Angular Correlation for $(e, 2e)$ Reactions on Atoms*

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The angular correlation for $(e, 2e)$ experiments involving knock out of the least-bound electrons in helium and argon is compared with theory. A distorted-wave off-shell impulse approximation is derived and shown to fit the data within experimental error. Outstanding features are that the shape of the angular correlation at energies from 200 to 800 eV depends only on the momentum transfer. Hence the angular correlation is directly related to the momentum wave function of the struck electron. The reaction is sensitive enough to distinguish between different approximations for the wave function.

I. INTRODUCTION

The 400-eV $(e, 2e)$ experiment on argon of Weigold, Hood, and Teubner[1] promises to inaugurate a wide range of applications to discover new knowledge of the structure of atoms and molecules. Before this knowledge can be reliably extracted from the experimental data, we must have a theory that is capable of correctly describing the shape of the angular correlation between the two emerging electrons (i.e., the distribution of momentum transfer $\vec{q}$) which is measured in the experiments. A schematic representation of the experiment is given in Fig. 1. An electron with momentum $\vec{k}_0$ is incident on an atomic system (atom, molecule, or solid) with a kinetic energy E_0 greater than the ionization potential. The two outgoing electrons are detected in coincidence by two electron detectors A and B capable of measuring both the direction and energy of the electrons. The angular variable ϕ, the azimuth of one of the outgoing electrons, is measured from the plane defined by the incident electron, and the other electron (A).

Earlier theoretical studies[2] of the $(e, 2e)$ reaction have been based on plane-wave Born, impulse, and binary-encounter approximations. In this paper we derive a theoretical framework based on a distorted-wave off-shell impulse approximation and test it by treating the simplest application, namely, the knock out of one of the least-bound electrons in the shell-model description of an atom, leaving the residual ion in its ground state. In Sec. II we give a brief outline of the model which is developed in Secs. III and IV. In Sec. V we present the experimental results, and compare them with the theory in Sec. VI.

II. THE MODEL

We will assume in our model that the ion plays the role of an inert particle, to which the knocked-out electron is initially bound, as far as the $(e, 2e)$ reaction is concerned. Many other reactions such as elastic and inelastic scattering and ionization leaving other residual ion states can occur. These are described by complex potentials in the interactions V_0, V_A, and V_B between the ion and the incident electron and the electrons measured in the detectors A and B, respectively. Approximate values of these optical-model potentials are known from analyses of elastic scattering, for example, that of Furness and McCarthy.[3]

The model is thus one of a quasi-three-body system, where the bodies interact through the

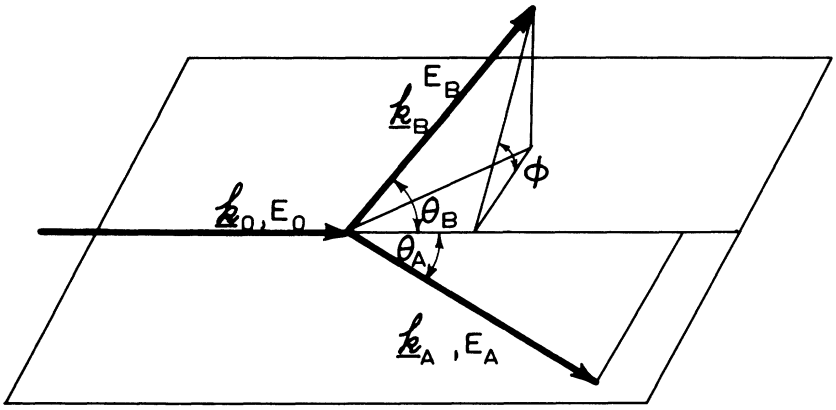

FIG. 1. Experimental arrangement for the $(e, 2e)$ reaction.

optical-model potentials and the Coulomb potential between the two electrons. To describe breakup in this system, we will derive an approximation to be called the distorted-wave off-shell impulse approximation.

III. DISTORTED-WAVE OFF-SHELL IMPULSE APPROXIMATION

The approximation has been derived by Dodd and Greider[4] as the first term of a multiple scattering series for a pure three-body problem. We will give a derivation more suitable to the quasi-three-body problem in which the optical-model potentials depend on the relative energy in the appropriate two-body subsystem.

