Signatures of target *e*-*e* correlations in the angular distribution of (*e*,3*e*) differential cross sections for the ionization of helium by fast electrons

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The effect of target *e*-*e* correlations on the angular distribution of fivefold differential cross section for the double ionization of helium by fast electrons has been studied. The helium ground-state wave functions due to Byron and Joachain [Phys. Rev. **146**, 1 (1966)], Silverman, Platas, and Matsen [J. Chem. Phys. **32**, 1402 (1960)], and Tweed and Langlois [J. Phys. B **20**, 5213 (1987)] have been employed. The calculation has been done in the first-order Born approximation with the two ejected electrons being described by a product of two Coulomb waves. The correlations in the final state have been accounted for by suitable effective charges and the Gamow correlation factor. Kinematics corresponding to or close to the Bethe ridge and with small momentum transfer and low ejected electron energies has been chosen. When one (energetic of the two) of the electrons is ejected along the momentum transfer direction, the angular distribution of the other for angles in the range 180°±60° with respect to the first is found to bear clear signatures of *e*-*e* correlations in the ground-state wave function. [S1050-2947(96)07605-6]

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I. INTRODUCTION

Since the fully differential (*e*,3*e*) experiments of Lahmam-Bennani *et al.* [1,2], there has been an increasing interest in the study of this process because of its potential in obtaining information about target electron-electron correlations. Just as the triple differential ionization cross section under appropriate conditions in a (*e*,2*e*) experiment is proportional to the square of the one-electron Fourier amplitude, the fivefold differential double ionization cross section (FDCS) in an (*e*,3*e*) experiment under suitable conditions is proportional to the square of the corresponding two-electron Fourier amplitude. This study may therefore be regarded as an extension of the (*e*,2*e*) spectroscopy pioneered by Weigold and McCarthy [3] and Giardini-Guidoni *et al.* [4]. One attempts to investigate the dependence of the angular distribution of the FDCS on the correlations (in the target) between the two ejected electrons. However, the extraction of the information on correlation from FDCS measurements is made difficult by several complicating factors. One of the factors relates to the mechanism of double ionization. In general, it is the result of (i) the so-called shake-off (SO) mechanism in which the projectile is assumed to interact once with and ejects only one of the target electrons [5]. The ejection of the two electrons is caused only by their mutual correlation in the initial state, (ii) a two-step (TS1) process in which the incident particle interacts successively with two different target electrons, ejecting them one by one and (iii) another two-step (TS2) process in which the incident particle ejects one target electron, which then interacts with and ejects the second one [6]. A calculation of all these processes is quite difficult. The final continuum state has three electrons in the field of the residual ion. A proper accounting of *e*-*e* correlations in the final state and eliminating their influence on the FDCS angular distribution is another complicating factor. Some of these difficulties get partly alleviated if the incident energy is fairly high, the scattering angle is small, and the scattered electron takes away most of the energy. In this situation the incident and the scattered electron wave functions may be taken as plane waves and the process is amenable to the Born treatment. The experiments of Lahmam-Bennani *et al.* correspond to such a kinematics.

Several calculations, within the first-order Born approximation, have been reported during the past few years. These consider only the shake-off process, which is known to be dominant [7]. The two ejected electrons in the field of the residual ion have been described by (i) orthogonalized plane waves [8,9], (ii) Coulomb waves with effective charges [10–12], (iii) orthogonalized Coulomb waves [11,13], (iv) the three-Coulomb wave function [14,15] of Brauner, Briggs, and Klar [16,17], and (v) an approximation to the Brauner-Briggs-Klar (BBK) model [18–20]. Becker, Jetzke, and Faisal [21] have considered a first-order multiple-scattering approach. The role of *e*-*e* correlations in the initial bound-state wave function has also been investigated to some extent [13,15,20,22,23]. In order to limit the range of the kinematical variables and to facilitate the analysis of the results, a study of the symmetry properties of the FDCS angular distribution with respect to the incident direction, scattering plane, momentum transfer direction, and electron exchange has also been carried out [15.] All these calculations have brought out the importance of including correlations in the description of both the initial state and the final state.

