PHYSICAL REVIEW A VOLUME 9, NUMBER 1 JANUARY 1974

Structure of atoms from the $(e,2e)$ reaction*

S. T. Hood, I. E. McCarthy, P. J. O. Teubner, and E. Weigold
School of Physical Sciences, The Flinders University of South Australia, S. A. 5042, Australia

(Received 2 July 1973)

A model is derived for the differential cross section for $(e,2e)$ reactions on atoms, leaving the residual ion in an excited state. The eigenstates of the ion are described by the shell model with configuration interaction. In the case of argon, $3s^{-1}$ spectroscopic factors are independently determined. They describe the probability that each of the three ion eigenstates whose $(e,2e)$ angular correlation has the $3s^{-1}$ shape, contain the $3s^{-1}$ configuration. Two Hartree-Fock single-particle models are compared. The spectroscopic factors add to 1 for both, but only one correctly predicts the experimental single-hole energy level.

I. INTRODUCTION

In a previous paper by Hood, McCarthy, Teubner, and Weigold[1] hereafter referred to as I, we showed that the angular correlation, or momentum transfer distribution, measured in 400- and 800-eV $(e, 2e)$ experiments on argon and helium can be extremely well understood in terms of a model for the atomic structure and the quantum mechanics of reactions. In that case the simplest spectroscopic situation—the removal of an electron from the topmost single-particle state leaving the ion in its ground state—was considered in order to concentrate on the reaction aspect of the problem.

Now that the validity of the reaction model has been established, it is interesting to consider the use of the reaction as a probe for the structure of eigenstates of the ion Hamiltonian other than the ground state.

In the first experiments at 400 eV by Weigold, Hood, and Teubner,[2] at least three states of Ar II were observed in addition to the ground state. The ionization energies were 29.3 eV for one state and about 40 eV for two (or more) unresolved states. Two ion states near 40 eV are known in photon spectroscopy and the data are consistent with the excitation of these states. The coincidence counting rate as a function of binding energy of the ejected electron, as reported in Ref. 2, is shown in Fig. 1.

We will specifically consider the formalism for the ionization of closed-shell atoms, with argon as an example. The formalism is easily extended to open-shell atoms. We will show that the $(e, 2e)$ reaction enables us to find the spectroscopic factors, which relate the single-particle wave functions to the actual eigenstates of the ion Hamiltonian. The position of the single-hole energy level can be found as the centroid of the corresponding ion eigenstates weighted by the spectroscopic factors.

II. SHELL MODEL FOR ATOMIC STRUCTURE

Our discussion of atomic structure will be presented in the language of the shell model with interparticle interactions. In this model the energy eigenvalues E_ρ and eigenstates $|\rho\rangle$ of the many-body system (atom or ion) are found theoretically by diagonalizing the Hamiltonian in a basis of independent-particle wave functions $\Phi_\rho(\alpha)$. The wave function Ψ_ρ for the atomic eigenstate $|\rho\rangle$ is expanded thus

$$\Psi_\rho = \sum_\alpha a_\rho(\alpha)\Phi_\rho(\alpha). \tag{1}$$

We will denote the corresponding expansion for the ion by

$$\Psi'_\sigma = \sum_\beta b_\sigma(\beta)\Phi'_\sigma(\beta). \tag{2}$$

The primed wave functions describe a system with Z-1 electrons; the unprimed functions refer to Z electrons.

Each independent-particle wave function $\Phi_\rho(\alpha)$ is a Slater determinant of single-particle wave functions ψ^m_{nlj} with the Z electrons distributed over them. The situation for the ion is analogous. An independent-particle basis wave function is called a configuration. Different configurations (different α) correspond to different ways of occupying the single-particle states. Each basis configuration must have the same total angular momentum and parity as the corresponding eigenfunction.