We must first remind the reader of the formulation of general three-body scattering theory (Gell-Mann and Goldberger[5]). The three-body Hamiltonian H for the problem is split into two arbitrary portions $\mathcal{K}+\mathcal{U}$, where $\mathcal{K}$ contains the three-body kinetic-energy operator K. Wave functions are defined as follows

$$\begin{aligned} &H=\mathcal{K}+\mathcal{U}\,,\\ &(E^{(\pm)}-H)\Psi^{(\pm)}=0\,,\\ &(E^{(\pm)}-\mathcal{K})\Phi^{(\pm)}=0\,. \end{aligned} \tag{1}$$

The three-body wave functions $\Psi^{(\pm)}$ satisfy the Lippmann-Schwinger equation

$$\Psi^{(\pm)}=\Phi^{(\pm)}+\frac{1}{E^{(\pm)}-H}\,\mathcal{U}\Phi^{(\pm)}=\Phi^{(\pm)}+\frac{1}{E^{(\pm)}-\mathcal{K}}\,\mathcal{U}\Psi^{(\pm)}\,, \tag{2}$$

where

$$E^{(\pm)}=\lim_{\epsilon\to 0+}(E\pm i\epsilon)\,. \tag{3}$$

The plus and minus superscripts correspond to boundary conditions with outgoing spherical waves (entrance channel) and ingoing spherical waves (exit channel), respectively. The inverse Shrödinger operators (Green's functions) are integral operators.

The amplitude for a reaction defined by the boundary conditions of $\Psi^{(\pm)}$ and $\Phi^{(\pm)}$ is

$$M=\langle\Psi^{(-)}\,|\,\mathcal{U}\,|\,\Phi^{(+)}\rangle=\langle\Phi^{(-)}\,|\,\mathcal{U}\,|\,\Psi^{(+)}\rangle\,. \tag{4}$$

The Lippmann-Schwinger equation (2) relates $\Psi^{(\pm)}$ to $\Phi^{(\pm)}$ by means of the three-body t-matrix.

$$\begin{aligned} &\mathcal{U}\,|\,\Psi^{(+)}\rangle=T^{(+)}\,|\,\Phi^{(+)}\rangle\,,\\ &\langle\Psi^{(-)}\,|\,\mathcal{U}=\langle\Phi^{(-)}\,|\,T^{(-)}\,, \end{aligned} \tag{5}$$

where

$$T^{(\pm)}=\mathcal{U}+\mathcal{U}\,\frac{1}{E^{(\pm)}-H}\,\mathcal{U}\,. \tag{6}$$

In the application to the present breakup problem, we will first treat the entrance channel in which the potentials are V_0, previously defined, and the single-particle potential U which binds the electron to the ion. It will be seen that the chief utility of the angular-correlation measurement is to provide a very sensitive test for the potential U. In addition the two electrons interact through the Coulomb potential v.

We first define our partitioning of the Hamiltonian

$$\mathcal{K}=K+V_0+U\,,\quad \mathcal{U}=v\,. \tag{7}$$

The breakup amplitude, according to (4) is

$$M=\langle\Psi^{(-)}\,|\,v\,|\,\Phi^{(+)}\rangle\,, \tag{8}$$

where

$$(E-K-V_0-U)\Phi^{(+)}=0\,. \tag{9}$$

We next turn our attention to the exit channel, where the electrons interact with the ion through potentials V_A and V_B. We now define $\mathcal{K}$ and $\mathcal{U}$ by

$$\mathcal{K}=K+V_A+V_B\,,\quad \mathcal{U}=v\,. \tag{10}$$

Equation (5) defines our formal expression for the breakup amplitude:

$$M=\langle\Phi^{(-)}|\,T^{(-)}\,|\Phi^{(+)}\rangle\,, \tag{11}$$

where

$$(E-K-V_A-V_B)\Phi^{(-)}=0\,, \tag{12}$$

$$T^{(-)}=v+v\,\frac{1}{E^{(-)}-K-V_A-V_B-v}\,v\,. \tag{13}$$

Equation (11) is exact, in the context of the quasi-three-body model. It is defined in terms of three-body operators operating in the space of three-body wave functions. We must reduce the problem to one in terms of two-body operators, which can be defined in terms of the two-body potentials of the problem. It will be convenient (but not necessary) to make the approximation that the ion is infinitely massive. We will attach the coordinate $\vec{r}_1$ to the electrons 0 and A and the coordinate $\vec{r}_2$ to the bound electron and the electron B. Antisymmetrization in these coordinates will be performed later. The canonically conjugate momenta are $\vec{p}_1$ and $\vec{p}_2$, respectively.