Two of us have recently made an attempt to look for kinematical situations in which the differences in *e*-*e* correlations in the helium ground-state wave function lead to a qualitative difference in the angular correlation of the ejected electrons [24]. It is found that the variation in the cross sec-

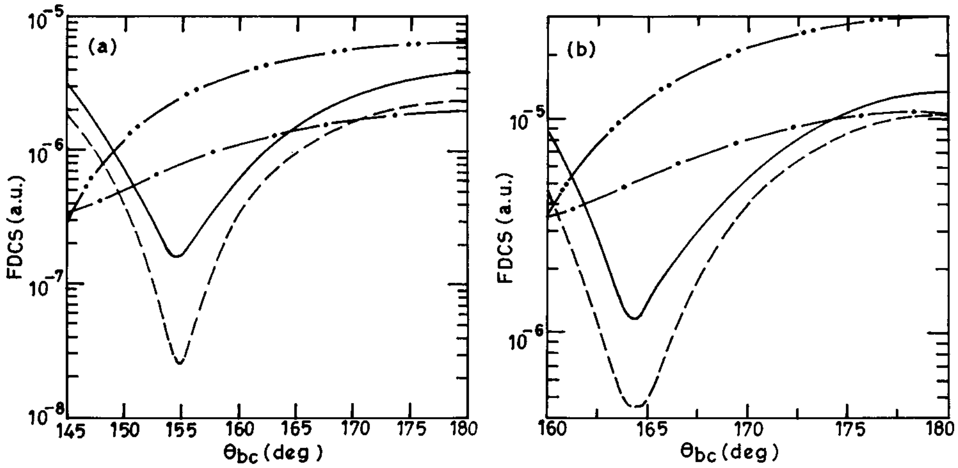

FIG. 1. Coplanar fivefold differential cross section (in a.u.) for double ionization of helium by electron impact at $E_0=5$ keV, $\theta_a=0.5°$ plotted against θ_{bc} in Bethe ridge kinematics. The angles θ_b and θ_c and the energies E_b and E_c for different values of θ_{bc} are given in Table I. θ_b and θ_c are measured with respect to the momentum transfer direction. Theoretical results: - · · - · · -, the BJ wave function; - · - · -, the OS wave function; ----, the SPM wave function; —, the TL wave function. E_b+E_c is equal to (a) 4 eV and (b) 10 eV.

tion is quite sensitive to the target e-e correlations when (i) the two low-energy ejected electrons are detected at fixed angles (θ_b and θ_c) but their energies E_b and E_c are varied such that the sum E_b+E_c is held fixed or (ii) one of the electrons is detected at some large fixed angle (say 90°) and the other angle θ_c is varied at fixed energies. However, in these studies no attempt has been made *a priori* to suitably choose kinematics (i) to minimize two-step ionization so that the model used may be more appropriate and (ii) to minimize the final-state e-e correlations so that the results are less dependent on uncertainties in properly accounting for it in the choice of the final-state wave function.

Berakdar and Klar [25] have investigated structures in the FDCS angular distribution and have pointed out kinematical situations where very little momentum is transferred to the target. They have also identified the associated ionization mechanisms. It has been shown that under these Bethe ridge conditions [26], the effect of initial- and final-state correlations of the target electrons can be separately considered. The contribution of various mechanisms (SO, TS1, and TS2) to the double ionization has recently been studied and analyzed by Popov *et al.* [27].

In the light of these studies, we, in the present paper, have considered kinematical arrangements that would ensure that (i) the process dominantly corresponds to shake-off with a soft binary collision between the incident electron and a target electron and (ii) the e-e correlation in the final state in minimal. Consider the situation where no momentum is transferred to the residual ion ($\vec{k}_r=\vec{0}$). The energy-momentum conservation equations are

$$E_0-I-E_a=E_b+E_c, \tag{1}$$

$$\vec{k}_0-\vec{k}_a=\vec{q}=\vec{k}_b+\vec{k}_c. \tag{2}$$

Here E_0, E_a, E_b, and E_c are the energies of the incident, scattered, and the two ejected electrons, respectively, $\vec{k}_0$, $\vec{k}_a$, $\vec{k}_b$, and $\vec{k}_c$ are their respective momenta, and I stands for the double-ionization threshold energy. At a given incident energy E_0 and fixed energy E_a of the scattered electron and fixed scattering angle θ_a (or momentum transfer $\vec{q}$), Eqs. (1) and (2) yield the values of E_b and E_c. These values naturally depend on the angle θ_{bc} and correspond to the Bethe ridge. We calculate the FDCS in coplanar kinematics for quite high incident energies for events in which the scattered electron takes away most of the energy and is scattered through a small angle. One of the electrons is assumed to be ejected with low energy along the momentum transfer ($\vec{q}$) direction corresponding to a soft binary collision. The other electron is ejected with still lower energy along the opposite direction as a result of shake-off, which is expected to be dominant in this kinematics. The variation in the FDCS is studied in two ways.

