Factorized distorted-wave approximation for the $(e,2e)$ reaction on atoms: Noncoplanar symmetric*

A. J. Dixon, I. E. McCarthy, C. J. Noble, and E. Weigold
Institute for Atomic Studies, The Flinders University of South Australia, Bedford Park, South Australia 5042, Australia
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Angular and energy correlations for electrons produced in the ionization of neon and xenon by electrons with energies between 400 eV and 2.5 keV have been measured using symmetric noncoplanar kinematics. The reaction yields information about the atomic orbitals and their correlations when analyzed with the distorted-wave off-shell impulse approximation. In the past, either plane waves or various eikonal approximations have been used for the distorted waves, and in the cases where the eikonal parameters are approximately related to elastic scattering, the spectroscopic sum rule has been approximately verified. In the present work, calculations have also been carried out using partial-wave-expanded optical-model wave functions which describe the elastic scattering in detail. The detailed calculation confirms the spectroscopic sum rule, and hence the validity of the structure determination in the case of neon. For xenon the full distorted-wave calculation gives a much improved fit to the shape of the cross section, but overestimates the effect of absorption, and hence underestimates the cross section for ejecting an electron from the valence s state. The plane-wave and eikonal approximations considerably overestimate the magnitude of the valence s-orbital cross section relative to the probability of ejecting an outer p electron. The latter two approximations improve as the energy is increased, but they are still inadequate for neon at 2.5 keV.

I. INTRODUCTION

The $(e,2e)$ reaction, particularly in the noncoplanar symmetric arrangement,[1] has been used for several years[1,2] as a probe for independent-particle wave functions of atoms and their correlations. An approximation for the differential cross section, the distorted-wave off-shell impulse approximation, has been derived from first principles with certain explicit approximations.[2] Essentially the reaction amplitude is treated as a linear combination of quasi-three-body amplitudes with coefficients given by the overlap of the atom and ion wave functions, expressed in terms of configuration interaction between different basis configurations built on the Hartree-Fock wave function. The three bodies are two electrons and a core.

The electron-electron interaction is included in the form of the Mott-scattering t matrix. The electron-core interactions are optical-model potentials. The electron-atom optical model has been derived by Furness and McCarthy[3] and applied with success to inert-gas atoms at incident energies from 20 to 3000 eV.[4] The distorted waves are thus quite thoroughly understood, and we have confidence in the calculation of optical-model potentials for ions, even though electron-ion elastic scattering experiments cannot be performed for confirmation.

Up to the present stage, simplified approximations have been made for the distorted waves in the form of an averaged eikonal approximation. They are treated as plane waves with a complex wave number whose values are obtained from optical-model wave functions.[5] In this approximation the reaction amplitude factorizes into the product of a distorted-wave transform of the atom-ion overlap function and the appropriate half-off-shell t-matrix element for Mott scattering.

While this approximation has proved by experience to yield the required structure information, the question remains whether the reaction mechanism can be thoroughly understood in terms of a better calculation.

The present work replaces the eikonal approximation for the distorted waves by fully partial-wave-expanded distorted waves calculated by solving the optical-model Schrödinger equation. The factorization into a distorted-wave transform and a t-matrix element is retained, since to remove it requires the evaluation at least of a nine-dimensional integral including the transformation from particle coordinates to relative and center-of-mass (c.m.) coordinates, because of the nonlocal nature of the t matrix. The present calculation involves a three-dimensional integration.

The object of the work is to see whether the spectroscopic value of the reaction is maintained with the more detailed calculation. In particular, it has been found[2] that the spectroscopic sum rule is not satisfied by comparison between s- and p-valence orbitals of inert gases when plane waves are used for analysis. In the eikonal approximation greater attenuation was needed for the more-tightly-bound s states. This is physically reasonable, but the eikonal-approximation parameters could not be directly derived from elastic scattering cross sections. An improved eikonal (phase-

distorted) approximation, which can be directly used to calculate elastic cross sections, was used to confirm the sum rule, but this was considered only as an interim measure, until the present calculation could be completed. The satisfaction of the spectroscopic sum rule is a very strict confirmation of the validity of the reaction theory and the structure ingredients of the theory. In order to provide a stringent test of the theory, experimental measurements have been carried out over a wide range of energies for both the light atom, neon, and the heavy atom, xenon.

