Application of the *J*-matrix method to problems of single ionization of atoms by fast electrons

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The *J*-matrix method, which is successfully used in atomic and nuclear physics to construct both many-particle wave functions of bound states and continuum states, is applied to the problem of the single ionization of the He atom by fast electrons, including the case when the residual ion is in the excited state. The theoretical calculations are compared with the available experimental data and also with the calculations of other authors. © *1996 American Institute of Physics.* [S1063-7761(96)00302-6]

1. INTRODUCTION

The process of single ionization of an atom by a fast electron that leaves the residual ion in an excited state has attracted the interest of experimentalists in recent years.[1,2] These processes, considered together with ordinary $(e,2e)$ collisions in which the residual ion remains in the ground state and double ionization [$(e,3e)$ collisions], make it possible to understand at a significantly deeper level the mechanisms and dynamics of electron interaction with complicated many-electron systems.

At the present time, most $(e,2e)$ experiments with excitation of the ions are made in the so-called dipolar coplanar geometry, in which the energies of the incident, E_0, and scattered, E_a, electrons are nearly the same and are of order a few kilo-electron-volts. Such kinematics is characterized by a small energy and momentum transfer to the atom. The typical differential cross section has the form of a two-hump curve symmetric with respect to the momentum transfer vector $\mathbf{Q}=\mathbf{p}_0-\mathbf{p}_a$. The peak around the positive direction of the vector $\mathbf{Q}$ is called the binary peak and arises largely from a direct collision of the incident and atomic electrons. The backward peak is the result of complicated interaction of the ejected electron with the residual ion. It is noteworthy that the backward peak in the case of $(e,2e)$ reactions with excitation is much stronger relative to the direct peak than in reactions that leave the ion in the ground state. This can be understood qualitatively, since in these reactions the greatest probability corresponds to the process in which an electron is excited in the ion as a result of slow secondary collisions of the ionized electron with the atomic electron. However, the quantitative description encounters appreciable computational difficulties associated with the need to include the contributions of a large number of virtual reaction channels.

If we consider helium, the simplest target, then the differential cross section of single ionization with excitation, or the triple differential cross section (TDCS), in the dipolar kinematics can be written in the form (in this paper, we use atomic units)

$$\frac{d^3\sigma_n}{d\Omega_a d\Omega_b dE_b}=\frac{8p_a p_b}{(2\pi)^3 p_0 Q^4}\times\sum_{lm}|A^{(1)}_{nlm}(\mathbf{p}_b,\mathbf{Q})+A^{(2)}_{nlm}(\mathbf{p}_b,\mathbf{Q})|^2, \tag{1}$$

where

$$A^{(i)}_{nlm}(\mathbf{p}_b,\mathbf{Q})=\int \phi^{-}_{nlm}{}^{*}(\mathbf{p}_b;\mathbf{r}_1,\mathbf{r}_2)\hat{T}_i\phi_0(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2. \tag{2}$$

Let $(E_0,\mathbf{p}_0)$, $(E_a,\mathbf{p}_a)$, and $(E_b,\mathbf{p}_b)$ be, respectively, the energies and momenta of the incident, scattered, and ejected electrons; the quantum numbers (nlm) describe the excited state of the ion—in the given case, a hydrogenlike atom with charge $Z=2$ of the nucleus. In writing down the expressions (1) and (2), we assumed that the fast electrons e_0 and e_a are described by plane waves and that the first Born approximation holds. This is more or less true in the case of ionization from the outer shell of the atom.

The transition operator $\hat{T}_i$ can be written both in the length representation (L representation),

$$\hat{T}_i=\exp(i\mathbf{Q}\cdot\mathbf{r}_i)-1.$$

and in the velocity representation (V representation):

$$\hat{T}_i=-\frac{i}{2\Delta E}[\exp(i\mathbf{Q}\cdot\mathbf{r}_i)(\nabla_i\cdot\mathbf{Q})+(\nabla_i\cdot\mathbf{Q})\exp(i\mathbf{Q}\cdot\mathbf{r}_i)],$$

where ΔE is the energy transfer to the atom. It is easy to show that the amplitudes (2) are the same in both representations if $\phi^{-}_{nlm}(\mathbf{p}_b;\mathbf{r}_1,\mathbf{r}_2)$ and $\varphi_0(\mathbf{r}_1,\mathbf{r}_2)$ are exact solutions of the many-particle Schrödinger equation

$$\left[\frac{1}{2}\Delta_1+\frac{1}{2}\Delta_2+E+\frac{2}{r_1}+\frac{2}{r_2}-\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\right]\phi=0 \tag{3}$$

and describe, respectively, a bound two-electron system (in the given case, the helium atom) and the two-electron system with one electron in the continuum. The function $\phi^{-}_{nlm}(\mathbf{p}_b;\mathbf{r}_1,\mathbf{r}_2)$ has the asymptotic behavior

