Semiclassical description of correlation effects in binary ionization processes

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A description is given of a new model proposed for the description of binary reactions of the $(e, 2e)$ type. It is a logical extension of the impulse approximation, which retains its simplicity and at the same time is valid in a much wider range. The advantages of this model compared with the currently popular eikonal impulse approximation are discussed. The results of the calculations are compared with a large amount of data on the $(e, 2e)$ scattering on atoms of helium and other rare gases. The wave function of the Ne^{2p} state is found to deviate somewhat from the Hartree-Fock function.

1. INTRODUCTION

The present paper deals with some theoretical aspects of the $(e, 2e)$ reactions which is a topic in atomic physics that has been growing explosively in the last fifteen years. At present many research terms in Australia, West Germany, Italy, Canada, U.S.A., and France are engaged in precision measurements of the various characteristics of the target itself and of the many-body scattering processes manifested in coincidence experiments. Large amounts of experimental data have been accumulated. However, a theoretical description of the ionization processes still shows inadequacy of our ability to represent these complex many-body reactions by simple models in a wide range of angles and energies.

Two types of the $(e, 2e)$ reactions are distinguished in the cases when the energy E of an ion incident on a target is much greater than the binding energy of an electron is an atom (we speak here of the outer shells of the atoms). In the case of binary reactions the energies of the final electrons E_1 and E_2 are close to one another and approximately equal to half the energy of the incident particle. The scattering angles of the final electrons are within the range 30–60° relative to the line of incidence, i.e., they are within the quasielastic peak. These reactions are characterized by a large momentum transfer $Q = \mathbf{p}_0 - \mathbf{p}_1$ and are described reasonably well by the simple impulse approximation.

In the second type of reaction the energy of one of the electrons E_1 is close to E and the angle of scattering of this electron lies within the range 0–10°. Such reactions are characterized by a small transfer of a momentum to a target atom. Theories based on various modifications of the impulse approximation fail to describe satisfactorily the various features of these reactions, particularly the profile and position of a recoil peak.

A detailed description of the state of experiments and a theory of fast ionization processes can be found, for example in Refs. 1–3. It is worth noting also the great practical importance of the $(e, 2e)$ methods in quantum chemistry, plasma physics, and surface physics.

Our aim will be to extend the impulse approximation, which describes well binary reactions at high (of the order of 1–2 keV) energies of the incident electrons, to much lower energies by allowing for the interaction of electrons in the final state. We shall see later that such an allowance makes it possible to describe not only the behavior of the differential cross section curve in relative units, but also on the absolute scale.

2. THEORY

Various theoretical models used to describe the binary $(e, 2e)$ reactions are based on the theory of scattering of three particles. Reduction of the many-body reactions, such as the general case of the ionization

$$A+e\rightarrow A^{+}+e+e, \tag{1}$$

to the three-body case is possible only at sufficiently high energies of the emitted electrons. We may assume that during the time of quasieleastic knocking out, the residual ion whose field affects the electron being knocked out remains in the same state, i.e., $A = (A^{+} + e)$. In other words, we shall consider the equation (here, and later, we shall assume for convenience that $2m_e = 1$)

$$(E-H_{10}-H_{20}-V_1-V_2-V_{12})\,|\psi\rangle=0, \tag{2}$$

to which the many-body equation reduces under the above assumption. In the coordinate representation we have $H_{i0} = -\partial^2/\partial\mathbf{r}_i^2$, $V_i(r) = -e^2Z(r)/r$ is the Hartree-Fock potential, $V_{12} = e^2/|\mathbf{r}_1 - \mathbf{r}_2|$. The effective charge $Z(r)$ is calculated in the usual way:

$$Z(r)=N-r\sum_{\lambda}{}' n_\lambda \int d^3\mathbf{r}'\,\varphi_\lambda^2(\mathbf{r}')/|\mathbf{r}-\mathbf{r}'|. \tag{3}$$

Here, N is the total number of electrons in an atom; n_λ is the number of electrons in a shell λ; $\varphi_\lambda(\mathbf{r}')$ is the wave function of the shell. The sum with a prime in Eq. (3) means that one electron is lost from the shell λ', i.e., $Z(\infty) = 1$.

Since the mass of the residual ion is $m_A \gg m_e$, the laws of conservation of energy and momentum in a reaction of the (1) type can be written in the form

$$E=E_1+E_2+\varepsilon_0, \quad \mathbf{p}_0=\mathbf{p}_1+\mathbf{p}_2+\mathbf{q},$$

where ε_0 is the binding energy of an electron in the investi-

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gated shell and q is the momentum of the residual ion or the recoil momentum.

