2$, $\xi_{12}=1/(2k_{12})$, and $Z_T=2$ is the helium nuclear charge. In Eq. (5), $\mathscr{P}_{12}=(1+P_{12})/\sqrt{2}$, where P_{12} is the exchange operator.

The C2 model is also referred to as the independent-particle approximation because no interaction between the two electrons is incorporated, it is given by

$$\psi_{\mathrm{C2}}^-(\mathbf{k}_1,\mathbf{k}_2|\mathbf{r}_1,\mathbf{r}_2)=\mathscr{P}_{12}\psi_{\mathbf{k}_1}^-(Z_T;\mathbf{r}_1)\psi_{\mathbf{k}_2}^-(Z_T;\mathbf{r}_2). \quad (7)$$

This set of wave functions lets us turn on and off the correlation in the final and initial channels [18]. For example, we can construct the C2-SH approximation (C2 and SH used as final and initial wave functions, respectively) having a small (large) correlation in the final (initial) channel; on the contrary, we can construct C3-GS1. Due to computational complexity we have not considered C3-SH; however, C3-GS2 is instead the best approximation that we can employ incorporating correlation in both channels.

The photon plane wave $\exp(i\mathbf{k}_p\cdot\mathbf{r})$ was incorporated into the programs previously developed by us that evaluate the 5DCS in closed form when the C2 model is employed [19] and numerically when the C3 model is used [6]. The evaluation of the double integral of Eq. (3) over $d\Omega_2$ requires a high number of grid points (θ_2,φ_2) due mostly to the peaked structure of the 5DCS for photon energies higher than 1.0 keV. A grid with a minimum of $N_{\theta_2}\times N_{\varphi_2}=150$ points was employed for these calculations.

III. RESULTS

A. Asymmetry parameter β in the dipole approximation

Before proceeding to tackle the influence of retardation on angular distributions, we first want to show the substantial

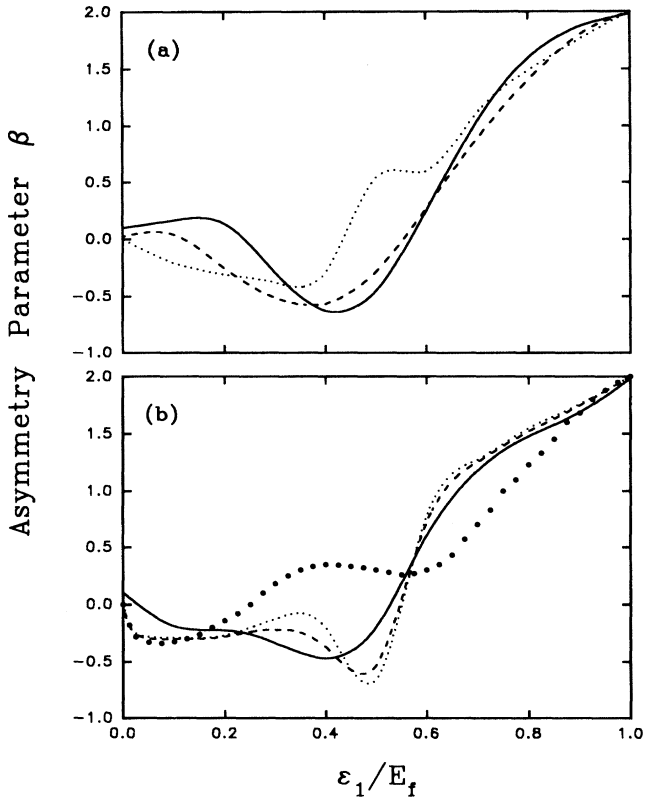

FIG. 2. Asymmetry parameter β calculated in the dipole velocity approximation for three different photon energies: E_γ= 1.0 keV (solid line), 3.0 keV (dashed line), and 5.0 keV (dotted line) using (a) C2-SH states and (b) C3-GS2 states. The solid dots (●) in (b) are the results obtained in Ref. [8] at 2.8 keV.

sensitivity of the asymmetry parameter β to the wave functions employed. In the dipole approximation the 3DCS is given by the formula [8]

$$\frac{d^3\sigma^{2+}_{\rm DIP}}{d\epsilon_1 d\Omega_1}=\frac{1}{4\pi}\frac{d\sigma^{2+}_{\rm DIP}}{d\epsilon_1}[1+\beta(\epsilon_1)P_2(\cos\theta_1)], \qquad (8)$$

where only the parameter β enters for the description of the angular distributions. Calculations of the 3DCS at different angles θ_1 permits extracting the value of the asymmetry parameter.

In Fig. 2 we show our calculated asymmetry parameter β with the C2 model [Fig. 2(a)] and with the C3 model [Fig. 2(b)] for three different photon energies E_γ= 1.0, 3.0, and 5.0 keV, using highly correlated ground-state wave functions. Note that since the velocity gauge was employed, $\sigma^{2+}_{\rm C2}\simeq\sigma^{2+}_{\rm C3}$ for $E_\gamma\geq$1.0 keV [6,20]. For 1.0 keV the limiting behavior of the asymmetry parameter is $\beta\rightarrow 0.1(1.98)$ as $\epsilon_1\rightarrow 0(E_f)$, although the behavior of this quantity differs in some form depending on the value of the electron energy ϵ_1. For higher photon energies the situation is clear: $\beta\rightarrow 0.0(2.0)$ as $\epsilon_1\rightarrow 0(E_f)$. The physical meaning of these limits has been explained previously [8]: when $\epsilon_1\simeq 0$ the slow electron is produced by a shakeoff process and emerges

