Double ionization of atoms by electron impact as a source of information on electron-electron correlations in targets

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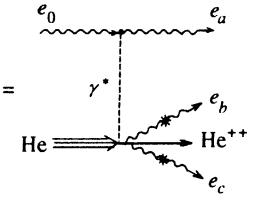
The quality of the information on the structure of the two-electron wave function of a target extracted from $(e,3e)$ experiments involving fast electrons in various kinematic situations has been surveyed. It has been shown that, as in the case of binary $(e,2e)$ experiments, the most direct information on the target structure can be obtained from reactions with a large momentum transfer. © *1995 American Institute of Physics.*

1. INTRODUCTION

The ionization of a target (an atom, a molecule, a thin film etc.) by an electron with the formation of several electrons, whose angular and energetic distributions are measured during the experiment, is a very complete quantum-mechanical experiment. It was shown more than 25 years ago in the work of Neudachin *et al.*[1,2] that the differential cross section for single ionization [a so-called $(e,2e)$ process] in cases in which the final scattered and ejected electrons comprise a symmetric pair, i.e., have similar energies and scattering angles relative to the incident electron beam, contains direct information on the structure of the one-electron wave function in the atom. Since the time of the first $(e,2e)$ experiments,[3,4] electron spectroscopy has become an independent field of scientific study, which is of practical significance in quantum chemistry and in the physics of plasmas, molecules, and thin films.

The design and performance of experiments on double ionization [so-called $(e,3e)$ processes] are considerably more complicated; therefore, the first measurements of the differential cross sections of $(e,3e)$ processes were performed only in 1989,[5] although theoretical arguments supporting the possibility of extracting information on electron correlations in a target from experimental data were advanced in the mid-seventies.[6,7]

The theory of $(e,3e)$ collisions involves the scattering of four charged quantum particles, i.e., a complicated quantum mechanical problem, especially with respect to carrying out specific calculations. The presence of fast electrons permits some simplification of the calculations and, in some cases, reduction of the problem to the three-particle case. This is possible, for example, when the incident and scattered electrons have similar energies, i.e., the energy transfer to the target is much smaller than the energy of the initial beam:

$T_{bc}^{FBA}(SO) =$ 

(D1)

The process described by diagram (D1) presupposes the exchange of only one virtual photon γ^* between the incoming electron and the target, and the diagram itself corresponds to a matrix element written in the first Born approximation (FBA). In principle, the momentum transfer $\mathbf{Q}=\mathbf{p}_0-\mathbf{p}_a$ take on any value allowed by the laws of the conservation of energy and momentum; however, $(e,3e)$ and $(\gamma,2e)$ (double ionization by a photon) processes have been described historically on a single theoretical basis. Therefore, it was assumed that the momentum transfer $\mathbf{Q}$ is relatively small not only in comparison with the momentum of the scattered electron $\mathbf{p}_a$, but also compared with the momenta of the ejected electrons $\mathbf{p}_b$ and $\mathbf{p}_c$. In this case the matrix elements of $(e,3e)$ and $(\gamma,2e)$ processes in the limit $Q\to 0$, which have a definite physical meaning, could be compared.

It was shown in Ref. 6 that if the kinematic conditions $E_0 \simeq E_a \gg E_b$ and $E_c \gg \Delta\varepsilon_0$, are satisfied, where $\Delta\varepsilon_0$ is the binding energy of the pair of the ejected electrons e_b and e_c in the target, the matrix element described by diagram (D1) contains direct information even about a two-particle wave function [by analogy to a $(e,2e)$ reaction]. However, it was theorized that e_b and e_c can be properly represented by orthogonalized plane waves (accordingly, this approximation is currently called the OPW approximation in the non-Russian literature), which at first glance seems logical when E_b and E_c are large.

The orthogonalized plane wave (OPW) approximation of the wave functions of the electrons e_b and e_c in the field of

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the A^{++} ion does not include their interactions in the final state. Back when $(e,2e)$ collisions were studied it was noted that consideration of the postinteraction state of the electrons even when their ejection energies are comparatively large (say, of the order of 200–300 eV for the ionization of hydrogen) results in an appreciable angular shift and distortion of the characteristic peaks in cross section.[8,9] In recent years, a model wave function of the final state, which is known by the abbreviation BBK from the first letters in the names of the authors[10] who first applied it to calculations of ionization processes, has been widely used to describe $(e,2e)$ processes.[1)] One special feature of this function is the "democratic" presence of all three interactions: both electron-ion interactions and the electron-electron interaction. This function was used in Ref. 12 in calculations of double ionization of the helium atom. The results were in complete disagreement with the angular distributions of the final electrons of the OPW model and even the more realistic distorted-wave model[13] when the same model was used for the wave function of the helium atom. In other words, the consideration of electron correlation in the function of the final state has a significant influence on the result of calculations of $(e,3e)$ processes, which is not observed (except for some small corrections) in calculations of $(e,2e)$ ionization.