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$$\phi^-_{nlm}(\mathbf{p}_b;\mathbf{r}_1,\mathbf{r}_2)|_{r_1\to\infty}$$

$$\approx\varphi_{nlm}(\mathbf{r}_2)\exp\left[i\mathbf{p}_b\mathbf{r}_1+\frac{i}{p_b}\ln(p_br_1+\mathbf{p}_b\mathbf{r}_1)\right]. \quad (4)$$

The use of the approximate expressions ϕ_0 and ϕ^-_{nlm} [in view of the impossibility of exact analytic solution of Eq. (3)] leads to a difference between the results obtained in the L and V representations. The extent of the difference can indicate the quality of the calculation of the wave functions.

Note that in the expression (2) the function ϕ_0 is symmetric with respect to interchange of the coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$, while the function ϕ^-_{nlm} is not symmetric on account of the choice of the asymmetric asymptotic behavior (4). Then the amplitude $A^{(1)}_{nlm}$ describes the mechanism of ionization by direct impact, while the amplitude $A^{(2)}_{nlm}$ corresponds to the so-called shake-off mechanism, when the incident electron "shakes off" one of the atomic electrons to an excited orbital, and the second atomic electron is ejected from the atom as a result of the abrupt change of the intra-atomic field.

Most theoretical calculations of the amplitudes $A^{(1)}_{nlm}$ and $A^{(2)}_{nlm}$ are based above all on some model representation of the ground-state function ϕ_0, namely, either in the form of a sum of Hartree–Fock orbitals or in the form of a certain variational sum of the type

$$\phi_0(\mathbf{r}_1,\mathbf{r}_2)=\sum_{ij}c_{ij}r_1^{\mu_i}r_2^{\nu_j}r_{12}^{\kappa_{ij}}\exp(-a_ir_1-b_jr_2-\lambda_{ij}r_{12}),$$

where $r_{12}=|\mathbf{r}_1-\mathbf{r}_2|$. In its turn, the representation of the final-state function ϕ^-_{nlm} varies from a simple product of two functions, which is obvious from (4), to more serious forms obtained by calculating by the coupled-channel method, by means of bispherical harmonics, etc. Without discussing the advantages and shortcomings of the existing theoretical calculations, we mention the recent paper of Kheifets *et al.* (Ref. 3), and also the earlier studies of Burkov *et al.*,[4] O'Mahoney and Mota-Furtado,[5] Dupre *et al.*,[2] Robaux *et al.*,[6] and Tweed.[7]

A feature common to most of the calculations is insufficient accuracy in the calculation of the wave function ϕ^-_{nlm}. This leads to a strong discrepancy between the curves of the differential cross sections in the L and V representations. In particular, it leads to a loss of orthogonality of the functions ϕ_0 and ϕ^-_{nlm}.

To calculate in this paper the differential cross sections of processes of single ionization with excitation, we use the well-known method of pseudostates in conjunction with the J-matrix method,[8–10] which has proved itself well in nuclear and atomic physics and makes it possible to use the fairly well studied diagonalization scheme to solve problems involving the continuous spectrum.

2. THEORY

In the J-matrix method, the wave functions of both the continuous spectrum and of the bound states are represented in the form of expansions with respect to basis functions. To facilitate the calculations, it is desirable to keep the set of basis functions as small as possible. In the given case, it is convenient to use basis functions symmetrized with respect to interchange of the coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$ and, therefore, determine immediately a symmetrized function (all calculations are made only for singlet states):

$$\psi^-_{nlm}(\mathbf{p}_b;\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{\sqrt{2}}[\phi^-_{nlm}(\mathbf{p}_b;\mathbf{r}_1,\mathbf{r}_2)$$

$$+\phi^-_{nlm}(\mathbf{p}_b;\mathbf{r}_2,\mathbf{r}_1)]. \quad (5)$$

The use of the symmetrized wave function (5) makes it possible to obtain an expression for calculation of the differential cross section in the form

$$\frac{d^3\sigma_n}{d\Omega_a d\Omega_b dE_b}=\frac{16p_ap_b}{(2\pi)^3p_0Q^4}$$

$$\times\sum_{lm}|\langle\psi^-_{nlm}|\exp(i\mathbf{Q}\mathbf{r}_1)-1|\phi_0\rangle|^2.$$