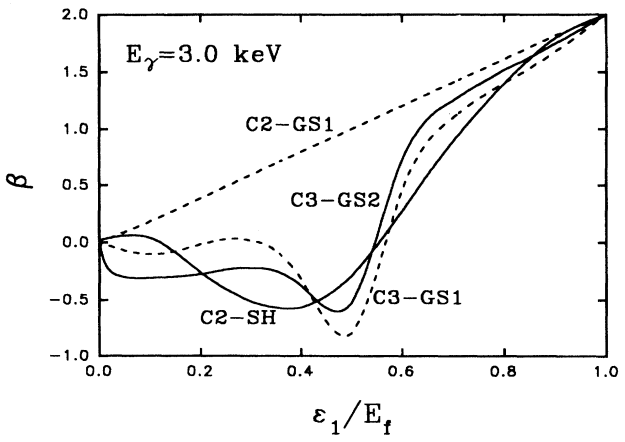

FIG. 3. Asymmetry parameter β calculated in the dipole velocity approximation at a photon energy of E_γ= 3.0 keV using the approximations indicated in the figure.

into the continuum isotropically by an $s\rightarrow s$ transition for which $\beta\simeq 0$; when $\epsilon_1\simeq E_f$ the fast electron absorbs the photon and acquires one unit of angular momentum from the zero angular momentum of the bound state, the angular distribution $(d^3\sigma^{2+}_{\rm DIP}/d\epsilon_1 d\Omega_1)$ is of the form $\cos^2\theta_1$, as in the single photoionization of an s subshell electron [21], and so $\beta\simeq 2$.

A comparison of the β curves of Fig. 2 for a given photon energy shows that the differences in using the C2 or C3 model are not very substantial except for a given range of energies ϵ_1, depending on the photon energy considered. For example, for 1.0 and 3.0 keV the main differences occur for $\epsilon_1\simeq 0$, where the C2 model predicts a positive β value while the C3 model a negative one. At 5.0 keV, the main substantial differences are at nearly equal electron energies, where the C2 model predicts a relative maximum while the C3 model a dip minimum. It is of interest to compare the behavior of the asymmetry parameter for the case $\epsilon_1\simeq 0$. When the C3 model is used, β is negative at nearly zero electron energy, which reflects that the final-state correlation is still important for the case $\epsilon_1\simeq 0$ and $E_f\rightarrow\infty$; the uncorrelated final state C2 gives a positive asymmetry parameter for $\epsilon_1\simeq 0$, although for E_γ=5.0 keV the ground-state correlation alone produces a negative β value for $\epsilon_1\simeq 0$.

Figure 2(b) shows also the result obtained by Teng and Shakeshaft [8] at E_γ= 2.8 keV. These authors have considered a correction of the C3 model based on a short-range correction factor determined by orthogonalization with respect to the initial bound state $\psi_i(\mathbf{r}_1,\mathbf{r}_2)$. Clearly, this correction alters the angular distribution especially for the case of nearly equal electron energies, although the low and high electron-energy limits are conserved. A correction for the C3 model could be necessary, even at high energies, because this model accounts correctly only for the asymptotic form of the wave function. However, a correction that alters the angular patterns could only be sustained by experimental verification. The theory to be compared with the experiments should also include effects arising from retardation, as will be shown in Sec. III B.

In Fig. 3 we present the asymmetry parameter β for a

photon energy of 3.0 keV and where the correlation in the final and initial state has been turned on and off. The main feature of these results is that whatever the final or initial states considered for the calculation, the limits $\beta \rightarrow 0.0(2.0)$ as $\epsilon_1 \rightarrow 0(E_f)$ are, nevertheless, obtained. The use of C2-GS1 states produces nearly a straight line. This approximation is the only one for which an analytical evaluation of the asymmetry parameter was found possible to manage (see Appendix A) and it could be expressed in the form

$$\beta_w(\epsilon_1) = \frac{2|\mathscr{A}|^2}{(|\mathscr{A}|^2 + |\mathscr{B}|^2)} , \tag{9}$$

where the expressions for the quantities $\mathscr{A}$ and $\mathscr{B}$ are given in Appendix A. The subscript w is introduced to indicate that this approximation introduces a weak correlation in the final and in the initial state. As properly stated in Ref. [8], when a weak correlation is introduced in both channels, the following relation holds:

$$\beta_w(\epsilon_1/E_f = 0.5) = 1.0 \tag{10}$$

for any final energy E_f, although the converse is not true: for example, we have obtained $\beta(\epsilon_1/E_f = 0.5) = 1.0$ using the C2-SH models at $E_\gamma = 12.0$ keV (not shown in the figure). Finally, it must be emphasized that when a high correlated ground state is used (solid lines) the C2 and C3 models do not produce remarkable disagreements even in the asymmetry parameter β, which is supported by the fact that in the velocity form of the T matrix the error introduced in the final state diminishes as E_f^{-1} [3].

B. Retardation effects on angular distributions

The angular distributions given by the 3DCS in the dipole approximation depend only on one parameter β, as given by Eq. (8). This makes the analysis simpler than when retardation is considered. Also, in the dipole approximation, the 3DCS does not depend on the azimuthal angle φ_1 and because of its functional dependence on the Legendre polynomial P_2 there is a magic angle ($\theta_1 = 54.73°$) where the intensity is independent of the angular distribution. The following relation holds:

$$\frac{d\sigma^{2+}_{\mathrm{DIP}}}{d\epsilon_1} = 4\pi \frac{d^3\sigma^{2+}_{\mathrm{DIP}}}{d\epsilon_1 d\Omega_1}(\theta_1 = 54.73°). \tag{11}$$

In Fig. 4 we present our calculations of the 3DCS at the magic angle in the dipole velocity approximation and with retardation taken into consideration, for $E_\gamma = 1.0$ keV with C2-SH states and with C3-GS2 states. It has been scaled by the factor 4π because in the dipole case it coincides with the differential cross section $d\sigma^{2+}_{\mathrm{DIP}}/d\epsilon_1$. Calculations with retardation at forward ($\varphi_1 = 0°$) and backward ($\varphi_1 = 180°$) scattering show deviations from dipole calculations. For brevity we shall denote $d^3\sigma^{2+}_{\mathrm{RET}}(0°) = d^3\sigma^{2+}_{\mathrm{RET}}/d\epsilon_1 d\Omega_1(\theta_1 = 54.73°, \varphi_1 = 0°)$ and a similar notation for $d^3\sigma^{2+}_{\mathrm{RET}}(180°)$.