Section II introduces the basic formalism. Section III deals with the computational details. Section IV discusses the experimental arrangement, and Sec. V, the noncoplanar symmetric reactions. The applicability of the spectroscopic sum rule is verified for neon, so that the value of the reaction as a spectroscopic tool is confirmed for light elements. In the case of xenon, the full calculation overestimates the absorption of electron waves for the valence s state.

II. FORMALISM FOR THE $(e,2e)$ AMPLITUDE

Previous derivations of the $(e,2e)$ amplitude[2] have concentrated on the optical-model aspect of the problem. A multichannel formalism was used to show how the potentials for the electron-atom entrance channel and the electron-ion distorted waves are related to the optical-model potential for elastic scattering in the appropriate two-body subsystems. The approximation of using the optical model for free two-body elastic scattering at the two-body energy involved in the $(e,2e)$ reaction was justified. Antisymmetry was treated in rather an *ad hoc* fashion and core excitation, i.e., inelastic scattering of the incident and scattered electron by the ion, was, of course, ignored.

It is possible to shed some light on the question of antisymmetry by dropping consideration of real and virtual excitations into channels other than $(e,2e)$ and considering ionization simply as a Hartree-Fock problem in which independent-particle states in the continuum are allowed for the two electrons concerned in the knockout process, but the remaining electron core remains in its ground state.

The ionization amplitude in this approximation has been given by Rudge.[6] It is, in a distorted-wave representation,

$$f(\vec{k}_A,\vec{k}_B) = -(2\pi)^{-5/2} n_j^{1/2} \int dx_1,\ldots,dx_n \left[\psi^*(x_3,\ldots,x_{n+1})(1-P_{12})\chi_A^{(-)*}(\vec{k}_A,x_1)\chi_B^{(-)*}(\vec{k}_B,x_2)\right.$$
$$\left. + (n_j-1)\psi^*(x_1,x_4,\ldots,x_{n+1})\chi_A^{(-)*}(\vec{k}_A,x_2)\chi_B^{(-)*}(\vec{k}_B,x_3)\right]$$
$$\times V\Psi^{(+)}(\vec{k}_0,x_1,\ldots,x_{n+1}) . \tag{1}$$

In this equation n_j is the number of equivalent electrons of angular momentum j that can be knocked out, V is the difference between the total Hamiltonian and the distorted-wave Hamiltonian, the coordinates x_i include position and spin, and P_{12} is the exchange operator. The momenta of the electrons in detectors A and B are $\vec{k}_A, \vec{k}_B$ and the incident momentum is $\vec{k}_0$. The effective charges Z_A, Z_B introduced by Rudge[6] to take account of the Coulomb forces in the three-body final state will be discussed in the following paper.[7] They make a negligible difference with noncoplanar symmetric kinematics.

The first term in Eq. (1) may be reduced to the factorized distorted-wave off-shell impulse approximation by the methods of Ref. 2. Making the Hartree-Fock approximation for the closed-shell target state

$$f(\vec{k}_A,\vec{k}_B) = [S_j^{(f)} n_j]^{1/2} \langle \vec{k}' \,|\, T_M(E_{k'}) \,|\, \vec{k}\rangle$$
$$\times \langle \chi_A^{(-)}(\vec{k}_A)\chi_B^{(-)}(\vec{k}_B) \,|\, \psi_j(\epsilon_f)\chi_0^{(+)}(\vec{k}_0)\rangle , \tag{2}$$

where the spectroscopic factor $S_j^{(f)}$ is the probability for finding the single-hole configuration $\psi_j^\dagger$ in the many-body wave function of the final ion state f. The final state is experimentally identified by its separation energy ϵ_f. The momentum variables in the matrix element of the Mott-scattering t matrix T_M are