Contributions from Hamiltonian matrix elements for configurations involving the occupation of single-particle states far removed from the lowest possible ones are small. Hence, in a practical calculation the basis is truncated to include only a finite number of configurations, in which only

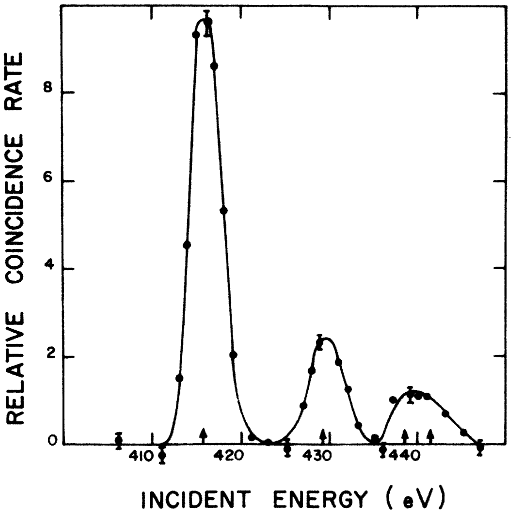

FIG. 1. Coincidence counting rate vs energy of the incoming electron for $\phi = 10°$, $\theta_1 = \theta_2 = 45°$ and $E = E_A + E_B = 400$ eV, $E_A = E_B$. The geometry for the reaction is discussed in full in I. The arrows indicate the positions of the states discussed in the text.

single-particle states near the lowest possible ones are occupied.

Single-particle states will be denoted by the old spectroscopic notation. Spin-orbit degeneracy will not be explicitly referred to except when it is necessary for counting states. We will call the configuration, in which all the single-particle states lowest in energy are occupied, the filled configuration. The actual lowest-energy eigenstate may contain different configurations (ground-state correlations) with electrons excited into higher single-particle states.

Each configuration will be described by a set of single-particle states with occupation numbers denoted by superscripts. Negative superscripts denote holes in the filled configuration. For example, two configurations involved in the expansion (1) of the ground state of Ar are the filled configuration and the $3s^{-2}3d^2$ two-particle two-hole configurations $1s^2 2s^2 2p^6 3s^2 3p^6$ and $1s^2 2s^2 2p^6 3s^{-2} 3p^6 3d^2$. Single-particle states which will never be occupied by particles or holes in our truncated basis are usually suppressed in the notation for simplicity.

In a calculation of the Ar II ion by Luyken,[3] which we will use for reference, only the states with $n = 3$ or 4 were considered in the basis. The ground-state Ψ_0' of Ar II was found to consist entirely of the configuration $3s^2 3p^5$, denoted alternatively by $3p^{-1}$. Thus the amplitude $b_0(3p^{-1})$ in Eq. (2) is 1 and all other amplitudes are negligible.

A single-particle basis is of course defined with respect to a single-particle potential $U(r)$. The "best" single-particle potential has two definitions that concern us. The theoretical definition is the potential that minimizes the number of configurations in the expansion (1) or (2). It is possible to construct a nonlocal potential by requiring that all amplitudes of one-particle one-hole configurations are zero. This is the Hartree-Fock potential. Different numerical approximations yield different Hartree-Fock potentials and wave functions. An equivalent definition of the Hartree-Fock potential is that it produces self-consistency between the potential used to calculate the wave functions and the potential derived from the resultant charge density. Antisymmetrization is responsible for the nonlocality.

The second definition is an experimental one. It is the potential $U(r)$ that gives the best fit to the (e, 2e) angular correlation, which is very sensitive to the potential shape. We showed in I that these definitions are consistent for some Hartree-Fock calculations when describing the (e, 2e) reaction to the ground states of argon and helium ions. This gives us confidence in using the single-particle wave functions from these calculations to construct our basis.

In the (e, 2e) reaction we are mainly concerned with states of the ion. In the shell-model calculation of Luyken, the argon-ion states with total angular momentum and parity $\frac{3}{2}-$ and $\frac{1}{2}-$ (which are not distinguished in the model because spin-orbit coupling is omitted) had only one numerically significant configuration, $3p^{-1}$. Ion states with total angular momentum and parity $\frac{1}{2}+$ had three numerically significant configurations. Luyken's example is the eigenstate at 29.3 eV. The coefficients $b_\sigma(\beta)$ for these configurations are shown in Table I. Other coefficients are numerically insignificant.

The Hamiltonian matrix is essentially a 3×3 matrix, so it has three eigenstates. Three energy levels whose (e, 2e) angular correlations correspond to the knockout of a 3s electron were observed by Weigold, Hood, and Teubner.[2] We will assume that they correspond to the three $\frac{1}{2}+$ eigenstates in the model. Since the numerical values of the coefficients depend on the details of the single-particle wave functions used in the basis, we could expect some differences for dif-

TABLE I. Coefficients $b_{29}(\beta)$ for the three numerically significant configurations in the $\frac{1}{2}+$ eigenstate at 29.3 eV in Ar II, as calculated by Luyken (Ref. 3).

