

Double photoionization of He by circularly polarized light: A QED approach

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Quantum electrodynamics is used to calculate the angle- and energy-resolved triple differential cross section for double photoionization of He by circularly polarized light for electrons emitted in a plane perpendicular to the incident beam direction. In the present work, the effect of chirality of the circularly polarized light in producing dichroism is obtained. Results are compared with the existing experimental results and theoretical calculations.

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I. INTRODUCTION

Double photoionization (DPI) of He is consistently attracting a great deal of attention both experimentally and theoretically [1–10]. DPI of the free atom is a manifestation of electron-electron correlation. There are a good number of theoretical and experimental works on double photoionization of He by linearly polarized light. Up until now, calculations on DPI were based on the first-order perturbation theory and dipole approximation for radiation fields [1,2,7–10]. Berakdar and Klar [2] calculated DPI by *circularly polarized light* (CPL) using the dipole approximation, correlated wave functions, and Coulomb distortions in the final state. In particular, Klar and collaborators [1] used tensorial calculus and a laboratory-fixed frame in the independent-particle approach to derive a general expression of the triple differential cross section (TDCS) from which the helicity dependence of the DPI cross section by CPL was obtained. Huetz and collaborators [7(a),7(b),8] used a body-fixed frame collective-coordinate approach in the dipole approximation to establish an alternative expression of the TDCS. Malegat and collaborators [9(a),9(b)] linked the above two approaches and obtained a generalized version of the TDCS which can be applied to DPI by CPL. Berakdar and Klar [2] predicted the helicity signature in the TDCS by photons of right-handed (RH) and left-handed (LH) circular polarization. Klar and collaborators [1] have shown that photoionization of a randomly oriented free atom by CPL produces photoelectron pairs with the ability to distinguish a RH from a LH coordinate frame. Results of their numerical calculations on He [1] show the amount of circular dichroism to depend strongly (i) on the choice of wave function used, (ii) on the energy distribution of photoelectrons, and (iii) on the relative angle of emission. Berakdar in his latest work [10] has shown that although helicity of CPL has no dynamical effect on DPI, phase differences in the amplitudes can be obtained by variation of the helicity of the absorbed photon. The circular dichroism was subsequently verified [5]. It was found that the necessary conditions to observe nonvanishing dichroism are (a) the two electrons unevenly share the excess

energy and (b) the direction of incident light and the direction of the two ejected electrons are not lying in one plane. The experimental results [5] compared well with the theoretical computations of Berakdar and Klar (Figs. 3–5).

This paper is an attempt to see the same effect from the perspective of QED and Feynman diagrams. So far the field theory and Feynman diagrams are successfully used in bound-state problems to calculate *charge transfer* [11], *ionization excitation* [12], and *below threshold excitation by electrons and photons* [13]. We are tempted to use the QED technique in the present bound-state problem to calculate DPI by CPL. Use is made of the covariant Lorentz gauge from the onset as well as Dirac spinors and relativistic wave functions for the interacting particles. We wish to clarify that while we will restrict ourselves to low-order perturbation theory with regard to radiation field (orders e and e^3 S matrices), we can obtain results accurate to all orders in Coulomb coupling by a suitable choice of the wave function. To estimate the effect of Coulomb coupling over the s -matrix particle-radiation field coupling, we multiply the unperturbed final wave function by the Coulomb distortion factor [12,13]. The Feynman diagrams contributing to DPI arise (i) due to the shake-off (SO) process and (ii) due to the two-step (TS) process. The SO process is one in which the photon striking the target ionizes one of the bound electrons and, subsequently, due to a change in the static correlation causing a change in the Coulomb field of the nucleus, the remaining electron is shaken off. The process is given by the first-order Feynman diagram [Fig. 1(a)]. This diagram can be identified with the first-order Born term (order e S matrix) from which the usual dipole approximation can be obtained. In the TS process, the photon striking the target ionizes one of the bound electrons and, subsequently, due to dynamic correlation the ionized electron exchanges a virtual photon with the remaining bound electron to dislodge it from the nucleus. The corresponding Feynman diagram [Fig. 1(b)] is of third order. The TS process can be identified with a third-order Born term (order e^3 S matrix). The interference between SO and TS terms is significant.