Equation (2) has to be supplemented by the boundary conditions. In the case of a breakup reaction and short-range potentials, it is of the form

$$\langle r_1 r_2|\psi\rangle \approx [(-2iE^{1/2})^{5/2}/32\pi^{5/2}]T_0(\mathbf{p}_0;\ \mathbf{p}_1\mathbf{p}_2)\exp(iE^{1/2}\rho)/\rho^{5/2} \quad (4)$$

in the limit $r_1, r_2 \to \infty$ for $\rho = (r_1^2 + r_2^2)^{1/2}$.

The majority of the theoretical models used to analyze the experimental data on the $(e, 2e)$ scattering are based on the hypothesis of the short-range nature of the potentials occurring in Eq. (2). In this case this equation can be solved by the Faddeev method, expanding the function $|\psi\rangle$ as a sum of the wave functions of the individual channels followed by reduction of Eq. (2) to a system of coupled differential equations. Solving this system by, for example, the method of successive approximations, we find that in the first order with respect to the ee interaction we can obtain a simple expression for the amplitude $T_0(\mathbf{p}_0;\ \mathbf{p}_1\mathbf{p}_2)$ of the ionization process:

$$T_0(\mathbf{p}_0;\ \mathbf{p}_1\mathbf{p}_2) = \langle \varphi_1(\mathbf{p}_1)\varphi_2(\mathbf{p}_2)|t_{12}|\varphi_{01}\varphi_2(\mathbf{p}_0)\rangle. \quad (5)$$

Allowing for the identity of electrons, the observed cross section can be calculated from the formula

$$\frac{d^3\sigma}{dE\,d\Omega_1\,d\Omega_2} = \frac{p_1 p_2}{p_0}\{|T_0(\mathbf{p}_0;\ \mathbf{p}_1\mathbf{p}_2) + T_0(\mathbf{p}_0;\ \mathbf{p}_2\mathbf{p}_1)|^2 + 3|T_0(\mathbf{p}_0;\ \mathbf{p}_1\mathbf{p}_2) - T_0(\mathbf{p}_0;\ \mathbf{p}_2\mathbf{p}_1)|^2\}. \quad (6)$$

The functions $|\varphi_i\rangle$ in Eq. (5) are the functions of discrete or continuous spectra in the potentials V_1 and V_2 of the residual ion.

Equation (5) can be regarded as the starting point of the majority of approximations used in the theory of ionization. The simplest impulse approximation (plane-wave impulse approximation—PWIA) is obtained from Eq. (5) by the substitution $|\varphi_i(\mathbf{p})\rangle \to |\mathbf{p}\rangle$, i.e., by substituting a plane wave. In this case, we have

$$T_0 \approx \varphi_{01}(\mathbf{q})t_{12}[\mathbf{p}_0 - (\mathbf{p}_1+\mathbf{p}_2)/2,\ (\mathbf{p}_2-\mathbf{p}_1)/2;\ 2(\mathbf{p}_2-\mathbf{p}_1)^2/4], \quad (7)$$

where $\varphi_{01}(\mathbf{q})$ is the Fourier transform of the function of a bound state; t_{12} is the so-called seminonenergy amplitude of the free ee scattering, dependent on three arguments: the relative momenta in the initial and final states, and the relative energy of an electron pair the explicit form of which is given, for example, in Ref. 4. Therefore, in the PWIA approximation the amplitude is factorized into a product of two factors, one of which describes the structure of the target atom and the other the process of scattering in the final state.

A model of the eikonal-wave impulse approximation—EWIA (Ref. 5)—has been proposed in order to retain simplicity of Eq. (5) and at the same time to allow for the influence of the residual ion in the hope of removing the discrepancies between the experimental data and their description in terms of the PWIA at lower energies E. In accordance with this approximation, $|\varphi_i(\mathbf{p})\rangle$ is described by a plane wave but the quantum numbers p are then calculated allowing for the distorting potential of the ion $\bar{\nabla} + i\bar{W}$, where $\bar{\nabla}$ and $\bar{W}$ are free parameters. A comparison of a large amount of experimental data with the EWIA theory can be found in Refs. 6 and 7.

Attempts have been made to calculate Eq. (2) using Coulomb wave functions[8] and other variants of more physical allowance for the influence of the residual ion within the framework of the distorted-wave impulse approximation (DWIA) have been proposed, but considerable mathematical difficulties are then encountered and the attractive nature of Eq. (7) is lost.

In spite of the considerable improvement in the description of some details of the experimental curves representing reactions with rare gases in terms of the EWIA model, some dissatisfaction has been expressed with the results for the range of angles $\theta \sim 30$–$40°$ and with the description of the absolute values of the cross sections (6), which had been measured quite recently.

Characteristic features of the observed cross sections are as follows. Firstly, the cross sections at angles 40–70° for energies $E \gtrsim 300$ eV agree on the whole quite well with the impulse approximation (7). Secondly, they seem to be shifted relative to the impulse approximation in the direction of higher angles and this shift increases on reduction in the energy. Thirdly, the absolute values of these cross sections are smaller than those predicted theoretically. All these features are used as the basis of the model described below.