(a) The angle θ_{bc} is varied from 180° to lower values, say, 120°. The energies E_b and E_c of the two electrons (subject to the sum E_b+E_c held constant) and the angles θ_b and θ_c for every θ_{bc} are obtained from Eqs. (1) and (2). Note that $\vec{k}_r$ is zero.

(b) One of the two electrons (say, b) is assumed to be always emitted along the direction of $\vec{q}$ ($\theta_b=0°$). The angle of ejection of the other electron is varied from $\theta_c=180°$ to, say, $\theta_c=120°$. The energies E_b and E_c are held fixed at values obtained from Eqs. (1) and (2) for $\theta_{bc}=180°$. Note that in this case k_r varies from zero at $\theta_c=180°$ to $k_r=k_c$ at $\theta_{bc}=120°$. The value of k_r is thus quite small. The Bethe ridge condition is exactly satisfied only for $\theta_{bc}=180°$.

In both of the above two cases the e-e correlations in the final state shall be minimal as θ_{bc} is never smaller than 120°.

In the next section we present details of the calculation. Section III contains the results and their discussion. The results are summarized in Sec. IV.

II. THEORY

The FDCS (in a.u.) is given by

$$\frac{d^5\sigma}{dE_b dE_a d\Omega_a d\Omega_b d\Omega_c}=\frac{k_a k_b k_c}{k_0}|F_{fi}|^2, \tag{3}$$

where

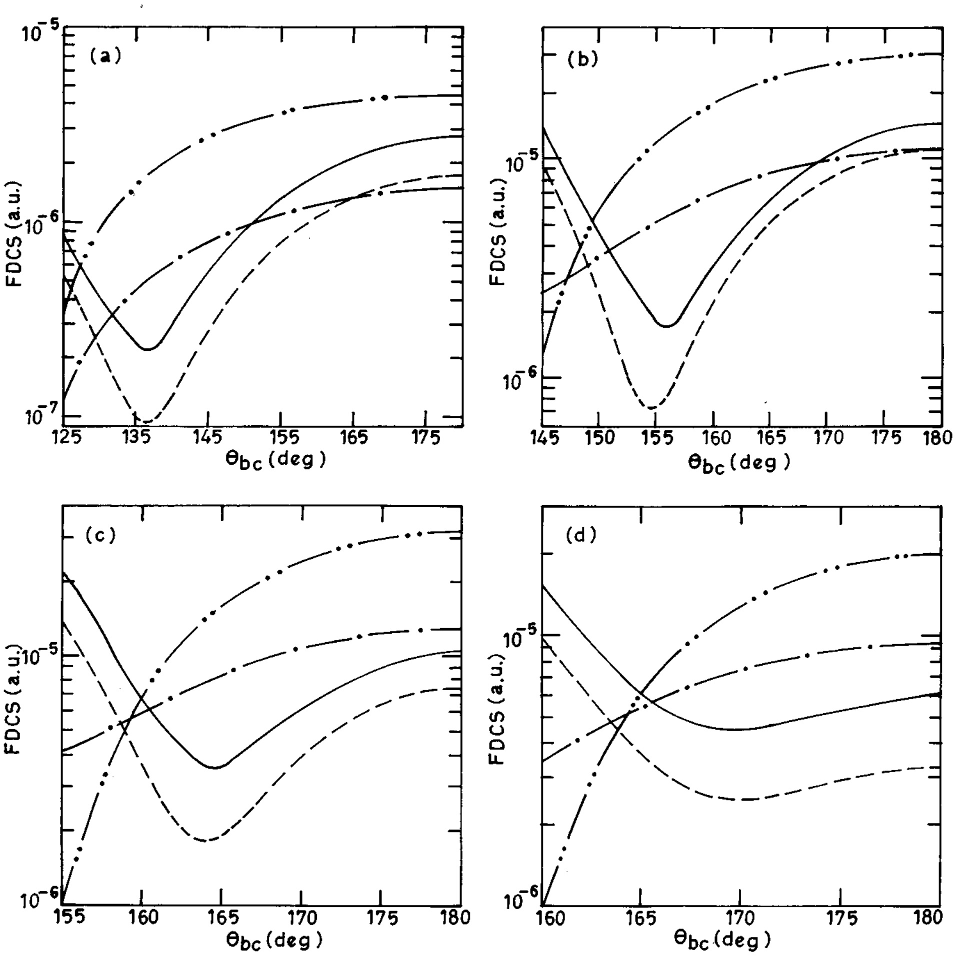

FIG. 2. Coplanar fivefold differential cross section (in a.u.) for double ionization of helium by electron impact at $E_0=5$ keV, $\theta_a=1°$ plotted against θ_{bc} in Bethe ridge kinematics. The angles θ_b and θ_c and the energies E_b and E_c for different values of θ_{bc} are given in Table II. θ_b and θ_c are measured with respect to the momentum transfer direction. Theoretical results: - ·· - ·· -, the BJ wave function; - · - · -, the OS wave function; ----, the SPM wave function; —, the TL wave function. E_b+E_c is equal to (a) 4 eV, (b) 10 eV, (c) 20 eV, and (d) 30 eV.