Configuration	$3s^{-1}$	$3p^{-2}\,3d$	$3p^{-2}\,4d$
Configuration index β	0	1	2
Coefficient $b_{29}(\beta)$	0.787 64	−0.555 73	−0.264 16

ferent single-particle models, but they are not expected to be appreciable if the model is valid.

There is a sum rule involving the coefficients $b_\sigma(\beta)$ with which we will be particularly concerned. Multiplying Eq. (2) on the left-hand side by $\Phi'^{*}_\sigma(\alpha)$ and integrating over all space, we use the orthonormality of the independent-particle wave functions $\Phi'_\sigma(\beta)$ to give

$$b_\sigma(\alpha) = \langle \Phi'_\sigma(\alpha) | \Psi'_\sigma \rangle . \qquad (3)$$

The closure relation for the eigenstates Ψ'_σ gives

$$\sum_\sigma [b_\sigma(\alpha)]^2 = \sum_\sigma \langle \Phi'_\sigma(\alpha) | \Psi'_\sigma \rangle \langle \Psi'_\sigma | \Phi'_\sigma(\alpha) \rangle = 1. \qquad (4)$$

We are interested also in defining the single-hole energy level. Denoting the single-hole configuration in the ion by $\beta = 0$, we define the single-hole energy level for states of the same total angular momentum and parity as the expectation value of the ion Hamiltonian H_{ion} for this configuration:

$$E_0 = \langle \Phi'_\sigma(0) | H_{\text{ion}} | \Phi'_\sigma(0) \rangle . \qquad (5)$$

Using the closure relation for the ion eigenstates Ψ'_σ and Eq. (3), we have

$$\begin{aligned} E_0 &= \sum_{\rho\rho'} [\langle \Phi'_\sigma(0) | \Psi'_\rho \rangle \langle \Psi'_\rho | H_{\text{ion}} | \Psi'_{\rho'} \rangle \langle \Psi'_{\rho'} | \Phi'_\sigma(0) \rangle] \\ &= \sum_\sigma [b_\sigma(0)]^2 E_\sigma . \qquad (6) \end{aligned}$$

In view of the sum rule (4), the definition of the single-hole energy level is the average of the eigenstates with the same total angular momentum and parity, weighted by the factors $[b_\sigma(0)]^2$.

The factors $[b_\sigma(0)]^2$ clearly play an important part in the shell model of the ion. They are called the spectroscopic factors.

III. DIFFERENTIAL CROSS SECTIONS

In order to write a Schrödinger equation for the system consisting of the incident electron and the atom, we will label the incident and struck electrons and their associated coordinates and potentials by subscripts 0 and 1, respectively. Antisymmetrization between these particles will be performed later. We will neglect overlaps between these particles and the core of the ion (i.e., the electrons with total quantum numbers $n = 1$ and 2), so that further antisymmetry involving them will not be performed. Independent-particle wave functions are of course antisymmetrized within the set of ion electrons, whose coordinates are collectively denoted by ξ.

The Schrödinger equation for the whole system is

$$\{E - [H_{\text{ion}}(\xi) + K_1 + K_0 + V_1 + V_0 + V_{01}]\} \Psi_{\text{tot}} = 0. \qquad (7)$$

The equation for the ion is

$$[\epsilon_\rho - H_{\text{ion}}(\xi)] \Psi'_\rho = 0. \qquad (8)$$

The kinetic-energy operators for particles 0 and 1 are K_0 and K_1, respectively. The two-electron potential is V_{01}. The potentials between particles 0 and 1 and the ion are, respectively, $V_0(\vec{r}_0, \xi)$ and $V_1(\vec{r}_1, \xi)$. These potentials depend on the ion internal coordinates ξ, since each particle is (weakly) capable of exciting the ion inelastically. We are neglecting the recoil of the ion for simplicity of notation. This is not a necessary approximation.