For a low-energy electron ($\epsilon_1 \simeq 0$) retardation plays a minor role and $d^3\sigma^{2+}_{\mathrm{RET}}(0°) \simeq d^3\sigma^{2+}_{\mathrm{RET}}(180°)$, as in the case of the single photoionization close to threshold. However, for higher electron energies the differences could be substantial.

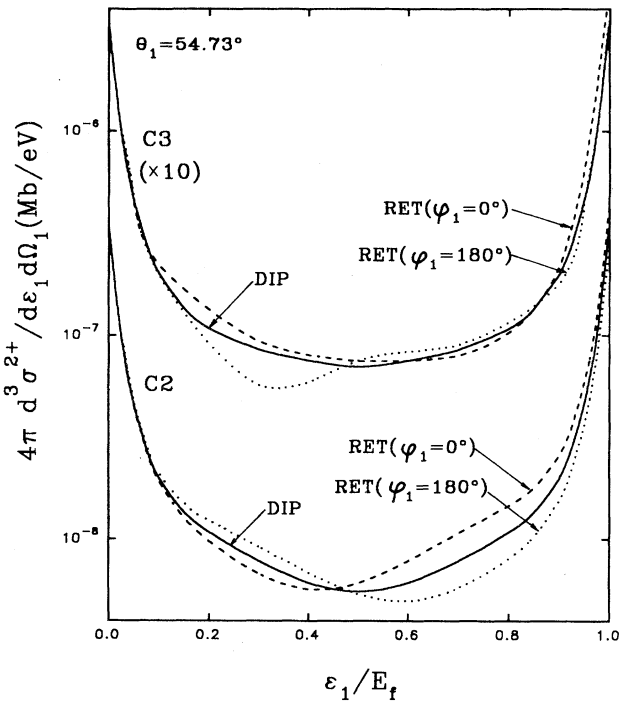

FIG. 4. 3DCS as a function of the energy of an electron calculated at the angle $\theta_1 = 54.73°$ for a photon energy of 1.0 keV. Solid line, dipole velocity approximation; dashed line, calculation with retardation at forward ($\varphi_1 = 0°$) scattering; dotted line, calculation with retardation at backward ($\varphi_1 = 180°$) scattering. Calculations were made with C2-SH states and with C3-GS2 states.

For a high-energy electron ($\epsilon_1 \simeq E_f$), we observe that $d^3\sigma^{2+}_{\mathrm{RET}}(0°) > d^3\sigma^{2+}_{\mathrm{RET}}(180°)$, using either model. This could be explained by considering that the behavior of the fast electron resembles the case of the single photoionization of an s subshell electron. In this case the first-order retardation correction for the $\cos^2\theta_1$ behavior of the 3DCS at $\epsilon_1 \simeq E_f$ is given by

$$\left(\frac{d^3\sigma^{2+}_{\mathrm{RET}}}{d\epsilon_1 d\Omega_1}\right)_{\epsilon_1 \simeq E_f} \simeq \frac{3}{4\pi}\left(\frac{d\sigma^{2+}_{\mathrm{DIP}}}{d\epsilon_1}\right)_{\epsilon_1 \simeq E_f} \times \cos^2\theta_1\{1 + \kappa \sin\theta_1 \cos\varphi_1\}, \tag{12}$$

where κ is a retardation correction as in the case of an s subshell electron [11]. Since for a high-energy single photoelectron $\kappa > 0$ [11], the relation $d^3\sigma^{2+}_{\mathrm{RET}}(0°) > d^3\sigma^{2+}_{\mathrm{RET}}(180°)$ is fulfilled using this interpretation. The validity of Eq. (12) will be discussed below.

The other features of the spectrum, apart from the end points of the electron energies recently discussed, could not be explained easily from physical grounds. Differences appear in how retardation affects the spectrum. One sees that in some regions the spectra invert depending on whether C2 or C3 final states are considered. For example, for $\epsilon_1/E_f = 0.7$ we observe in Fig. 4 that $d^3\sigma^{2+}_{\mathrm{RET}}(0°)/d^3\sigma^{2+}_{\mathrm{RET}}(180°) \simeq 1.9$ using the C2 model, whereas this ratio is 0.8 with the C3 model. These results imply that measurements of electron

spectra taken at the magic angle for these energies could not be directly related to the differential cross section $d\sigma^{2+}/d\epsilon_1$, as already done for low photon energies [22,23]. We note that although the 3DCS presents an asymmetry in φ_1 at $\theta_1=54.73°$, when properly integrated over $d\Omega_1$, the differential cross section $d\sigma^{2+}_{\rm RET}/d\epsilon_1$ is symmetric about the midpoint $E_f/2$, as required by exchange.

