PHYSICAL REVIEW A VOLUME 13, NUMBER 2 FEBRUARY 1976

Differential cross sections for electron-impact ionization of helium

Tom Burnett, Steven P. Rountree, and Gary Doolen
Physics Department, Texas A&M University, College Station, Texas 77843

W. Derek Robb*
Joint Institute for Laboratory Astrophysics, University of Colorado and National Bureau of Standards, Boulder, Colorado 80302
(Received 6 March 1975; revised manuscript received 29 September 1975)

In an earlier paper a general formulation of differential cross sections for electron-impact ionization of atomic systems, in the Born approximation, was presented. The present work uses this formulation, with simple correlated wave functions, to evaluate various differential cross sections for electron-impact ionization of helium. The results are compared with previous experimental and theoretical data. The favorable agreement obtained with experiment for high incident-electron energies and low ejected-electron energies in both double- and single-differential cross sections is indicative of the agreement which can be expected when the same procedure is applied to the electron-impact ionization of other atoms.

I. INTRODUCTION

Several papers have recently been published on experimental studies of energy and angular distributions in electron-impact ionization of atomic helium. This has stimulated theoretical studies of single- and triple-differential cross sections. Bell, Freeston, and Kingston[1] have used Born and classical impulse approximations to calculate cross sections which are differential in the energy of the secondary electron. Jacobs[2] has calculated the triple-differential cross section using the Born approximation with accurate atomic-state wave functions. However, this calculation involves the uncertain problem of nonorthogonality of initial- and final-state wave functions. Geltman[3] has used the Coulomb-projected Born approximation to calculate similar cross sections, and Schulz[4] has used a product of Coulomb wave functions in the final state with a simplified helium ground-state wave function. He determines the exchange and capture amplitudes as well as the direct amplitude and studies the effect of varying nuclear-screening parameters on the ionization cross section. Kim and Inokuti[18] have extrapolated to threshold the Born cross section for discrete excitations and obtained results for differential ionization cross sections for the ejection of zero-energy electrons. Other calculations in the Born approximation at a restricted number of energies have been performed by Sloan[5] and Omidvar, Kyle, and Sullivan.[6] A review of theoretical and experimental double-differential cross sections is given by Oda.[7]

In the present work we make a detailed comparison with the abovementioned theoretical work, and also with the experimental results of Ehrhardt *et al.*,[8] Opal, Beaty, and Peterson,[9] Crooks,[10] and Oda, Nishimura, and Tahira,[11] and Grissom, Compton, and Garrett.[19] In Sec. II we give a brief discussion of the numerical techniques and physical approximations used, and in Sec. III we present, under separate headings, our results for triple-, double-, and single-differential cross sections.

II. DISCUSSION OF COMPUTATIONAL PROCEDURES

In an earlier paper[12] (hereafter referred to as I) we presented a detailed derivation for Born-approximation triple, single and total ionization cross sections. This theory was applied to the calculation of continuum generalized oscillator strengths for electron-helium ionization, using two sets of atomic-state wave functions.

The better set of wave functions consisted of a four-configuration initial target-state wave function of the form $c_1 1s^2 + c_2 1s\overline{2s} + c_3 \overline{2s}^2 + c_4 \overline{2p}^2$ and a close-coupling final-state continuum wave function. The $1s$ orbital was that of He^+ and the Slater exponents of the $\overline{2s}$ and $\overline{2p}$ orbitals were optimized on the $1\,^1S$ He energy. In the close-coupling wave function the $1s$ channel was included, together with all possible bound-orbital configurations. So we have made significant allowance for electron-correlation effects in the ground state (the present wave function gives 78% of the $1\,^1S$ correlation energy), and because we have used the He^+ $1s$ function, we have allowed for core relaxation in the final state.

In the present work we take the reduced multipole matrix elements evaluated for this set of atomic wave functions and manipulate them, in Eqs. (17) and (18) of I, to obtain triple-, double-, and single-differential cross sections. The reduced matrix elements (like those in Table IV of I), which are a function of momentum transfer K

and energy of the ejected electron, k^2, are fitted by cubic splines. These two-dimensional fits are then used in the interpolations and integrations which are encountered in the calculation of the various cross sections.