In order to compute the differential cross section we will expand the total wave function in ion eigenstates $\Psi'_\rho(\xi)$:

$$\Psi_{\text{tot}} = \sum_\rho u_\rho(\vec{r}_0, \vec{r}_1) \Psi'_\rho(\xi). \qquad (9)$$

Substituting (9) into (7), multiplying the left-hand side by Ψ'^{*}_σ, and integrating over ξ, we obtain a set of coupled equations for the channel wave functions $u_\sigma(\vec{r}_0, \vec{r}_1)$:

$$\{E - \epsilon_\sigma - K_1 - K_0 - V_{01}\} u_\sigma(\vec{r}_0, \vec{r}_1) = \sum_\rho V_{\sigma\rho} u_\rho, \qquad (10)$$

where

$$V_{\sigma\rho} = \langle \Psi'_\sigma | V_0(\vec{r}_0) + V_1(\vec{r}_1) | \Psi'_\rho \rangle . \qquad (11)$$

In our model we will neglect the coupling between channels ρ and σ, except insofar as it is included in optical-model potentials $\tilde{V}_0(\vec{r}_0)$ and $\tilde{V}_1(\vec{r}_1)$, which are assumed to be the same for all channels of interest. Optical-model potentials for argon are defined and semiphenomenologically evaluated by Furness and McCarthy.[4] The neglect of explicit coupling between ion excitations is well justified in atomic physics where inelastic cross sections and collective effects such as $E2$ photon transitions are small. The ion excitations are of course described in the optical-model potential for each channel.

In this approximation we have a set of uncoupled equations for each channel σ.

$$(E - \epsilon_\sigma - K_1 - K_0 - \tilde{V}_0 - \tilde{V}_1 - V_{01}) u_\sigma(\vec{r}_0, \vec{r}_1) = 0. \qquad (12)$$

The evaluation of each channel wave function u_σ is a quasi-three-body problem of the type discussed in I. In the $(e, 2e)$ experiment each channel σ is separately excited and is identified by the ion energy level ϵ_σ.

For the entrance channel the wave function for the atom in its ground state may be written

$$\Psi_0(\vec{r}_1, \xi) = A \sum_\rho a_\rho \psi_\rho(\vec{r}_1) \Psi'_\rho(\xi). \qquad (13)$$

In the independent-particle (Hartree-Fock) approximation the sum (13) contains only particle-hole terms, that is, terms in which $\Psi'_\rho(\xi)$ is described only by configurations involving a hole ρ [left by removing the particle whose wave function is $\psi(\rho)$] in the filled configuration of the ion. Other terms in Ψ_0 are called ground-state correlations. If they are negligible the spectroscopic amplitude a_ρ is 1. Otherwise a_ρ is less than 1.

In terms of the expansion (2) of the ion eigenstates ρ we can write

$$\Psi_0 = A \sum_\rho a_\rho \psi_\rho(\vec{r}_1) \sum_\beta b_\rho(\beta) \Phi'_\rho(\beta), \tag{14}$$

where the Hartree-Fock terms are the ones involving only the single-hole configurations $\beta = 0$ corresponding to the ion state ρ.

We will assume that the Hartree-Fock approximation is good for the argon atom (although we will briefly discuss what happens if it is not). In this approximation

$$\Psi_0 = A \sum_\rho \psi_\rho(\vec{r}_1) \Phi'_\rho(0). \tag{15}$$

For the exit channel, in the optical-model approximation (12), where $\vec{k}_A$ and $\vec{k}_B$ denote the momenta of the outgoing electrons,

$$\Psi^{(-)}_{\text{tot}}(\vec{k}_A, \vec{k}_B) = u^{(-)}_\sigma(\vec{k}_A, \vec{k}_B) \Psi'_\sigma(\xi). \tag{16}$$

We can now write the matrix element for the $(e, 2e)$ reaction which is, apart from kinematic factors,

$$M^m_{J\pi} = \langle \Psi^{(-)}_{\text{tot}}(\vec{k}_A, \vec{k}_B) | V_0 + V_{01} | \vec{k}_0, \Psi_0 \rangle. \tag{17}$$

This amplitude can be written immediately from the formal theory of scattering.[5] The ket vector of the matrix element (17) is the state vector of the separated electron-atom system which is the solution of the Schrödinger equation involving all the potentials except V_0 and V_{01}.

Using the approximations (15) and (16) in (17) and factorizing the integral into an integral involving the ion coordinates ξ and a three-body integral, we have

$$M^m_{J\pi} = A \sum_\rho \langle \Psi'_\sigma | \Phi'_\rho(0) \rangle \langle u^{(-)}_\sigma(\vec{k}_A, \vec{k}_B) | V_0 + V_{01} | \vec{k}_0, \psi_\rho \rangle. \tag{18}$$

In the Hartree-Fock approximation for the atom, the index ρ stands for the single-particle indices n, l, j, m in which j and l give the total angular momentum J and parity π of the ion state ρ and m gives the magnetic substate.