We are also interested in the center-of-mass and relative-electron coordinates

$$\vec{R}=\tfrac{1}{2}(\vec{r}_1+\vec{r}_2)\,,\quad \vec{r}=(\vec{r}_1-\vec{r}_2)\,, \tag{14}$$

and the conjugate momenta

$$\vec{P}=\vec{p}_1+\vec{p}_2\,,\quad \vec{p}=\tfrac{1}{2}(\vec{p}_1-\vec{p}_2)\,. \tag{15}$$

The kinetic-energy operator is

$$K = K_1 + K_2 = K_r + K_R , \tag{16}$$

where

$$K_1 = p_1^2/2m , \quad K_2 = p_2^2/2m ,$$
$$K_r = p^2/2\mu , \quad K_R = P^2/2m , \tag{17}$$
$$\mu = \tfrac{1}{2}m , \quad M = 2m .$$

The Schrödinger equation (9) for $\Phi^{(\pm)}$ separates in the coordinates $\vec{r}_1, \vec{r}_2$:

$$[E - K_1 - V_0(r_1) - K_2 - U(r_2)]\Phi(\vec{r}_1, \vec{r}_2) = 0 ,$$
$$[E_0 - K_1 - V_0(r_1)]\chi_0^{(+)}(\vec{r}_1) = 0 ,$$
$$[\epsilon - K_2 - U(r_2)]\psi_{nlj}^m(\vec{r}_2) = 0 , \tag{18}$$
$$\Phi^{(+)}(\vec{r}_1, \vec{r}_2) = \chi_0^{(+)}(\vec{k}_0, \vec{r}_1)\psi_{nlj}^m(\vec{r}_2) .$$

The incident distorted wave is $\chi^{(+)}(\vec{k}_0, \vec{r}_1)$, where the $\hbar\vec{k}_0$ is the momentum of the incident electron. The bound-state single-particle wave function is $\psi_{nlj}^m(\vec{r}_2)$ for the potential $U(r_2)$.

The expression (11) that we want to reduce to a tractable form is written explicitly as

$$M = \int d^3r_1 \int d^3r_2\, \Phi^{(-)}(\vec{r}_1, \vec{r}_2)\left(v(r) + v(r)\frac{1}{E - K_R - K_r - V_A(r_1) - V_B(r_2) - v(r)}\, v(r')\right)\chi_0^{(+)}(\vec{r}_1')\psi_{nlj}^m(\vec{r}_2') . \tag{19}$$

The coordinates after the operator are primed because the nonlocal Green's-function operator $(E\text{-}H)^{-1}$ involves integrations over $\vec{r}_1'$ and $\vec{r}_2'$. The term in large parentheses has the explicit form

$$\int d^3r_1' \int d^3r_2' [v(r)\delta(\vec{r} - \vec{r}')\delta(\vec{R} - \vec{R}') + G(\vec{r}, \vec{R}, \vec{r}', \vec{R}')] .$$

In the approximation to be derived the explicit form of G is not required.

A similar procedure to (18) may be followed for separating $\Phi^{(-)}(\vec{r}_1, \vec{r}_2)$:

$$\Phi^{(-)}(\vec{r}_1, \vec{r}_2) = \chi_A^{(-)}(\vec{k}_A, \vec{r}_1)\chi_B^{(-)}(\vec{k}_B, \vec{r}_2) . \tag{20}$$

The distorted waves for the electrons A and B are $\chi_A^{(-)}$ and $\chi_B^{(-)}$, computed from the two-body Schrödinger equations:

$$[E_A - K_1 - V_A(r_1)]\chi_A^{(-)}(\vec{k}_A, \vec{r}_1) = 0 ,$$
$$[E_B - K_2 - V_B(r_2)]\chi_B^{(-)}(\vec{k}_B, \vec{r}_2) = 0 . \tag{21}$$

The momenta of the electrons A and B are $\hbar\vec{k}_A$ and $\hbar\vec{k}_B$.

The second term in the three-body t matrix in (19), however, cannot be separated exactly. We must take the first terms in the Taylor expansions of $V_A(r_1)$ and $V_B(r_2)$, respectively, about $\vec{R}$. This is a good approximation since in an ion the gradients of the single-particle potentials are small, except near the nucleus. Our reaction is unlikely to occur near the nucleus, since the absorptive potentials reduce the absolute values of the distorted waves there, also the volume of this part of space is small compared with that of the periphery of the atom.