The cross section that is differential in the energy and angle of the ejected electron is obtained by integrating Eq. (17) of I over momentum transfer, using analytic formulas for the integrals of cubic splines. The cross section that is singly differential in ejected-electron energy is obtained by using a cubic spline fit to the integrand of Eq. (18) in I. In both cases a spline fit of the matrix elements, in the variable k^2, was performed prior to the spline fit in the variable K, where necessary.

III. DISCUSSION OF RESULTS

A. Triple-differential cross sections

Equation (17) of I can be expressed as an expansion in terms of the spherical-harmonic functions $Y_L^0(\hat{k})$. In Table I we present our values for the coefficients $\beta_{1s,L}(k^2, K)$ of this expansion, for several values of k^2 and K, and compare them with equivalent values of Jacobs.[2] The two calculations agree well, except for low ejected-electron energies in the $L=1$ coefficients. This discrepancy probably arises because we explicitly orthogonalize our continuum $\Psi_j(^1S)$ [see Eq. (22) of I] wave function to the initial state wave function $\Phi_0(^1S)$, while Jacobs retains the nuclear potential in the corresponding Born matrix element to compensate for nonorthogonality of his initial and final ^1S states. We would point out however, that Jacobs[2] obtains more favorable agreement with the experimental binary-to-recoil peak ratio.

TABLE I. The angular-distribution expansion coefficients $\beta_{1s,L}(k^2, K)$ for ionization of helium. The coefficients in square brackets are those of Jacobs (Ref. 2).

k^2 (Ry)	$L=1$	$L=2$	$L=3$	$L=4$	$L=5$
		$K=0.2$ a.u.			
0.2	0.588	2.025	0.449	0.038	0.001
	[0.227]	[1.958]	[0.347]	[0.0346]	[0.003]
0.6	0.641	2.062	0.586	0.097	0.008
	[0.381]	[1.999]	[0.489]	[0.073]	[0.009]
1.0	0.656	2.074	0.640	0.119	0.011
	[0.436]	[2.018]	[0.529]	[0.087]	[0.012]
2.0	0.583	2.070	0.574	0.111	0.010
	[0.458]	[2.034]	[0.529]	[0.089]	[0.012]
		$K=0.4$ a.u.			
0.2	1.068	2.094	0.824	0.142	0.012
0.6	1.162	2.206	1.079	0.323	0.048
1.0	1.190	2.249	1.189	0.407	0.068
2.0	1.092	2.250	1.132	0.412	0.070
		$K=0.6$ a.u.			
0.2	1.446	2.194	1.108	0.289	0.038
0.6	1.562	2.368	1.441	0.568	0.115
1.0	1.606	2.452	1.606	0.732	0.170
2.0	1.535	2.479	1.629	0.808	0.196

In Fig. 1 we show experimental and theoretical triple-differential cross sections for 256.5 eV incident-electron energy. For such an incident energy the Born approximation is marginal. Further, one would expect that there is considerable difficulty in detecting the 3-eV ejected electron. However, we would expect the agreement between the Born results and experiments to be best for higher incident-electron energies ($k_0^2 \geq 500$ eV) and moderate energies of ejection ($k^2 \geq 15$ eV). Consequently, we also present in Fig. 1 the triple-differential cross sections for 500-eV and 1000-eV incident electrons and for 20-eV ejected electrons. This choise of energies is based on the following facts: (a) In our calculation, the overlap between the ^1S initial and final states is small (Table II of I); (b) the ^1S e^-+He^+ phase shifts at these energies are in good agreement with those obtained by Sloan[13] and Burke and Taylor[14]; and (c) comparison between experimental and theoretical double-differential cross sections (Sec. III B) indicate that the experimental difficulties encountered in the detection of the ejected electron at these energies are minimal. Experimental values obtained at these energies would provide a better test of the Born approximation, particularly for electrons ejected about the recoil peak.