In the pseudostate method, it is assumed that one of the electrons can be in a pseudostate characterized by quantum numbers $(n'l'm')$. The number of pseudostates is finite. The second electron is in a state that can belong to either the discrete or the continuous spectrum. The total wave function of the two-electron system is sought approximately in the form

$$\psi^-_{nlm}(\mathbf{p}_b;\mathbf{r}_1,\mathbf{r}_2)=\mathscr{P}\sum_{n'l'm'}a^{n'l'm'}_{nlm}(\mathbf{r}_1)\frac{1}{r_2}\chi_{n'l'}(r_2)$$

$$\times Y_{l'm'}(\hat{\mathbf{r}}_2),$$

where $\mathscr{P}$ is the symmetrization operator, $\chi_{n'l'}(r_2)$ are the radial wave functions of the pseudostates, and $a^{n'l'm'}_{nlm}(\mathbf{r}_1)$ are coefficients that can nominally be regarded as wave functions of the second electron.

The wave functions of the pseudostates are found by expanding in square-integrable basis functions:

$$\chi_{nl}(\rho)=\sum_{n'=0}^{N_l}d^l_{n'n}\Phi_{n'l}(\xi_l\rho),$$

where the functions $\Phi_{nl}(x)$ form a Laguerre basis,

$$\Phi_{nl}(x)=\sqrt{\frac{n!}{(n+2l+l)!}}x^{l+1}\exp\left(-\frac{x}{2}\right)L_n^{2l+1}(x), \quad (6)$$

ξ_l is the basis parameter, and $L^\alpha_n(x)$ are the associated Laguerre polynomials.

The number N_l determines the accuracy of the calculation of the wave functions.[10] This parameter can be chosen independently for each partial wave.

For numerical calculation of the wave function $\psi^-_{nlm}(\mathbf{p}_b;\mathbf{r}_1,\mathbf{r}_2)$, it is convenient to separate the total orbital angular momentum L of the two electrons and its projection M and write the final-state wave function of the He^+ ion and the ejected electron in the form of an expansion

$$|\psi^-_{nlm}(\mathbf{p}_b)\rangle=\frac{1}{p_b}\sum_{\substack{\lambda\mu\\ \nu'\Gamma'LM}}\alpha^L_{\nu'\Gamma'\Gamma}(E)\langle lm\lambda\mu|LM\rangle$$

$$\times Y_{\lambda\mu}(\hat{\mathbf{p}}_b)|(n'l')(\nu'\lambda'):LM\rangle,$$

where (nlm) are the quantum numbers of the He^+ ion in the final state, $(\lambda\mu)$ are the quantum numbers of the ejected electron, $\Gamma' \equiv (n'l'\lambda')$ is the index of the reaction channel, $E = p_b^2/2 + \epsilon_{nl}$ is the total energy, $\varepsilon_{nl'}$ is the energy of the pseudostate, and the basis vectors $|(\nu\lambda)(nl):LM\rangle$ in the coordinate representation have the form

$$\langle \mathbf{r}_1, \mathbf{r}_2 | (nl)(\nu\lambda):LM\rangle = \begin{cases} \dfrac{1}{r_1 r_2} \mathscr{P}[\chi_{nl}(r_2)\chi_{\nu\lambda}(r_1)\mathscr{Y}_{l\lambda LM}(\hat{\mathbf{r}}_2, \hat{\mathbf{r}}_1)], & n \leq N_l, \\ \dfrac{1}{r_1 r_2} \mathscr{P}[\chi_{nl}(r_2)\Phi_{\nu\lambda}(\xi_\lambda r_1)\mathscr{Y}_{l\lambda LM}(\hat{\mathbf{r}}_2, \hat{\mathbf{r}}_1)], & n > N_l, \end{cases} \tag{7}$$

where

$$\mathscr{Y}_{l\lambda LM}(\hat{\mathbf{r}}_2, \hat{\mathbf{r}}_1) = \sum_{m\mu} \langle lm\lambda\mu | LM\rangle Y_{lm}(\hat{\mathbf{r}}_2) Y_{\lambda\mu}(\hat{\mathbf{r}}_1).$$

The expansion coefficients $a^L_{\nu'\Gamma'\Gamma}(E)$ are the solution of the infinite system of algebraic equations

$$\sum_{M\Gamma'} \sum_{\nu'=0}^{\infty} a^L_{\nu'\Gamma'\Gamma}(E) \langle (n'l')(\nu'\lambda'):LM | H - E | (n''l'') \times (\nu''\lambda''):LM\rangle = 0, \tag{8}$$

where H is the Hamiltonian corresponding to Eq. (3).