When retardation is considered, the angular distributions given by the 3DCS cannot be described by a single parameter as in the dipole case. In single photoionization the differential cross section $d\sigma^{+}/d\Omega$ requires, in principle, an infinite number of terms [24]; however, for relatively small energies a first order retardation correction could generally be used. We analyze in the following the form that a first-order retardation correction has for the case of double photoionization. In this case we expand, as usual, the photon plane wave in the form

$$\exp(i\mathbf{k}_p\cdot\mathbf{r})\simeq 1+i\mathbf{k}_p\cdot\mathbf{r}. \tag{13}$$

The matrix element of Eq. (1) is now given by

$$\mathbf{T}_{\rm RET}(\mathbf{k}_1,\mathbf{k}_2|\mathbf{k}_p)\simeq\mathbf{T}_{\rm DIP}(\mathbf{k}_1,\mathbf{k}_2)+\mathbf{T}^{(1)}_{\rm RET}(\mathbf{k}_1,\mathbf{k}_2|\mathbf{k}_p), \tag{14}$$

where

$$\mathbf{T}^{(1)}_{\rm RET}(\mathbf{k}_1,\mathbf{k}_2|\mathbf{k}_p)=\langle\psi_f^-|(i\mathbf{k}_p\cdot\mathbf{r}_1)\nabla_1+(\,i\mathbf{k}_p\cdot\mathbf{r}_2)\nabla_2|\psi_i\rangle, \tag{15}$$

and the 5DCS, first order in k_p, is then given by

$$\frac{d^5\sigma^{2+}_{\rm RET}}{d\epsilon_1 d\Omega_1 d\Omega_2}\simeq\left(\frac{4\pi^2}{c}\right)\frac{k_1k_2}{E_\gamma}\,(|\hat{\mathbf{e}}\cdot\mathbf{T}_{\rm DIP}(\mathbf{k}_1,\mathbf{k}_2)|^2 +2{\rm Re}\{[\hat{\mathbf{e}}\cdot\mathbf{T}_{\rm DIP}(\mathbf{k}_1,\mathbf{k}_2)]\times[\hat{\mathbf{e}}\cdot\mathbf{T}^{(1)*}_{\rm RET}(\mathbf{k}_1,\mathbf{k}_2|\mathbf{k}_p)]\}). \tag{16}$$

Integrating the 5DCS given by Eq. (16) over $d\Omega_2$ leads to the 3DCS also to first order in k_p. As in the case of the asymmetry parameter β, the only model for which we could find an analytic expression for this first-order retardation correction is the one given by C2-GS1 and in this case the 3DCS is given by (see Appendix B)

$$\frac{d^3\sigma^{2+}_{\rm RET}}{d\epsilon_1 d\Omega_1}\simeq\frac{1}{4\pi}A_w(\epsilon_1)\{1+\beta_w(\epsilon_1)P_2(\cos\theta_1) +\sin\theta_1\cos\varphi_1[a_w(\epsilon_1)+2a_w(\epsilon_1)P_2(\cos\theta_1)]\}, \tag{17}$$

where $A_w(\epsilon_1)$ and $\beta_w(\epsilon_1)$ are given in Appendix A and the retardation correction coefficient $a_w(\epsilon_1)$ is given in Appendix B. From this formula we note that (i) the C2-GS1 model introduces a first-order retardation correction with one additional parameter a_w and (ii) this retardation correction is of the same form as that for single photoionization [11], although in that case the retardation correction depends in general on two independent additional coefficients, not one.

Since an analytical evaluation is not possible when more complicated wave functions are employed, we analyze in the following a first-order retardation correction given by

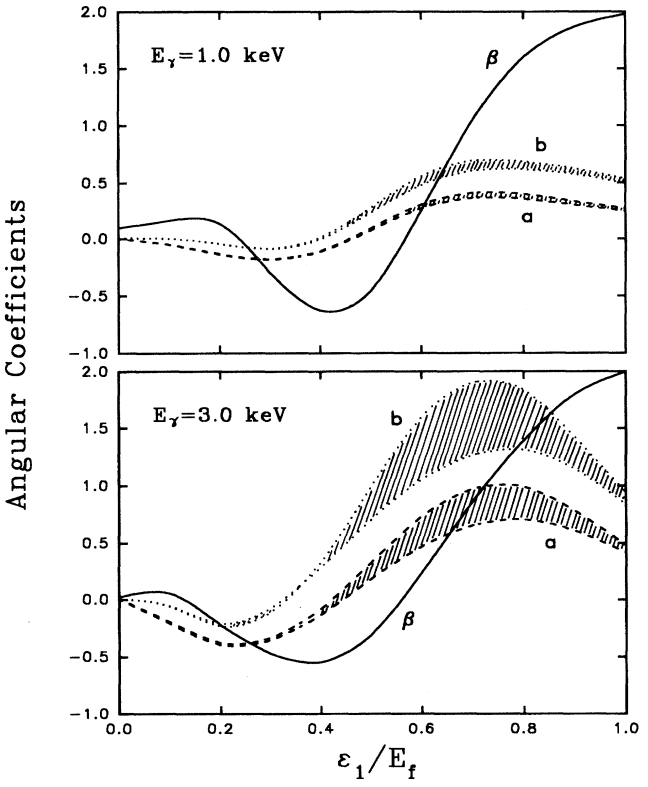

FIG. 5. Angular coefficients β, a, and b of Eq. (18) for a photon energy of 1.0 keV and 3.0 keV with C2-SH states. The shaded area corresponds to the uncertainty in the determination of the coefficients.

$$\frac{d^3\sigma^{2+}_{\rm RET}}{d\epsilon_1 d\Omega_1}\simeq\frac{1}{4\pi}A(\epsilon_1)\{1+\beta(\epsilon_1)P_2(\cos\theta_1) +\sin\theta_1\cos\varphi_1[a(\epsilon_1)+b(\epsilon_1)P_2(\cos\theta_1)]\}, \tag{18}$$

where we have introduced two independent additional coefficients $a(\epsilon_1)$ and $b(\epsilon_1)$ and $A(\epsilon_1)=d\sigma^{2+}_{\rm DIP}/d\epsilon_1$ in the case Eq. (18) represents a good approximation for the 3DCS. We note that, for the C2-GS1 model, these additional parameters are simply related by $b=2a$. It should be pointed out that the first-order retardation correction for the 3DCS given by Eq. (18) is expressed in the coordinate system of Fig. 1 and if another coordinate system is employed the equation would look different [25].