B. Double-differential cross sections

In Fig. 2 we present cross sections which are doubly differential in the angle and energy of the ejected electron. In Fig. 2(a) we compare directly with the experimental results of Opal *et al.*[15] and Oda *et al.*[11] of 500 eV incident-electron energy, and ejected electron energies of 27.8, 35.1, and 44.2 eV. In Figs. 2(b)–2(d) we present a comparison with Opal *et al.*[15] for ejected-electron energies of the 4.13, 20.1, and 50.9 eV, and incident energies of 500, 1000, and 2000 eV, respectively. Similar comparisons are made in Fig. 2(e) with the data of Crooks.[10]

For incident energies of 1000 eV and 2000 eV and ejected-electron energies of 20.1 eV and 50.9 eV [Figs. 2(c) and 2(d)], the agreement between experiment and the present work is very good near the maximum. For the ejected-elec-

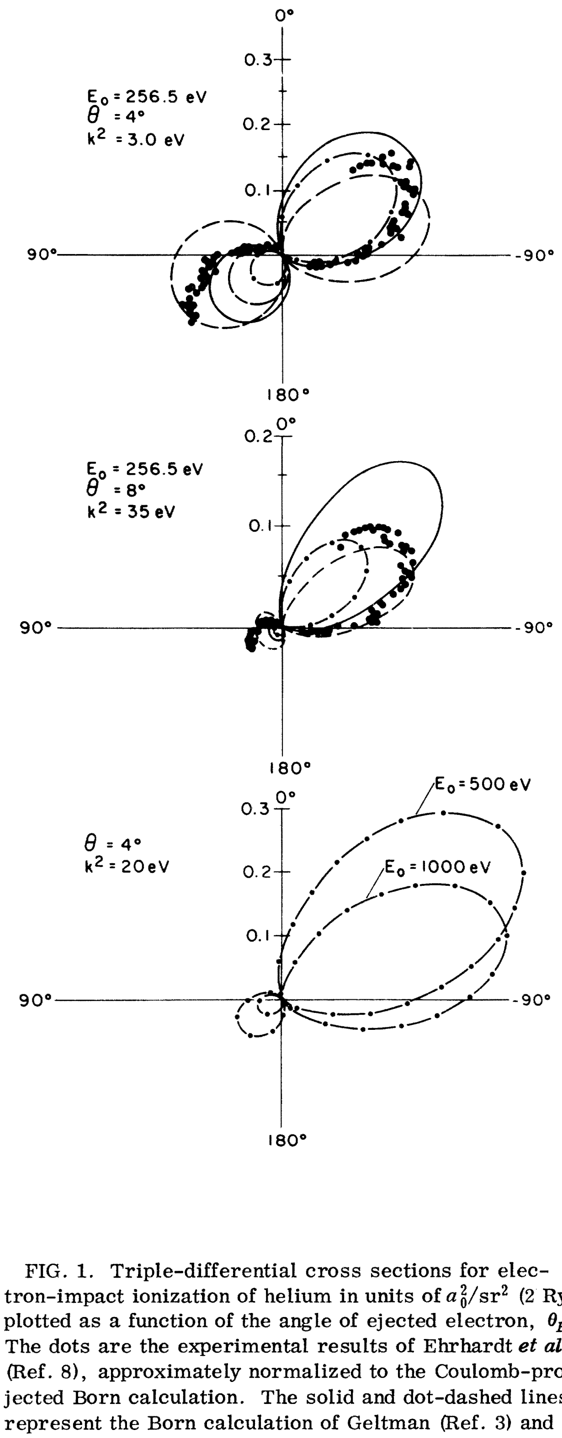

FIG. 1. Triple-differential cross sections for electron-impact ionization of helium in units of a_0^2/sr^2 (2 Ry) plotted as a function of the angle of ejected electron, θ_E. The dots are the experimental results of Ehrhardt ***et al.*** (Ref. 8), approximately normalized to the Coulomb-projected Born calculation. The solid and dot-dashed lines represent the Born calculation of Geltman (Ref. 3) and the present work, respectively; (— - —) represents the work of Jacobs (Ref. 2) which is indistinguishable from the present work in the forward peak; and the long dashed line (— — —) indicates Geltman's Coulomb-projected Born calculation. k^2 is the energy of ejected electron; θ is the angle through which the incident electron is scattered.

tron energy of 4.13 eV, however, we find that the agreement is not quite so good. Since the present approximation is obviously appropriate for the lower ejected-electron energies and high incident-electron energy, we feel that the difference between theory and experiment at these lower ejected-electron energies is attributable to experimental difficulties. The experimental cross sections peak at a slightly greater angle than the Born cross section. This is probably due in part to our neglect of final-state interactions between the continuum electrons.