The work in Refs. 12 and 13 had a purely theoretical character. In this paper we describe a qualitative physical investigation of this phenomenon and comparative evaluations of the cross sections in various regions of the characteristic peaks. It is shown, in particular, that the kinematics of the $(e,3e)$ reaction represented by diagram (D1) are not entirely successful from the point of view of the extraction of direct information on two-electron correlations in a target from an experiment in the case of small values of the momentum transfer Q. Unlike $(\gamma,2e)$ reactions, $(e,3e)$ reactions offer more suitable kinematics for this purpose with greater momentum transfer.

For simplicity, a helium atom is considered as the target below.

2. THEORY

2.1. General formulas

In the case of $\mathrm{He}(e,3e)\mathrm{He}^{++}$ collisions, the energy and momentum conservation laws have the following forms:

$$E_0+\varepsilon_0^{\mathrm{He}}=E_a+E_b+E_c, \tag{1}$$

$$\mathbf{p}_0=\mathbf{p}_a+\mathbf{p}_b+\mathbf{p}_c+\mathbf{q}. \tag{2}$$

Here $(E_0,\mathbf{p}_0)$, $(E_a,\mathbf{p}_a)$, $(E_b,\mathbf{p}_b)$, and $(E_c,\mathbf{p}_c)$ are, respectively, the energy and momentum of the incident electron, the scattered electron, and the first and second ejected electrons; $\varepsilon_0^{\mathrm{He}}=-79$ eV is the ground-state energy of the helium atom; $\mathbf{q}$ is the recoil impulse of the ion. The previously mentioned energy transfer $\Delta E=E_0-E_a$ and the momentum transfer $\mathbf{Q}=\mathbf{p}_0-\mathbf{p}_a$ are also considered.

Below we shall mainly consider the following kinematic conditions:

1) the incident and scattered electrons have large energies (for example, of the order of 5–10 keV), i.e., $E_0,E_a\gg\Delta E$;

2) the energy transfer to the helium atom is much greater than the binding energy of the electrons in the atom, i.e., $\Delta E\gg|\varepsilon_0^{\mathrm{He}}|$ (for example, on the order of 300–500 eV);

3) the ejected electrons have approximately equal ejection energies;

4) the momentum transfer is much smaller than the energy transfer, i.e., $Q^2\ll\Delta E$.

Such kinematics have not yet been realized experimentally: the requirement for large ejection energies is basically not satisfied; however, this model reveals the physics of the interaction mechanisms.

In atomic units the differential cross section has the form

$$d^5\sigma=\frac{p_a p_b p_c}{(2\pi)^6 p_0}\left|\frac{T_{bc}}{2\pi}\right|^2 dE_b dE_c d\Omega_a d\Omega_b d\Omega_c. \tag{3}$$

Such a form of the cross section is a consequence of the fact that the spin part of the wave function of the helium atom is antisymmetric and the coordinate part is accordingly symmetric. In the absence of spin-spin and spin-orbit coupling, the same symmetry requirements are imposed on the final wave function.

The amplitude T_{bc} in the first Born approximation, which is depicted in diagram (D1), has the following analytical expression

$$T_{bc}^{\mathrm{FBA}}=\frac{4\pi}{Q}M(\mathbf{p}_b,\mathbf{p}_c;\mathbf{Q}), \tag{4}$$

where

$$M(\mathbf{p}_b,\mathbf{p}_c;\mathbf{Q})=\frac{1}{\sqrt{2}Q}\int\int d\mathbf{r}_1 d\mathbf{r}_2[\phi^{-*}(\mathbf{p}_b,\mathbf{p}_c;\mathbf{r}_1,\mathbf{r}_2)+\phi^{-*}(\mathbf{p}_c,\mathbf{p}_b;\mathbf{r}_1,\mathbf{r}_2)][\exp(i\mathbf{Q}\mathbf{r}_1)+\exp(i\mathbf{Q}\mathbf{r}_2)-2]\phi_0(\mathbf{r}_1,\mathbf{r}_2). \tag{5}$$

The functions $|\phi^-(\mathbf{p}_b,\mathbf{p}_c)\rangle$ and $|\phi_0\rangle$ in (5) are eigenfunctions of the Schrödinger equation

$$\left[\frac{1}{2}\frac{\partial^2}{\partial\mathbf{r}_1^2}+\frac{1}{2}\frac{\partial^2}{\partial\mathbf{r}_2^2}+E+\frac{2}{r_1}+\frac{2}{r_2}-\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\right]\langle\mathbf{r}_1\mathbf{r}_2|\phi\rangle=0. \tag{6}$$