$$F_{fi}=-\frac{1}{2\pi}T_{fi}=-\frac{1}{2\pi}\langle\psi_f^{(-)}|V|\psi_i^{(+)}\rangle. \qquad (4)$$

The projectile-target interaction V is given by

$$V=-\frac{2}{r_0}+\frac{1}{r_{01}}+\frac{1}{r_{02}}, \qquad (5)$$

where $\vec{r}_0$, $\vec{r}_1$, and $\vec{r}_2$ are, respectively, the coordinates of the incident and the two target electrons with respect to the target nucleus and $r_{0i}=|\vec{r}_0-\vec{r}_i|$. The final-state wave function $\psi_f^{(-)}$ has been taken as a product of a plane wave for the fast scattered electron and two (symmetrized) Coulomb waves for the slow ejected electrons multiplied by the Coulomb correlation factor C:

$$\psi_f^{(-)}=e^{i\vec{k}_a\cdot\vec{r}_0}\frac{C}{\sqrt{2}}[\phi_{k_b}(Z_b,\vec{r}_1)\phi_{k_c}(Z_c,\vec{r}_2)+\phi_{k_b}(Z_b,\vec{r}_2)\phi_{k_c}(Z_c,\vec{r}_1)], \qquad (6)$$

with

$$C=\exp(-\pi\eta/2)\Gamma(1-i\eta), \quad \eta=1/|\vec{k}_b-\vec{k}_c| \qquad (7)$$

$$\phi_k(Z,\vec{r})=\frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}}e^{\pi Z/2k}\Gamma(1+iZ/k)\times{}_1F_1(-iZ/k,1,-i(kr+\vec{k}\cdot\vec{r})), \qquad (8)$$

where $\Gamma(1+iZ/k)$ and ${}_1F_1(-iZ/k,1,-i(kr+\vec{k}\cdot\vec{r}))$ are, respectively, the usual gamma and confluent hypergeometric functions. The effective charges Z_b and Z_c are given by [28,29]

$$Z_b=2-k_b(k_b^2-\vec{k}_b\cdot\vec{k}_c)/|\vec{k}_b-\vec{k}_c|^3, \qquad (9)$$

$$Z_c=2-k_c(k_c^2-\vec{k}_b\cdot\vec{k}_c)/|\vec{k}_b-\vec{k}_c|^3. \qquad (10)$$

This approximation to the BBK wave function for the final state has been used earlier [17,18,30,31] and is quite convenient even with complicated initial-state wave functions. It is found that the angular distribution obtained by this choice and the exact BBK wave function are essentially identical [17,18]. The results differ only in the magnitude. In the present study we are primarily interested in the relative magnitude and angular distribution for $\theta_{bc}\geqslant 120°$ and therefore the model used here for the final-state wave function is good enough.

The initial-state wave function $\psi_i^{(+)}$ is given by

$$\psi_i^{(+)}=e^{i\vec{k}_0\cdot\vec{r}_0}\phi_0(\vec{r}_1,\vec{r}_2), \qquad (11)$$

TABLE I. Angles θ_b and θ_c and energies E_b and E_c [obtained from Eqs. (1) and (2)] for different values of θ_{bc} at scattering angle $\theta_a=0.5°$ and $E_b+E_c=4$ and 10 eV.

θ_{bc}	E_b (eV)	θ_b (deg)	E_c (eV)	θ_c (deg)
		$E_b+E_c=4$ eV		
145	2.065	69.549	1.935	75.45
150	2.652	42.979	1.348	107.021
155	2.858	32.034	1.142	122.966
160	2.981	23.911	1.018	136.089
165	3.061	17.127	0.939	147.873
170	3.111	11.082	0.888	158.918
175	3.139	5.448	0.861	169.552
180	3.148	0.000	0.852	180.000
		$E_b+E_c=10$ eV		
160	5.960	51.217	4.040	108.783
165	6.487	33.371	3.513	131.629
170	6.754	20.778	3.246	149.222
175	6.891	10.036	3.109	164.964
180	6.933	0.000	3.067	180.000

where for the helium ground-state wave function $\phi_0(\vec{r}_1,\vec{r}_2)$ we have taken the following four forms: (a) the closed-shell-type Hartree-Fock wave function (BJ) of Byron and Joachain [32]; (b) the open-shell (OS) -type wave function of Silverman, Platas, and Matsen [33] that includes only radial correlations; (c) another wave function (SPM) of Silverman, Platas, and Matsen [33] that includes both radial and angular correlations; and (d) the configuration-interaction wave function (TL) of Tweed and Langlois [34] that includes $1s$, $2s$, $3s$, $2p$, $3p$, and $3d$ terms.