In both the forward direction (0°–45°) and the backward direction (135°–180°), the agreement between our results and experiments is poor. However, the spread in the experimental results is large and does not yet offer conclusive proof of the failure of the Born approximation for the energies which we have considered.

C. Single-differential cross sections

In Figs. 3(a) and 3(b) we present cross sections which are differential in the energy of the ejected electron alone. Apart from the discrepancies at low ejected-electron energies (0–10 eV), the agreement between our results and the data of Opal *et al*. and Crooks is very good. Below 10 eV the agreement between the present results and the data of Opal *et al.* is within the experimental errors, but it is not very satisfactory. A better indication of the quality of the present results is given by comparison with Kim and Inokuti[18] and Grissom *et al.*[19] Kim and Inokuti extrapolated the cross sections for excitation of discrete levels, to the continuum, and obtained cross sections for ejection of zero-energy electrons. Their results are shown as open circles on Fig. 3(a) and are in excellent agreement with the present results. The total accord of our completely *ab initio* predictions and these semiempirical predictions is a good testimony to the accuracy and adequacy of our wave functions. In particular, we feel that our Born values are much more accurate than the abovementioned experimental values for the differential cross sections involving ejected electrons with less than 10 eV energy.

To lend more weight to this conclusion, we next compare our results with the experimental work of Grissom *et al*. They used a trapped-electron technique specifically designed to collect very low-energy secondary electrons, thus overcoming difficulties and uncertainties encountered in the double-differential cross-section experiments. So we would expect that our results, if correct, would agree closely with the results of this experiment. In order to compare our results, we must calculate