Let us turn once again to Eq. (5). Its derivation presumes a rapid fall of the potentials V_1, V_2, and V_{12} at infinity, which does not correspond to reality. Lifting of this restriction results in divergence not only of the iteration series of perturbation theory but also of the integrals corresponding to the separate forms.[9,10] Moreover, the function (4) has an incorrect asymptote with respect to ρ (there are no logarithmic terms in the argument of the exponential function). This makes it necessary to look for a model closer to reality. In particular, we have to allow more accurately for the long-range of electrons in the final state. Such attempts have been made before.[11–13] For example,the long-range effects of the reaction products are allowed for in Ref. 12 by quasiclassical methods, resulting in a considerable reduction in the discrepancy between the theory and experiment in a wide range of angles and energies.

We shall consider the model called the plane-wave semiclassical approximation (PWSC) in greater detail. Mathematically this model is based on the work of Merkuriev.[14] Following this work we shall divide the six-dimensional space $\rho = (\mathbf{r}_1, \mathbf{r})$ so as to include the Coulomb "tails" of the potentials in the free Hamiltonian, for example,

$$H_0^c = -\frac{\partial^2}{\partial \mathbf{r}_1^2} - \frac{\partial^2}{\partial \mathbf{r}_2^2} + [V_1(r_1) + V_2(r_2) + V_{12}(\mathbf{r}_1-\mathbf{r}_2)]\theta(\rho-\rho_0). \quad (8)$$

Then, Eq. (2) becomes

$$[E - H_0^c - (V_1+V_2+V_{12})\theta(\rho_0-\rho)]\langle \mathbf{r}_1\mathbf{r}_2|\psi\rangle = 0. \quad (9)$$

For convenience, we shall introduce V^{out} for the potentials occurring in Eq. (8) and V^{in} for the potentials in Eq. (9). Therefore, V^{in} is a short-range potential.

We shall next expand the function $|\psi\rangle$ as a sum of two

components:

$$|\psi\rangle=|\psi_{12}\rangle+|\psi_{(1,2)}\rangle, \tag{10}$$

corresponding to the channels 12 and (1, 2). By definition, we have

$$(E-H_0^c)\,|\psi_{12}\rangle=V_{12}^{in}|\psi\rangle, \quad (E-H_0^c)\,|\psi_{(1,2)}\rangle=(V_1^{in}+V_2^{in})\,|\psi\rangle. \tag{11}$$

Such a division is indicated by an analogy with the case when one of the three particles participating in the scattering (in this case, the residual ion) has an infinitely large mass.[15]

Substituting Eq. (10) into Eq. (11), we obtain

$$\begin{aligned}(E-H_0^c-V_{12}^{in})\,|\psi_{12}\rangle&=V_{12}^{in}|\psi_{(1,2)}\rangle,\\ (E-H_0^c-V_1^{in}-V_2^{in})\,|\psi_{(1,2)}\rangle&=(V_1^{in}+V_2^{in})\,|\psi_{12}\rangle,\end{aligned} \tag{12}$$

which yields

$$|\psi_{(1,2)}\rangle=|\Phi_0(\mathbf{p}_0)\rangle+g_{(1,2)}^c(V_1^{in}+V_2^{in})\,|\psi_{12}\rangle,$$

$$|\psi_{12}\rangle=g_{12}^c V_{12}^{in}|\psi_{(1,2)}\rangle,$$

where $g_{(1,2)}(E)$ and $g_{12}^c(E)$ are Green functions of the type

$$g_{(1,2)}^c(E)=(E-H_0^c-V_1^{in}-V_2^{in}+i0)^{-1},$$

$$g_{12}^c(E)=(E-H_0^c-V_{12}^{in}+i0)^{-1}.$$

In turn, $|\Phi_0(\mathbf{p}_0)\rangle$ represents the solution of the equation

$$(E-H_{10}-H_{20}-V_1-V_2-V_{12}^{out})\,|\Phi_0(\mathbf{p}_0)\rangle=0 \tag{13}$$

which describes the initial state of an atom and an electron. If we ignore the "tail" in Eq. (13) described by V_{12}^{out}, then $|\Phi_0(\mathbf{p}_0)\rangle\to|\varphi_{01}\varphi_2(\mathbf{p}_0)\rangle$, i.e., this expression degenerates to a product of functions describing a bound electron and a free electron in the field of the residual ion. The equation (13) carries more information than the neglected term V_{12}^{out} and, in particular, this equation can be used to allow for the dipole interaction between the incident electron and an atom.