We calculate the TDCS for DPI of He for the same geometric configuration (Fig. 2) as was done in the coincidence experiment [5]. There, the two electrons ionized by a 93.5 eV photon moving in the z direction were viewed in the x - y plane. One of the photoelectrons, a , is viewed in a fixed direction x . The second photoelectron, b , is collected in the

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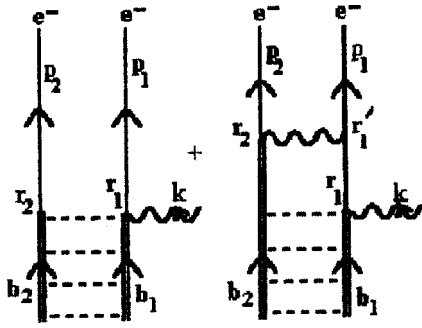


FIG. 1. Feynman diagrams for (a) shake-off process and (b) two-step process. The bound electrons are represented by a thick line with arrow, the ionized electrons are represented by a thin line with arrow, the dashed line represents the Coulomb photon, and the wavy line with arrow is the transverse photon while the wavy line without arrow is the virtual photon.

x - y plane. Although the cross section has no dynamical dependence on helicity, its effect on DPL is obtained here from a kinematical consideration. From the physical point of view, the electric-field vectors of the polarized light directed along the directions of polarization are effective in the ionization of the atoms. With the change of chirality of the circularly polarized light, the electric-field vectors rotate [14]. As the mutually perpendicular polarization vectors [9] in the circularly polarized light rotate with the change of helicity, the two ionized electrons that are scattered at a certain angle between them for a particular helicity will reverse in their role in sharing the kinetic energy and momentum with the change of helicity. Eventually, the electrons a and b (Fig. 2) with momenta p_1 and p_2 , respectively, for positive helicity will have momenta p_2 and p_1 , respectively, when the helicity becomes negative. Thus the source of dichroism is due to an exchange of momentum distribution with the change of chirality of the circularly polarized photon. The dichroism, however, will not exist if the two electrons share equal energy because of the indistinguishability of the electrons. The present results of the TDCS are compared with the existing experimental and theoretical results (Figs. 3–5) for incident CPL of positive and negative helicity with energy 93.5 eV for the rela-

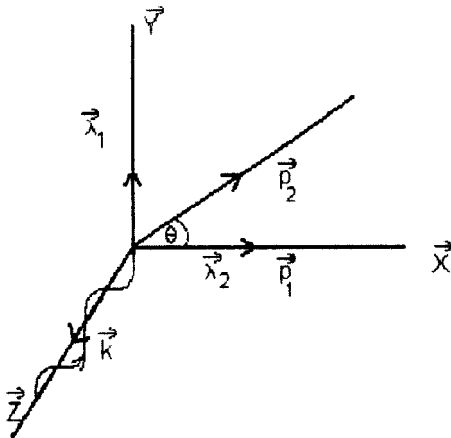


FIG. 2. Representative diagram showing the geometry of interaction (see text).

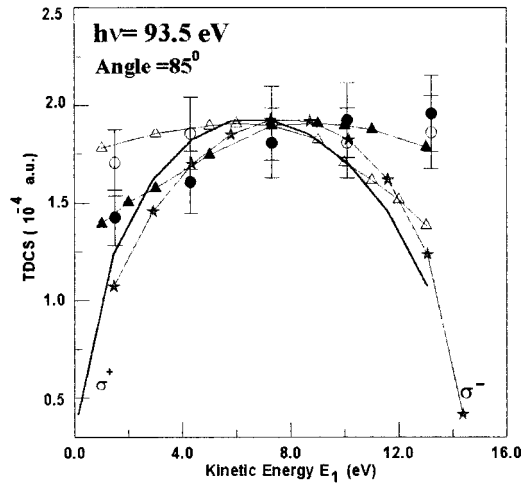


FIG. 3. Triple differential cross section (TDCS) for double photoionization of He ($1s$) by a right circularly polarized (RCP) and left circularly polarized (LCP) photon of energy 93.5 eV with relative angle of emission 85° . Present theory: RCP light, solid line; LCP light, line with stars. Other theory as in Ref. [5] having a multiplying factor 0.27: RCP light, line with solid triangles; LCP light, line with open triangles. Experiment [5]: RCP light, solid circles; LCP light, open circles.

tive scattering angles 85° , 125° , and 150° between the outgoing electrons. It is interesting to note that, in the present case, the dichroism vanishes at an equal sharing of energy between the two electrons, as it does in the existing experimental and theoretical results. The TDCS curve with respect to the energy of an electron in a particular direction for light with positive helicity appears as the mirror image of the similar curve by light with negative helicity about the line of equal energy sharing.

II. THEORETICAL FORMALISM

In QED a composite system of bound particles is represented by a string of field operators operating on a particle vacuum and multiplied by the unperturbed solution of the

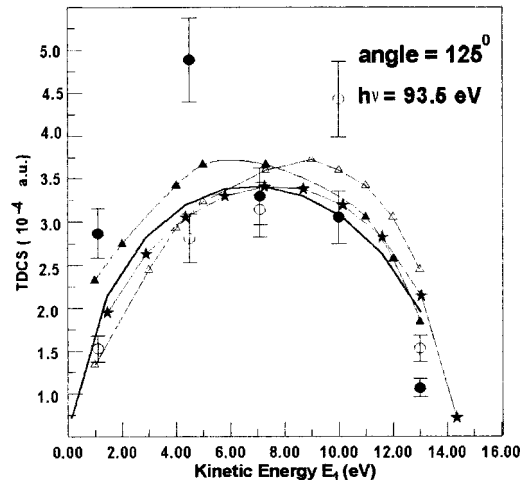


FIG. 4. Same as in Fig. 3 for angle of emission 125° .