To make an analysis of Eq. (18), we note that our numerical programs introduce retardation to all orders in the multipole expansion, so that we can investigate three things: (a) whether the formula of the first-order retardation correction given by Eq. (18) is still valid, (b) whether the retardation coefficients a and b have a relation as in the case of the C2-GS1 model, and (c) the validity of Eq. (18) as the photon energy increases.

In Fig. 5 we present our calculated coefficients a and b using the C2-SH states for two photon energies of 1.0 keV and 3.0 keV. To assess the quality of Eq. (18) to describe the

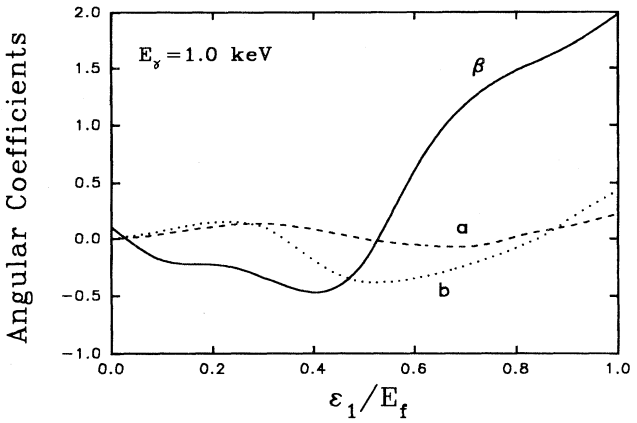

FIG. 6. Angular coefficients β, a, and b of Eq. (18) for a photon energy of 1.0 keV with C3-GS2 states.

3DCS, we have calculated the correction coefficients a and b, choosing different sets of grid points (θ_1,φ_1) for their determination; the shaded area in the figure corresponds to the uncertainty in the value of the coefficients for the approximations employed. We stress that this uncertainty corresponds to how well the 3DCS could be parametrized using Eq. (18) and *not* to a physical uncertainty in the parameters a and b. At a photon energy of 1.0 keV the deviations from the average are very low and have a maximum of 5%, but for low electron energies ϵ_1 the approximation of a first-order retardation correction is excellent. However, at a photon energy of 3.0 keV the approximation given by Eq. (18) deteriorates and the deviations in the coefficients are up to 25%, although for $\epsilon_1/E_f<0.4$ the approximation is still a very good one. On this basis, we can consider that the approximation of the 3DCS by Eq. (18) is a good one for electron energies $\epsilon_1<1.0$ keV, whereas for higher electron energies it will be necessary to introduce more than three parameters (β, a, and b) to describe the angular distributions [26]. We observed also that the relation $b=2a$ is in general not valid as more correlation is introduced.

In Fig. 6 we present the correction coefficients a and b at the photon energy of 1.0 keV using the C3 model. A comparison with the results presented in Fig. 5 using the C2 model at the same photon energy shows that these coefficients have different values, even considering the uncertainty in their determination. However, the limiting values of these coefficients are similar. For a low-energy electron ($\epsilon_1\simeq 0$) we observe that $a=b=0$. This is explained physically in the following manner. For a total asymmetry energy sharing ($\epsilon_1\simeq 0$ and $\epsilon_2\simeq E_f$) the full photon momentum ($\mathbf{k}_p$) is imparted to the fast electron, leaving no trace of $\mathbf{k}_p$ for the slow electron; the retardation corrections vanish for the slow electron. As mentioned before, the fast electron resembles the case of the single photoionization of an s subshell electron; the formula previously introduced for the retardation correction of the 3DCS at $\epsilon_1\simeq E_f$, given by Eq. (12), could be written in the form of Eq. (18), with $\beta=2.0$, $b=2.0\kappa$, and $a=\kappa$, or equivalently $b=2a$. Coincidently, for the fast electron behavior we indeed observe $b=2a$, using either model for the final state in Figs. 5 and 6.

Comparing the results of Figs. 5 and 6 at 1.0 keV, it can be observed that the retardation coefficients approach the values $a\simeq 0.25$ and $b\simeq 0.50$ as $\epsilon_1\rightarrow E_f$. We can explain the independence of the final state for this case as follows. As $E_f\rightarrow\infty$ and $\epsilon_1\rightarrow E_f$, the Sommerfeld parameter $\xi_{12}\rightarrow 0$ and the effect of the correlation of the C3 model, embodied in the multiplicative term $D^-(\xi_{12},\mathbf{k}_{12};\mathbf{r}_{12})$ of Eq. (5), tends to disappear and $\psi^-_{C3}\simeq\psi^-_{C2}$. The results using both models will be very similar to the case of a complete asymmetric energy sharing at high total energy.

In conclusion, our calculations favor the picture that, in a complete asymmetric energy sharing, the angular distribution of the fast electron resembles the case of an s subshell electron in a single-photoionization process, even when considering the retardation effects, while the slow electron emerges isotropically, without a trace of the polarization direction of the photon or of its momentum.