$$\vec{k} = \tfrac{1}{2}(\vec{k}_A - \vec{k}_B), \quad \vec{k}' = \tfrac{1}{2}(\vec{k}_0 + \vec{q}) , \tag{3}$$

where $\vec{q}$ is the measured recoil momentum

$$\vec{q} = \vec{k}_0 - \vec{k}_A - \vec{k}_B . \tag{4}$$

The spectroscopic sum rule, which we regard as a crucial test of the theory is

$$\sum_f S_j^{(f)} = 1 . \tag{5}$$

Before antisymmetrization, the incident electron is labeled by 1, the knocked-out electron by 2, and the remaining (core) electrons by $3,\ldots,n+1$. The interaction V consists mainly of the Cou-

lomb potential v_{12}. The second term in Eq. (1) involves the knock-on of particle 3 from the core by particle 1. This amplitude involves the overlap of a continuum function $\chi_B^{(-)}(\vec{k}_B, x_3)$ with a Hartree-Fock orbital $\psi_3(x_3)$. Since the optical-model potential consists mainly of the Hartree-Fock potential (with exchange and polarization potentials added), this overlap is small. The second term is dropped from the calculation. The amplitude is computed according to Eq. (2).

III. COMPUTATIONAL DETAILS

The second factor in the matrix element (2) is expanded in partial waves to give

$$\langle \chi_A^{(-)}(\vec{k}_A)\chi_B^{(-)}(\vec{k}_B) \,|\, \psi_j(\epsilon_f)\chi_0^{(-)}(\vec{k}_0)\rangle = (4\pi)^{3/2}\sum_{l_1}\hat{l}_1\exp(i\sigma_{l_1})\sum_{l_2}\hat{l}_2\exp(i\sigma_{l_2})$$
$$\times\sum_{l}\hat{l}^{-2}C^{l_1 l_2 l}_{000}Y^{l_1 l_2}_{lM}\sum_{l_0} i^{l_0-l_1-l_2}\hat{l}_0^2 C^{l_0 L l}_{0MM}C^{l_0 L l}_{000}\hat{L}v^{l_1 l_2}_{l_0 L}\,, \qquad (6)$$

where the Coulomb phase shift is σ_l, $C^{l_1 l_2 l_3}_{m_1 m_2 m_3}$ is a Clebsch-Gordan coefficient, $\hat{l}=(2l+1)^{1/2}$, and the distorted waves are written, ignoring spin-orbit coupling, as

$$\chi_0^{(+)}(\vec{k},\vec{r}) = (4\pi)^{1/2}\sum_l i^l R_l(k,r)\hat{l}Y_l^0(\hat{r})\,,$$
$$\chi_l^{(-)*}(\vec{k},\vec{r}) = 4\pi\sum_{l,m} i^{-l}\exp(i\sigma_l)R_l(k,r)Y_l^m{}^*(\hat{k})Y_l^m(\hat{r})\,. \qquad (7)$$

The radial integrals are

$$v^{l_1 l_2}_{l_0 L}(k_A,k_B,k_0) = \int_0^\infty r^2\,dr\,R_{l_1}(k_A,r)R_{l_2}(k_B,r)$$
$$\times R_{l_0}(k_0,r)R_{nLj}(r)\,. \qquad (8)$$

The bound-state orbital is also written by neglecting spin-orbit coupling as

$$\psi_j(\epsilon_f,\vec{r}) = R_{nLj}(r)Y_L^M(\hat{r})\,, \qquad (9)$$

and the bispherical harmonic for the final state is

$$Y^{l_1 l_2}_{lM}(\hat{k}_A,\hat{k}_B) = \sum_m C^{l_1 l_2 l}_{mM-mM}Y_{l_1}^m(\hat{k}_A)Y_{l_2}^{M-m}(\hat{k}_B)\,. \qquad (10)$$

The atomic bound-state wave functions are the Hartree-Fock orbitals of Clementi and Roetti.[8] They are used, not only for the bound-state orbitals in (2), but also for computing the optical-model potentials[4] for the distorted waves. For entrance-channel distorted waves we use the Hartree-Fock orbitals for the neutral atom. For exit-channel distorted waves we use the Hartree-Fock orbitals for the ion with the hole in the appropriate orbital.