This system of equations is solved numerically by means of the J-matrix method.[8] The main approximation of the J-matrix formalism as applied to the given problem[9,10] consists of the neglect of the matrix elements of the residual interaction

$$V = \frac{1}{r_1} - \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

for $\nu' > N_{\lambda'}$, and (or) $\nu'' > N_{\lambda''}$. As a result, the system of equations (8) is decomposed into two parts—an interior ($\nu'' \leq N_{\lambda''}$) and an exterior ($\nu'' > N_{\lambda''}$). The infinite system of equations for $\nu'' > N_{\lambda''}$ can be solved exactly analytically, and its solution is given essentially by the exact Coulomb functions of the ejected electron in the chosen discrete representation multiplied by the wave functions of the pseudostates of the residual ion. For $\nu'' \leq N_{\lambda''}$, the system of equations (8) can be solved by the diagonalization method. The matching of the interior and exterior solutions makes it possible to determine the characteristics of the continuous spectrum of the two-electron atomic system.

The ground-state wave function of the He atom is found by expanding in the basis set (7):

$$|\phi_0\rangle = \sum_{\lambda l} \sum_{n=0}^{N_l} \sum_{\nu=0}^{N_\lambda} \alpha^{(0)}_{n\nu l\lambda} |(nl)(\nu\lambda):00\rangle.$$

Therefore, to determine $\phi_0(\mathbf{r}_1, \mathbf{r}_2)$ it is sufficient to diagonalize the matrix of the Hamiltonian H in the basis (7).

The obtained wave functions of the ground state and continuous spectrum make it possible to calculate the so-called double differential cross section (DDCS) for scattering of fast electrons by the He atom for the case when the He ion is left in the state (nl) and integration is performed over the angle of the ejected electron,

$$\frac{d^2\sigma_{nl}}{d\Omega_a dE_b} = \frac{16 p_a p_b}{(2\pi)^3 p_0 Q^4} \sum_{L\lambda} |J^\Gamma_L(Q)|^2,$$

and also the partial differential cross section of single ionization:

$$\frac{d^3\sigma_{nl}}{d\Omega_a d\Omega_b dE_b} = \frac{1}{4\pi} \frac{d^2\sigma_{nl}}{d\Omega_a dE_b} \times \left[1 + \sum_{\Lambda=1}^{\infty} \beta^\Lambda_{nl} P_\Lambda(\cos(\widehat{\mathbf{Q}\mathbf{p}_b})) \right], \tag{9}$$

where β^Λ_{nl} is the anisotropy coefficient:

$$\beta^\Lambda_{nl} = (-1)^l \frac{\sum_{L'\lambda'} \Pi_{L\lambda L'\lambda'} \langle \lambda 0 \lambda' 0 | \Lambda 0\rangle \langle L 0 L' 0 | \Lambda 0\rangle \{ {}^{l\lambda L}_{\Lambda L'\lambda'} \} J^{\Gamma'}_{L'}(Q)^* J^\Gamma_L(Q)}{\sum_{L\lambda} |J^\Gamma_L(Q)|^2},$$

$$J^\Gamma_L(Q) = \sum_{\nu'\Gamma'} \alpha^L_{\nu'\Gamma'\Gamma}(E) \langle (n'l')(\nu'\lambda'): \times LM \| 1 - i^L \sqrt{4\pi} j_L(Qr) Y_L(\hat{\mathbf{r}}) \| \psi_0\rangle.$$

$$\prod_{L\lambda L'\lambda'} = \sqrt{(2L+1)(2\lambda+1)(2L'+1)(2\lambda'+1)}.$$

Summed over the orbital angular momenta l, the cross section (9) has the form

$$\frac{d^3\sigma_n}{d\Omega_a d\Omega_b dE_b} = \frac{1}{4\pi} \frac{d^2\sigma_n}{d\Omega_a dE_b} \left[1 + \sum_{\Lambda=1}^{\infty} \beta^\Lambda_n P_\Lambda(\cos(\widehat{\mathbf{Q}\mathbf{p}_b})) \right], \tag{10}$$