The problem is that the operator $V_A + V_B$ cannot be commuted through the operator $v(r)$ on the left-hand side in Eq. (19) to act on the wave function $\Phi^{(-)}(\vec{r}_1, \vec{r}_2)$, since it depends on the coordinate $\vec{r}$.

For the second term (but not the first term) we must put

$$V_A(r_1) \cong V_A(R) , \quad V_B(r_2) \cong V_B(R) . \tag{22}$$

The three-body Schrödinger equation now separates thus:

$$[E - K_R - V_A(R) - V_B(R) - K_r - v(r)]\Phi^{(-)}(\vec{r}, \vec{R}) = 0 ,$$
$$[E_A + E_B - K_R - V_A(R) - V_B(R)]\chi^{(-)}(\vec{R}) = 0 ,$$
$$[\epsilon - K_r - v(r)]\phi(\vec{r}) = 0 , \tag{23}$$
$$\Phi^{(-)}(\vec{r}, \vec{R}) = \phi(\vec{r})\chi^{(-)}(\vec{R})$$
$$\cong \phi(\vec{r})\chi_A^{(-)}(\vec{k}_A, \vec{r}_1)\chi_B^{(-)}(\vec{k}_B, \vec{r}_2) .$$

The operator in large parentheses in (19) becomes (when operating on $\Phi^{(-)}$)

$$\left(v(r) + v(r)\frac{1}{\epsilon - K_r - v(r)}\, v(r')\right)\delta(\vec{R} - \vec{R}')$$
$$\equiv \int d^3r_1' \int d^3r_2'\; t_C(\epsilon, r, r')\delta(\vec{R} - \vec{R}') . \tag{24}$$

The function $t_C(\epsilon, r, r')$ is the two-body Coulomb t matrix in coordinate space calculated for the energy

$$\epsilon = E_0 - E_A - E_B , \tag{25}$$

which is the separation energy of the electron that is removed.

The distorted-wave off-shell impulse approximation is

$$M = A\langle\chi_A^{(-)}(\vec{k}_A)\chi_B^{(-)}(\vec{k}_B)\,|\,t_C(\epsilon)\,|\,\chi_0^{(+)}(\vec{k}_0)\psi_{nlj}^m\rangle , \tag{26}$$

where A denotes antisymmetrization in $\vec{r}_1$ and $\vec{r}_2$.

It is clearly a very close approximation to an exact solution of the quasi-three-body problem. It is exact up to first order in v. Higher-order terms involve only the neglect of gradients of the atomic single-particle potentials near the periphery of the atom where they are small.

IV. EVALUATION OF THE MATRIX ELEMENT

The matrix element (26) will be evaluated with the aid of the eikonal approximation for the distorted waves

$$\chi^{(+)}(\vec{k}, \vec{r}) = e^{-\gamma_k R_N} e^{i\vec{\kappa}\cdot\vec{r}},$$
$$\chi^{(-)*}(\vec{k}, \vec{r}) = e^{-\gamma_k R_N} e^{-i\vec{\kappa}\cdot\vec{r}}, \tag{27}$$
$$\vec{\kappa} = (1+\beta+i\gamma)\vec{k}.$$

This approximation was first tried and found to be excellent for the inelastic scattering of 40-MeV α particles from nuclei by McCarthy and Pursey.[6] It has had great success[7] in describing the reaction $C^{12}(p, 2p)B^{11}$ at 400 MeV, and has been verified by comparison with plots of nuclear wave functions by Amos.[8] At first sight its success in nuclear theory may seem irrelevant to the case of atomic reactions. However, one must remember that the radial optical-model equation is written in terms of the dimensionless variable $\rho = kr$ as

$$\left(\frac{d^2}{d\rho^2} + \frac{K(\rho)^2}{k^2} - \frac{l(l+1)}{\rho^2}\right) u_l(\rho) = 0, \tag{28}$$

where the local wave number $K(\rho)$ is defined by

$$K(\rho)^2 = (2m/\hbar^2)[E - V(\rho)]. \tag{29}$$

Values of K^2/k^2 are very similar (and quite close to 1) for the atomic case at a few hundred eV and the nuclear case at a few hundred MeV. The relevant real atomic potentials are of the order of 20 eV (in the interaction region). The imaginary parts[3] are of the order of 10 eV. The nuclear potentials are of the order $(10+10i)$ MeV. Hence it is seen that the wave functions (as functions of ρ) are very similar.