C. Contribution of retardation on total cross sections

As pointed out in the Introduction, a common feature of the calculations of the ratio $R=\sigma^{2+}/\sigma^{+}$ in the high-energy regime is the use of the dipole approximation. This is not automatically justified because the wavelength of the photon is about the same as the size of the He target at about 4.0 keV; thus the use of higher multipole radiation would be required. For the single photoabsortion cross section σ^+ it is known that cross sections that do not neglect retardation differ from dipole results by quantities of the order $(v/c)^2$ (see, for example, Ref. [27]). It should be mentioned that corrections of this order also result from the use of the relativistic Dirac formulation, therefore the results of the nonrelativistic cross sections including retardation should be taken with care.

We investigate in this section the contribution of retardation on the total cross section σ^{2+} and its influence on the ratio R. As mentioned before, in the dipole approximation the integration of the 5DCS to obtain the total cross section could be simplified due to the symmetries of the dipole operator. When retardation is considered these simplifications are not valid and the integration of the 5DCS becomes a formidable task if complex wave functions are considered. For this reason we have limited ourselves to the simple C2-GS1 models to calculate σ^{2+} without neglecting retardation. In Ref. [6] more elaborate wave functions have been employed within the dipole approximation (see Table II of Ref. [6]). For the single-photoionization cross section σ^+ the same initial state GS1 was employed, whereas the final state is described as a product of a bound $1s$ state with charge 2 and a continuum state with effective charge 1 (Coulomb approximation [28]).

Results in the dipole velocity approximation and with retardation taken into consideration are shown in Table I. As the same states are employed in both calculations, this serves as an examination of the influence of retardation on the total cross section. It accounts for only 0.4% at 1.0 keV and for 4.8% at 12.0 keV on σ^{2+}. However, a comparison of the ratio R shows that

$$\frac{\sigma^{2+}_{\mathrm{RET}}}{\sigma^{+}_{\mathrm{RET}}}=\frac{\sigma^{2+}_{\mathrm{DIP}}}{\sigma^{+}_{\mathrm{DIP}}}, \tag{19}$$

TABLE I. Total cross sections of single and double ionization of helium by photons of energy E_γ. The wave functions employed are the Coulomb approximation (see the text) and GS1 for single ionization and C2-GS1 for double ionization. DIP, calculation in dipole velocity approximation; RET, calculation with retardation. The last column is the relative difference of $\sigma^{2+}_{\rm RET}$ and $\sigma^{2+}_{\rm DIP}$.

E_γ (keV)	$\sigma^{+}_{\rm DIP}$ (Mb)	$\sigma^{+}_{\rm RET}$ (Mb)	$\sigma^{2+}_{\rm DIP}$ (Mb)	$\sigma^{2+}_{\rm RET}$ (Mb)	$\frac{\sigma^{2+}_{\rm RET}-\sigma^{2+}_{\rm DIP}}{\sigma^{2+}_{\rm RET}}$ (%)
1.0	3.711×10^{-4}	3.724×10^{-4}	6.516×10^{-6}	6.542×10^{-6}	0.38
2.0	3.772×10^{-5}	3.799×10^{-5}	6.384×10^{-7}	6.434×10^{-7}	0.79
3.0	9.673×10^{-6}	9.783×10^{-6}	1.633×10^{-7}	1.652×10^{-7}	1.18
4.0	3.655×10^{-6}	3.711×10^{-6}	6.188×10^{-8}	6.287×10^{-8}	1.59
6.0	9.195×10^{-7}	9.409×10^{-7}	1.569×10^{-8}	1.607×10^{-8}	2.39
8.0	3.436×10^{-7}	3.545×10^{-7}	5.908×10^{-9}	6.098×10^{-9}	3.21
10.0	1.598×10^{-7}	1.661×10^{-7}	2.764×10^{-8}	2.875×10^{-9}	4.03
12.0	8.537×10^{-8}	8.946×10^{-8}	1.483×10^{-9}	1.555×10^{-9}	4.86

which indicates that previous calculations [3,5,6] may give the same result for the ratio R when retardation effects are taken into account, although the separate values of the cross sections σ^{2+} and σ^{+} slightly increase. Of course, the wave functions employed for this evaluation do not give a good value for the asymptotic ratio due mainly to the poor cusp ratio of the initial state GS1 ($R_{\rm cusp}=-1.685$). At 12.0 keV our calculation gives a ratio of 1.73%, to be contrasted with the shake calculation of Åberg [2], which, using the same initial state GS1, gives a ratio of 1.75% (while the exact one is 1.67%).

A simple analysis of the results of Table I shows that the single-photoionization cross section behaves as $\sigma^{+}_{\rm RET}/\sigma^{+}_{\rm DIP}=1+(v/c)^2$, where v is the velocity of the ejected electron. This is in accordance with analytic results valid for the K shell [27]. The double-photoionization cross section behaves similarly $\sigma^{2+}_{\rm RET}/\sigma^{2+}_{\rm DIP}=1+(v_m/c)^2$, where v_m is the maximum velocity of an electron. The fact that corrections of the same order appear in both single- and double-photoionization cross sections appears to be the clue for the validity of Eq. (19).

Finally, we point out that the retardation contribution at the level of the total cross section σ^{2+} could be competitive with the inclusion of relativistic effects, as is the case for σ^{+}. At $E_\gamma=12.0$ keV the maximum electron velocity is about $v_m/c=0.2$ and relativistic effects should be noticeable. No estimate of σ^{2+} is available within a relativistic framework, so deviations from the ratio of 1.67% due to relativity are uncertain.