The ground-state function $|\phi_0\rangle$ and the function $|\phi^-(\mathbf{p}_b,\mathbf{p}_c)\rangle$ describe two electrons in the field of a point source with a charge $Z=2$ and have the energies $E=\varepsilon_0^{\mathrm{He}}$ and $E=E_b+E_c$. Owing to the property of orthogonality $\langle\phi^-(\mathbf{p}_b,\mathbf{p}_c)|\phi_0\rangle=0$, the presence of the double integral in (5) is not of fundamental significance; however, it is usually retained, since during the construction of some models this property may be violated and the finite character of the function M may accordingly be violated in the limit $Q\to0$ with the resultant appearance of false peaks in the cross section.

The integral (5) is nonzero specifically because Eq. (6) contains the electron-electron interaction $V_{12}=-|\mathbf{r}_1-\mathbf{r}_2|^{-1}$, which is responsible for the electron-electron correlations investigated here.

2.2. Qualitative physical model

If we consider the classical "billiard ball" model in the case of $E_b = E_c$ and a small value of Q, the angle of emission of a pair that was at rest before impact relative to the direction of the momentum transfer vector $\mathbf{Q}$ would be equal to $\theta_{Qp_b} = \theta_{Qp_c} \simeq \pi/2 - Q/2\sqrt{\Delta E}$. A similar result follows from (1) and (2), if the binding energy in (1) is neglected and the recoil impulse $\mathbf{q}$ in (2) is set equal to zero. There would then be no residual ion. Hence it follows that in the case of fast particles the region $q \sim 0$ gives the largest possible value for the double-ionization amplitude. The same conclusion is also valid for $(e,2e)$ processes, but $(e,3e)$ collisions are far more informative with respect to the kinematics of the momenta, as was noted in the early work of Neudachin *et al.*

In the general case the wave function of two interacting "free" electrons in the field of a residual He^{++} ion may be represented in the form

$$\phi^-(\mathbf{p}_b,\mathbf{p}_c;\mathbf{r}_1,\mathbf{r}_2) = D(\mathbf{p}_b,\mathbf{p}_c)[\varphi^-(\mathbf{p}_b,\mathbf{r}_1)\varphi^-(\mathbf{p}_c,\mathbf{r}_2) + I(\mathbf{p}_b,\mathbf{p}_c;\mathbf{r}_1,\mathbf{r}_2)]. \quad (7)$$

In Eq. (7) the coefficient $D(\mathbf{p}_b,\mathbf{p}_c)$ appears as a result of renormalization of the divergent terms of the perturbation theory series with respect to V_{12}, and its absolute value equals

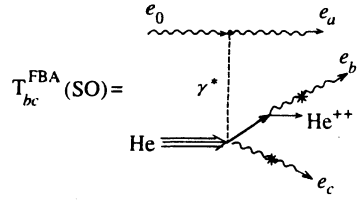
$$|D(\mathbf{p}_b,\mathbf{p}_c)|^2 = \frac{2\pi x}{e^{2\pi x}-1}, \quad x = |\mathbf{p}_b - \mathbf{p}_c|^{-1}. \quad (8)$$

The details were presented in Refs. 14 and 15. The functions $\varphi^-(\mathbf{p},\mathbf{r})$ are functions of the continuous spectrum of the one-particle Coulomb Hamiltonian with a charge $Z=2$ and satisfy the equation

$$\left(\frac{1}{2}\frac{\partial^2}{\partial \mathbf{r}^2} + \frac{p^2}{2} + \frac{2}{r}\right)\varphi^-(\mathbf{p},\mathbf{r}) = 0$$

(the superscript minus sign points out the characteristics of the converging wave at $r \to \infty$). Finally, the function I includes information on the rescattering of the ejected electrons in the final state.

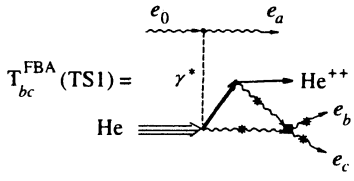
The first term in (7) actualizes the so-called "shake-off" (SO) mechanism, which was described earlier by Migdal for nuclear particles and was examined for atomic reactions in Refs. 16 and 17. In our case it may be described by the diagram



(D2)

As in diagram (D1), the asterisks on the wavy lines show that the electrons e_b and e_c are described by distorted waves.