Taking the expansion (2) for the observed ion state Ψ'_σ and using the orthonormality of the basis configurations $\Phi'_\sigma(\beta)$ we have

$$M^m_{lj} = b_\sigma(0)(2j+1)^{1/2} T^m_{lj}. \tag{19}$$

The factor $(2j+1)^{1/2}$ comes from the normalization and antisymmetrization of the first factor in (18). The factor T^m_{lj} is the distorted-wave off-shell impulse-approximation amplitude of I.

Note that in the Hartree-Fock approximation for the atom there is no term in the overlap $\langle \Psi'_\sigma | \Phi'_\rho(0) \rangle$ involving basis configurations in Ψ'_σ other than the simple one-hole configurations that we have labeled by $\beta = 0$. If there are ground-state correlations, they give additional terms in (19) with coefficients $a_\rho b_\rho(\beta)$ from the expansion (14) of Ψ_0. Since a_ρ is small, these terms are not expected to be very important in the cross section, but their possibility will not be overlooked.

The differential cross section is given by

$$\sigma = \sum\nolimits_{\text{av}} |M^m_{lj}|^2, \tag{20}$$

where $\sum_{\text{av}}$ denotes the average over initial magnetic substates and the sum over final magnetic substates.

The final form used for computation is

$$\sigma = (2j+1)^2 S_\sigma(0) \sigma_{\text{dw}}, \tag{21}$$

where

$$S_\sigma(0) = [b_\sigma(0)]^2 \tag{22}$$

is the spectroscopic factor for the configuration $\beta = 0$ in the ion state σ, and σ_{dw} is the cross section for the knockout of a single particle in the distorted-wave off-shell impulse approximation:

$$\sigma_{\text{dw}} = f \left| \langle \tfrac{1}{2}(\vec{\kappa}_A - \vec{\kappa}_B) | t_C\{\tfrac{1}{4}|\vec{\kappa}_A - \vec{\kappa}_B|^2\} \right. \\ \left. \times | \tfrac{1}{2}(\vec{\kappa}_0 + \vec{\kappa}) \rangle \right|^2 |\phi_{nl}(\vec{\kappa})|^2. \tag{23}$$

In the absence of a measurement of the absolute cross section, we will ignore the kinematic factor f. The distorted momenta $\vec{\kappa}_j$ are closely related to the experimental momenta $\vec{k}_j$. In fact it was shown in I that they may be equated to $\vec{k}_j$ without loss of accuracy, provided the distortion is accounted for by an over-all attenuation factor, which is again undetermined by the present experiment.

The first factor in (23) is the square of an off-shell Coulomb t-matrix element,[6] which is independent of the azimuthal angle ϕ in the present experimental kinematics in which the energies of the outgoing particles are kept constant and their momenta make constant and equal angles θ with the incident direction. The shape of the differential cross section is thus a direct (and very sensitive) measure of the Fourier transform $\phi_{nl}(\vec{\kappa})$ of the single-particle wave function $\psi_{nl}(\vec{r}_1)$ of the struck electron. [The sum in (20) removes the quantum numbers m by the addition theorem of spherical harmonics and the neglect of spin-orbit coupling makes j a redundant subscript]. These facts were demonstrated in I.

The additional information available here concerns the relative magnitudes of differential cross sections for excitations of different ion eigenstates in the same experiment. These quantities are experimentally measured. Cross sections for ion eigenstates of the same total angular momentum and parity are proportional to the spectroscopic factor $S_\sigma(0)$ which describes the probability of finding the appropriate single-hole configuration in the eigenstate. They can also be compared with cross sections for ion eigenstates of different total angular momentum, where the comparison involves an additional factor $(2j+1)^2$. We can consider that there is one factor of $2j+1$ since there are $2j+1$ chances of removing an electron with angular momentum j. There is another such factor since there are $2j+1$ possible angular momentum projections of the final state.

Essentially we have a means of directly measuring the spectroscopic factors $S_\sigma(0)$, which give us the coefficients $b_\sigma(0)$ in the shell-model expansions (2) of the eigenstates σ. Similar reactions (stripping and pickup) have long been used for a similar purpose in nuclear physics.[7]

IV. SPECTROSCOPIC FACTORS FOR THE ARGON ION

We will assume that the wave function of the ground state of the argon ion consists purely of the configuration $3p^{-1}$. This is suggested by the fact that only one energy level with a $3p^{-1}$ angular correlation is observed in this experiment and also predicted by the shell-model calculation of Luyken.[3] We are therefore assuming that $S_{15.76}(3p^{-1})=1$.