where

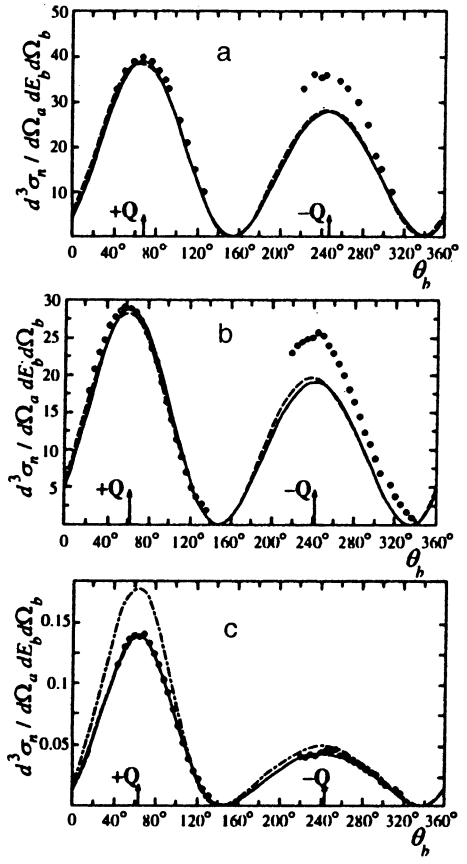

FIG. 1. Differential cross section $d^3\sigma_n/d\Omega_a d\Omega_b dE_b$ (in atomic units) for the He$(e,2e)$He$^+$ reaction $(n=1)$. The kinematic conditions are as follows: $E_a=5500$ eV; a) $E_b=5$ eV, $\theta_a=0.35°$; b) $E_b=10$ eV, $\theta_a=0.32°$; c) $E_b=75$ eV, $\theta_a=1°$. The experimental points are taken from Ref. 2. The solid curve represents our calculations, the dashed curve is the calculation by the coupled-channels method,[3] and the dot–dash curve is the calculation in the model of orthogonalized Coulomb waves.[2]

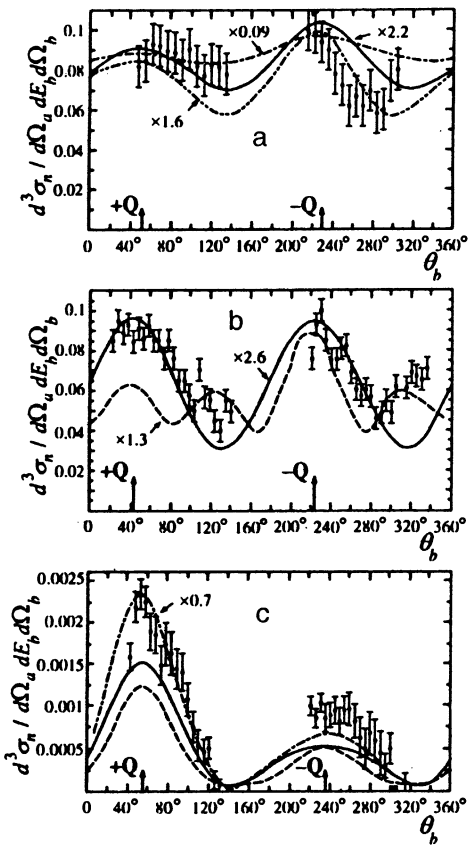

FIG. 2. Differential cross section $d^3\sigma_n/d\Omega_a d\Omega_b dE_b$ (in atomic units) for the He$(e,2e)$He$^+$ reaction $(n=2)$. The kinematic conditions are as follows: $E_a=5500$ eV; a) $E_b=5$ eV, $\theta_a=0.35°$; b) $E_b=10$ eV, $\theta_a=0.32°$; c) $E_b=75$ eV, $\theta_a=1°$. The experimental points are taken from Ref. 2. The solid curve gives the results of our calculations, the dashed curve the results obtained by the coupled-channel method,[3] the dot–dash curve the calculations in the model of orthogonalized Coulomb waves,[2] and the curve with two dots gives the result of calculation in R-matrix form of the strong-coupling method.[5] The multiplication coefficients for the theoretical curves are indicated in the figure.

$$\frac{d^2\sigma_n}{d\Omega_a dE_b}=\sum_l \frac{d^2\sigma_{nl}}{d\Omega_a dE_b},$$

$$\beta_n^\Lambda=\sum_l \beta_{nl}^\Lambda \frac{d^2\sigma_{nl}}{d\Omega_a dE_b} \Big/ \frac{d^2\sigma_n}{d\Omega_a dE_b}. \qquad (11)$$

3. CONCLUSIONS AND DISCUSSION

In Figs. 1–3, we give the results of calculations made in accordance with the scheme presented in the previous section. The experimental data are taken from the studies of the group of Lahmam-Bennani[2] (Figs. 1 and 2) and Stefani's group[1] (Fig. 3). In Table I, we give our calculated values of the double differential cross sections and the anisotropy parameters corresponding to Figs. 1–3.