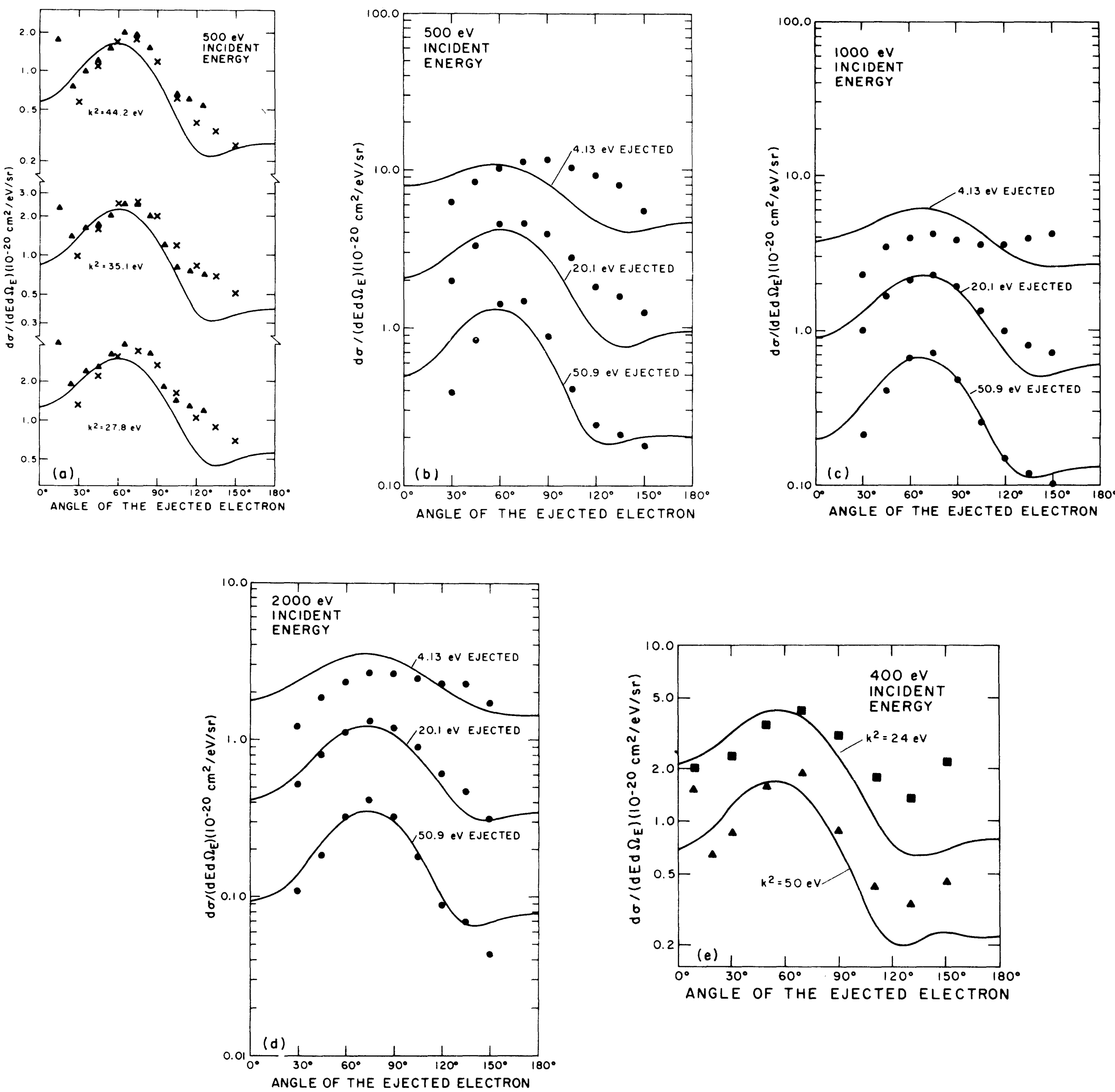

FIG. 2. Double-differential cross sections for electron-impact ionization of helium. In (a) the crosses are the experimental results of Opal *et al.* (Ref. 15), the triangles are the experimental results of Oda *et al.* (Ref. 11), and the solid line is the present work. In (b)-(d), the dots are the experimental results of Opal *et al.* (Ref. 15) and the solid line is the present work. In (e), the squares and triangles are, respectively, the experimental results of Crooks (Ref. 10) for 24-eV and 50-eV ejected electrons.

$$\sigma(E_0,W)=\int_0^W \frac{d\sigma(E_0,\epsilon)}{d\epsilon}\,d\epsilon\,,$$

where E_0 is the energy of the primary electron, $d\sigma(E_0,\epsilon)/d\epsilon$ is the differential cross section for ejection of secondary electrons of energy ϵ, and W is the depth of the trap. We have computed $\sigma(E_0,W)$ for a trap depth of 0.095 eV and our results, which are given in Fig. 3(c), are in excellent agreement with those of Grissom *et al.*

On the basis of this comparison, we conclude that the Born results for ejection of zero-energy electrons breaks down only for incident-electron energies less than 200 eV. The authors of Ref. 20 claim that the Born approximation breaks down for 2000-eV incident electrons and ejected-electron energies less than 13 eV. This is contradictory to the present results and indeed is incor-