Using a familiar operator relationship $g_i V_i = g_0 t_i$ between the potential V and the scattering amplitude t, we obtain

$$\begin{aligned}|\psi_{(1,2)}\rangle&=|\Phi_0(\mathbf{p}_0)\rangle+g_0^c(E)\,\tau_{12}^{in}(E)\,|\psi_{12}\rangle,\\ |\psi_{12}\rangle&=g_0^c(E)\,t_{12}^{in}(E)\,|\psi_{(1,2)}\rangle.\end{aligned} \tag{14}$$

Here, $g_0^c(E)=(E-H_0^c+i0)^{-1}$ is a quasifree Green function, and the operators τ_{12}^{in} and t_{12}^{in} satisfy the formal equations

$$\begin{aligned}\tau_{12}^{in}&=(V_1^{in}+V_2^{in})+(V_1^{in}+V_2^{in})\,g_0^c\tau_{12}^{in},\\ t_{12}^{in}&=V_{12}^{in}+V_{12}^{in}g_0^c t_{12}^{in}.\end{aligned}$$

Iteration of the system of equations (14) gives the following expression for the function $|\psi\rangle$:

$$|\psi\rangle=|\Phi_0(\mathbf{p}_0)\rangle+g_0^c(E)\,[1+T^c(E)\,g_0^c(E)\,]\,t_{12}^{in}|\Phi_0(\mathbf{p}_0)\rangle, \tag{15}$$

where

$$T^c(E)=\tau_{12}^{in}+t_{12}^{in}g_0^c\tau_{12}^{in}+\tau_{12}^{in}g_0^c t_{12}^{in}g_0^c\tau_{12}^{in}+\ldots. \tag{16}$$

Retaining only the first terms in the sum (16), we can rewrite Eq. (15) in the coordinate representation:

$$\langle\mathbf{r}_1\mathbf{r}_2|\psi\rangle=\langle\mathbf{r}_1\mathbf{r}_2|\Phi_0(\mathbf{p}_0)\rangle+\langle\mathbf{r}_1\mathbf{r}_2|g_0^c(1+\tau_{12}^{in}g_0^c)\,t_{12}^{in}|\Phi_0(\mathbf{p}_0)\rangle. \tag{17}$$

Outside the region bounded by the radius ρ_0, i.e., if r_1, $r_2>r_0=\rho_0/\sqrt{2}$, we find from Eq. (17) that

$$(E-H_0^c)\,\langle\mathbf{r}_1\mathbf{r}_2|\psi\rangle=0 \tag{18}$$

subject to the boundary conditions

$$\langle\mathbf{r}_1\mathbf{r}_2|\psi\rangle_{\rho=\rho_0}=\langle\mathbf{r}_1\mathbf{r}_2|g_0^c(1+\tau_{12}^{in}g_0^c)\,t_{12}^{in}|\Phi_0(\mathbf{p}_0)\rangle, \tag{18'}$$

because the first term in Eq. (17) is exponentially small for $r_1, r_2, > r_0$ due to the bound state if r_0 is not less than the Bohr radius.

We should mention in passing that the expression $g_0^c+g_0^c\tau_{12}^{in}g_0^c$ in Eq. (18') can also be represented by a Green function:

$$g^c(E)\equiv g_{(1,2)}^c(E)=(E-H_{10}-H_{20}-V_1-V_2-V_{12}^{out}+i0)^{-1},$$

i.e., by means of an operator which is the reciprocal of that which occurs in Eq. (13).

In the case of symmetric or slightly asymmetric kinematics of the $(e, 2e)$ experiments for initial energies E of the order of several hundreds of electron volts and for higher orbitals we can usually expect the following inequalities:

$$e^2Z(r_0)/E_i r_0\ll 1, \quad e^2/E_{12}r_0\ll 1, \quad E_\alpha^{1/2}r_0\gg 1, \tag{19}$$

where E_i and E_{12} are the absolute and relative energies of the final electrons. Under these conditions we can expect that the approximation of the geometric optics for Eq. (18) is valid, i.e., if

$$\langle\mathbf{r}_1\mathbf{r}_2|\psi\rangle=[(-2iE^{1/2})^{3/2}/32\pi^{5/2}]\,A(\boldsymbol{\rho})\exp[i\chi(\boldsymbol{\rho})], \tag{20}$$

we obtain a system of first-order differential equations for the quantity A and the eikonal χ:

$$(\nabla_\rho\chi)^2=E-V_1^{out}-V_2^{out}-V_{12}^{out}, \tag{21}$$

$$\mathrm{div}_\rho(A^2\nabla_\rho\chi)=0. \tag{21'}$$

It follows from the theory of first-order differential equations that a solution of Eqs. (21) and (21') depends on a certain parameter t and it determines the $\boldsymbol{\rho}(t)$ curve in the six-dimensional space or the $\mathbf{r}_i(t)$ curves in the ordinary three-dimensional space. The parameter t can be the length of a path S_ρ or the "time." In the latter case the characteristic equations appear as ordinary equations of classical mechanics and govern, subject to suitable boundary conditions, the electron paths in the outer region. If $\mathbf{r}_i(0)=(r_0, \theta_{0i})$, then $\mathbf{r}_i(\infty)$ is the coordinate of the ith electron at the observation point. A system of classical equations of motion, identical with the system of characteristic equations equivalent to the differential equation (21), makes it possible to calculate corrections to the rectilinear paths of electrons in the range $r_1, r_2>r_0$, subject to the inequalities of Eq. (19). Obviously, the sum of the force of attraction of an electron to the residual ion and of the force of the mutual repulsion of electrons in the outer region results in some bending of the paths in the direction of increasing angles compared with the angles of emergence from the region $\rho\leqslant\rho_0$. A calculation of these corrections can be found in Ref. 12 and the explicit form of the angular shift is given below by Eq. (32). When