In the calculations of the present paper, we have used basis functions with total orbital angular momenta $L=0, 1, 2, 3, 4$. The number of basis functions N_l taken into account in each partial wave l for each value of the total orbital angular momentum L and also the parameters ξ_l of the Laguerre basis are given in Table II. The diagonalization calculation of the ground state in the chosen basis (see Table II) gave a fairly accurate value of the ground-state energy: $E_0=-2.90362$ a.u (the more accurate theoretical calculation in the nonrelativistic model with infinitely heavy nucleus that we employed is $E_0=-2.90372$ a.u; the experimental value is $E_0=-2.90370$ a.u, see Ref. 11).

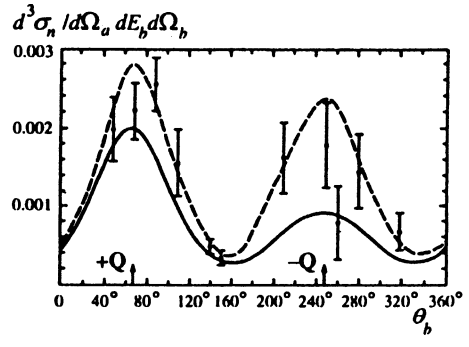

FIG. 3. Differential cross section $d^3\sigma_n/d\Omega_a d\Omega_b dE_b$ (in atomic units for the He$(e,2e)$He$^+$ reaction $(n=2)$. The kinematic conditions are as follows: $E_a=1200$ eV, $E_b=20$ eV, $\theta_a=4°$. The experimental points are taken from Ref. 1. The solid continuous curve gives our calculations, and the dashed curve gives the results of one of the potential models.[6,7]

TABLE I. Differential cross sections $d^3\sigma_n/d\Omega_a d\Omega_b dE_b$ and anisotropy parameters (for $\Lambda \leqslant 4$).

Kinematic conditions	n, l	Cross section	Anisotropy parameters			
			$\Lambda = 1$	$\Lambda = 2$	$\Lambda = 3$	$\Lambda = 4$
$E_a = 5500$ eV	$1s$	139.6	0.2161	1.981	0.2899	$2.538 \cdot 10^{-2}$
$E_b = 5$ eV	$2s$	0.2236	−0.1859	1.996	−0.1513	$4.434 \cdot 10^{-3}$
$\theta_a = 0.35°$	$2p$	0.2234	$-8.73 \cdot 10^{-2}$	−0.9969	$8.751 \cdot 10^{-2}$	$-3.082 \cdot 10^{-3}$
	$2s + 2p$	0.4470	−0.1366	0.5001	$-3.194\ 10^{-2}$	$6.778 \cdot 10^{-4}$
$E_a = 5500$ eV	$1s$	98.98	0.2736	1.999	0.3268	$3.403 \cdot 10^{-2}$
$E_b = 10$ eV	$2s$	0.1532	−0.0290	1.962	$5.909 \cdot 10^{-2}$	$9.070 \cdot 10^{-3}$
$\theta_a = 0.32°$	$2p$	0.1011	$-9.409 \cdot 10^{-2}$	−0.9370	$8.309 \cdot 10^{-2}$	$-5.359 \cdot 10^{-3}$
	$2s + 2p$	0.2543	$-5.488 \cdot 10^{-2}$	0.8092	$6.864 \cdot 10^{-2}$	$3.331 \cdot 10^{-3}$
$E_a = 5500$ eV	$1s$	0.3442	0.8105	2.094	0.8945	0.2232
$E_b = 75$ eV	$2s$	$4.134 \cdot 10^{-3}$	0.6701	1.978	0.8045	0.1459
$\theta_a = 1°$	$2p$	$4.493\ 10^{-4}$	0.1715	−0.9293	−0.1608	$-7.203 \cdot 10^{-3}$
	$2s + 2p$	$4.583 \cdot 10^{-3}$	0.6212	1.693	0.7099	0.1309
$E_a = 1500$ eV	$2s$	$6.201 \cdot 10^{-3}$	0.5884	1.655	0.4268	0.2530
$E_b = 20$ eV	$2p$	$1.419 \cdot 10^{-3}$	0.1646	−0.7955	−0.2074	−0.1411
$\theta_a = 4°$	$2s + 2p$	$7.620 \cdot 10^{-3}$	0.5095	1.199	0.3087	0.1796

The calculations were compared with other theoretical results, in particular with the model of orthogonalized Coulomb waves (OCW in foreign publications), the model based on a multichannel R matrix (FBMC: first Bohr multichannel), and the coupled-channel method proposed recently in studies of McCarthy's group (CC: close coupling).