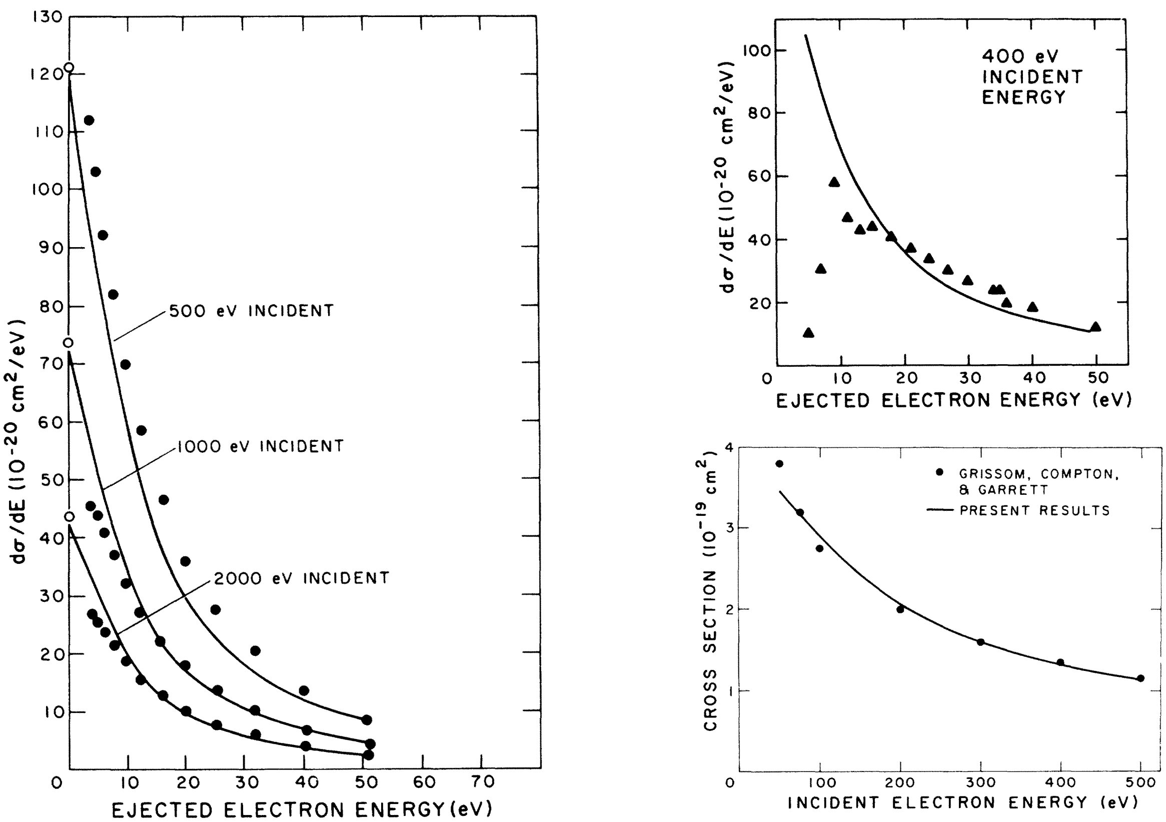

FIG. 3. Single-differential cross sections for electron-impact ionization of helium. The dots are the experimental results of Opal *et al.* (Ref. 15) and the triangles are the experimental results of Crooks (Ref. 15). The open circles are theoretical results of Kim and Inokuti (Ref. 18) for 500-, 1000-, and 2000-eV incident electrons.

rect. The fact that their results are poor in this case is not due to any failure of the Born approximation, but rather to (a) the extreme inadequacy of their Hartree-Fock–Slater wave functions to allow for core relaxation, correlation, and exchange effects in the low-energy ejected-electron situation, and (b) experimental difficulties in the experiment of Opal *et al.*[15]

IV. CONCLUDING REMARKS

It is obvious that the Born approximation has some severe limitations. In particular, initial- and final-state interactions and exchange are neglected. However, the effects of these limitations cannot be studied or fully understood when physically inadequate wave functions are used. The wave functions used in the present work are a considerable improvement over most previous work and they adequately describe such physical effects as initial-state electronic correlation, core relaxation and exchange, distortion, and correlation between the ionic and ejected electrons.

Thus we draw the following conclusions about the Born approximation for e^- +He ionization, on the basis of our results:

(1) For cross sections which are differential in the ejected-electron energy alone, the Born approximation is in excellent agreement with experiment and semiempirical theory, for all ejected-electron energies, even at incident-electron energies of 200 eV.