The second term actualizes the two-step (TS1) mechanism, which has been described, for example, in Ref. 18. Its matrix element in a first approximation with respect to V_{12} is depicted in the diagram



(D3)

When E_b and E_c are large, the one-particle function $\varphi^-(\mathbf{p},\mathbf{r})$ may be represented in the eikonal approximation: $\varphi^-(\mathbf{p},\mathbf{r}) = \exp(i\mathbf{pr})\zeta(\mathbf{p},\mathbf{r})$, i.e., in the form of a rapidly oscillating function and a smooth function. Plugging the first term from (7) into integral (5), we see that the rapidly oscillating character of the integrand is maintained, since $\mathbf{p}_b$ and $\mathbf{p}_c$ are not compensated by $\mathbf{Q}$. The shake-off mechanism does not realize the classical condition $q=0$ in this case, and a small contribution of its matrix element to the total amplitude T_{bc}^{FBA} should be expected. A more detailed, although simple, investigation shows that the characteristic peak in the cross section $d^5\sigma$ from diagram (D2) is concentrated around the direction of $\mathbf{Q}$ and

$$d^5\sigma(\mathrm{SO}) \sim (\Delta E)^{-7}, \quad (9)$$

although just this term represents the double Fourier transform of the function of the initial state $\phi_0(\mathbf{r}_1,\mathbf{r}_2)$, i.e., it gives the most direct information on the wave function of the target.

The second term in (7) allows mixing of $\mathbf{p}_b$ and $\mathbf{p}_c$ during the interaction of the electrons with one another in such a manner that the condition $q \sim 0$ is realized. This is possible when $\mathbf{Q} \sim \mathbf{p}_b + \mathbf{p}_c$. The angle of the peak from the second term differs from the angle of the peak of the shake-off mechanism, and at large ejection energies they scarcely interfere. Evaluation of the contribution of the two-step mechanism gives

$$d^5\sigma(\mathrm{TS1}) \sim (\Delta E)^{-3}. \quad (10)$$

Details on the derivation of estimates (9) and (10) are given in Appendix 1.

To confirm the estimates obtained from the model of successive approximations, which is fairly crude for Coulomb potentials, as well as to visualize the situation, Fig. 1 presents the results of calculations of the differential cross section $d^5\sigma(3)$ for the following three models of the wave function of the final state, which are presently widely used:

a) the orthogonalized plane wave (OPW) approximation: $\phi^-(\mathbf{p}_b,\mathbf{p}_c;\mathbf{r}_1,\mathbf{r}_2) = [\exp(i\mathbf{p}_b\mathbf{r}_1) - \langle \mathbf{p}_b|\tilde{\varphi}_0\rangle\tilde{\varphi}_0(r_1)][\exp(i\mathbf{p}_c\mathbf{r}_2) - \langle \mathbf{p}_c|\tilde{\varphi}_0\rangle\tilde{\varphi}_0(r_2)]$,

b) the orthogonalized Coulomb wave (OCW) approximation: $\phi^-(\mathbf{p}_b,\mathbf{p}_c;\mathbf{r}_1,\mathbf{r}_2) = [\varphi^-(\mathbf{p}_b,\mathbf{r}_1) - \langle \varphi^-(\mathbf{p}_b)|\tilde{\varphi}_0\rangle\tilde{\varphi}_0(r_1)] \times [\varphi^-(\mathbf{p}_c,\mathbf{r}_2) - \langle \varphi^-(\mathbf{p}_c)|\tilde{\varphi}_0\rangle\tilde{\varphi}_0(r_2)]$,

c) the Brauner–Briggs–Klar (BBK) approximation: $\phi^-(\mathbf{p}_b,\mathbf{p}_c;\mathbf{r}_1,\mathbf{r}_2) = |D(\mathbf{p}_b,\mathbf{p}_c)|^2\varphi^-(\mathbf{p}_b,\mathbf{r}_1)\varphi^-(\mathbf{p}_c,\mathbf{r}_2)F[i/2p_{bc}; 1; -i(p_{bc}r_{12} + \mathbf{p}_{bc}\mathbf{r}_{12})]$.

Here $\mathbf{p}_{bc} = (\mathbf{p}_b - \mathbf{p}_c)/2$; $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$; F is a confluent hypergeometric function. In all three cases the target function ϕ_0 was chosen in the simplest approximation in the form of the product of two exponential functions [see (A8)]. The kine-