The optical model has two parameters, the static polarizability α and the energy-dependent imaginary potential W. For neutral atoms these have been determined[4] from elastic scattering. For the ion we assume that they are the same as for the neutral atom at the same energy.

For very high energies it is not possible to include enough partial waves in the calculation to obtain complete convergence. Convergence is complete at 400 eV, and even at 800 eV for angles where the cross section is large. A correction is applied for higher energies, which is based on the fact that the plane-wave amplitude can be computed exactly. The corrected amplitude T_C is given in terms of the partial-wave-expanded distorted- and plane-wave amplitudes $T_{\rm DW}$ and $T_{\rm PW}$, and the exact plane-wave amplitude $T_{\rm PWEX}$, by

$$T_C = T_{\rm DW} + (T_{\rm PWEX} - T_{\rm PW})\,. \qquad (11)$$

Where the correction term is small, we may expect T_C to be a good approximation to the distorted-wave amplitude.

The averaged eikonal approximation has been computed for comparison purposes. Here the distorted waves are approximated by

$$\chi^{(\pm)}(\vec{k},\vec{r}) = \exp(-\gamma kR)\exp[i(1+\beta\pm i\gamma)\vec{k}\cdot\vec{r}]\,. \qquad (12)$$

The wave-number modification and attenuation parameters β and γ are given in terms of effective constant optical-model potentials $\overline{V}$ and $\overline{W}$ by

$$\beta + i\gamma = (\overline{V} + i\overline{W})/2E\,. \qquad (13)$$

The parameter R normalizes the wave function to 1 on the scattering axis just before the beam enters the potential. Experience with the coplanar symmetric reaction[7] suggests that reasonable parameter values are

$$R = 3.8 \text{ a.u.},\quad \overline{V} = 10 \text{ eV},\quad \overline{W} = 5 \text{ eV}\,.$$

These values are used throughout the work.

In the experimental data one normalization constant is not measured at each incident energy. All data at a given energy are determined relative to each other. Theory and experiment are normalized to the same value at the forward p-state peak in all cases since the p-state spectroscopic factors are 1.

IV. EXPERIMENTAL METHOD

The experiments were carried out using the noncoplanar symmetric geometry, first used by Weigold *et al.*,[1] in which the two emitted electrons have equal energies and make equal angles with respect to the incident direction. Since the experimental apparatus and technique have been described in detail in Ref. 2, a description need not be repeated here. In brief, electrons from an electron gun crossed a beam of neon or xenon (>99.99% purity), and the two outgoing electrons passed through detectors at an angle of 42.3° relative to the incident direction. Each detector consisted of a retarding lens, cylindrical mirror analyzer, and channel electron multiplier. The angular correlations between the emitted electrons were then obtained by changing the azimuth of one of the detectors. The angular resolution was approximately 1.5° FWHM. In any experimental run the total energy $E = E_A + E_B = E_0 - \epsilon$ was kept fixed. Separation energy spectra were obtained by varying the incident energy keeping the angles fixed.

Owing to the large number of spurious collisions, it is necessary to detect the two electrons in coincidence. The fast coincidence technique used has also been fully described in Ref. 2.

V. RESULTS AND INTERPRETATION

The first example chosen is neon, since its spectroscopy is extremely simple. In all inert gas ions the valence p-orbital is not detectably split among ion eigenstates.[2] In neon the valence s-orbital is not significantly split either and it is therefore ideal for testing the spectroscopic sum rule.

