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Elastic scattering of electrons from singly ionized argon

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Recently, Greenwood *et al.* [Phys. Rev. Lett. **75**, 1062 (1995)] reported measurements of large-angle elastic scattering of electrons from singly ionized argon at an energy of 3.3 eV. They compared their results for the differential cross section with cross sections determined using phase shifts obtained from two different scattering potentials and found large discrepancies between theory and experiment at large angles. They state that these differences may be due to the effects of polarization of the target, which are not included in their calculations, as well as inaccurate representations of electron exchange in the local scattering potentials that are employed to determine the phase shifts. In order to test these proposed explanations of the discrepancies, we have carried out calculations of elastic scattering from Ar^+ using the R-matrix method. We compare both a single-state calculation, which does not include polarization, and a 17-state calculation, in which the effects of dipole polarizability are included through the use of polarization pseudostates within the close-coupling expansion, to each other and with the measurements. We find some differences between the two calculations at intermediate scattering angles, but very close agreement at angles above 100°. Although the calculated cross sections agree with experiment between 120° and 135°, large discrepancies persist at angles above 135°. We conclude that the differences between the measurements and theory cannot be explained on the basis of an inaccurate representation of electron exchange or polarization of the target.

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Greenwood, Williams, and McGuinness [1] have recently reported on experimental measurements of large-angle elastic scattering of electrons from Ar^+ at an electron energy of 3.3 eV. Their experiment measures the partial elastic cross section from some initial angle through 180° as a function of the initial angle. They extracted the angular differential cross section by fitting a curve to the experimental partial cross section and taking the derivative with respect to the initial angle. They compared their differential cross section with theoretical cross sections determined using phase shifts calculated from the Herman-Skillman potential by Manson [2] and those calculated by Szydlik, Kutcher, and Green [3], using the potential of Green, Sellin, and Zachor [4]. They then folded the calculated cross sections with a 0.250 meV [full width at half maximum (FWHM)] Gaussian function over energy to simulate the experimental energy spread and an angular Gaussian function, for which the angular width varies linearly from 15° at 120° to 5° at 170°, to simulate the experimental angular spread. Although they obtained reasonable agreement between theory and experiment in the angular range between 120° and approximately 135°, the theory is found to be much larger than the measured cross section at larger angles. Greenwood, Williams, and McGuinness [1] propose that the discrepancies are most likely due to problems with the scattering potential used to generate the phase shifts. In particular, they mention possible inaccurate descriptions of electron exchange in the local potentials and the lack of any representation of polarization of the target by the continuum electron within these potentials.

We have already reported on extensive R-matrix calculations of elastic and inelastic scattering in neutral argon and chlorine [5]. For the elastic and excitation cross sections, we employed target orbitals determined using Fischer's multiconfiguration-Hartree-Fock programs [6]. We also calculated a set of polarization pseudoorbitals using a technique similar to that first proposed by Dalgarno and Lewis [7]. These were in turn used to generate a set of polarization pseudostates, which when included in the close-coupling expansion of the target, provide an approximate representation of the effect of polarization on the scattering event. The R-matrix calculations were carried out using extensively modified versions of the R-matrix programs developed for the opacity project [8].

Here, in order to investigate the discrepancy between theory and experiment for elastic scattering in Ar^+, we use the same methods employed earlier for neutral Ar and Cl. The basis set for the target states used in the 17-state calculation for Ar^+ is identical in form to that employed in neutral Cl [5], and is described in Table I. The single-state calculation includes only the $3p^5\,{}^2P$ term in the close-coupling expansion. Both R-matrix calculations, of course, include nonlocal continuum Hartree-Fock exchange terms, while only the 17-state calculation includes the effects of the dipole polarization of the core.