The parameters in the eikonal approximation are easily approximated by solving a one-dimensional Schrödinger equation as

$$\beta + i\gamma = \overline{V}/2E, \tag{30}$$

where $\overline{V}$ is the average complex potential in the interaction region (the periphery of the atom). The normalization parameter R_N ensures that the absolute value of the distorted wave is 1 at a distance R_N before it enters the interaction region. A good approximation for R_N is the distance inside which 99% of the atomic charge density is concentrated. In practice both β and γ are less than 0.1 and R_N is about 1.1 Å for argon.

The impulse approximation matrix element (26) becomes

$$M = NA\int d^3r_1 \int d^3r_2 \int d^3r_1' \int d^3r_2'\; e^{-i\vec{\kappa}_A\cdot\vec{r}_1} e^{-i\vec{\kappa}_B\cdot\vec{r}_2} \times t_C(r, r')\delta(\vec{R} - \vec{R}') e^{i\vec{\kappa}_0\cdot\vec{r}_1'} \psi_{nlj}^m(\vec{r}_2'), \tag{31}$$

where

$$N = e^{-(k_0\gamma_0 + k_A\gamma_A + k_B\gamma_B)R_N}. \tag{32}$$

It is straightforward to show (see, for example, McCarthy and Tandy[9]) that (31) reduces to

$$M = NA\langle \tfrac{1}{2}(\vec{\kappa}_A - \vec{\kappa}_B)|\, t_C(\tfrac{1}{4}|\vec{\kappa}_A - \vec{\kappa}_B|^2)\,|\, \tfrac{1}{2}(\vec{\kappa}_0 + \vec{q})\rangle \phi_{nlj}^m(\vec{\kappa}),$$

where $\phi_{nlj}^m(\kappa)$ is the Fourier transform of $\psi_{nlj}^m(\vec{r})$ with respect to $\vec{\kappa}$.

$$\vec{\kappa} = \vec{\kappa}_0 - \vec{\kappa}_A - \vec{\kappa}_B. \tag{34}$$

The differential cross section is proportional to

$$\sigma = N^2 \sum_{av} |A(\tfrac{1}{2}(\vec{\kappa}_A - \vec{\kappa}_B)|\, t_C(\tfrac{1}{4}|\vec{\kappa}_A - \vec{\kappa}_B|^2) \times |\, \tfrac{1}{2}(\vec{\kappa}_0 + \vec{q})\rangle|^2 |\, \phi_{nlj}^m(\vec{\kappa})|^2. \tag{35}$$

The notation $\sum_{av}$ denotes a sum over final and an average over initial magnetic degeneracies.

The t-matrix elements required are half off the energy shell. A convenient computational form for them has been given by Ford.[10]

The final computational formula is

$$\sigma(\kappa) = N^2 \left(\frac{2me^2}{\hbar^2}\right)^2 \frac{2\pi\eta}{e^{2\pi\eta} - 1} \left\{ \frac{1}{|\vec{k} - \vec{k}'|^4} + \frac{1}{|\vec{k} + \vec{k}'|^4} - \frac{1}{|\vec{k} - \vec{k}'|^2} \frac{1}{|\vec{k} + \vec{k}'|^2} \cos\left[\eta \ln\left(\frac{|\vec{k} + \vec{k}'|^2}{|\vec{k} - \vec{k}'|^2}\right)\right] \right\} \left[\int r\,dr\, j_l(\kappa r) u_{nl}(r)\right]^2. \tag{36}$$

$$\vec{k} = \tfrac{1}{2}(\vec{\kappa}_0 + \vec{\kappa}), \quad \vec{k}' = \tfrac{1}{2}(\vec{\kappa}_A - \vec{\kappa}_B), \quad \eta = me^2/\hbar^2 k'. \tag{37}$$

The radial single-particle function is $u_{nl}(r)$.

Since $\vec{\kappa}$ is very nearly equal to the momentum transfer $\vec{q}$ which is measured in the experiment, it is clear that the momentum-transfer distribution $\sigma(\kappa)$ looks like a Mott scattering factor (off-shell) multiplying the momentum distribution of the electron in the atom before it was knocked out.