Figure 1 shows the separation energy spectrum obtained for neon at 1200 eV. The energy resolution has been set at 3.5 eV FWHM. Two $\frac{1}{2}+$ ion states are observed, with dominant configurations of $1s^2 2s 2p^6$ and $1s^2 2s^2 2p^4 3d^1$ with, respectively, 96% and 4% of the $2s^{-1}$ strength. The $1s^2 2s^2 2p^4 3s$ ion state is not measurable excited. Of the negative parity ion states, only the $2p^{-1}$ ground state is significantly excited.

Figure 2(a) shows the momentum distribution (angular correlation) for the $2p$ state of neon at 2500, 1200, and 600 eV. The distorted-wave (full line) and eikonal and plane-wave approximations are arbitrarily normalized to the forward (in c.m.) maximum in the $2p$ q distribution at each energy. Since the experiment does not measure absolute cross sections, the distorted-wave calculation is used to give the absolute scale, except at 2500 eV, where the absolute scale is given by the plane-wave calculation. Although the magnitudes of the cross sections calculated by the eikonal and plane-wave

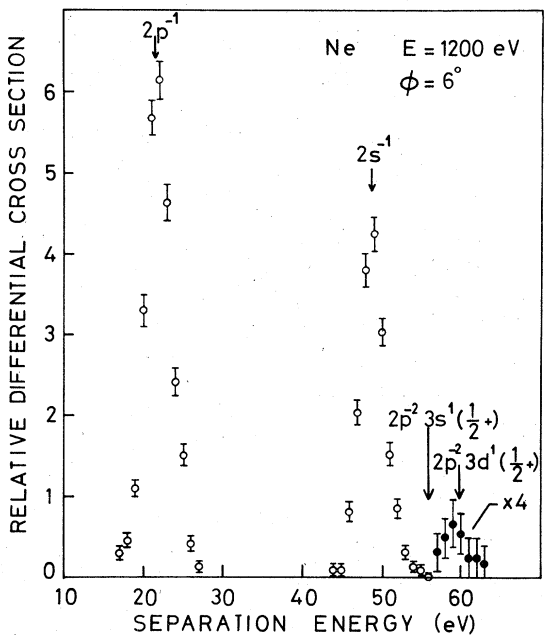

FIG. 1. Differential cross section for the 1200-eV $(e,2e)$ reaction on neon at $\phi = 6°$ and $\theta = 42.3°$ plotted against separation energy. The arrows indicate the positions of various ion states, labeled by the configuration with the largest CI coefficient.

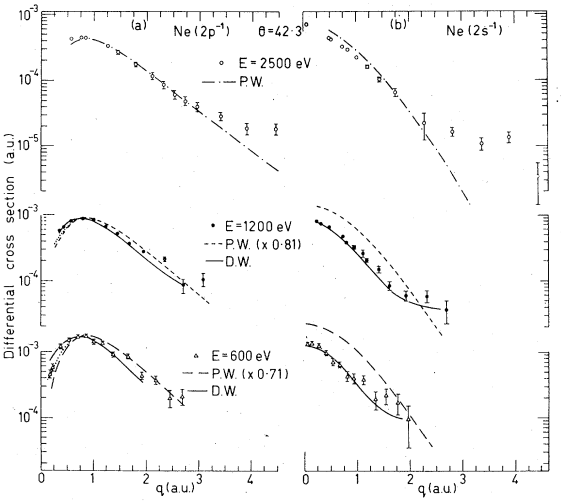

FIG. 2. Neon $2p$ and $2s$ cross sections (in units of a_0^2/hartree sr^2) at 600, 1200, and 2500 eV in the noncoplanar symmetric geometry plotted as a function of the recoil momentum q (in units of a_0^{-1}). The $2p$ data have been normalized to the forward $2p$ peak in the distorted-wave (DW) calculation at 600 and 1200 eV, and to the plane-wave (PW) calculation at 2500 eV. The eikonal approximation gives a cross section whose magnitude is less than that given by the plane-wave approximation but the shapes are nearly indistinguishable except at low energy and q for the $2p$ transition, where the dotted curve indicates the eikonal result.

approximations are different, they give nearly indistinguishable shapes, and therefore only the plane-wave calculation is shown in detail in Fig. 2. At low q, the eikonal approximation shape is given by the dotted curve. The shape of the distorted-wave approximation fits the data excellently. The eikonal and plane-wave approximations are slightly worse at forward angles, but essentially equivalent. At 2500 eV, only the eikonal and plane-wave calculations (indistinguishable) were carried out, since the full distorted-wave calculation would require too many partial waves for convergence. The finite experimental angular resolution has not been included in the calculations shown in Fig. 2. Its inclusion leads to a small increase in the cross section at values of q close to zero.