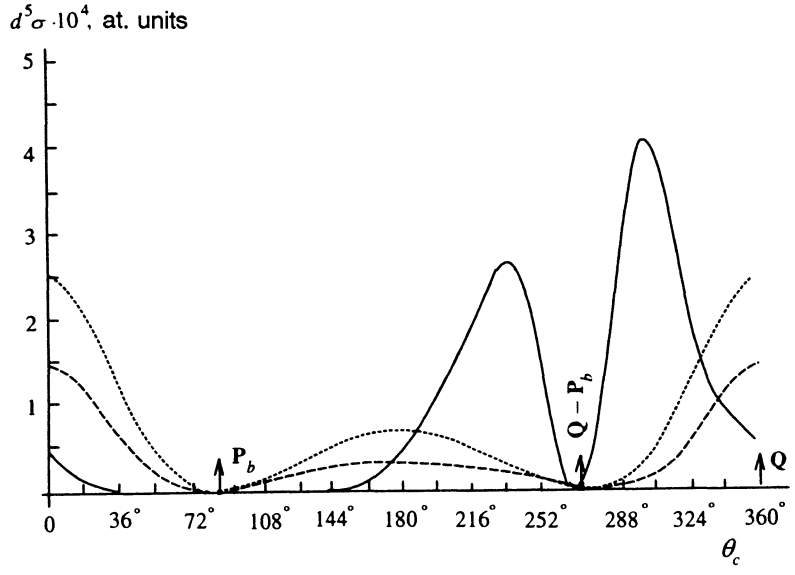


FIG. 1. Differential cross section ($d^5\sigma$) of the He(e,3e)He^{++} reaction as a function of θ_c for fixed values of θ_a and θ_b (E_0=5279 eV, E_a=5000 eV, θ_a=0°, θ_b=84.4°; E_b=E_c=100 eV). The angle θ_c is measured from the direction of $\mathbf{p}_0$, which coincides in the present kinematic situation with the direction of $\mathbf{p}_a$ and $\mathbf{Q}$. Notation used: solid trace—Brauner–Briggs–Klar (BBK) model; dashed trace—orthogonalized Coulomb wave (OCW) approximation (×1000); dotted trace—orthogonalized plane wave (OPW) approximation.

matic conditions are as follows: E_b=E_c; the vector $\mathbf{p}_b$ is fixed in space, and its angle with respect to the momentum transfer vector $\mathbf{Q}$ is specified by the relation

$$\cos\theta_{Qp_b}=\frac{Q}{2p_b},$$

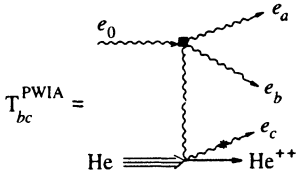
which allows the condition q=0 when $\mathbf{p}_c$ rotates in the plane of $\mathbf{Q}$ and $\mathbf{p}_b$. It is clearly seen from the figure that the addition of a correlator to the BBK model in the form of a hypergeometric function significantly alters the structure of the differential cross section, and the system of peaks is again concentrated around the direction of the recoil impulse, while the contribution of the OCW model in the scale chosen may be neglected.

Thus, the contributions of the shake-off and two-step mechanisms differ by four orders of magnitude in the amount of energy transferred. However, the size and shape of the peak of the two-step mechanism depend on both the model of the initial wave function $|\phi_0\rangle$ and the model of the final wave function $|\phi^-(\mathbf{p}_b,\mathbf{p}_c)\rangle$, i.e., "the two-model dependence" of this peak should be specified.

This implies that if any model of the target wave function gives a theoretical result agreeing with experiment, say, in the OPW or OCW approximation, the BBK function or another function including the postinteraction state of the electrons may utterly destroy this agreement, and the conclusion regarding the target structure would then be untrue. Therefore, in our opinion, the process described by diagram (D1) with a small momentum transfer is not entirely satisfactory from the point of view of obtaining direct information on the target structure, and other kinematic schemes are required.

2.3. Binary kinematics

A theory on a hierarchy of momenta, i.e., a phenomenon in which the energy transfer ΔE is redistributed in a highly asymmetric manner between e_b and e_c and permits the extraction of new information regarding correlations in the target, was formulated in the cited papers by Neudachin *et al.* However, this idea, as well as Berkadar's interesting arguments on this subject,[19] were discussed on the basis of kinematics with a small momentum transfer Q, i.e., on the basis of similarity between (e,3e) and (γ,2e) collisions. But, a (e,3e) process permits consideration particularly of the opposite case of large momentum transfers that are comparable to the momentum of the scattered electron p_a. An example of such a reaction in the plane-wave impulse approximation (PWIA) is depicted in the diagram



(D4)

The differential cross section in this case may be written in the following form, which differs somewhat from (3):

$$d^5\sigma(\mathrm{PWIA})=2\,\frac{p_a p_b p_c}{(2\pi)^6 p_0}\left|\frac{t_{ee}}{2\pi}\right|^2\rho(\mathbf{p}_c,\mathbf{p}_c+\mathbf{q}). \qquad (11)$$