V. EXPERIMENTAL RESULTS

The apparatus used in the present experiment is, in the main, identical to that employed by Weigold, Hood, and Teubner[1] and is shown schematically in Fig. 2. Electrons are accelerated in an electron gun to the desired impact energy and are scattered from a gas beam produced by allowing the target gas to effuse through a stainless-steel tube 0.2 mm in diam-

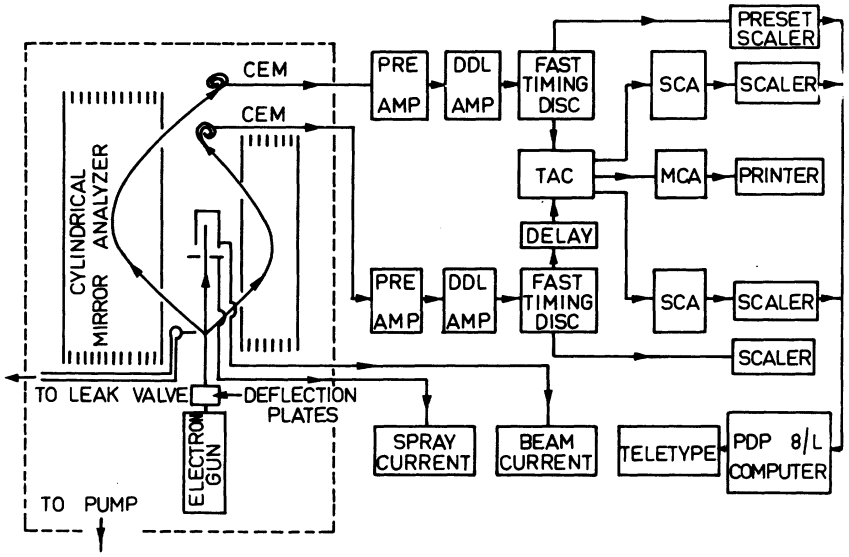

FIG. 2. Schematic diagram of the apparatus. For details see the text.

eter. The scattered electrons are then energy analysed by two cylindrical mirror analyzers. Although the entrance aperture on the larger analyzer could be rotated in azimuth by ±75°, the present measurements were all taken in the angular range ±40°. The acceptance angles of the detectors are approximately 7° and their combined energy resolution is of the order of 1%. Two channel electron multipliers (CEM) are used to detect the two electrons in coincidence. The time resolution of the coincidence equipment (consisting of double delay-line amplifiers, zero-level cross-over discriminators, and a time-to-amplitude converter) is monitored by a multichannel analyzer (MCA) and is typically 10 nsec. The background accidental coincidence counting rate is constant, being independent of the time difference between the two pulses. Two single-channel analyzers (SCA) are used to route the coincidence and background pulses into separate scalers.

The background gas pressure, electron-gun current, and singles counting rates are all monitored continuously. Care is taken to reduce stray electric and magnetic fields. The effect of the earth's magnetic field is minimized by means of Helmholtz coils. All conducting surfaces are coated with colloidal graphite to reduce production of secondary electrons. Data taking has been partially automated, since several days are often required to obtain sufficient statistics for one angular correlation.

In the symmetric noncoplanar geometry used in the present series of experiments, the angular variable is the azimuth ϕ of one of the outgoing electrons measured from the plane defined by the incident electron and the other outgoing electron. Both electrons are emitted at an angle θ of 45° relative to the incident direction, and both are selected to have the same energy, i.e.,

$$\theta_A = \theta_B = \theta = 45^\circ \text{ and } k_A = k_B .$$

Then the magnitude of the momentum transfer $\vec{q} = \vec{k}_A + \vec{k}_B - \vec{k}_0$ is given by

$$q = |(2k_A \cos\theta - k_0)^2 + 4k_A^2 \sin^2\theta \sin^2\tfrac{1}{2}\phi|^{1/2} .$$

Figure 3 shows the angular correlations obtained for the ejection of a $1s$ electron from helium leaving the helium ion in its ground state for total energies ($E = E_0 - \epsilon = E_A + E_B$) of 800,