the path of a ray has been determined, the eikonal can be found from Eq. (21) in the form of a curvilinear integral along the ray path.

We shall now consider Eq. (21'). We can write down

$$\nabla_\rho \chi = n(\rho)\mathbf{l}, n(\rho) = (E - V_1^{out} - V_2^{out} - V_{12}^{out})^{1/2},$$

where l is a unit vector tangential to the $\rho(t)$ curve at a point l. It follows from the Gaussian theorem that

$$\int_V \operatorname{div}(A^2 n\mathbf{l})\, dV = \oint nA^2 \mathbf{l}\mathbf{m}\, d\sigma. \tag{22}$$

If in the six-dimensional space we select a volume bounded from the sides by the rays $\rho(t)$ and on the ends by elements of areas $d\sigma_1$ and $d\sigma_2$ of the surfaces $\chi_1 = \text{const}$ and $\chi_2 = \text{const}$, we find from Eq. (22) that

$$nA^2 d\sigma = \text{const}. \tag{23}$$

This is simply the law of conservation of energy. It follows From Eq. (23) that

$$A^2(t) = A^2(0)\,[n(0)/n(t)\,][d\sigma(0)/d\sigma(t)\,].$$

Since $d\sigma$ is an element of a spherical surface in the six-dimensional space, it follows that when the inequalities of Eq. (19) are satisfied, we have $d\sigma(t) \propto \rho^5$, i.e.,

$$A^2(t) = A^2(0)\,[n(0)/n(t)\,](\rho_0/\rho)^5. \tag{24}$$

It should be stressed that, in accordance with Eq. (22), we determine the density of the current along rays $\rho(t)$, i.e., along classical electron paths. This means that if $A^2(0) = f(\theta_{10}, \theta_{20})$, then $A^2(\infty) = f(\theta_{10} + \Delta\theta_1, \theta_{20} + \Delta\theta_2)$. It should also be noted that $n(\infty) = E^{1/2}$ or

$$\frac{n(0)}{n(\infty)} = \left\{1 + \frac{2e^2}{Er_0}\left[Z(r_0) - 1/4 \sin\left(\frac{\theta_{10}+\theta_{20}}{2}\right)\right]\right\}. \tag{25}$$

It now remains to relate the quantity $A(0)$ in Eq. (24) to the boundary condition (18'). This can be done using Eq. (18') to construct a model of the function $\langle \mathbf{r}_1\mathbf{r}_2|\psi\rangle$ at $\rho = \rho_0$ either by simplifying the operators occurring in Eq. (18') or phenomenologically on the basis of certain physical considerations. Next, matching this model function to the representation described by Eq. (20), we can determine $A(0)$.

We shall ignore in Eq. (18') the Coulomb "tails" occurring in the quasifree Green function $g_0^c(E)$, i.e., we shall assume that $g_0^c = g_0$, where $g_0(E)$ is a free-motion propagator. Then, in the coordinate representation, writing down the matrix element in the form of an integral, we obtain

$$\langle \mathbf{r}_1\mathbf{r}_2|\psi\rangle_{\rho=\rho_0} = \int \frac{d^3\mathbf{p}_1}{(2\pi)^3}\frac{d^3\mathbf{p}_2}{(2\pi)^3}\frac{\exp(i\mathbf{p}_1\mathbf{r}_1 + i\mathbf{p}_2\mathbf{r}_2)}{E - p_1^2 - p_2^2 + i0} \times \langle \mathbf{p}_1\mathbf{p}_2|(1+\tau_{12}^{in} g_0)\, t_{12}^{in}|\varphi_{01}\varphi_2(\mathbf{p}_0)\rangle, \tag{26}$$

where φ_i are the wave functions of the spectrum of the V_i^{in} operators. Calculating Eq. (26) by the constant phase method, which is justified at high values of E, we obtain the principal term in the form of a diverging spherical wave:

$$\langle \mathbf{r}_1\mathbf{r}_2|\psi\rangle^{out} \approx \frac{(-2iE^{1/2})^{3/2}}{32\pi^{5/2}\rho^{5/2}} T_0(\mathbf{p}_0; \mathbf{p}_1\mathbf{p}_2)\exp(iE^{1/2}\rho), \tag{26'}$$

where

$$T_0(\mathbf{p}_0; \mathbf{p}_1\mathbf{p}_2) = \langle \mathbf{p}_1\mathbf{p}_2|(1+\tau_{12}^{in} g_0)\, t_{12}^{in}|\varphi_{01}\varphi_2(\mathbf{p}_0)\rangle = \langle \varphi_1(\mathbf{p}_1)\varphi_2(\mathbf{p}_2)|\, t_{12}^{in}|\varphi_{01}\varphi_2(\mathbf{p}_0)\rangle. \tag{27}$$