The corresponding 2s information is shown in Fig. 2(b). The experimental points are those obtained for the 48.5-eV $2s^{-1}$ ion eigenstate, which contains $96 \pm 2\%$ of the 2s strength. The 2s cross section is measured relative to the 2p cross section at any energy. We see the essential improvement in shape and magnitude introduced by the distorted waves. With respect to shape, the eikonal and plane-wave approximations are again very similar and they underestimate the high-q cross section, but the distorted-wave approximation is essentially correct. The normalization of the theoretical curves was determined by fitting the 2p peaks. Therefore the magnitude fit of the 2s theoretical curves is significant. In fact it is the most important information available from the present work, since it tells us whether the spectroscopic sum rule is satisfied.

Table I lists the 2p:2s cross section ratios at 400 eV at several angles ϕ. The corresponding q values are also included in the table. The distorted-wave calculation is in very good agreement with the data, whereas the plane-wave and eikonal approximations are in serious disagreement with the data, the eikonal approximation being marginally better. Since the 2s and 2p strengths in neon are not significantly split, the excellent cross-section ratios given by the distorted waves at 400 eV

TABLE I. Observed and calculated neon 2p:2s (e, 2e) noncoplanar symmetric cross-section ratios at 400 eV as a function of the azimuthal angle ϕ. The finite angular resolution of approximately 1.5° full width at half maximum (FWHM) has not been included in the calculations.

ϕ (deg)	$q(2p)$ (a.u.)	$q(2s)$ (a.u.)	$\sigma(2p^{-1})/\sigma(2s^{-1})$ Expt.	DW	PW	Eik.
0	0.1	0.07	0.38 ±0.08	0.66	0.03	0.09
5	0.25	0.23	1.0 ±0.2	1.04	0.17	0.21
15	0.68	0.67	2.64 ±0.25	2.83	0.89	0.97

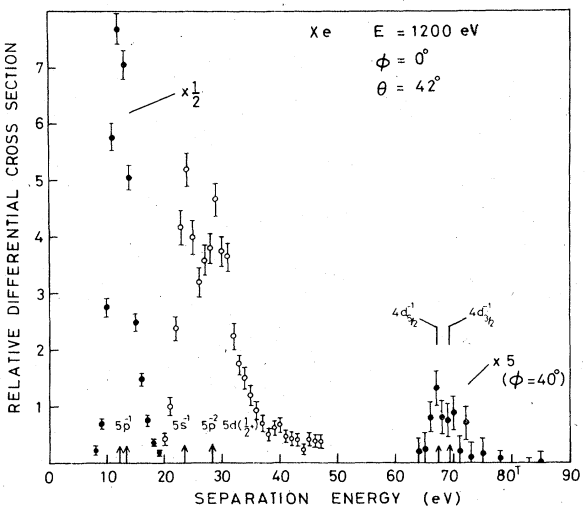

FIG. 3. Differential cross section for the 1200-eV symmetric (e, 2e) reaction on xenon at $\phi = 0°$ (and 40°) plotted against the separation energy. The positions of various ion states, labeled by their dominant CI configuration, are indicated by arrows.

(Table I) and at 600 and 1200 eV (Fig. 2), confirm the spectroscopic sum rule and thus the whole analysis.