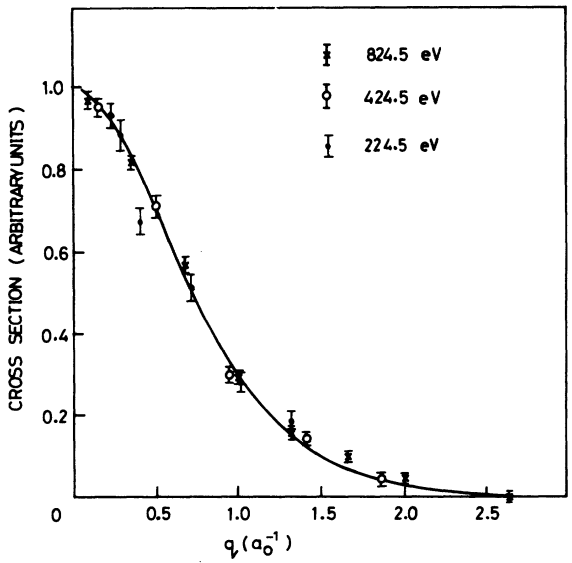

FIG. 3. Angular correlation for helium at incident energies of 824.5, 424.5, and 224.5 eV. The theoretical curve is calculated for 824.5 and 424.5 eV, in which cases the curves are indistinguishable.

400, and 200 eV. The lowest and highest incident energies are, respectively, approximately 9 and 34 times the binding energy of the ejected electron.

From Fig. 3 it can be seen that the three angular correlations observed over this wide energy range are indistinguishable when plotted as a function of the momentum transfer q. This is obviously not the case if they are plotted as a function of the angular variable ϕ.

No excitation of the first excited state of the helium ion could be observed. The cross section for the excitation of the $n=2$ level is $(0.1 \pm 1.3\%)$ of that leading to the ground state. This is certainly consistent with the theoretical value of 1% for the ratios of total cross sections expected from electron correlations in helium.[11]

Figures 4 and 5 show the angular correlations obtained at total energies of 800 and 400 eV, respectively, for the ejection of an outer $3p$ electron from argon leaving the argon ion in its ground state. Electrons leaving the ion in its ground state could be clearly differentiated from electrons ejected from more deeply bound states, leaving the ion in more highly excited states (cf. Weigold, Hood, and Teubner[1]).

VI. COMPARISON OF THEORY AND EXPERIMENT

The angular correlations for $(e, 2e)$ reactions on helium and argon, leaving the residual ion in its ground state, were calculated by Eq. (36). An experimental uncertainty of 7° in the direction of each electron in the final state was folded into the calculation. In each case the function $u_{nl}(r)$ was taken from tables of Hartree-Fock wave functions. With the geometry of the present experiment, the shape of the angular correlation depends only on the momentum transfer if distortion of the ingoing and outgoing waves is negligible. Values of the distortion parameters used were $\beta=\gamma=0.01$ for $E=800$ eV and $\beta=\gamma=0.02$ for $E=400$ eV.

Figure 3 shows the result for helium plotted as a function of momentum transfer. In this case both theory and the various experimental results for total energies of 800, 400, and 200 eV are indistinguishable. The Hartree-Fock wave functions of Herman and Skillman[12] and Fischer[13] gave indistinguishable curves.

The cases of argon at 800 and 400 eV are shown in Fig. 4 and 5, respectively. In these cases the sharp minimum for the kinematic situation where all three electrons are coplanar (zero momentum transfer) is washed out by the angular-resolution factor. This factor has a greater effect on the momentum-transfer distribution at 800 than at 400 eV. In both cases the theoretical curves using the wave functions of Herman and Skillman[12] and Fischer[13] are indistinguishable. The curves calculated for different energies without the angular-resolution factor are also indistinguishable, indicating that the difference in the experiments at the two energies is due

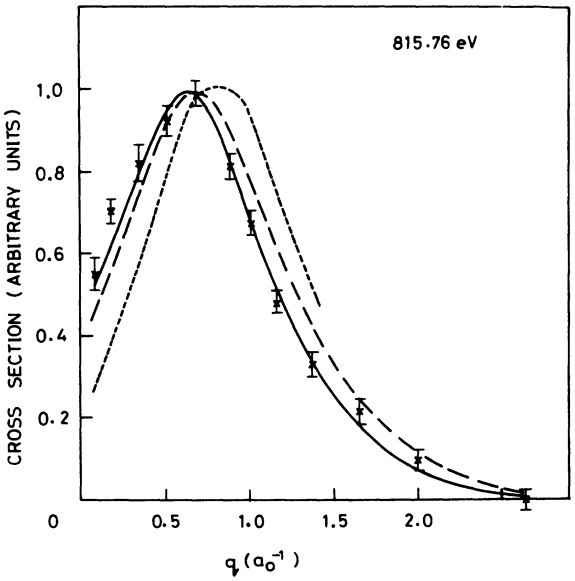

FIG. 4. Angular correlation for argon at an incident energy of 815.76 eV. The full curve is calculated with the HF wave functions of Herman and Skillman (Ref. 12) and of Fischer (Ref. 13) (indistinguishable). The dashed line is calculated with the HF wave function of Lu *et al.* (Ref. 14). The dotted line is calculated with an effective hydrogen-atom wave function.