In order to determine meaningful spectroscopic factors we must use a single-particle model and a reaction model that adequately reproduce the angular correlation shape. In Fig. 2 we show that the Hartree-Fock models of Herman and Skillman[8] (HS) and of Fischer[9] (CF), which give indistinguishable theoretical curves, both fit the $3s^{-1}$ data very well for all but the highest measured momentum transfer values. These Hartree-Fock models also gave an excellent fit to the $3p^{-1}$ angular correlation in I. An experimental acceptance angle of 7° has been folded into these calculations.

In order to compare relative magnitudes of cross sections we have chosen to consider $3s^{-1}$ angular correlations at minimum momentum transfer ($\phi=0$) and the $3p^{-1}$ angular correlation at $q=0.717a_0^{-1}$ ($\phi=15°$ for $E=400$ eV). These points are both in the region where the shape is excellently reproduced by the model and they are near maxima so that the effect of folding in the experimental acceptance angle is minimized.

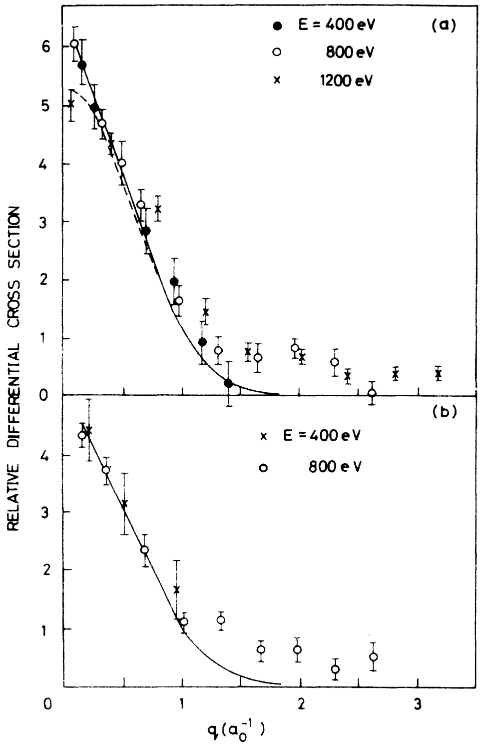

FIG. 2. Relative differential cross sections for the (e,2e) reaction exciting (a) the 29.3-eV level and (b) the two levels at 40 eV. The solid line is the theoretical curve for $E=E_A+E_B=400$ and 800 eV, for which the 7° angular uncertainty has similar effects. The broken line is for $E=1200$ eV, which is more affected by the angular uncertainty.

The $3s^{-1}$ spectroscopic factor for the ion eigenstate at 29.3 eV and the sum of the spectroscopic factors for the two unresolved eigenstates at 40 eV are shown in Table II for both single-particle models. The spectroscopic factor $S_{29.3}$ of Luyken's calculation is 0.62.

The sum of the spectroscopic factors is 0.92 ± 0.07 for CF and 0.96 ± 0.07 for HS. Both satisfy the sum rule within experimental error. We may in fact expect the sum of the spectroscopic factors to be less than 1 for two reasons. First, there may be appreciable ground-state correlations in the argon atom. Second, there certainly are more than three ion eigenstates with a contribution from the $3s^{-1}$ independent-particle configuration, although these contributions are small. It remains to be seen whether such effects can be identified in more accurate future experiments.

So far the CF and HS Hartree-Fock calculations give indistinguishable results. However they can

TABLE II. Relative cross sections and spectroscopic factors [assuming $S_{15.76}(3p^{-1})=1$]. The different single-particle models are described by CF [Fischer (Ref. 9)] and HS [Herman and Skillman (Ref. 8)].

Ion state	Relative cross section (Expt., $E=400$ eV)	S_{CF}	S_{HS}
$3p^{-1}$	0.945 ($\phi=15°$)	1	1
$3s^{-1}_{29.3}$	0.34 ($\phi=0°$)	0.50 ± 0.05	0.52 ± 0.05
$3s^{-1}_{40}$	0.26 ($\phi=0°$)	0.42 ± 0.04	0.44 ± 0.04

be distinguished by applying Eq. (6) for the experimental single-hole energy level, which can be rewritten as

$$E_0=\sum_\sigma S_\sigma(0)E_\sigma.$$

The experimental $3s^{-1}$ level, computed as the centroid of the relevant ion levels using HS spectroscopic factors, is 34 ± 1 eV, while the HS Hartree-Fock eigenvalue is 28.7 eV. These are inconsistent. The corresponding values for CF are consistent. They are, respectively, 34 ± 1 and 34.8 eV.