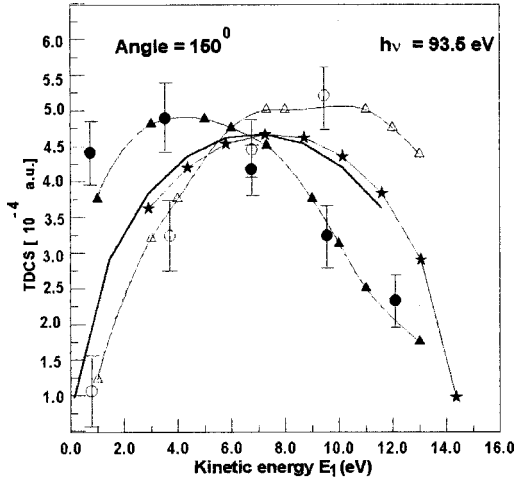
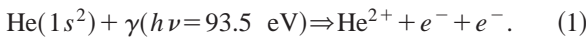


FIG. 5. Same as in Fig. 3 for angle of emission 150° , the other theoretical curves [5] having a multiplying factor 0.48.

Schrödinger equation [11–13]. Creation and annihilation operators of the particles bound to the Coulomb field of the nucleus obey equal-time commutation relations. There will be no loss of generality to represent the bound electrons by the Feynman directed lines. The amplitude for DPI reaction under consideration is given by the sum of the amplitudes of the SO and TS processes. The first-order S matrix [Fig. 1(a)] contains electron current and the incident circularly polarized photon. The second electron is shaken off due to a change in the static correlation, i.e., a change in the Coulomb field of the nucleus. In the TS process corresponding to the third-order Feynman diagram [Fig. 1(b)], double ionization occurs due to dynamic correlation between the two electrons. The third-order S matrix contains an electron propagator, a photon propagator, electron current, and a circularly polarized photon. The reaction under consideration is



A. Shake-off process

The amplitude for the SO process [Fig. 1(a)] is given by

$$S_{\text{SO}} = \frac{1}{4} \left(\frac{e^2}{\hbar c} \right)^{1/2} [\bar{\Psi}_f(r_1, r_2, R) \gamma_\mu A_\mu(r_1, k) \Psi_i(r_1, r_2, R)]. \quad (2)$$

γ_μ is the Dirac matrix and $A_\mu(r_1)$ is the wave function for the circularly polarized photon. r_1 , r_2 , and R are the space-time four-coordinates of the two bound electrons and the nucleus, respectively. The initial wave function of the system of bound electrons in the He atom is given as in [13],

$$\begin{aligned} \Psi_i(r_1, r_2, R) &= \phi_{1s^2}(x, y) \frac{1}{(2\pi)^3} \\ &\times \left(\frac{m^2}{\varepsilon_1 \varepsilon_2} \right)^{1/2} u(b_1, r_1) u(b_2, r_2) \\ &\times \exp(iRL_i) \exp(ib_1 r_1 + ib_2 r_2), \end{aligned} \quad (3)$$

where $u(b_i, r_i)$ is the Dirac spinor for the bound electron with four-momentum b_i at the position r_i ($i=1,2$) $\varepsilon_1, \varepsilon_2$ are the binding energies of the two bound electrons, and L_i is the CM momentum. The space coordinates of the electrons relative to the nucleus are

$$\vec{x} = \vec{r}_1 - \vec{R} \quad \text{and} \quad \vec{y} = \vec{r}_2 - \vec{R},$$

$$\Phi_{1s^2}(x, y) = X_{1s}(x) X_{1s}(y) \quad (3a)$$

is the ground-state wave function of the He atom [13],

$$X_{1s}(x) = A e^{-z_1 x} + B e^{-z_2 x}, \quad A = 0.7349, \quad B = 0.799,$$

$$z_1 = 1.41, \quad z_2 = 2.61.$$

The final wave function of the system of two free electrons and the nucleus is

$$\begin{aligned} \Psi_f(r_1, r_2, R) &= \frac{1}{(2\pi)^3} \left(\frac{m^2}{p_{10} p_{20}} \right)^{1/2} u(p_1, r_1) u(p_2, r_2) \\ &\times \exp(iRL_f) F_c(\vec{p}_1, \vec{p}_2) \exp(ip_1 r_1 + ip_2 r_2). \end{aligned} \quad (4)$$