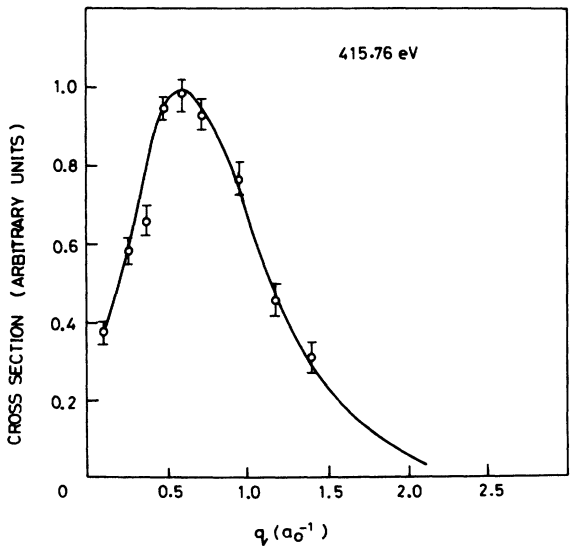

FIG. 5. Angular correlation for argon at an incident energy of 415.76 eV. The theoretical curve is calculated with the HF wave functions of Herman and Skillman (Ref. 12) and of Fischer (Ref. 13) (indistinguishable).

to angular resolution, not to a breakdown of the impulse approximation.

A Hartree-Fock wave function due to Lu *et al.*[14] was also tried in the case of argon at 800 eV (dashed line in Fig. 4). The experiment clearly distinguishes this wave function from the other two. In order to illustrate further the sensitivity of the experiment to the choice of the single-particle wave function, we have illustrated on the same diagram (dotted line in Fig. 4) the angular correlation calculated for a $3p$ hydrogen-atom wave function with an effective charge determined by the Hartree-Fock screening factor ($Z_{\text{eff}} = 7.517$). This is often used as a rough approximation to a single-particle wave function, but it is clearly inadequate in the present reaction.

VII. CONCLUSIONS

In order to verify our description of the $(e, 2e)$ reaction mechanism, we have chosen cases where the structure of the atomic states involved is well known. In the noncoplanar symmetric geometry chosen for the present experiment, the shape of the angular correlation in the off-shell impulse approximation depends only on the momentum transfer, and not independently on the energies of ingoing or outgoing electrons. In other words, the shape of the angular correlation is given directly by the momentum-space wave function of the knocked-out electron. This is true if distortion is negligible in determining the shape. The absorptive effect of other channels, which is included in the distortion, is noticed only in the magnitude of the differential cross section, which is not measured in the present experiments. In a later paper relative magnitudes for excitation of different final states in the same experiment, which are measured, will be discussed.

The experimental data for both helium and argon, when the effect of finite angular resolution is taken into account, verify that the momentum-transfer distribution is independent of the energies of the ingoing and outgoing electrons. It is worth noting that for helium this is still true at an incident energy of only 225 eV, in marked contrast with the results of Ehrhardt *et al.*[15] at 256.5 eV. In our noncoplanar symmetric situation the momentum transfer to the "scattered" and "ejected" electrons is very large, whereas the very asymmetric coplanar situation employed by Ehrhardt *et al.* is characterized by low momentum transfer to the ejected electron. Since in such experiments the ejected electron is emitted with a very low energy at a relatively large angle, large distortion effects are to be expected.

The validity of Hartree-Fock wave functions as a description of the relevant atomic structure is verified. In a structure calculation, spectroscopic amplitudes are defined with respect to a single-particle potential. The experiment provides a very sensitive definition of the "best" single-particle potential. It is capable of distinguishing Hartree-Fock wave functions calculated in different numerical approximations. In summary, $(e, 2e)$ experiments such as those reported here and of Weigold, Hood, and Teubner yield directly, to a very good approximation, the momentum-space wave function of an electron ejected from an atomic system.

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