Determination of complex scattering amplitudes in low-energy elastic electron-sodium scattering

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Measurements of spin-resolved elastic electron-sodium scattering have been carried out at incident energies of 4.1 and 12.1 eV, and the ratio of triplet to singlet scattering cross sections has been obtained at each energy. The ratio is used to provide a determination of not only the magnitudes of the triplet and singlet amplitudes, but also the cosine of the relative phase difference between them. These determinations of magnitude and relative phase represent the most detailed characterization to date of electron-atom scattering from a "one-electron" target.

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In a seminal paper in 1969, Bederson [1] discussed a class of experiments in electron-atom scattering that would allow complete determination of the scattered wave function in elastic scattering from a one-electron atom. These proposed measurements were conceived around an "ideal" alkali-metal atom, that is, one in which nuclear spin, core effects, and the spin-orbit interaction can be ignored during the collision. A description of the scattered wave function in a collision with such an "ideal" atom requires two scattering amplitudes because of the possibility of exchange between the target and incident electrons. Hence a simple (i.e., unpolarized) differential cross-section measurement, which consists of an average over these amplitudes, is insufficient to give all the experimentally accessible information. However, by conducting experiments in which the spins of the atom and the electron are resolved, it is possible, as Bederson pointed out, to extract from the measurements of the spin-dependent cross sections both the magnitudes and the relative phase of the complex scattering amplitudes.

Though complete experiments have been reported for closed-shell atoms [2], a complete scattering-amplitude determination as proposed by Bederson in a one-electron target has not yet been realized. A number of studies with some degree of spin resolution have been reported [3–10], but so far all the complementary information has not been available for a single system. In this Brief Report we present new spin-resolved measurements on sodium which are combined with existing measurements to provide the most complete determination to date. Our results, in conjunction with differential cross-section measurements [11], allow individual determination of the magnitudes of the two scattering amplitudes necessary to describe the scattering. Combined with recent spin-polarized scattering results from Hegemann *et al.* [9], our results also allow determination of the cosine of the phase angle between these two complex amplitudes. But for an evaluation of the sign of the relative phase, we have with these determinations effected a complete characterization of the scattered wave function for low-energy electron-sodium scattering. When compared with theory, the experimental determinations presented here lead to insights into where improvements in the calculations might be made.

In a theoretical treatment of collisions between electrons and one-electron atoms of the sort discussed by Bederson, allowance must be made for the fact that there are two channels associated with the spin states of the electron and atom [12]. The two complex scattering amplitudes corresponding to these two channels are commonly expressed as either direct and exchange amplitudes f and g [13] or, alternatively, as singlet and triplet amplitudes S and T. S and T correspond to the two possible total-spin channels $S = 0, 1$ of the composite two-electron system.

The two sets of amplitudes are related via $T = f - g$ and $S = f + g$, and both provide an equivalent description of the scattering process. Because, in the absence of spin-orbit interaction, the singlet and triplet channels do not mix, we choose for the present work to describe our results in terms of the singlet and triplet amplitudes.

The first experiments resolving spin in low-energy-electron–alkali-metal scattering were performed on potassium. Collins *et al.* [4] prepared spin-polarized atoms and measured the polarization of the atoms after scattering from an unpolarized electron beam. Hils *et al.* [5] reported measurements using unpolarized electrons incident upon spin-polarized atoms and measuring the polarization of the scattered electrons. Though in principle the results of these two experiments could be combined to yield more complete information, direct combination is prevented because different incident energies were used.

More recently, a number of experiments have been carried out with spin-polarized electrons incident upon spin-polarized target atoms, without spin resolution after scattering. Hydrogen [6], lithium [7], and sodium [8, 10] have been studied in varying amounts of detail.

The experiments we report here, with polarized incident particles and without spin analysis after scattering, give experimental results which can be presented as a ratio of triplet-to-singlet scattering cross sections $r = |T|^2/|S|^2$. The ratio is determined from experiment by

$$r = \frac{I_{\rm par}(1+P_eP_a) - I_{\rm anti}(1-P_eP_a)}{I_{\rm anti}(3+P_eP_a) - I_{\rm par}(3-P_eP_a)}, \quad (1)$$

where $I_{\rm par}$ and $I_{\rm anti}$ are the measured scattering intensities with incident electron and atomic spins parallel and antiparallel, respectively, and P_e and P_a are the electron and atomic beam polarizations.

Once an experimental determination of the ratio r is available, it can be used together with an experimental measurement of the spin-averaged differential cross section $\sigma_0 = \frac{1}{4}|S|^2 + \frac{3}{4}|T|^2$ to provide a determination of the magnitudes of the individual scattering amplitudes $|S|$ and $|T|$:

$$|S| = \left(\frac{4\sigma_0}{1+3r}\right)^{1/2}, \quad (2)$$

$$|T| = \left(\frac{4r\sigma_0}{1+3r}\right)^{1/2}. \quad (3)$$

If the cross-section measurement is on an absolute scale, $|S|$ and $|T|$ will also be determined absolutely. If, as is often the case, the differential cross-section measurement is relative, some form of normalization must be carried out before $|S|$ and $|T|$ are derived.