L_f is the CM momentum of the interacting system in the final state. The Coulomb distortion factor $F_c(p_1, p_2)$ is given as in [12]. λ_1, λ_2 are the polarization vectors of the two mutually perpendicular plane-polarized light with potentials $A_{1\mu}(r_1, k)$ and $A_{2\mu}(r_1, k)$. The circularly polarized photon $A_\mu(r_1, k)$ is given by

$$\begin{aligned} A_\mu(r_1, k) &= A_{1\mu}(r_1, k) \pm i A_{2\mu}(r_1, k) \\ &= (\lambda_1 \pm i \lambda_2) \exp(ikr_1) / \sqrt{2k_0 (2\pi)^3}. \end{aligned} \quad (5)$$

The + (−) sign indicates right (left) circular polarization. p_1 and p_2 are the four-momenta of the two electrons and k is the momentum of the photon. The geometry of the reaction (1) is taken similar to that in the experiment [5] such that $\vec{K} \perp \vec{p}_1$, \vec{p}_2 , $\vec{\lambda}_1$, and $\vec{\lambda}_2$, where $\lambda_1 = (0; 0, 1, 0)$, $\lambda_2 = (0; 1, 0, 0)$, $k = (k_0; 0, 0, \vec{K})$, $p_1 = (p_{10}; p_1, 0, 0)$, and $p_2 = (p_{20}; p_{2x}, p_{2y}, 0)$. θ is taken as the angle between the two ionized electrons. On substitution from Eqs. (3)–(5) in Eq. (2),

$$\begin{aligned} S_{\text{SO}} &= C_1 \frac{1}{4} \left(\frac{e^2}{\hbar c} \right)^{1/2} F_c(p_1, p_2) \int \bar{u}(p_2) \bar{u}(p_1) \\ &\times \exp(-ip_1 r_1 - ip_2 r_2 - iRL_f) \gamma_\mu (\lambda_1 \pm i \lambda_2) \\ &\times \exp(-ikr_1) u(b_1) u(b_2) \exp(ib_1 r_1 + ib_2 r_2 + iRL_i) \\ &\times \phi_{1s^2}(x, y) d^4 r_1 d^4 r_2 d^4 R. \end{aligned}$$

Taking $L = \lambda_1 \pm i \lambda_2$, and knowing that at equal time $r_{10} = r_{20} = R_0 = r_0$,

$$\begin{aligned}
S_{\text{SO}} &= \Lambda [\bar{u}(p_2)u(b_2)][\bar{u}(p_1)\gamma_\mu L u(b_1)] \int dr_0 \\
&\times \exp[i r_0(-p_{20}-p_{10}+k_0+b_{10}+b_{20}+L_{i0}-L_{f0})] \\
&\times \int \Phi_{1s^2}(x,y) \exp(i\vec{p}_2 \cdot \vec{r}_2 + i\vec{p}_1 \cdot \vec{r}_1 - i\vec{k} \cdot \vec{r}_1 \\
&+ i\vec{R} \cdot \vec{L}_f) d^3 r_1 d^3 r_2 d^3 R, \tag{6}
\end{aligned}$$

where

$$\Lambda = \frac{1}{4} \left(\frac{e^2}{\hbar c} \right)^{1/2} \frac{1}{\sqrt{(2\pi)^3 2\omega}} C_1, \tag{7}$$

$$C_1 = \frac{1}{(2\pi)^3} \sqrt{\frac{m^2}{\varepsilon_1 \varepsilon_2}} \frac{1}{(2\pi)^3} \sqrt{\frac{m^2}{p_{10} p_{20}}} F_c(p_1, p_2),$$

and

$$\begin{aligned}
F_c(p_1, p_2) &= (2\pi)^3 \sqrt{\eta_1 \eta_2}, \quad \eta_1 = \frac{z e m^2}{\hbar |p_1|} \\
\eta_2 &= \frac{z e m^2}{\hbar |p_2|}.
\end{aligned}$$

The products of the spinors are taken as follows:

$$T_3 = \bar{u}(p_1) L u(b_1), \quad T_4 = \bar{u}(p_2) u(p_2), \tag{8}$$

and $L = \lambda L$.

After equal time integration over r_0 ,

$$\begin{aligned}
S_{\text{SO}} &= \Lambda T_3 T_4 (2\pi) \delta(b_{10} + b_{20} + k_0 + L_{i0} \\
&- p_{10} - p_{20} - L_{f0}) I_{\text{SO}}. \tag{9}
\end{aligned}$$

I_{SO} is the overlap integral,

$$\begin{aligned}
I_{\text{SO}} &= \int \Phi_{1s^2}(x,y) \\
&\times \exp(i\vec{p}_2 \cdot \vec{r}_2 + i\vec{p}_1 \cdot \vec{r}_1 - i\vec{k} \cdot \vec{r}_1 \\
&+ i\vec{R} \cdot \vec{L}_f - iR L_i) d^3 r_1 d^3 r_2 d^3 R.
\end{aligned}$$