III. RESULTS

We have calculated the FDCS at an incident energy of 5000 eV. Figures 1 and 2 show the results plotted against the separation angle θ_{bc} between the two ejected electrons, at scattering angles $\theta_a=0.5°$ and 1°, respectively, for various fixed values of the sum E_b+E_c in the coplanar kinematics indicated in (a) above. Tables I and II show the angles θ_b and θ_c made by the ejection directions of electrons b and c with the direction of momentum transfer $\vec{q}$ and their energies E_b and E_c [obtained from Eqs. (1) and (2)] for different values of θ_{bc}. For a given E_0, θ_a, and E_b+E_c, the minimum value of θ_{bc} is fixed by Eqs. (1) and (2). Note that in this kinematical setup, the momentum transfer to the residual ion is always zero. It is observed that a smaller value of θ_a leads to a larger FDCS, but restricts the permissible range of θ_{bc} for a given E_b+E_c. This is the reason why only two cases with $E_b+E_c=4$ and 10 eV have been considered at $\theta_a=0.5°$. It is found that in all the cases considered here the FDCS at $\theta_{bc}=180°$ obtained by using BJ wave function is largest, indicating thereby that the ejection of the second electron is relatively an easier process with BJ wave function. As the separation angle θ_{bc} decreases from 180°, the BJ and OS results decrease quite slowly over about two-thirds the range shown in the figures compared to the SPM and TL results. The later results show a similar angular distribution and indicate a preference for the emission of the second electron (the slower one) at $\theta_{bc}=180°$. This is a reflection of the e-e angular correlation present in SPM and TL wave functions of helium.

TABLE II. Same as Table I, but for $\theta_a=1°$ and $E_b+E_c=4$, 10, 20, and 30 eV.

θ_{bc}	E_b (eV)	θ_b (deg)	E_c (eV)	θ_c (deg)
		$E_b+E_c=4$ eV		
125	2.715	42.943	1.285	82.057
130	3.105	32.112	0.894	97.888
135	3.305	25.616	0.694	109.384
140	3.430	20.864	0.570	119.136
145	3.513	17.077	0.487	127.923
150	3.571	13.895	0.428	136.105
155	3.613	11.118	0.387	143.882
160	3.643	8.621	0.357	151.379
165	3.664	6.317	0.336	158.683
170	3.678	4.144	0.322	165.856
175	3.686	2.053	0.314	172.947
180	3.689	0.000	0.311	180.000
		$E_b+E_c=10$ eV		
145	5.782	58.494	4.218	86.506
150	6.783	40.468	3.217	109.532
155	7.253	30.460	2.747	124.540
160	7.543	22.830	2.457	137.170
165	7.731	16.388	2.269	148.612
170	7.851	10.617	2.149	159.383
175	7.917	5.223	2.083	169.777
180	7.938	0.000	2.062	180.000
		$E_b+E_c=20$ eV		
155	11.188	62.453	8.812	92.547
160	12.879	40.165	7.120	119.835
165	13.634	27.485	6.366	137.515
170	14.062	17.400	5.938	152.600
175	14.289	8.464	5.711	166.536
180	14.361	0.000	5.639	180.000
		$E_b+E_c=30$ eV		
160	17.176	57.528	12.823	102.472
165	19.067	36.121	10.933	128.879
170	19.945	22.289	10.055	147.711
175	20.386	10.728	9.613	164.272
180	20.523	0.000	9.477	180.000

Figures 3 and 4 correspond to the kinematics described in (b) above. The arrangements at $\theta_c=180°$ are identical to the corresponding ones in Figs. 1 and 2. The energetic of the two electrons is emitted along the direction $\vec{q}$ and their energies E_b and E_c are held fixed. The results are symmetric about $\vec{q}$. The kinematics is thus easier to handle experimentally. The recoil momentum to the residual ion is nonzero except at $\theta_c=180°$. However, its maximum value is equal to k_c if θ_c is restricted to the range 120°–180° in which the model used for the final-state wave function is known to work. At smaller values of θ_c, two-step processes, which are not con-