In Eq. (27), we have $\mathbf{p}_i = E^{1/2}\mathbf{r}_i/\rho$, i.e., $\mathbf{p}_i$ are the momenta of particles at the exit of a sphere $\rho = \rho_0$ and $p_1^2 + p_2^2 = E$. The last equality in Eq. (27) follows from the results of Ref. 15, since τ_{12}^{in} is the scattering operator in independent systems and this operator transforms plane waves into distorted waves in the relevant scattering channels.

We can obtain a complete representation of the function (26) if Eq. (26') is supplemented by a similar converging wave, i.e.,

$$\langle \mathbf{r}_1\mathbf{r}_2|\psi\rangle_{\rho\sim\rho_0} \approx \frac{(-2iE^{1/2})^{3/2}}{32\pi^{5/2}\rho^{5/2}}[T_0(\mathbf{p}_0; \mathbf{p}_1\mathbf{p}_2)\exp(iE^{1/2}\rho) + \gamma\exp(-iE^{1/2}\rho)]. \tag{28}$$

Matching Eqs. (28) and (20) at the boundary $\rho = \rho_0$ and assuming that $\chi(0) = E^{1/2}\rho_0$, we obtain

$$A(0) = \frac{2T_0(\mathbf{p}_0; \mathbf{p}_1\mathbf{p}_2)}{\rho_0^{5/2}}\left[\left(1 + \frac{n(0)}{E^{1/2}}\right) - \frac{i}{E^{1/2}}\left(\frac{A'(0)}{A(0)} + \frac{5}{2\rho_0}\right)\right]^{-1}. \tag{29}$$

On the basis of Eq. (24) and the inequalities of Eq. (19) we can readily show that the imaginary part of the denominator of the last formula has a higher order of smallness than the corrections to the real parts, so that the former can be ignored. Collecting now Eqs. (20), (24), and (29) we obtain the following expressions for $\langle \mathbf{r}_1\mathbf{r}_2|\psi\rangle$ in the limit $\rho \to \infty$ ($t \to \infty$):

$$\langle \mathbf{r}_1\mathbf{r}_2|\psi\rangle \approx \frac{(-2iE^{1/2})^{3/2}}{32\pi^{5/2}\rho^{5/2}} f\left(\frac{n^{1/2}(0)}{E^{1/4}}\right) \times T_0[(\mathbf{p}_0; \mathbf{p}_1(\infty)\mathbf{p}_2(\infty)]\exp[i\chi(\rho)]. \tag{30}$$

Here, we have

$$f(x) = 2x/(1+x^2), \quad \chi(\rho)_{\rho\to\infty} \approx E^{1/2}\rho - \nu \ln(2E^{1/2}\rho),$$
$$\nu = -e^2/2p_1 - e^2/2p_2 + e^2/2|\mathbf{p}_1 - \mathbf{p}_2|.$$

It follows from the above that the quantity $T_0[\mathbf{p}_0; \mathbf{p}_1(\infty)\mathbf{p}_2(\infty)]$ differs from $T_0(\mathbf{p}_0; \mathbf{p}_1, \mathbf{p}_2)$ in Eq. (27) by angular displacements $\Delta\theta_1$ and $\Delta\theta_2$ of electrons. It should be noted also that the wave function (30) has the correct asymptote, corresponding to the spherical eikonal the form of which was determined by Merkuriev.[14]

Equation (30) gives the following expression for the differential cross section in the PWSC model:

$$\frac{d^3\sigma(\theta_1, \theta_2)}{dE\, d\Omega_1\, d\Omega_2} = C\left[\frac{d^3\sigma(\tilde\theta_1, \tilde\theta_2)}{dE\, d\Omega_1\, d\Omega_2}\right]_{\text{PWIA(DWIA)}}, \tag{31}$$

where θ_i is the angle of observation in coplanar kinematics, $\tilde\theta = \theta_i - \Delta\theta_i$, and

$$\Delta\theta_i = 2\frac{\varepsilon_H r_H}{E_i r_0}\frac{p_i \cos\chi[\,|\mathbf{p}_1 - \mathbf{p}_2| + 2p_j \sin\chi]}{4|\mathbf{p}_1 - \mathbf{p}_2|\sin\chi[\,|\mathbf{p}_1 - \mathbf{p}_2| + (p_1 + p_2)\sin\chi]},$$
$$e^2 = 2\varepsilon_H r_H, \quad \chi = {}^1/_2(\theta_1 + \theta_2), \quad \varepsilon_H = 13.6 \text{ eV}, \tag{32}$$

r_H is the radius of the first Bohr orbit of the hydrogen atoms. The coefficient C is symmetric with respect to r_1 and r_2 be-