It is interesting to see the improvement of the plane-wave (and eikonal) approximation as the energy increases and the distorted waves become more nearly plane waves. The shape of the eikonal approximation profile reflects the region of space in which $\overline{V} = 10$ eV is a good approximation to the distorting potential. This is in the long-range (low-momentum) region. The deep interior distorting potential introduces high recoil momentum components due to transfer of momentum to the ion by elastic interaction with the ingoing and outgoing electrons. The eikonal and plane-wave approximations seriously underestimate this effect, but it is well described by distorted waves. This is particularly noticeable for the 2s state.

Figure 3 shows the separation energy spectrum obtained for xenon at 1200 eV. The strength of the 5p orbital is essentially all contained in the $5p^{-1}_{3/2}$ and $5p^{-1}_{1/2}$ ion eigenstates. The spin orbit splitting of 1.3 eV between the $5p^{-1}(3/2-)$ ion ground state and the $5p^{-1}(1/2-)$ state has been observed, and the cross-section ratio has been measured,[2,9] to be 2:1, in agreement with the relative statistical weights. The 5s orbital is, however, significantly split between a number of ion eigenstates, with separation energies extending up to at least 48 eV. The $\frac{1}{2}+$ ion state of lowest energy ($\epsilon = 23.3$ eV) contains only 34% of the $5s^{-1}$ orbital strength. This is found to be independent of energy over the range of energies 200 to 1200 eV.[2] Higher-resolution

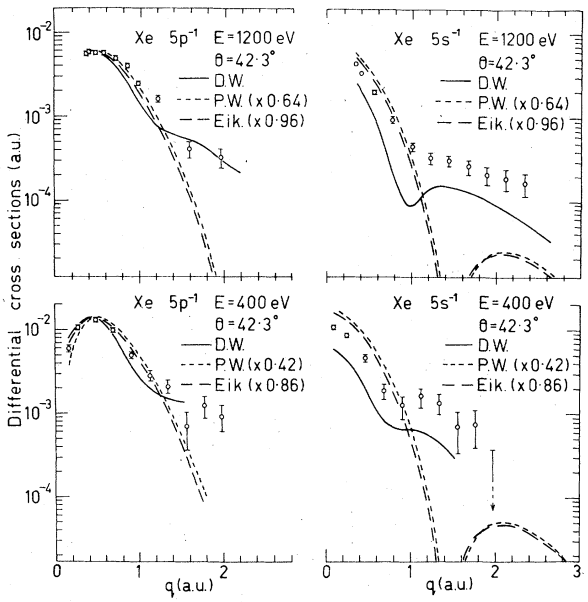

FIG. 4. Differential cross section (in a_0^2/hartree sr^2) for the 400- and 1200-eV noncoplanar symmetric $(e,2e)$ $5p$ and $5s$ xenon transitions plotted as a function of the recoil momentum q (in units of a_0^{-1}). The experimental data have been normalized by fitting the peak in the $5p$ data to the corresponding distorted-wave result (full curve). The results of the plane wave (PW) and eikonal (Eik.) approximations have also been normalized to the maximum in the $5p^{-1}$ DW cross section.

separation-energy spectra[2,9] identify some of the higher-energy $\frac{1}{2}+$ ion eigenstates excited in the reaction. At high q and separation energies of approximately 70 eV excitation of ion eigenstates can be observed corresponding to the removal of an electron from the $4d$ orbital. These states will not be further discussed in the present work.

Figure 4 shows the momentum distributions obtained at 400 and 1200 eV for electrons ejected from the $5p$ and $5s$ orbitals of xenon. The data are again compared with the cross sections calculated with the distorted-wave (full line) and eikonal and plane-wave approximations. The data have been normalized to the $5p^{-1}$ distorted-wave calculations. The $5s^{-1}$ experimental cross section (summed over all the states belonging to the $5s^{-1}$ representation) has been measured relative to the corresponding $5p^{-1}$ cross section.

The q distribution for the $5p^{-1}$ state at both 400 and 1200 eV is fitted very well by the distorted-wave calculation at low and high momenta, but at intermediate momenta the distorted waves underestimate the cross section. On the other hand, at 400 eV the plane-wave and eikonal approximations overestimate the cross section at intermediate momenta. This is particularly so for the plane-wave approximation. Both seriously underestimate the high-q cross section at 400 and 1200 eV.