We describe briefly the main characteristics of the models.

The model of orthogonalized Coulomb waves[12] is currently widely used for estimates and uses a "good" ground-state wave function of the helium atom, in particular the function from the handbook of Clementi and Roetti[13] for $n=1$ and the function of Tweed and Langlois[14] for $n=2$. The ejected electron in the final state is described by a Coulomb function with charge $Z=1$ for $n=1$ and an adjustable parameter $1 \leqslant Z \leqslant 2$ for $n=2$.

In the method of strong channel coupling, the initial and final states are described by means of the multichannel R matrix,[15] and this automatically leads to their orthogonality. The calculations differ in the number of channels taken into account and include either three or five pseudostates.

In the coupled-channel method,[3] a multiconfiguration Hartree–Fock wave function of the He atom is used, and the final wave function is calculated by the coupled-channel method in the momentum representation in the first approximation in accordance with perturbation theory. In this sense, the model of orthogonalized Coulomb waves is a zeroth approximation.

We note some general features characteristic of practically all types of calculations.

First, all calculations for $n=1$ give practically the same picture: The binary peak (around $+\mathbf{Q}$) is more powerful than the backward peak, and for low energies E_b the calculated values are approximately the same amount below the experimental values in the region of the backward peak, although with increasing energy E_b this difference is eliminated.

Second, in the case $n=2$ the binary-peak–backward-peak ratio is definitely less than for $n=1$. At the same time, most calculations give results that are low relative to the experiment, although the coefficient of "multiplication" decreases with increasing E_b. The only exception is the model of orthogonalized Coulomb waves, which in various modifications gives results that are much too large or gives strong fluctuations of the theoretical curves[16] in poor agreement with the experiment.

We now consider the physics of the processes that make it possible to explain qualitatively the observed effects. Figure 4 is an approximate scheme of the electron orbits in the He atom (the energy of the single-particle state is 24.6 eV) and in the He^+ ion (energies 54.4 eV for $n=1$ and 13.6 eV for $n=2$). The essence of the first Born approximation, which is used to obtain the expressions (1) and (2), is a single direct collision of a fast incident electron with one of the helium electrons.

Suppose that we even "switch off" the interaction between electrons 1 and 2 in the final state. Then the following

TABLE II. Number of basis functions taken into account and the parameters of the Laguerre basis (6) for different partial waves used in the calculation of the ground state and excited states of the He atom (for different total angular momenta L).

	s	p	d	f	g	h	i	j
Ground state	12	12	12	12	11	10	8	6
ξ	6.50	9.00	10.30	13.00	14.10	15.00	5.00	5.00
$L=0$	12	12	12	12	11	10	8	6
ξ	2.00	2.00	1.00	1.00	0.50	0.50	0.50	1.00
$L=1$	12	11	11	10	8	6	0	0
ξ	2.00	2.00	1.00	0.50	0.50	0.50	–	–
$L=2$	12	11	9	7	5	4	0	0
ξ	2.00	2.00	1.30	1.00	0.50	0.50	–	–
$L=3$	7	7	7	5	5	3	0	0
ξ	2.00	2.00	1.30	1.00	0.50	0.50	–	–
$L=4$	4	4	4	4	4	4	0	0
ξ	2.00	2.00	1.30	1.00	0.50	0.50	–	–

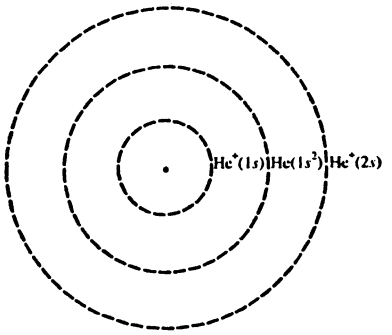

FIG. 4.

development of the events is the only one possible: The electron with respect to which the impact occurred leaves the atom, and the second electron "descends" to the inner orbit with the ground-state energy of the He^+ ion solely as a result of interaction with the nucleus. This process, described by the term $A^{(1)}_{nlm}$ (2), corresponds to ionization with transition of the residual ion to the ground state ($n=1$) and leads to a strong binary peak in the cross section. Here all the models of the final state, even the simplest, give similar results, since the process is almost classical.