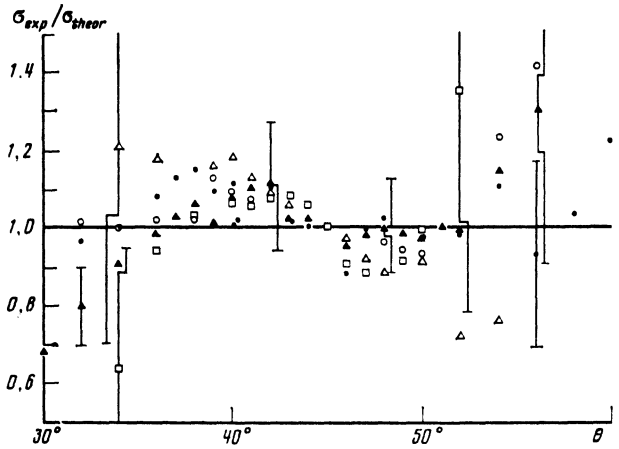

FIG. 1. Ratio of the absolute differential cross sections $\sigma_{exp}/\sigma_{theor}$ for the He^{1s} orbital plotted for a wide range of energies (the experimental points were taken fom Ref. 6): ●) 200 eV; ▲) 400 eV; ○) 800 eV; △) 1600 eV; □) 2500 eV.

cause it is governed entirely by the quantity $n(0)$, and it is identical for the direct and exchange amplitudes, amounting to

$$C=\frac{4\xi}{(1+\xi)^2}, \quad \xi=\left\{1+4\frac{\varepsilon_H r_H}{Er_0}\left[Z(r_0)-\frac{1}{4\sin\chi}\right]\right\}^{1/2}.$$

A comparison with the experimental results shows that the cross section on the right-hand side of Eq. (31) can easily be calculated in the approximation of plane waves up to $E \gtrsim 200$ eV, so that we shall confine our treatment to this case.

We shall now make several comments before presenting the results. It follows from Eqs. (15)–(30) that three important approximations were made. Firstly, we retained only the first term of the sum of Eq. (16); secondly, we simplified Eq. (18); thirdly, we replaced (18′) with Eq. (28). We obtained corrections to $(d^3\sigma)_{PWIA}$ of the order of ε_H/E. It can be shown that the first two simplifying assumptions are of higher orders of smallness in respect to this ratio, but this is not true of the third, since $g_0^c - g_0 \sim \varepsilon_H/E$. Therefore, we cannot expect Eq. (31) to be in 100% agreement with the results of absolute measurements, especially as these measurements are not yet too accurate. On the other hand, Eq. (31) reproduces quite satisfactorily the experimentally observed angular shift of the binary peak relative to calculations based on the PWIA model, which is due to the bending of electron paths in the outer region. This occurs because the peak is fairly sharp and even a small correction (32) shifts it greatly.

3. RESULTS

In this model there is one parameter r_0 which in principle is free. However, the physical meaning of the quantity r_0 is that it is of the order of the shell radius in which the ionization occurs. In fact, Fig. 1 shows the ratio $\sigma_{exp}/\sigma_{theor}$ for a large number of data obtained by determination of the absolute cross sections for He^{1s} in the energy range 200 eV $\lesssim E \lesssim$ 2.5 keV. It is then found that $r_0 = 0.7$ a.u., which is practically equal to the average radius of the 1s shell taken from the tables.[16] The ratio $\sigma_{exp}/\sigma_{theor}$ is the best of those used in other models. Figure 2 shows the results of a symmetric experiment on He^{1s} at $E = 200$ eV (in general, such an energy is fairly low) and the results of calculations carried out using various models. An increase in the energy alters the curves approximately in such a way that the difference between them and the experimental points disappears. For $E \gtrsim 1.5$ keV all models reproduce the experimental results.

Similar results were obtained for the differential cross sections for the ionization of the outer shells of other rare gases. The experimental results were taken from Ref. 6. The values of r_0 once again were close to the average radius of the shell being ionized.