(2) For cross sections which are differential in both ejected-electron energy and angle, the qualitative agreement between the Born approximation and experiment is excellent. The major quantitative discrepancies occur for ejection angles of less than 30° and greater than 150°, and for low energies of ejection. The angular discrepancy is possibly due to the experimental problems of accurately measuring the lower ejected-electron current in these regions. As for the low-energy discrepancy, there is no reason to suspect that

the Born approximation, with a close-coupling final-state wave function, is invalid for a 2000-eV incident electron and a 4.13-eV ejected electron, and it appears that the problem lies with field effects in the experiments of Refs. 9–11.

(3) For cross sections which are triply differential in the energy and angle of the ejected electron, and the angle of scattering of the incident electron, experiments have not been performed at incident energies high enough to allow fair comparison with Born-approximation results. Where comparison is available, at 256.5 eV incident energy, the agreement (after appropriate normalization of the experimental values) is worst with regard to the size of the backward lobe. This, however, is only significant for low-energy ejected electrons (3 eV) and improves for higher ejected energies. We have presented results for 500-eV and 1000-eV incident electrons and 20-eV ejected electrons with scattering of the incident electrons through 4°. If experiments could be performed at these values, then meaningful statements could be made about the validity of the Born approximation for evaluating triply differential cross sections.

ACKNOWLEDGMENTS

We would like to acknowledge useful discussions with Dr. M. E. Rudd, Dr. N. Oda, Dr. Earl Beaty, Dr. Karl Heinz Hesselbacher, and Dr. Sydney Geltman. This work would not have been possible without a grant of computer time from the National Center for Atmospheric Research, Boulder, which is sponsored by the National Science Foundation. The work was supported in part by the U. S. Air Force Office of Scientific Research under Grant No. AFOSR-73-2484 and by the National Science Foundation under Grant No. 39308X.

*Present address: Los Alamos Scientific Laboratory, P.O. Box 1663, Los Alamos, N. M. 87545.

[1]K. L. Bell, M. W. Freeston, and A. E. Kingston, J. Phys. B 3, 959 (1970).
[2]V. Jacobs, Phys. Rev. A 10, 499 (1974).
[3]S. Geltman, J. Phys. B 7, 1994 (1974).
[4]M. Schulz, J. Phys. B 6, 2580 (1973).
[5]I. H. Sloan, Proc. Phys. Soc. 85, 435 (1965).
[6]K. Omidvar, H. L. Kyle, and E. C. Sullivan, Phys. Rev. A 5, 1174 (1972).
[7]N. Oda, in *Proceedings of the Eighth International Conference on the Physics of Electronic and Atomic Collisions, Belgrade, 1973*, edited by B. C. Čobić and M. V. Kurepa (Institute of Physics, Belgrade 1973), pp. 443–463.
[8]H. Ehrhardt, K. H. Hesselbacher, K. Jung, E. Schubert, and K. Willmann, J. Phys. B 7, 69 (1972).
[9]C. B. Opal, E. C. Beaty, and W. K. Peterson, At. Data 4, 209 (1972).
[10]G. B. Crooks, Ph.D. thesis (University of Nebraska 1972) (unpublished).
[11]N. Oda, F. Nishimura, and S. Tahira, J. Phys. Soc. Jpn. 33, 462 (1972).
[12]W. D. Robb, S. P. Rountree, and T. Burnett, Phys. Rev. A 11, 1193 (1975).
[13]I. H. Sloan, Proc. R. Soc. A 281, 151 (1964).
[14]P. G. Burke and J. Taylor, Proc. Phys. Soc. 88, 549 (1966).
[15]C. B. Opal, W. K. Peterson, and E. C. Beaty, J. Chem. Phys. 55, 4100 (1971).
[16]W. K. Peterson, C. G. Opal, and E. C. Beaty, J. Phys. B 4, 1020 (1971).
[17]G. Peach, Proc. Phys. Soc. 87, 381 (1966).
[18]Yong-ki Kim and Mitio Inokuti, Phys. Rev. A 7, 1257 (1973).
[19]J. T. Grissom, R. N. Compton, and W. R. Garrett, Phys. Rev. A 6, 977 (1972).
[20]S. T. Manson, L. H. Thoburen, D. H. Madison, and N. Stolterfoht, Phys. Rev. A 12, 60 (1975).