Our results from the 17-state R-matrix calculation for the differential cross section at 3.3 eV from 100° to 180° are shown in Fig. 1 in comparison to the measurements of Greenwood, Williams, and McGuinness [1]. The solid curve is purely theoretical, while the dashed curve is our theoretical result convoluted with Gaussians to represent the energy spread and the angular spread given in Ref. [1]. As can be seen, there is quite good agreement between experiment and the convoluted cross section over the limited angular range from about 120° to about 135°. However, for angles above

TABLE I. The terms used for the 17-state calculation of elastic scattering in Ar^+, where the overbars represent nonspectroscopic pseudo-orbitals. The $1s$, $2s$, $2p$, $3s$, and $3p$ orbitals were determined from a single-configuration Hartree-Fock calculation. The $\overline{3d}$ pseudo-orbital was determined from Eq. (1) of Ref. [5] using the average potential of Boyle [12]. The $\overline{4s}$ pseudo-orbital was determined from Eq. (1) of Ref. [5] using the average potential of Boyle [12]. The $\overline{4p}$ pseudo-orbital was determined from Eq. (1) of Ref. [5] for the $3s3p^5(^3P)\overline{4p}\,^2D^e$ term.

$3s^23p^5\ ^2P^o$			
$3s3p^6\ ^2S^e$,	$3s^23p^4(^1D)\overline{3d}\ ^2S^e$,	$3s^23p^4(^1S)\overline{4s}\ ^2S^e$,	$3s3p^5(^3P)\overline{4p}\ ^2S^e$
$3s3p^5(^1P)\overline{4p}\ ^2S^e$,	$3s^23p^4(^3P)\overline{3d}\ ^2P^e$,	$3s^23p^4(^1D)\overline{3d}\ ^2P^e$,	$3s^23p^4(^3P)\overline{4s}\ ^2P^e$
$3s3p^5(^3P)\overline{4p}\ ^2P^e$,	$3s3p^5(^1P)\overline{4p}\ ^2P^e$,	$3s^23p^4(^1S)\overline{3d}\ ^2D^e$,	$3s^23p^4(^3P)\overline{3d}\ ^2D^e$
$3s^23p^4(^1D)\overline{3d}\ ^2D^e$,	$3s^23p^4(^1D)\overline{4s}\ ^2D^e$,	$3s3p^5(^3P)\overline{4p}\ ^2D^e$,	$3s3p^5(^1P)\overline{4p}\ ^2D^e$

135°, there is a large disagreement between the theoretical curves and the experimental measurements. This is similar to the disagreement seen in the comparisons presented in Ref. [1].

A few comments concerning the convolution are called for. As one might expect, the effect of the energy and angular spread on the differential cross section is clearly visible near the minimum in Fig. 1. However, it is completely negligible at large angles, since the variation of the differential cross section with both energy and angle is very small at large angles. On the other hand, the pure and convoluted theoretical curves for the differential cross section presented in Ref. [1] diverge for angles greater than 170°, a result that we cannot explain.

The most significant result of the present calculation is that the inclusion of the effects of polarization and the proper nonlocal exchange contributions has no significant effect on the discrepancy between experiment and theory. This is also seen in Fig. 2, where we present partial cross sections from an initial angle to 180° as a function of the initial angle. Both the theoretical curves (with and without convolutions) are much larger than the measured cross section. This is, of course, primarily due to the large differences between experiment and theory for the differential cross section above 135°.

In order to support our thesis that these calculations show that the difference between the experimental and theoretical results in Ar^+ cannot be explained on the basis of target polarization or electron exchange, we also present our results for elastic scattering from neutral Ar and Cl. In Fig. 3, we compare differential cross sections for Ar and Cl with those for Ar^+; the dashed curves are obtained from single-state calculations, without target polarization, while the solid curves are from calculations that include polarization effects through coupling with a set of polarized pseudostates. The Ar and Cl calculations were performed at an energy of 3.0 eV, because of the existence of experimental results for this energy in Ar, while the Ar^+ calculations were carried out at 3.3 eV. In the case of Ar, the inclusion of dipole polarization requires only three additional states, compared to Cl where the sixteen additional states listed in Table I are necessary. Again, nonlocal exchange terms are part of all these calculations.