The only exception was the Ne^{2p} state (Fig. 3). This state had been investigated by various authors under various kinematic conditions[6,18] and it was always found that there was some discrepancy between the experimental results and calculations when the wave function was taken from Ref. 16. This was checked by assuming that at $E = 2.6$ keV, when—in principle—all the above models are practically identical with the results of the PWIA model and with the experimental data, we can determine $\varphi_{01}(\mathbf{q})$ from Eqs. (7) and (6). This information was then used in Eqs. (31) to analyze the experimental data already at $E = 800$ eV. The results are

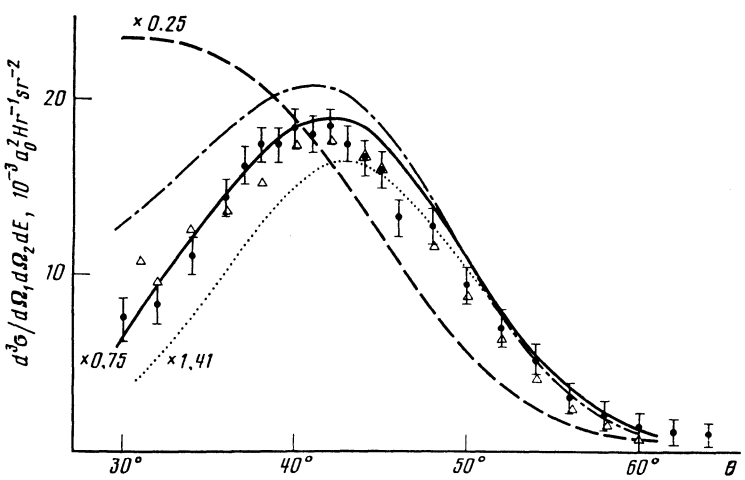

FIG. 2. Comparison of the experimental data for He^{1s} at $E = 200$ eV (Ref. 6) with calculations carried out using various theoretical models: the dashed curve represents the PWIA model, the chain curve represents EWIA, the dotted curve represents DWIA,[17] and the continuous curve corresponds to PWSC.

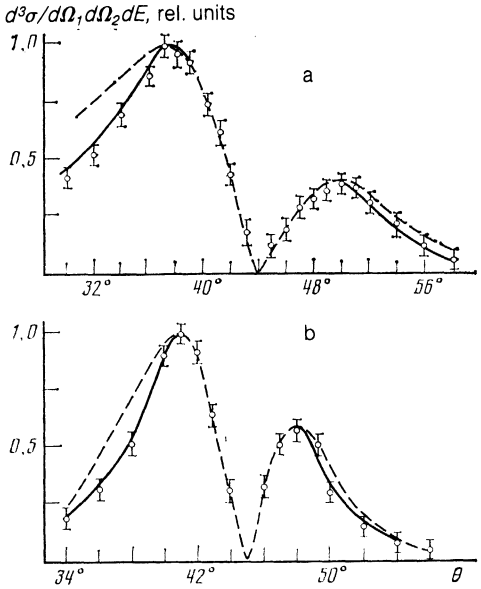

FIG. 3. Symmetric experiments[6] and calculations for Ne^{2p}: a) $E = 800$ eV; b) $E = 2600$ eV. The dashed curve corresponds to the Hartree-Fock wave function and the continous curve to the wave function calculated using the PWSC model.

presented in Fig. 3. Therefore, in all probability neon is characterized by some static correlation beween closely spaced $2s$ and $2p$ shells, resulting in deviation of the wave function of the ground state from the Hartree-Fock function. This is esentially the first constructive prediction of the new effects found by the $(e, 2e)$ method.

4. CONCLUSIONS

The results of an analysis of a large number of binary experiments based on Eq. (31) showed that it is a natural generalization of the plane-wave impulse approximation, which makes it possible to extend the range of its validity to much lower initial energies and to angles $\theta \lesssim 40°$. In principle, the plane-wave semiclassical approximation can be used also to explain the processes of ionization from inner shells when $Z(r_0) > 1$. In particular, it accounts reasonably for the observed reduction in the ionization cross section in the case of the Ne^{2s} orbital compared with calculations carried out using the plane-wave impulse approximation and this is because of the coefficient in Eq. (31). Clearly, Eq. (31) becomes invalid at low initial energies and for strongly asymmetric kinematics, and also for angles $\theta < 30°$.

In spite of the undoubted success of the plane-wave semiclassical approximation, it is worth noting its competition with the eikonal-wave impulse approximation model, in which (in contrast to the plane-wave semiclassical treatment) an allowance for the interaction between an electron and an ion is basically made by a small metric distortion of the values of the momenta which occur in the reaction, i.e., $p_i = (E_i + \overline{V})^{1/2}$. Recent reports generalize this effect and make it possible to use the impulse approximation in describing the capabilities of the plane-wave impulse approximation.[19] In the case of Eq. (31), an allowance for the first Born term in the wave functions of Eq. (27), i.e., a slight deviation from plane waves, distorts the plane-wave representations when the recoil momenta are $q \gtrsim 2$ a.u. This circumstance sets the limits to reliable predictions of the function $\varphi_{01}(\mathbf{q})$ on the basis of the $(e, 2e)$ experimental data.

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[1)]If we ignore not the whole Coulomb "tail" but only the residue V_{12}^{out}, we can drop this restriction and regard φ_i as the eigenfuctions of a Hamiltonian with a potential V_i.

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