On substituting $\vec{r}_1 = \vec{x} + \vec{R}$ and $\vec{r}_2 = \vec{y} + \vec{R}$ in I_{SO} ,

$$\begin{aligned}
I_{\text{SO}} &= \int \Phi_{1s^2}(x,y) \exp\{i\vec{p}_2 \cdot (\vec{y} + \vec{R}) + i\vec{p}_1 \cdot (\vec{x} + \vec{R}) \\
&- i\vec{k} \cdot (\vec{x} + \vec{R}) + i\vec{R} \cdot \vec{L}_f - iR L_i\} d^3 x d^3 y d^3 R \\
&= (2\pi)^3 \delta^3(\vec{p}_1 + \vec{p}_2 + \vec{L}_f - \vec{k} - L_i) \int \Phi_{1s^2}(x,y) \\
&\times \exp\{i\vec{p}_2 \cdot \vec{y} + i\vec{p}_1 \cdot \vec{x} - i\vec{k} \cdot \vec{x}\} d^3 x d^3 y.
\end{aligned}$$

Using Eq. (3a) and integrating over x and y ,

$$I_{\text{SO}} = (2\pi)^3 \delta^3(\vec{p}_1 + \vec{p}_2 + \vec{L}_f - \vec{k}) F(z_1, z_2, p_1, p_2, k), \tag{10}$$

where

$$\begin{aligned}
F(z_1, z_2, p_1, p_2, k) &= \left\{ \frac{8\pi z_1 A}{(z_1^2 + p_2^2)^2} + \frac{8\pi z_2 B}{(z_2^2 + p_2^2)^2} \right\} \\
&\times \left\{ \frac{8\pi z_1 A}{(z_1^2 + p_1 - k^2)^2} + \frac{8\pi z_2 B}{(z_2^2 + p_1 - k^2)^2} \right\}.
\end{aligned}$$

Finally, the amplitude for the shake-off process is

$$\begin{aligned}
S_{\text{SO}} &= \delta(b_{10} + b_{20} + k_0 + L_{i0} - p_{10} - p_{20} - L_{f0}) \\
&\times \delta^3(\vec{p}_1 + \vec{p}_2 + \vec{L}_f - \vec{k}) \Lambda T_3 T_4 I_{\text{SO}} (2\pi)^4. \tag{11}
\end{aligned}$$

B. Two-step (TS) process

The amplitude for the TS process [Fig. 1(b)] is given by

$$\begin{aligned}
S_{\text{TS}} &= \frac{1}{4} \left(\frac{e^2}{\hbar c} \right)^{3/2} F_c(p_1, p_2) \exp(iR L_f) \\
&\times [\bar{\psi}_e(p_1, r'_1) \gamma_\delta S(r'_1 - r_1) \gamma_\mu A_\mu(k, r_1) \Psi'_i(r_1, R)] \\
&\times D(r_2 - r'_1) [\bar{\psi}_e(p_2, r_2) \gamma_\mu \Psi_i(r_2, R)], \tag{12}
\end{aligned}$$

where $\psi_e(p_1, r_1)$ and $\psi_e(p_2, r_2)$ are the Dirac wave functions for the two outgoing electrons at the vertices r_1 and r_2 . $D(r_2 - r'_1)$ and $S(r'_1 - r_1)$ are the photon-propagator and electron-propagator, respectively,

$$\psi_e(r_1, p_1) = C_3 u(p_1) \exp(ip_1 r_1), \tag{13}$$

$$\psi_e(r_2, p_2) = C_4 u(p_2) \exp(ip_2 r_2), \tag{14}$$

$$D(r_2 - r'_1) = - \int \frac{d^4 q}{(2\pi)^4} \frac{\exp\{iq(r_2 - r'_1)\}}{q^2 + i\varepsilon}, \tag{14a}$$

$$S(r'_1 - r_1) = \int \frac{d^4 s}{(2\pi)^4} \frac{\exp\{is(r'_1 - r_1)\}}{s - m + i\varepsilon}. \tag{14b}$$

Wave functions $\Psi'_i(r_1, R)$ and $\Psi_i(r_2, R)$ of the bound electrons [Fig. 1(b)] at the vertices r_1 and r_2 are, respectively,

$$\psi'_i(r_1, R) = C'_3 u(b_1) \exp(ib_1 r_1) \Phi_{1s^2}(x,y) \exp(iR L_1), \tag{15}$$

$$\psi_i(r_2, R) = C'_4 u(b_2) \exp(ib_2 r_2) \Phi_{\text{He}^+}(y) \exp(iR L_2). \tag{16}$$

L_1, L_2 are the CM momenta such that $L_1 + L_2 = L_i$, and

$$C_3 = \frac{1}{(2\pi)^{3/2}} \sqrt{m/p_{10}}, \quad C_4 = \frac{1}{(2\pi)^{3/2}} \sqrt{m/p_{20}},$$

$$C'_3 = C'_4 = \frac{1}{(2\pi)^{3/2}} \sqrt{m/\varepsilon_{1s}},$$

$\Phi_{1s^2}(x,y)$ is as in Eq. (3a), and

$$\Phi_{\text{He}^+}(y) = N \exp(-\alpha y), \quad N = \frac{1}{\sqrt{\pi}} \frac{z}{a_0}, \quad \alpha = \frac{z}{a_0}. \quad (16a)$$

Z is the nuclear charge and a_0 is the Bohr radius.