As can be seen from Fig. 3(a), polarization has a very large effect on the cross section for Ar, except for angles above 160° where the two curves come together. It is also clear from the comparison with the experimental results of Srivastava *et al.* [9] that, when the effects of polarization are included, the theory does an excellent job of representing the

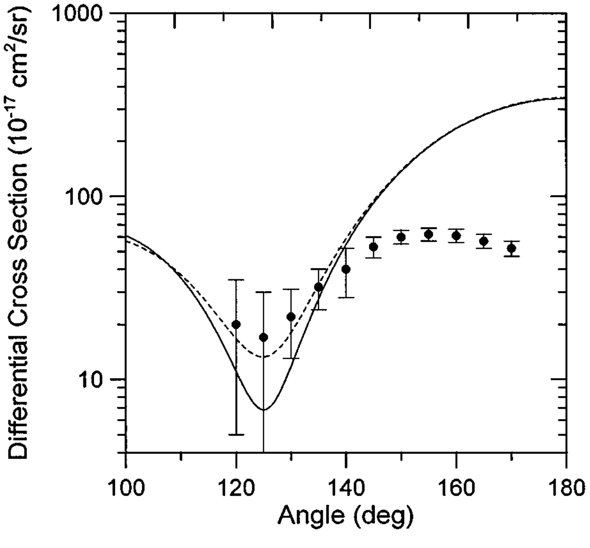

FIG. 1. Angular differential cross section for elastic scattering in Ar^+ at 3.3 eV. Solid curve: from a 17-state R-matrix calculation including polarized pseudostates; dashed curve: from a 17-state calculation convoluted over energy and angle using the energy and angular widths given in Ref. [1]; experimental points are from Ref. [1].

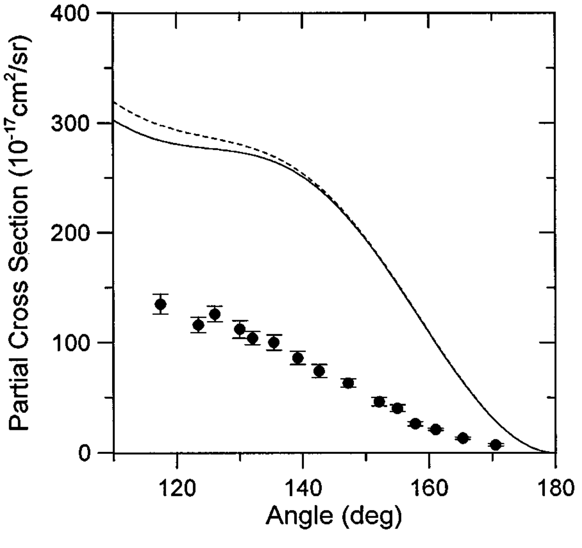

FIG. 2. Partial differential cross section for elastic scattering in Ar^+ at 3.3 eV from an initial angle through 180°, as a function of the initial angle. Solid curve: from 17-state R-matrix calculation; dashed curve: from a 17-state calculation convoluted over energy and angle before integration over the angle; experimental points: from Ref. [1].