In contrast, if the interaction of the helium electrons 1 and 2 in the final state is "switched on," the second electron goes over, with a very small probability and solely as a result of purely quantum tunneling effects, to the orbit further from the nucleus. This corresponds to excitation of the residual ion at the end of the reaction ($n=2$). Such a process is possible only if allowance is made for the potential V_{12} in the calculations of the final-state function when as a result of the secondary interaction of electrons 1 and 2 the bound electron goes over to the higher orbit. This immediately removes a model like the orthogonalized Coulomb wave model from among the "good" models. At the same time, there can also be another mechanism, in which the primary interaction of the incident electron and one of the helium electrons carries the latter into the excited state, while the second electron goes over at the same time into the continuum as a result of internal interactions. This mechanism corresponds to the term $A^{(2)}_{nlm}$ [the expression (2)]. The balance of $A^{(1)}_{nlm}$ and $A^{(2)}_{nlm}$ changes the binary-peak–backward-peak ratio in the case $n=2$. The observed lowering of the calculated values relative to the experiment in the region of the backward peak does not yet have a quantitative explanation and is apparently due to the behavior of the wave functions at intermediate distances from the nucleus.

Finally, the difference observed in the calculations of McCarthy's group between the cross sections obtained using the L and V formalisms (the latter gives somewhat better results) is due to the inadequate accuracy in the calculation of the wave functions and, in particular, reflects the nonorthogonality of the functions of the final and initial states. However, when the V formalism is used, the matrix elements tend to zero at $Q=0$, and this makes it possible to speak of a certain quasiorthogonality.[17]

Our calculations have been made in the L representation. We have established the convergence of the calculations with increasing number of values of the total orbital angular momentum, partial waves, and size of the basis (N_l) taken into account.

A certain discrepancy between the results of our calculations and the experimental data can, in our opinion, be explained by the inadequacy of the first Born approximation, since the analogous calculations of photoionization of the He atom[10] (for which the dipole approximation is entirely adequate) give excellent agreement with the experiment.

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[1] G. Stefani, L. Avaldi, and R. Camilloni, J. Phys. B **23**, L227 (1990).
[2] C. Dupre, A. Lahmam-Bennani, A. Duguet *et al.*, J. Phys. B **25**, 259 (1992).
[3] A. S. Kheifets, I. Bray, I. E. McCarthy, and Bo Shang, J. Phys. Rev. A **50**, 4700 (1994).
[4] S. M. Burkov, N. A. Letyaev, S. I. Strakhova, and T. M. Zajac, J. Phys. B **21**, 1195 (1988).
[5] P. F. O'Mahoney and F. Mota-Furtado, in *Proc. 3rd Eur. Conf. on* (*e*, 2*e*) *Collisions and Related Problems (Roma)*, edited by G. Stefani (1990), p. 1.
[6] O. Robaux, R. J. Tweed, and J. Langlois, J. Phys. B **24**, 4567 (1991).
[7] R. J. Tweed, Z. Phys. D **23**, 309 (1992).
[8] H. A. Yamani and L. Fishman, J. Math. Phys. **16**, 410 (1975).
[9] J. T. Broad and W. P. Reinhard, J. Phys. B **9**, 1491 (1976).
[10] Yu. F. Smirnov, L. Ya. Stotland, and A. M. Shirokov, Izv. Akad. Nauk SSSR, Ser. Fiz. **54**, 897 (1990).
[11] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Academic Press, New York, 1957) [Russ. transl., Fizmatgiz, Moscow, 1960].
[12] C. DalCapello, C. Tavard, A. Lahmam-Bennani, and M. C. DalCapello, J. Phys. B **17**, 4557 (1984).
[13] E. Clementi and C. Roetti, At. Data Tables **14**, 177 (1974).
[14] R. J. Tweed and J. Langlois, J. Phys. B **20**, L259 (1987).
[15] P. J. Burke and W. D. Robb, Adv. At. Mol. Phys. **11**, 143 (1975).
[16] J. Langlois, O. Robaux, and R. J. Tweed, in *Proc. 3rd Eur. Conf. on* (*e*, 2*e*) *Collisions and Related Problems (Roma)*, edited by G. Stefani (1990), p. 234.
[17] Yu. V. Popov and E. K. Shabalina, J. Phys. B **19**, L855 (1986).

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