The spinor parts of the amplitude are

$$T_1 = \bar{u}(p_2) \gamma_\mu u(b_2),$$

$$T_2 = \bar{u}(p_1)(\not{k} + m) \not{E} u(b_1),$$

and substituting

$$\Lambda'(k, p_1, p_2) = \frac{1}{4} \left(\frac{e^2}{\hbar c} \right)^{3/2} \frac{1}{\sqrt{(2\pi)^3 2\omega}} C_3 C_4 C'_3 C'_4 \\ \times \frac{1}{(2\pi)^8} F_c(p_1, p_2)$$

we get for the two-step amplitude (12),

$$S_{\text{TS}} = \int \Lambda'(K, p_1, p_2) T_2 T_1 \Phi_{1s^2 1s}(x, y) \Phi_{\text{He}^+}(y) \frac{1}{q^2} \frac{1}{s^2 - m^2} \\ \times \exp[ir'_1(-p_1 + s - q) + ir_1(-s + b_1 + k) \\ + ir_2(-p_2 + b_2 + q) + iR(L_1 + L_2)] \\ \times \exp(-iRL_f) d^4 r'_1 d^4 r_1 d^4 r_2 d^4 R d^4 q d^4 S. \quad (17)$$

After integrating over r'_1 and S and making equal-time integration as in Eq. (9) and changing \vec{r}_1, \vec{r}_2 in terms of the relative coordinates \vec{x} and \vec{y} , we get

$$S_{\text{TS}} = \Lambda'(k, p_1, p_2) \int T_2 T_1 \delta(b_{10} + b_{20} + k_0 + L_{i0} \\ - p_{10} - p_{20} - L_{f0}) \delta^3(\vec{k} - \vec{p}_1 - \vec{p}_2 - \vec{L}_f) \\ \times I_{\text{TS}} \frac{1}{q^2 (s^2 - m^2)} d^4 q d^3 \vec{x} d^3 \vec{y}, \quad (18)$$

where $q_0 = p_{20} - b_{20}$, $s = p_1 + q$, $\vec{L}_1 = \vec{0}$, and the overlap integral I_{TS} is given by

$$I_{\text{TS}} = \int \Phi_{1s^2 1s}(x, y) \Phi_{\text{He}^+}(y) \\ \times \exp[ix(\vec{p}_1 + \vec{q} - \vec{k}) + iy(\vec{p}_2 - \vec{q})] d^3 \vec{x} d^3 \vec{y}.$$

Using Eqs. (3a) and (16a) we get after integration over x and y ,

$$I_{\text{TS}} = [AF(z_1, \vec{p}_1 + \vec{q} - \vec{k}) + BF(z_2, \vec{p}_1 + \vec{q} - \vec{k})][ANF(z_1 \\ + \alpha, \vec{p}_2 - \vec{q}) + BNF(z_2 + \alpha, \vec{p}_2 - \vec{q})], \quad (19)$$

where

$$F(z_1, \vec{t}) = \frac{8\pi z_1}{(z_1^2 + \vec{t}^2)^2}.$$

C. Probability amplitude

The probability amplitude

$$|M_{fi}|^2 = \frac{1}{2} [(S_{\text{SO}} + S_{\text{TS}})(S_{\text{SO}} + S_{\text{TS}})^* \\ + (S_{\text{SO}} + S_{\text{TS}})^*(S_{\text{SO}} + S_{\text{TS}})] \\ = \frac{1}{2} [(S_{\text{SO}} S_{\text{SO}}^* + S_{\text{SO}}^* S_{\text{SO}} + S_{\text{TS}} S_{\text{TS}}^* + S_{\text{TS}}^* S_{\text{TS}}) \\ + (S_{\text{SO}} S_{\text{TS}}^* + S_{\text{TS}} S_{\text{SO}}^* + S_{\text{SO}}^* S_{\text{TS}} + S_{\text{TS}}^* S_{\text{SO}})]. \quad (20)$$

1. Shake-off term

From Eq. (10),

$$S_{\text{SO}} = \delta(b_{10} + b_{20} + k_0 + L_{i0} - p_{10} - p_{20} - L_{f0}) \\ \times \delta^3(\vec{p}_1 + \vec{p}_2 + \vec{L}_f - \vec{k}) \Lambda T_3 T_4 I_{\text{SO}} (2\pi)^4 S_{\text{SO}} S_{\text{SO}}^* \\ = \Lambda^2 T_3 T_3^* T_4 T_4^* I_{\text{SO}}^2 (2\pi)^8 \delta(E_i - E_f) \delta^3(P_i - P_f), \quad (21)$$

where energy conservation is given by

$$\delta(E_i - E_f) = \delta(b_{10} + b_{20} + k_0 + L_{i0} - p_{10} - p_{20} - L_{f0}).$$