V. CONCLUSIONS

We have derived a model for the (*e*, 2*e*) reaction leaving the ion in a particular resolved eigenstate. In the model the differential cross section is proportional to a spectroscopic factor describing the probability of finding a particular single-hole configuration in the ion eigenstate. The shape of the angular correlation is given by the distorted-wave off-shell impulse approximation.

The shape of the angular correlation has previously been shown to be very sensitive to the detailed shape of the single-particle wave function used in the calculation. This provides one criterion for the "correct" wave function.

Another criterion, which depends both on the validity of the reaction model and the single-particle model, is that the spectroscopic factors should sum to 1. The spectroscopic factors for $3s^{-1}$ configurations in the only three eigenstates of the argon ion that are observed to have the $3s^{-1}$ angular correlation shape are independently determined relative to that for the ground state, which is assumed to be 1, since only one such eigenstate is observed. Their sum is 1, within experimental error, for two sets of Hartree-Fock wave functions (CF and HS) that give equally good fits to angular correlations.

The experimental position of the single-hole energy level is defined to be the centroid of all the eigenstates containing the corresponding single-hole configuration, weighted by the spectroscopic factors. In the case of the argon ion the Hartree-Fock $3s^{-1}$ energy level is consistent with the experimental determination for the CF wave functions but not for HS.

This analysis leaves several questions to be answered. If the sum of the spectroscopic factors is 0.92, where is the missing 8%? If it is mostly in remaining ion eigenstates whose cross sections are too small to show up in the present experiments, more accurate future experiments may reveal it. If it is mostly in ground-state correlations of the argon atom, such terms would give $3d^{-1}$ and $4d^{-1}$ angular correlations, which would slightly distort the $3s^{-1}$ shape. It is unlikely that the small distortion due to an 8% effect could be experimentally distinguished.

A more serious problem is perhaps the fact that the theory gives a noticeably worse fit to high-momentum components for $3s^{-1}$ argon states than it does for the least-bound single-particle states in helium ($1s^{-1}$) and argon ($3p^{-1}$). In view of the accuracy of the theory in these cases it is difficult to see why it should be inaccurate in the $3s^{-1}$ case. It is tempting to believe the theory and speculate that the Hartree-Fock calculation gives an inferior 3*s* wave function for very small values of the radial coordinate, where the rapid oscillation of the function is responsible for high-momentum components. We have checked that sufficiently high-momentum components do not come from $3d^{-1}$ or $4d^{-1}$ excitations that could result from possible ground-state correlations of the argon atom.

Finally, it is worth noting that although the $3p^{-1}$ and $3s^{-1}_{29.3}$ excitations have been observed in photoelectron spectroscopy,[10] the ionic states with separation energy near 40 eV have not been observed.

---

[*] Work supported by the Australian Research Grants Committee. One of us (S.T.H.) acknowledges the receipt of a Commonwealth postgraduate research award.

[1] S. T. Hood, I. E. McCarthy, P. J. O. Teubner, and E. Weigold, Phys. Rev. A 8, 2494 (1973).

[2] E. Weigold, S. T. Hood, and P. J. O. Teubner, Phys. Rev. Lett. 30, 475 (1973).

[3] B. F. J. Luyken, Physica 60, 432 (1972).

[4] J. B. Furness and I. E. McCarthy, J. Phys. B (to be published).

[5] M. Gell-Mann and M. L. Goldberger, Phys. Rev. 91, 398 (1953).

[6] W. F. Ford, Phys. Rev. 133, B1616 (1964); J. Math. Phys. 7, 626 (1966).

[7] M. H. Macfarlane and J. B. French, Rev. Mod. Phys. 32, 567 (1960).

[8] F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, New York, 1963).

[9] C. Froese-Fischer, At. Data 4, 302 (1972).

[10] K. Siegbahn, C. Nordling, G. Johansson, J. Hedman, P. F. Hedén, K. Hamrin, U. Gelius, T. Bergmark, L. O. Werme, R. Manne, and Y. Baer, *ESCA Applied to Free Molecules* (North-Holland, Amsterdam, 1969).