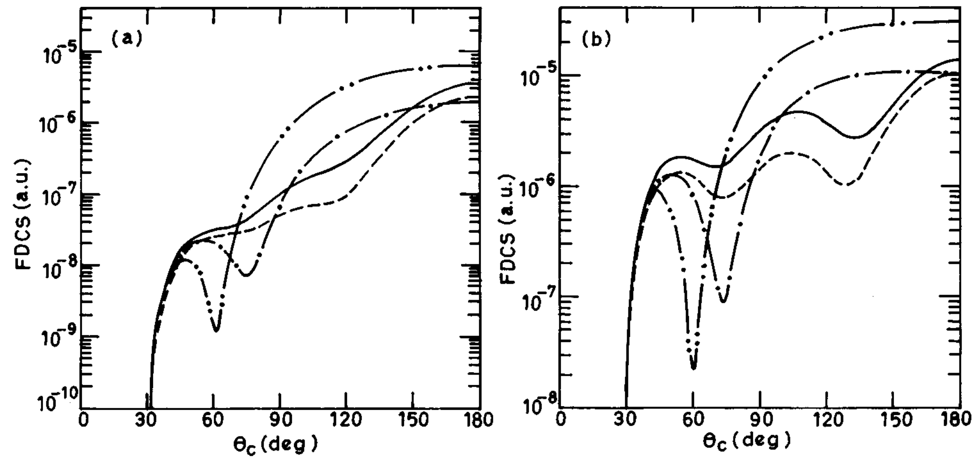

FIG. 3. Coplanar fivefold differential cross section (in a.u.) for double ionization of helium by electron impact at $E_0=5$ keV, $\theta_a=0.5°$, and $\theta_b=0°$ plotted against θ_c $(=\theta_{bc})$. θ_b and θ_c are measured with respect to the momentum transfer direction. Theoretical results: - ·· - ·· -, the BJ wave function; - · - · -, the OS wave function; -----, the SPM wave function; —, the TL wave function. (a) $E_b=3.15$ eV, $E_c=0.85$ eV and (b) $E_b=6.93$ eV, $E_c=3.07$ eV.