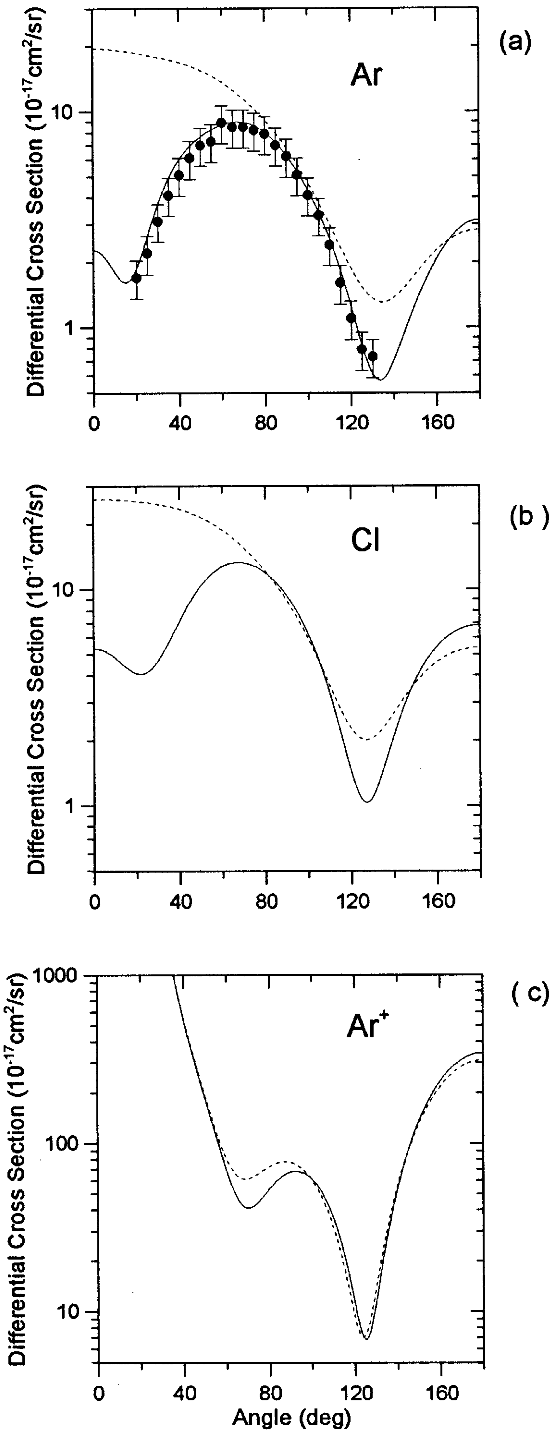

FIG. 3. (a) Angular differential cross section for Ar at 3.0 eV. Dashed curve: from a single-state R-matrix calculation without polarization; solid curve: from a four-state R-matrix calculation including the effects of polarization through the use of polarized pseudostates (see Ref. [5]); experimental points from Ref. [9]. (b) Angular differential cross section for Cl at 3.0 eV. Dashed curve: from a single-state R-matrix calculation without polarization; solid curve: from a seventeen-state R-matrix calculation including the effects of polarization through the use of polarized pseudo states (see Ref. [5]). (c) Angular differential cross section for Ar^+ at 3.3 eV. Dashed curve: from a single-state R-matrix calculation without polarization; solid curve: from a 17-state R-matrix calculation including the effects of polarization through the use of polarized pseudo states.

differential cross section. It is unfortunate that the experimental measurements were not carried out at higher angles. However, it is important to note that the theoretical methods employed here also yield results for the total cross section and the momentum-transfer cross section in Ar [5], which agree well with various experimental measurements. One would not expect this if the theoretical differential cross section was significantly larger than the measured cross section above 120°.

We also show our results for Cl in Fig. 3(b) to illustrate that the shape of the angular distribution is quite similar in this atom, which is isoelectronic to Ar^+. Finally in Fig. 3(c), we see that, except for the influence of the dominant contribution from the Coulomb field at forward angles, the shape of the cross section in Ar^+ shows a general similarity to that of the neutral atoms. However, here the effect of polarization is much less pronounced.

In general, one would expect that the effects of polarization would decrease as one goes from the neutral atom to the ion. This surely seems to be true for the species considered here. However, as pointed out by the authors in Ref. [1], calculations by Johnson and Guet [10], using relativistic many-body theory, indicate that the effects of polarization are more significant in Cs^+ than in the isoelectronic Xe atom. But even here, polarization appears to affect only the shape of the Cs^+ cross section at large angles and has a relatively small effect on the magnitude of the cross section.

Furthermore, a careful examination of the results presented in Ref. [10] indicates that the differences in the differential cross sections for Xe and Cs^+ at 10 eV are almost entirely due to the unusual nature of f-wave scattering in these species. At a momentum of 0.86 a.u., corresponding to an energy of 10 eV, the f wave in Xe will reside in the outer-well region of the effective potential and will not overlap strongly with the bound-state wave functions. However in Cs^+, the f wave should begin to penetrate the inner-well region at this momentum and interact more strongly with the bound wave funtions. When this occurs, the differential cross section becomes very sensitive to the details of the calculation and the difference between a pure Hartree-Fock calculation and one that includes polarization becomes more pronounced. The effect of this penetration can be seen in Fig. 6 of Ref. [10] in the relatively large variation in the f-wave phase shift in Cs^+ near this momentum. A similar effect occurs for d-wave scattering in Ar^+ [11]. However, at 3.3 eV, the d wave is still in the outer-well region, which explains why the differential cross section does not change significantly at this energy with the inclusion of polarization. Thus, the theoretical results in singly ionized Cs do not provide an explanation for the large discrepancies in magnitude between experiment and theory in Ar^+.

In conclusion, we do not find anything from our theoretical work on Ar^+ or neutral Ar and Cl that could explain the observed differences between the experimental and theoretical results for Ar^+. We would encourage additional theoretical calculations and measurements of this differential cross section.

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