Knowing that $L_\pm = \lambda_1 \pm i\lambda_2$ and since $b_1 = (b_{10}, 0)$, $b_2 = (b_{20}, 0)$, $\lambda_1 = (0; 0, 1, 0)$, $\lambda_2 = (0; 1, 0, 0)$, and $b_{10} = b_{20} = m - \varepsilon_{1s}$, we get

$$b_1 p_1 = b_{10} p_{10} = (m - \varepsilon_{1s})(m + E_1),$$

$L_\pm L_\pm^* = -2$, and $L_\pm b_1 = L_\pm b_2 = 0$. The trace part becomes

$$T_3 T_3^* = \bar{u}(p_1) \not{L}_\pm u(b_1) \bar{u}(b_1) \not{L}_\pm^* u(p_1) \\ = \text{Tr} \left(\not{L}_\pm \frac{b_1 + m}{2m} \not{L}_\pm^* \frac{p_1 + m}{2m} \right) \\ = \frac{4}{4m^2} [-(L_\pm L_\pm^*)(b_1 p_1) + m(L_\pm L_\pm^*)] \\ = \frac{4}{4m^2} [L_\pm L_\pm^* (-b_{10} p_{10} + m^2)] \\ = \frac{2}{m^2} [m(E_1 - \varepsilon_{1s}) - E_1 \varepsilon_{1s}] = T_3^* T_3. \quad (22)$$

Similarly,

$$T_4 T_4^* = \bar{u}(p_2) u(b_2) \bar{u}(b_2) u(p_2) \\ = \text{Tr} \left(\frac{b_2 + m}{2m} \frac{p_2 + m}{2m} \right) \\ = \frac{4}{4m^2} [b_{20} p_{20} + m^2] \\ = \frac{4}{4m^2} [2m^2 + m(E_2 - \varepsilon_{1s}) - E_2 \varepsilon_{1s}] = T_4^* T_4. \quad (23)$$

2. Two-step term

From Eq. (18),

$$\begin{aligned}
 S_{\text{TS}} &= \Lambda'(K, p_1, p_2) \int T_2 T_1 \delta(E_i - E_f) \\
 &\quad \times \delta^3(\vec{k} - \vec{p}_1 - \vec{p}_2 - \vec{L}_f) \frac{1}{q^2} \frac{1}{(p_1 + q)^2 - m^2} I_{\text{TS}} d^3 q, \\
 S_{\text{TS}} S_{\text{TS}}^* &= [\Lambda'(K, p_1, p_2)]^2 \int T_2 T_2^* T_1 T_1^* \\
 &\quad \times \delta(E_i - E_f) \delta^3(\vec{k} - \vec{p}_1 - \vec{p}_2 - \vec{L}_f) I(q)^2 d^3 q,
 \end{aligned} \tag{24}$$

where

$$I(q) = I_{\text{TS}} \frac{1}{q^2} \frac{1}{(p_1 + q)^2 - m^2}.$$

After some lengthy calculations, the trace parts

$$\begin{aligned}
 T_2 T_2^* &= T_2^* T_2 \\
 &= \frac{1}{4m^2} [(L_{\pm} L_{\pm}^*) \{-16(sb_1)(sp_1) - 8m^2(b_1 p_1) \\
 &\quad + 32m^2(sb_1) + 64m^2(b_1 p_1) + 16m^2 s^2 - 8m^2(sp_1) \\
 &\quad + 16m^4\} - 32(sb_1)(L_{\pm}^* p_1)(sL_{\pm})],
 \end{aligned} \tag{25}$$

where $s = p_1 + q$,

$$T_1 T_1^* = T_1^* T_1 = (4/m^2)[-2(b_2 p_2) + 4m^2]. \tag{26}$$

3. Interference term

$$\begin{aligned}
 S_{\text{SO}} S_{\text{TS}}^* &= S_{\text{SO}}^* S_{\text{TS}} = (2\pi)^4 \delta(E_i - E_f) \delta^3(P_i - P_f) \\
 &\quad \times (\Lambda T_3 T_4 I_{\text{SO}}) \left[\delta(E_i - E_f) \delta^3(\vec{P}_i - \vec{P}_f) \right. \\
 &\quad \left. \times \Lambda'(K, p_1, p_2) \int T_2 T_1 I(q) d^3 q \right]^*.
 \end{aligned} \tag{27}$$