IV. CONCLUSIONS AND PROSPECTS

In this work we have considered some aspects of the retardation effects that affect the cross sections in double photoionization. Several features have been exposed that are missing in dipole calculations of this process, which have tended to explain the data reported in synchrotron x-ray experiments [1,10]. The analysis of data of future experiments on the energy and angular distributions [29] might shed light on the dynamics of the two-electron escape. For this task inclusion of retardation effects in the theory will be necessary.

First, we have presented calculations of the asymmetry parameter β using the dipole velocity operator for a range of energies including the intermediate- and the high-energy regime. We have shown that for sufficiently high energies the limits $\beta\rightarrow0.0(2.0)$ as $\epsilon_1\rightarrow0(E_f)$ are satisfied, independently of the approximations employed for the final or initial state, although the detailed behavior of $\beta(\epsilon_1)$ depends sensitively on the choice of these approximations. These limits of the asymmetry parameter β are, in consequence, a fundamental feature of the high-energy regime of the process. In particular, the disagreement between our results and the ones presented by Teng and Shakeshaft [8] obtained using a short-range correction term for the C3 model should be investigated experimentally.

We have investigated the role of retardation on the differential cross sections. We have shown that the differential cross section $d^3\sigma^{2+}_{\rm RET}/d\epsilon_1 d\Omega_1$ could be described by a first-order retardation correction that introduces two additional parameters $a(E_f,\epsilon_1)$ and $b(E_f,\epsilon_1)$ besides the asymmetry parameter $\beta(E_f,\epsilon_1)$, with good confidence for electron energies $\epsilon_1<1.0$ keV. For higher electron energies more than three parameters will be necessary to parametrize this cross section; in this case a better coordinate system to describe the 3DCS appears to be one with the photon momentum $\mathbf{k}_p$ along the z axis, since in single photoionization this coordinate system is the one generally used [24].

Finally, an interesting feature is our numerical finding of the identity given by Eq. (19), which, although it has been obtained with simple models for the states considered, opens the way for a more general demonstration. This relation would imply that the asymptotic ratio σ^{2+}/σ^{+}, which in dipole approximation gives the value 1.67%, would be truly realized in a formalism that takes retardation into account. This formalism could be developed, in principle, under the same assumptions of the shake formalism of Åberg and Dalgarno. Since relativistic effects are also important for the energies considered, a complete formalism should be developed within the relativistic framework.

ACKNOWLEDGMENTS

The Instituto de Astronomía y Física del Espacio (IAFE) is affiliated with the Consejo Nacional de Investigaciones Científicas y Técnicas. We acknowledge discussions with R.

H. Pratt, T. Surić, and P. M. Bergstrom, Jr., within the IAFE–University of Pittsburgh collaboration program. We also appreciate correspondence with and comments by R. Wehlitz.

APPENDIX A: CALCULATION OF β WITH C2-GS1 STATES

In what follows we derive the asymmetry parameter β for the C2-GS1 model. The C2 model is given by Eq. (7) and the GS1 wave function reads

$$\psi_{\mathrm{GS1}}(\mathbf{r}_1,\mathbf{r}_2)=N_i(e^{-ar_1-br_2}+e^{-br_1-ar_2}). \tag{A1}$$

We use the Nordsieck-type integrals [30]

$$\int d\mathbf{r}e^{-i\mathbf{k}\cdot\mathbf{r}-\alpha r}{}_1F_1(-i\xi,1,ikr+i\mathbf{k}\cdot\mathbf{r})=I_1(k,\xi,\alpha), \tag{A2}$$

$$\int d\mathbf{r}e^{-i\mathbf{k}\cdot\mathbf{r}-\alpha r}\frac{z}{r}{}_1F_1(-i\xi,1,ikr+i\mathbf{k}\cdot\mathbf{r})=I_2(k,\xi,\alpha)\cos\theta, \tag{A3}$$

where θ is the polar angle of $\mathbf{k}$, $\xi=-Z_T/k$, and

$$I_1(k,\xi,\alpha)=\frac{8\pi i}{(k^2+\alpha^2)^2}A_{k,\alpha}^{i\xi}\left[-\alpha(i-\xi)-\frac{\xi(\alpha-ik)}{A_{k,\alpha}}\right], \tag{A4}$$

$$I_2(k,\xi,\alpha)=\frac{-8\pi i}{(k^2+\alpha^2)^2}A_{k,\alpha}^{i\xi}(1+i\xi)k, \tag{A5}$$

$$A_{k,\alpha}=\frac{\alpha^2-k^2-2i\alpha k}{(k^2+\alpha^2)}. \tag{A6}$$

The T matrix in the dipole velocity approximation [Eq. (4)] is then given by

$$\hat{\mathbf{z}}\cdot\mathbf{T}_{\mathrm{DIP}}(\mathbf{k}_1,\mathbf{k}_2)=C(\mathscr{A}\cos\theta_1+\mathscr{B}\cos\theta_2), \tag{A7}$$

where

$$C=\frac{\sqrt{2}}{(2\pi)^3}N_iN^*(\xi_1)N^*(\xi_2) \tag{A8}$$

and

$$\mathscr{A}=-aI_2(k_1,\xi_1,a)I_1(k_2,\xi_2,b)-bI_2(k_1,\xi_1,b)I_1(k_2,\xi_2,a), \tag{A9}$$

$$\mathscr{B}=-aI_2(k_2,\xi_2,a)I_1(k_1,\xi_1,b)-bI_2(k_2,\xi_2,b)I_1(k_1,\xi_1,a). \tag{A10}$$