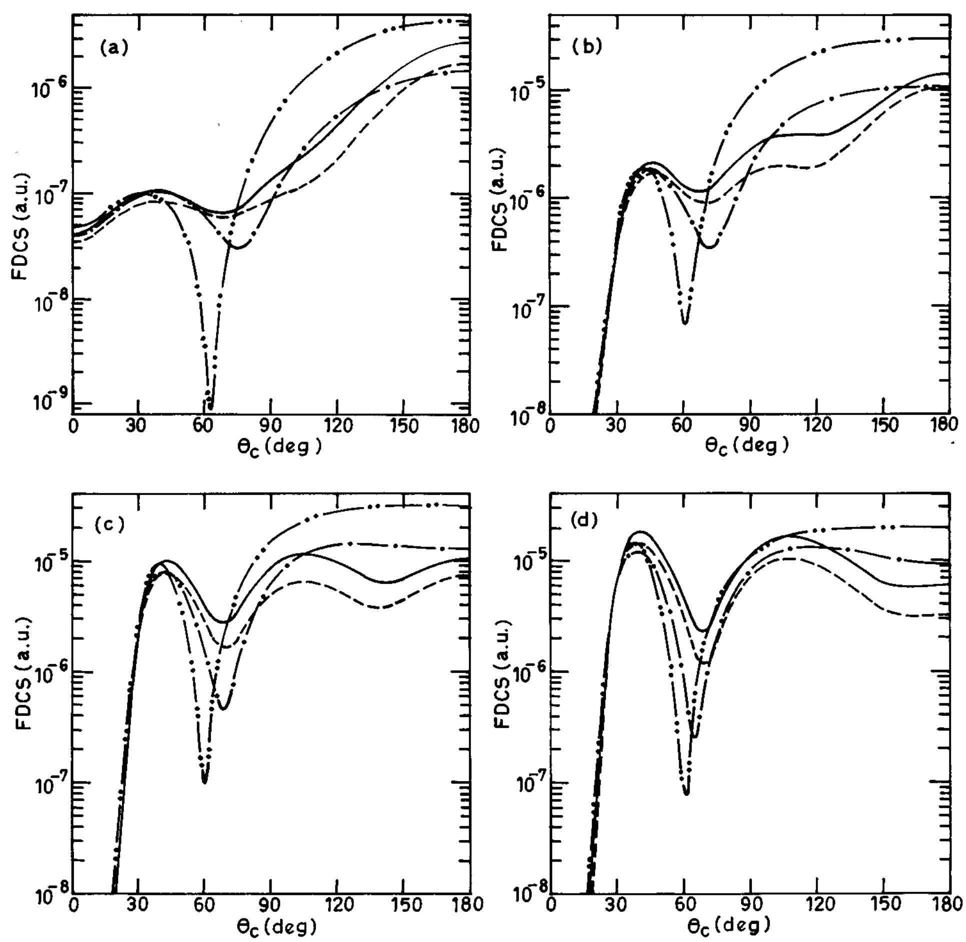

FIG. 4. Coplanar fivefold differential cross section (in a.u.) for double ionization of helium by electron impact at $E_0=5$ keV, $\theta_a=1°$, and $\theta_b=0°$ plotted against θ_c $(=\theta_{bc})$. θ_b and θ_c are measured with respect to the momentum transfer direction. Theoretical results: - ·· - ·· -, the BJ wave function; - · - · -, the OS wave function; ------, the SPM wave function; —, the TL wave function. (a) $E_b=3.69$ eV, $E_c=0.31$ eV; (b) $E_b=7.94$ eV, $E_c=2.06$ eV; (c) $E_b=14.36$ eV, $E_c=5.64$ eV; and (d) $E_b=20.52$ eV, $E_c=9.48$ eV.

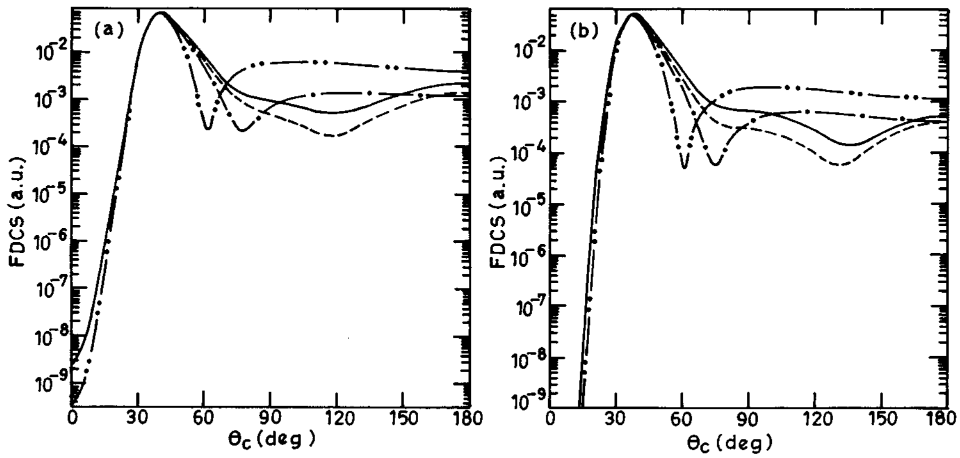

FIG. 5. Same as Fig. 3, but for the Coulomb correlation factor $C=1$.

sidered in the present study, also become relatively important. In the range $\theta_c=180°\pm60°$, the qualitative behavior of the FDCS in all the cases is essentially similar to that shown in Figs. 1 and 2. However, the near isotropic angular distribution of the BJ and OS results is more evident and highlights the usefulness of this kinematics in the study of target *e-e* correlations. If the Coulomb correlation factor C [Eq. (7)] is replaced by unity, the difference between various results becomes even more marked (Figs. 5 and 6).

An analysis of Figs. 3–6 shows that for θ_c in the range $180°\pm60°$, the BJ and OS results could be represented by $s_0^2|C|^2$ to a fair degree and SPM and TL results by $|\{s_0+s_1e^{it_1}P_1(\cos\theta_c)\}C|^2$. The real coefficients s_0, s_1, and t_1 depend on the helium ground-state wave function and are functions of k_b, k_c, q, and θ_c. This residual dependence on θ_c is, however, very weak. The need for s_1 and t_1 in the description of the angular distribution is a manifestation of the presence of the p orbitals in the SPM and TL wave functions. The strength of the d orbital in the TL wave function is, however, too weak to show up. The coefficient s_0 is larger in the case of the BJ wave function, indicating a lesser degree of *e-e* correlation in the ''closed shell''-type wave function.