The following notation was adopted in Eq. (11):

$$\left|\frac{t_{ee}}{2\pi}\right|^2=\frac{4}{Q^4}\,|D(\mathbf{p}_c,\mathbf{p}_b)|^2\left[1+y^4-y^2\cos\left(\frac{2}{|\mathbf{p}_a-\mathbf{p}_b|}\ln y\right)\right]$$

is the Mott cross section for ee scattering;

$$y=\frac{|\mathbf{p}_0-\mathbf{p}_a|}{|\mathbf{p}_0-\mathbf{p}_b|};$$

$$\rho(\mathbf{p}_c,\mathbf{p}_c+\mathbf{q})=\left|\int d\mathbf{r}\,\exp[i(\mathbf{p}_c+\mathbf{q})\mathbf{r}]\chi(\mathbf{p}_c,\mathbf{r})\right|^2$$

is the distribution density of the fluctuation function

$$\chi(\mathbf{p}_c,\mathbf{r})=\int d\mathbf{r}'\,\varphi^{-}{}^{*}(\mathbf{p}_c,\mathbf{r}')\phi_0(\mathbf{r},\mathbf{r}'), \tag{12}$$

whose properties were described in Ref. 20.

Some simple estimates obtained from (11) show that

$$d^5\sigma(\mathrm{PWIA})\sim(\Delta E)^{-3/2}. \tag{13}$$

According to the meaning of the approximation, the smaller the values of p_c and q, the better it should work. The maximum of the differential cross section (11) should be expected when the vector $\mathbf{p}_c$ is equal in magnitude to $\mathbf{q}$, but opposite in direction.

Diagram (D4) is equivalent to an $(e,2e)$ collision in so-called binary kinematics, which, as was stated in the introduction, is presently used in several applications as a tool for directly studying one-electron distributions. In our case a $(e,3e)$ process having binary kinematics with respect to e_a and e_b provides a similar possibility for studying the properties of the projection of the target ground state onto the continuum function $\varphi^{-}(\mathbf{p}_c,\mathbf{r})$ with the "soft" momentum $\mathbf{p}_c$.

Arguments advanced in Refs. 8 and 9 make it possible to search for corrections to Eq. (11) in the form of angular shifts of the cross section due to bending of the trajectories of e_a and e_b as a result of their interaction.

3. DISCUSSION AND CONCLUSIONS

Experiments with $\mathrm{A}(e,2e)\mathrm{A}^{+}$, $\mathrm{A}(e,2e)\mathrm{A}^{+}{}^{*}$, and $\mathrm{A}(e,3e)\mathrm{A}^{++}$ processes set up under binary kinematics, i.e., when the scattered and ejected electrons form a symmetric (or almost symmetric) fast pair with a large momentum transfer, yield the most direct information on the momentum distribution of one-particle fluctuations of the form

$$\chi_\alpha(\mathbf{r})=\int d\mathbf{r}'\,\varphi_\alpha^{-}(\mathbf{r}')\phi_0(\mathbf{r},\mathbf{r}'),$$

where φ_α^{-} is the spectral Coulomb function.

A combined study of the results of symmetric binary experiments with single and double ionization by a beam of fast electrons makes it possible to obtain new and, perhaps, unexpected information on the target structure.

A few words on the applicability of the conclusions drawn in this work to many-electron atoms are in order. For the He atom, Eq. (6) is exact in the context of dipolar kinematics. For heavier atoms, it should be assumed that the core is immobile during the collision and that the interaction of the impinging electron with the correlated atomic pair takes place on its background. It should also be roughly assumed that both the initial and final wave functions are products of the function of the pair and the function of the residual ion. This is a fairly strong assumption, especially in the case of small ejection energies, and is thus an additional argument against dipolar kinematics for $(e,3e)$ experiments. At the same time, binary kinematics, under which the ejection energies are large, permits consideration specifically of a (core +electron pair) system when, of course, the necessary symmetrization procedures are performed.

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APPENDIX

1. For the purpose of obtaining estimates (9) and (10), we utilize Eq. (7), in which we take into account the function $I(\mathbf{p}_c,\mathbf{p}_b;\mathbf{r}_1,\mathbf{r}_2)$ in the first order of the renormalized perturbation theory series with respect to V_{12}. In addition, we orthogonalize the function ϕ^{-} in (7) to ϕ_0, i.e., we consider the function

$$|\tilde{\phi}\rangle=|\phi^{-}\rangle-|\phi_0\rangle\langle\phi_0|\phi^{-}\rangle. \tag{A1}$$

Bearing in mind these two circumstances, we write the differential cross section (3) in the form

$$d^5\sigma=\frac{8|D(\mathbf{p}_c,\mathbf{p}_b)|^2}{(2\pi)^6}\frac{p_a p_b p_c}{p_0 Q^4}\,|A(\mathbf{p}_b,\mathbf{p}_c;\mathbf{Q}) +B(\mathbf{p}_b,\mathbf{p}_c;\mathbf{Q})+[\mathbf{p}_b\leftrightarrow\mathbf{p}_c]|^2. \tag{A2}$$