The plane-wave and eikonal approximations give a $5s^{-1}$ cross section which is significantly too large at low and intermediate q at both 400 and 1200 eV, but they far more seriously underestimate the cross sections at high q ($\gtrsim 1$ a.u.). The shape of the experimental cross section is however, very well described by the distorted-wave calculation, although the magnitude of the cross section is underestimated. At $q<1$ a.u., where the cross section is large, the data lie halfway between the plane and distorted-wave calculations.

The results for xenon show that the distorted-wave approximation is again far superior to the eikonal and plane-wave approximations at high q, which corresponds to the inner regions of the atom where distorting potentials are larger. The shape of the cross section given by the eikonal and plane-wave approximations are quite good at low q, that is the outer regions of the atom where the distorting potentials are relatively small. The plane-wave approximation again improves as the energy is increased and distortions become less important.

VI. SUMMARY

We have compared the experimental electron momentum distributions for the noncoplanar symmetric $(e,2e)$ reaction on neon and xenon with calculated momentum distributions over the energy range 400 to 2500 eV. The calculations are all based on the factorized distorted-wave off-shell impulse approximation, using either plane waves, an eikonal approximation, or full partial-wave-expanded optical-model wave functions for the distorted waves.

In the case of neon, the eikonal and plane-wave approximations give nearly indistinguishable results, the shape of the cross section being given by the square of the momentum-space wave function of the two valence orbitals investigated. Both significantly overestimate the magnitude of the $2s$ cross section relative to the $2p$ cross section. Although these approximations improve as the energy is increased, the discrepancy is still serious at 2500 eV. The full calculation, on the other hand, gives a much better fit to both the shape and relative magnitudes of the $2p$ and $2s$ cross sections even at the lowest energy of 400 eV confirming the spectroscopic sum rule. It also therefore confirms the validity of the structure determination in the case of neon.

For the much heavier atom xenon, theory and experiment do not agree as well as for neon. The plane-wave and eikonal approximations again seriously overestimate the valence-s cross section relative to that of the outer p orbital. However, at

high q ($\gtrsim$1.2 a.u.) they very much underestimate the magnitude of both the $5p$ and $5s$ cross sections. The full distorted-wave calculation gives a very good fit to the shapes of both the $5p$ and $5s$ cross sections, but it significantly underestimates the relative magnitude of the $5s$ cross section. This must be due to inadequacies either in the reaction model, or in the optical-model potentials used for deriving the distorted waves. The reaction could, for instance, be much more sensitive to the details of the imaginary potential than is the case for elastic scattering. The deficiency most likely arises from the factorization approximation. Although this approximation is valid in the plane-wave limit, it may not be adequate when using fully distorted waves, even in the noncoplanar case where the t matrix is approximately independent of angle. This conclusion is supported by the coplanar results reported in the following paper. We are at present undertaking a program designed to remove the necessity for assuming factorization of the amplitude.

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

[2]I. E. McCarthy and E. Weigold, Phys. Rep. 27C, 276 (1976).

[3]J. B. Furness and I. E. McCarthy, J. Phys. B 7, 541 (1974).

[4]I. E. McCarthy, C. J. Noble, B. A. Phillips, and A. D. Turnbull, Phys. Rev. A 15, 2173 (1977).

[5]A. Ugbabe, E. Weigold, and I. E. McCarthy, Phys. Rev. A 11, 576 (1975).

[6]M. R. H. Rudge, Rev. Mod. Phys. 40, 564 (1968).

[7]I. Fuss, I. E. McCarthy, C. J. Noble, and E. Weigold, following paper, Phys. Rev. A 17, 604 (1978).

[8]E. Clementi and C. Roetti, At. Data Nucl. Data Tables 14, 177 (1974).

[9]S. T. Hood, A. Hamnett, and C. E. Brion, J. Electron. Spectrosc. 11, 205 (1977).