Since

$$T_3 T_2^* = \bar{u}(p_1) \not{L} u(b_1) \bar{u}(b_1) \not{L} (\not{s} + m) \gamma_{\delta} u(p_1), \tag{28}$$

$$T_4 T_1^* = \bar{u}(p_2) u(b_2) \bar{u}(b_2) u(p_2), \tag{29}$$

$$T_3 T_4 T_2^* T_1^* = (T_3 T_2^*)(T_4 T_1^*) = A_2 q_0 + B_2 |q| + C_2, \tag{30}$$

where

$$\begin{aligned}
 A_2 &= -\frac{4}{m^3} [b_0 m^2 - b_0^2 p_{10} + m^2 p_{20} - p_{20} p_{10} b_0 \\
 &\quad + b_0 |p_1| |p_2| \cos \theta],
 \end{aligned}$$

$$\begin{aligned}
 B_2 &= \frac{1}{m^3} [6|p_2| \cos \theta (m^2 - b_0 p_{10}) \\
 &\quad + (b_0^2 + b_0 p_{20})(4|p_1| \cos \theta - |p_1|)],
 \end{aligned}$$

$$\begin{aligned}
 C_2 &= -\frac{1}{m^3} [(m^2 - b_0 p_{10}) \{8(b_0 p_{10} + p_{10} p_{20} \\
 &\quad - |p_1| |p_2| \cos \theta) - 2|p_1| |p_2| \cos \theta\} - 2(b_0^2 + b_0 p_{20}) |p_1^2|],
 \end{aligned}$$

and θ is the angle between \vec{p}_1 and \vec{p}_2 .

D. Cross section

The momenta of the photoelectrons being taken as p_1 and p_2 , and L_f being the momentum of the recoil ion, using Eq. (20) the cross section for double ionization can be written as

$$\begin{aligned}
 \sigma &= \int \frac{1}{|k|} |M_{fi}|^2 \frac{d^3 p_1}{(2\pi)^3} \frac{d^3 p_2}{(2\pi)^3} \frac{d^3 L_f}{(2\pi)^3} \\
 &= \frac{1}{(2\pi)^9} \int \frac{1}{|k|} |M_{fi}|^2 p_1^2 dp_1 p_2^2 dp_2 d\Omega_a d\Omega_b d^3 L_f.
 \end{aligned} \tag{31}$$

The electron a with momentum p_1 is taken in the x direction (Fig. 2) and the electron b with momentum p_2 is emitted at an angle θ relative to p_1 . On integration over energy and momentum δ functions, the triple differential cross section becomes

$$\begin{aligned}
 \frac{d^3 \sigma}{d\Omega_a d\Omega_b dE_1} &= \frac{1}{(2\pi)^9} \frac{1}{|k|} |M_{fi}|^2 m p_1 m p_2 \\
 &= \frac{1}{(2\pi)^9} \frac{1}{|k|} 2m^3 \sqrt{E_1 E_2} |M_{fi}|^2.
 \end{aligned} \tag{32}$$

III. RESULTS AND DISCUSSIONS

In the present computation, we have considered the geometry of double photoionization as in the experiment, where the plane containing the directions of the two outgoing electrons is taken perpendicular to the direction of propagation of the incident circularly polarized light (Fig. 2). The two outgoing electrons are collected in coincidence in the x - y plane. One electron a is collected in the x direction and the direction of collection of the other electron b is changed relative to the first one. The results of the TDCS are then compared with the existing experimental and theoretical data (Figs. 3–5) for an incident circularly polarized photon of positive and negative helicity having energy 93.5 eV, the relative scattering angles between the outgoing electrons being 85°, 125°, and 150°, respectively. It is interesting to note that, as in the experimental and theoretical results [5], the dichroism vanishes at equal sharing of energy by the two electrons. The curves are like mirror images about the point of vanishing dichroism. The dominant contribution comes from the TS term.

IV. CONCLUSION

In the present paper we have computed the TDCS for double photoionization using field theory and the Feynman diagram. Although the usual quantum-mechanical approach and the dipole approximation as mentioned in the Introduction can reproduce the experimental results [5], application of field theory in bound-state problems has its own intrinsic appeal. Of the two diagrams corresponding to the shake-off and two-step processes, the latter yields higher contribution. Like the existing theoretical works, in the present calculation also the absolute magnitude of the TDCS is dependent on a particular pair of energy (E_1, E_2) of the two emitted electrons and the angle of emission between them. Circular dichroism is obtained here from kinematical consideration. For equal sharing of energy, dichroism vanishes. However, for unequal sharing of energy, the TDCS graphs for $+ve$ and $-ve$ helicities become mirror images about the point of van-

ishing dichroism, as in the existing experimental and theoretical results. A slight discrepancy between the present result and the experimental results hopefully can be removed by using more accurate correlated wave functions [6] in the initial state and Coulomb distorted wave function [15] in the final state, which we shall include in our subsequent calculations. Finally, we would like to point out that, in principle, field theory and Feynman diagrams are suited to explain the phenomena of double photoionization and circular dichroism in a two-electron bound system.

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