The following notation was adopted in Eq. (A2):

$$A(\mathbf{p}_b,\mathbf{p}_c;\mathbf{Q})=\int d\mathbf{r}\varphi^{-}{}^{*}(\mathbf{p}_b,\mathbf{r})[\exp^{i\mathbf{Qr}} -\gamma(\mathbf{Q})]\chi(\mathbf{p}_c,\mathbf{r}), \tag{A3}$$

$$B(\mathbf{p}_b,\mathbf{p}_c;\mathbf{Q})=\sum\!\!\!\!\!\!\int\sum\!\!\!\!\!\!\int ds_\alpha ds_\beta \times\frac{\langle\varphi^{-}(\mathbf{p}_b),\varphi^{-}(\mathbf{p}_c)|V_{12}|\varphi_\alpha^{-}\varphi_\beta^{-}\rangle}{\Delta E-\varepsilon_\alpha^{\mathrm{He}^+}-\varepsilon_\beta^{\mathrm{He}^+}+\varepsilon_0^{\mathrm{He}}+i0} \times[A_{\alpha,\beta}(\mathbf{Q})-A(\mathbf{p}_b,\mathbf{p}_c;\mathbf{Q})], \tag{A4}$$

$$A_{\alpha,\beta}(\mathbf{Q})=\int d\mathbf{r}\varphi_\alpha^{-}{}^{*}(\mathbf{r})[\exp^{i\mathbf{Qr}}-\gamma(\mathbf{Q})]\chi_\beta(\mathbf{r}), \tag{A5}$$

$$\gamma(\mathbf{Q})=\int d\mathbf{r}_1 d\mathbf{r}_2\phi_0^2(\mathbf{r}_1,\mathbf{r}_2)\exp^{i\mathbf{Qr}}, \tag{A6}$$

$$\chi_\alpha(\mathbf{r})=\int d\mathbf{r}'\,\varphi_\alpha^{-}{}^{*}(\mathbf{r}')\phi_0(\mathbf{r},\mathbf{r}'). \tag{A7}$$

Each of the functions φ_α^{-} in (A3)–(A7) is a spectral hydrogenic wave function of a one-particle Coulomb Hamiltonian with a field charge $Z=2$ (the minus sign refers only to the continuum functions). The summation $\sum\!\!\!\!\!\!\int ds_\alpha$ is carried out over the entire spectrum of one-particle excitations, including the continuum.

2. In section 2.2 we were primarily interested in the influence of the correlations in the final state on the form of the differential cross section; therefore, we take the function $\phi_0(\mathbf{r}_1,\mathbf{r}_2)$ in the very simple separable approximation:

$$\phi_0(\mathbf{r}_1,\mathbf{r}_2)\simeq\tilde{\varphi}_0(\mathbf{r}_1)\tilde{\varphi}_0(\mathbf{r}_2), \tag{A8}$$

where $\tilde{\varphi}_0(\mathbf{r}_2)=\sqrt{\kappa^3/\pi}\exp(-\kappa r)$ and $\kappa=1.68$. Also, taking into account that $p_b=p_c\gg Q$, we set $\varphi^{-}(\mathbf{p},\mathbf{r})\simeq\exp(i\mathbf{pr})$.

In this case $\gamma(Q)=(1+Q^2/4\kappa^2)^{-2}$ and

$$A(\mathbf{p}_b,\mathbf{p}_c;\mathbf{Q})\approx\frac{2^6\kappa^5\pi}{(p_c^2+\kappa^2)^2}\left\{\frac{1}{[(\mathbf{Q}-\mathbf{p}_b)^2+\kappa^2]^2}-\frac{\gamma(Q)}{(p_b^2+\kappa^2)^2}\right\}. \quad \text{(A9)}$$

The asymptotic estimate (9) follows from (A9) when $E_b=E_c\gg\varepsilon_0^{\mathrm{He}}$.