The 5DCS is then given by

$$\frac{d^5\sigma^{2+}_{\mathrm{DIP}}}{d\epsilon_1 d\Omega_1 d\Omega_2}=C_0|\mathscr{A}\cos\theta_1+\mathscr{B}\cos\theta_2|^2, \tag{A11}$$

where $C_0=(4\pi^2/c)k_1k_2|C|^2/E_\gamma$. Integrating over $d\Omega_2$ leads to the 3DCS given by

$$\frac{d^3\sigma^{2+}_{\mathrm{DIP}}}{d\epsilon_1 d\Omega_1}=\frac{1}{4\pi}A_w(\epsilon_1)[1+\beta_w(\epsilon_1)P_2(\cos\theta_1)], \tag{A12}$$

where

$$A_w(\epsilon_1)=\frac{(4\pi)^2}{3}C_0(|\mathscr{A}|^2+|\mathscr{B}|^2) \tag{A13}$$

and

$$\beta_w(\epsilon_1)=\frac{2|\mathscr{A}|^2}{(|\mathscr{A}|^2+|\mathscr{B}|^2)}. \tag{A14}$$

A comparison of Eq. (A12) with Eq. (8) shows that $A_w(\epsilon_1)=d\sigma^{2+}_{\mathrm{DIP}}/d\epsilon_1$. From Eq. (A14) we see that $0\leq\beta_w\leq 2$, so that negative values of the asymmetry parameter are not allowed using the states considered. From the definition of the quantities $\mathscr{A}$ and $\mathscr{B}$ it is readily seen that $\mathscr{A}=\mathscr{B}$ when $\epsilon_1=E_f/2$ and so we obtain that $\beta_w(\epsilon_1/E_f=0.5)=1$ for any final energy E_f. Also, it could be seen that for $E_f\gg -E_0$ this asymmetry parameter observes the limits $\beta_w\to 0.0(2.0)$ as $\epsilon_1\to 0(E_f)$. But this is not the case for the near-threshold behavior; for example, for $E_\gamma=120$ eV we have $\beta_w\to 0.3(1.7)$ as $\epsilon_1\to 0(E_f)$.

APPENDIX B: CALCULATION OF THE FIRST-ORDER RETARDATION CORRECTION WITH C2-GS1 STATES

In what follows we consider, as in the text, $\hat{\mathbf{e}}=\hat{\mathbf{z}}$ and $\hat{\mathbf{k}}_p=\hat{\mathbf{x}}$. To evaluate the first-order retardation correction, we use the Nordsiek-type integral [31]

$$\int d\mathbf{r}e^{-i\mathbf{k}\cdot\mathbf{r}-\alpha r}\frac{xz}{r}{}_1F_1(-i\xi,1,ikr+i\mathbf{k}\cdot\mathbf{r})=I_3(k,\xi,\alpha)\cos\theta\sin\theta\cos\varphi, \tag{B1}$$

where θ and φ are the polar and azimuthal angles of $\mathbf{k}$, $\xi=-Z_T/k$, and

$$I_3(k,\xi,\alpha)=\frac{16\pi}{(k^2+\alpha^2)^3}A_{k,\alpha}^{i\xi}(i-\xi)(2i-\xi)k^2. \tag{B2}$$

Together with the integral given by Eq. (A2) we obtain

$$\hat{\mathbf{z}}\cdot\mathbf{T}^{(1)}_{\mathrm{RET}}=ik_pC(\mathscr{C}\cos\theta_1\sin\theta_1\cos\varphi_1+\mathscr{D}\cos\theta_2\sin\theta_2\cos\varphi_2), \tag{B3}$$

where C is given in Eq. (A8) and

$$\mathscr{C}=-aI_3(k_1,\xi_1,a)I_1(k_2,\xi_2,b)-bI_3(k_1,\xi_1,b)I_1(k_2,\xi_2,a), \tag{B4}$$

$$\mathscr{D}=-aI_3(k_2,\xi_2,a)I_1(k_1,\xi_1,b)-bI_3(k_2,\xi_2,b)I_1(k_1,\xi_1,a). \tag{B5}$$

Using Eqs. (A7) and (B3), it may then be easily proved that

$$\int d\Omega_2 2\mathrm{Re}\{[\hat{\mathbf{z}}\cdot\mathbf{T}_{\mathrm{DIP}}(\mathbf{k}_1,\mathbf{k}_2)][\hat{\mathbf{z}}\cdot\mathbf{T}^{(1)*}_{\mathrm{RET}}(\mathbf{k}_1,\mathbf{k}_2|\mathbf{k}_p)]\}=-k_p8\pi|C|^2\mathrm{Re}[i\mathscr{A}\mathscr{C}^*]\cos^2\theta_1\sin\theta_1\cos\varphi_1. \tag{B6}$$

Finally, using this result in the integration over $d\Omega_2$ of the first-order retardation correction of the 5DCS [Eq. (16)] gives

$$\frac{d^3\sigma^{2+}_{\rm RET}}{d\epsilon_1 d\Omega_1} \simeq \frac{1}{4\pi} A_w(\epsilon_1)\{1+\beta_w(\epsilon_1)P_2(\cos\theta_1) + \sin\theta_1\cos\varphi_1[a_w(\epsilon_1)+2a_w(\epsilon_1)P_2(\cos\theta_1)]\}, \tag{B7}$$

where $A_w(\epsilon_1)$ and $\beta_w(\epsilon_1)$ are given in Appendix A and

$$a_w(\epsilon_1)=k_p\frac{\mathrm{Im}[2\mathscr{A}\mathscr{C}^*]}{(|\mathscr{A}|^2+|\mathscr{B}|^2)} \tag{B8}$$

is the coefficient of the first-order correction. We note that at $E_\gamma=1.0$ keV this parameter has the limits $a_w\to 0.0(0.24)$ as $\epsilon_1\to 0(E_f)$. In general $a_w\to 0.0$ as $\epsilon_1\to 0$, for any final energy E_f.

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