In all the cases, FDCSs show some structure for smaller

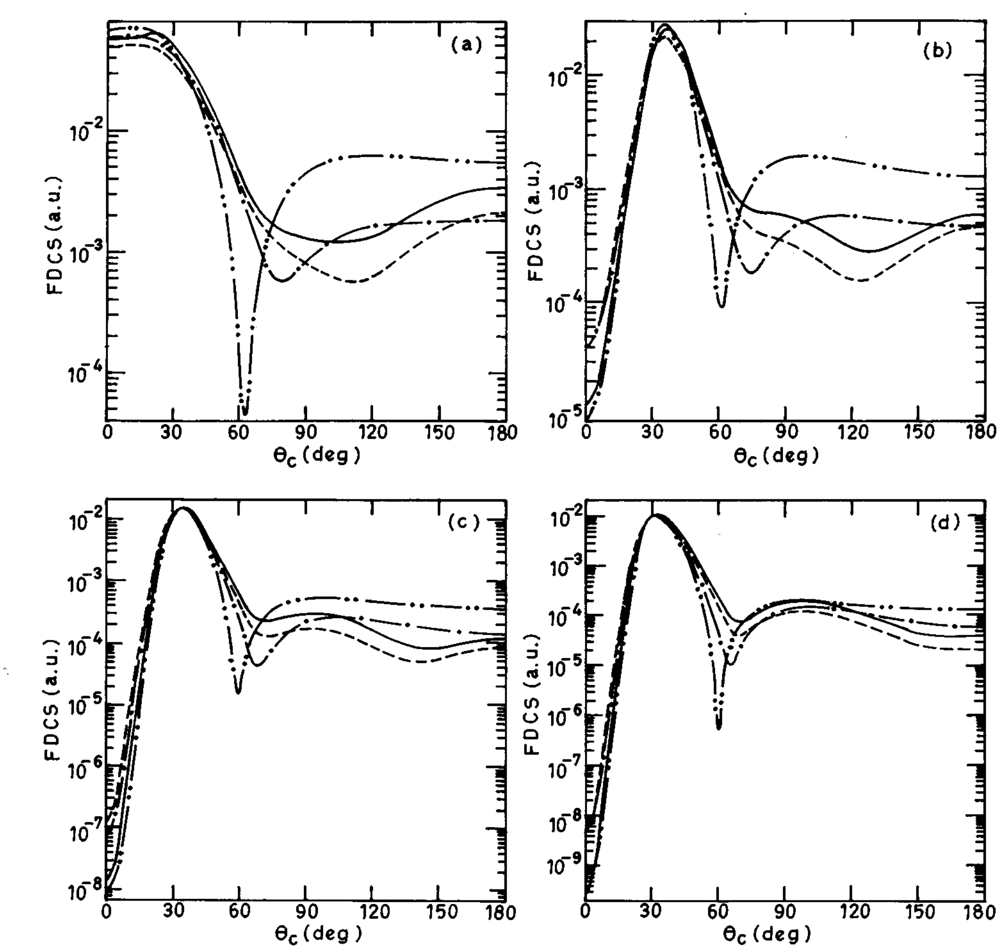

FIG. 6. Same as Fig. 4, but for the Coulomb correlation factor $C=1$.

θ_{bc} in Figs. 1 and 2 and smaller θ_c in Figs. 3–6. This structure quite strongly depends on the choice of the helium ground-state wave function. Yet it is not interpretable to provide meaningful information on target e-e correlations.

IV. SUMMARY

The differential cross section for the double ionization of helium by fast electrons has been calculated in the first-order Born approximation. The two ejected electrons have been described by a product of two Coulomb waves with suitable effective charges (satisfying the Rudge condition) and Gamow correlation factor. This choice of the final-state wave function is found to lead to a FDCS angular distribution similar to the one obtained by using the exact BBK wave function. A kinematical arrangement that makes the shake-off mechanism of double ionization more dominant has been chosen. Four choices for the ground-state wave function have been employed to study the manifestation of the target e-e correlations on the FDCS angular distribution. It is found that when one of the electrons is ejected with low energy along the momentum transfer direction, the angular distribution of the other slower electron in the angular range $180°\pm60°$ with respect to the first bears the signature of the e-e correlations in the ground state of helium. In the case of BJ and OS wave functions where the correlation is only radial, the FDCS is found to be almost proportional to the Gamow factor G $(=|C|^2)$, whereas in the case of SPM and TL wave functions, which contain p orbitals, it is found to vary as $|1+\lambda P_1(\cos\theta_c)|^2$ times G, where λ is a complex coefficient that is essentially constant for given energies of the two ejected electrons and given momentum transfer. The range of θ_c useful for the present analysis is, however, quite limited because the model used here ignores second-order mechanisms of ionization.

ACKNOWLEDGMENT

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