3. When (A8) is taken into account, the amplitude for the shake-off mechanism $A_{\alpha,\beta}(\mathbf{Q})$ takes on the form

$$A_{\alpha,\beta}(\mathbf{Q})=\int d\mathbf{r}\varphi_\alpha^{-}{}^*(\mathbf{r})[e^{i\mathbf{Q}\mathbf{r}}-\gamma(Q)]\tilde{\varphi}_0(r)\int d\mathbf{r}'\varphi_\beta^{-}{}^*(\mathbf{r}')\tilde{\varphi}_0(r'). \quad \text{(A10)}$$

It is not difficult to show that the integral with respect to $\mathbf{r}'$ in (A10) is proportional to $(2-\kappa)^{n_\beta-1}$, where n_β is the principal quantum number of the excited state, i.e., it should be expected that the main contribution to sum (A4) over β is made by the ground state with $\beta=0$. In this approximation the function B is written in terms of the one-electron Coulomb Green's function $g^{\mathrm{C}}(\mathbf{r},\mathbf{r}';E+i0)$ as

$$B(\mathbf{p}_b,\mathbf{p}_c;\mathbf{Q})\simeq\int d\mathbf{r}_1d\mathbf{r}_2\varphi^{-}{}^*(\mathbf{p}_b,\mathbf{r}_1)\varphi^{-}{}^*(\mathbf{p}_c,\mathbf{r}_2)\times|\mathbf{r}_1-\mathbf{r}_2|^{-1}\varphi_0(r_2)\int d\mathbf{r}'g^c(\mathbf{r}_1,\mathbf{r}';\times\Delta E-P_1+i0)[e^{i\mathbf{Q}\mathbf{r}'}-\gamma(\mathbf{Q})]\chi_0(\mathbf{r}'), \quad \text{(A11)}$$

where $P_1=-\varepsilon_0^{\mathrm{He}}+\varepsilon_0^{\mathrm{He}^+}=24.6$ eV is the ionization potential.

It was shown in Ref. 21 that for large values of E the Green's function $g^{\mathrm{C}}(\mathbf{r},\mathbf{r}';E+i0)$ may be described formally by

$$g^{\mathrm{C}}(\mathbf{r},\mathbf{r}';E)\approx\frac{C}{E+i0}\delta(\mathbf{r}-\mathbf{r}'),\qquad C=1+(i\nu-1)\exp(i\nu), \quad \text{(A12)}$$

where ν is a free parameter that is close to unity in the sense of an approximation. When (A12) is taken into account, expression (A11) takes the form

$$B(\mathbf{p}_b,\mathbf{p}_c;\mathbf{Q})\simeq\frac{C}{\Delta E}\int d\mathbf{r}_1d\mathbf{r}_2\varphi^{-}{}^*(\mathbf{p}_b,\mathbf{r}_1)\varphi^{-}{}^*(\mathbf{p}_c,\mathbf{r}_2)\times\frac{[\exp(i\mathbf{Q}\mathbf{r}_1)-\gamma(Q)]}{|\mathbf{r}_1-\mathbf{r}_2|}\chi_0(r_1)\varphi_0(\mathbf{r}_2), \quad \text{(A13)}$$

where $\chi_0(r_1)=\tilde{\varphi}_0(r_1)\int d\mathbf{r}'\varphi_0(r')\tilde{\varphi}_0(r')$.

With the asymptotic estimate (A13) we again take advantage of the plane-wave approximation and perform the replacement of variables $\mathbf{R}=(\mathbf{r}_1+\mathbf{r}_2)/2$, $\boldsymbol{\rho}=\mathbf{r}_1-\mathbf{r}_2$. Then

$$B(\mathbf{p}_b,\mathbf{p}_c;\mathbf{Q})\simeq\frac{C}{\Delta E}\int d\mathbf{R}\frac{d\boldsymbol{\rho}}{\rho}\exp\left[-\frac{i}{2}(\mathbf{p}_b-\mathbf{p}_c)\boldsymbol{\rho}\right]\times\{\exp(i\mathbf{q}\mathbf{R})-\gamma(Q)\times\exp[i(\mathbf{q}-\mathbf{Q})\mathbf{R}]\}\chi_0\left(\mathbf{R}+\frac{\boldsymbol{\rho}}{2}\right)\varphi_0\left(\mathbf{R}-\frac{\boldsymbol{\rho}}{2}\right). \quad \text{(A14)}$$

If Q is small and we consider the region $q\sim0$, the difference

$$\tfrac{1}{2}|\mathbf{p}_b-\mathbf{p}_c|=|\mathbf{p}_b+\tfrac{1}{2}(\mathbf{q}-\mathbf{Q})$$

is large. Therefore, since χ_0 and φ_0 are smooth functions, we can set $\rho=0$ in them, according to the rules for calculating rapidly oscillating integrals. From (A14) we ultimately obtain

$$B(\mathbf{p}_b,\mathbf{p}_c;\mathbf{Q})\simeq\frac{4\pi C}{\Delta Ep_b^2}\int d\mathbf{R}\times[1-\gamma(Q)e^{-i\mathbf{Q}\mathbf{R}}]e^{i\mathbf{q}\mathbf{R}}\chi_0(R)\varphi_0(R),$$

whence estimate (10) also follows in the vicinity of $q\sim0$.

[1)]This function was previously proposed in papers by Merkur'ev,[11] but was not used for specific calculations.

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