In the past year, Hegemann *et al.* [9] have reported experiments on sodium in which polarized electrons are incident upon unpolarized atoms and the polarization of the scattered electrons is analyzed. An angular range of 30°–110° was investigated at incident energies of 4.0 and 12.1 eV. The quantity P'/P was measured, where P and P' are the electron polarizations before and after collision, respectively. In terms of the triplet and singlet scattering amplitudes, P'/P can be expressed as follows:

$$P'/P = \frac{2r + 2\sqrt{r}\cos\gamma_{ST}}{1+3r}, \quad (4)$$

where γ_{ST} is the phase angle difference between the complex scattering amplitudes S and T and r is the ratio $|T|^2/|S|^2$. From Eq. (4) it is clear that a measurement of r can be used together with a measurement of P'/P to determine the cosine of γ_{ST}.

We note that from a measurement of $\cos\gamma_{ST}$ one can determine γ_{ST} to within its sign. To obtain the sign a measurement must be done in which three of the four polarizations in the experiment are prepared or analyzed along three mutually orthogonal axes [14]. Though such a measurement is experimentally difficult, given the present results it can now be done with relatively low precision since only the sign of the measured quantity is required.

For the present work, we have measured triplet-singlet ratios with polarized target atoms and polarized incident electrons in elastic scattering from sodium over the angular range 25°–135° at incident energies of 4.1 and 12.1 eV. These energies match very closely the energies at which differential cross sections have been measured [11], so determination of the scattering amplitudes can be carried out. Additionally, these energies match those measured by Hegemann *et al.*, so $\cos\gamma_{ST}$ can also be obtained.

Details of the apparatus and experimental methods are described elsewhere [15]. Briefly, the results were obtained with a crossed-beam electron scattering apparatus with polarized incident electrons and optically pumped, spin-polarized sodium atoms. Both the electron and atomic spins are oriented either "up" or "down," perpendicular to the scattering plane. The electron beam is produced with a GaAs photoemission source [16] with polarization $P_e = 0.32 \pm 0.02$, beam current 1–2 μA, and energy width 250 meV. The scattered electrons are detected with a channel electron multiplier equipped with a retarding-field analyzer and mounted on a rotating turntable. The angular acceptance of the detector is about ±3°, and the accuracy with which the scattering angle can be set is approximately ±0.5°.

The atom beam is produced in an effusive, recirculating oven with beam density $\sim 10^{15}$ atoms/m^3. The sodium atoms are spin polarized by optical pumping over a ~ 10-mm region of the atom beam located "upstream" from the collision region. Circularly polarized laser light from a single-frequency, stabilized ring dye laser, tuned to the $3S_{1/2}(F=2) \rightarrow 3P_{3/2}(F=3)$ transition, is used to carry out the polarization [17]. A second laser beam, generated from the first with an acousto-optical modulator, is tuned to the $3S_{1/2}(F=1) \rightarrow 3P_{3/2}(F=2)$ transition, separated from the main transition by 1712 MHz. The second beam optically pumps atoms from the $F=1$ ground state into the $F=2$ ground state via the $F=2$ excited state, allowing them to participate in the polarization process. By pumping with two frequencies of laser light, an atomic polarization of 0.98 ± 0.01 is produced in the collision region.

During the experiment, the electron detector was fixed at a specific angle and the electron and atomic spins were modulated between "up" and "down" so that the four scattering intensities corresponding to the four possible relative spin orientations were measured. We label these intensities $I_{\uparrow\uparrow}, I_{\downarrow\uparrow}, I_{\uparrow\downarrow}$, and $I_{\downarrow\downarrow}$, where the first subscript arrow corresponds to the electron spin, and the second to the atomic spin. The atom beam was also periodically blocked to measure a background. The electron beam polarization was modulated at 100 Hz with a Pockels cell, and the atom polarization was reversed periodically with a motorized quarter-wave plate. A measurement cycle consisted of 1–5 s for each atomic polarization and a background measurement of 1–5 s. Count rates varied from about 2 s^{-1} to over 100 s^{-1}, depending on incident energy and scattering angle. At each angle, the measurement cycle was repeated for up to 2 h, and counts were accumulated separately for each portion of the cycle.

The four background-corrected scattering intensities corresponding to the four possible relative spin orientations were combined into parallel and antiparallel intensities via $I_{\rm par} = I_{\uparrow\uparrow} + I_{\downarrow\downarrow}$ and $I_{\rm anti} = I_{\uparrow\downarrow} + I_{\downarrow\uparrow}$. These parallel and antiparallel intensities were combined to determine the ratio according to Eq. (1). Uncertainty estimates on the intensities were obtained from counting statistics, and these were propagated through the formulas in the standard way [18] to give one-standard-deviation uncertainty estimates for r.

Figure 1 shows our measurements of r at incident energies of 4.1 and 12.1 eV. At the lower energy, the data

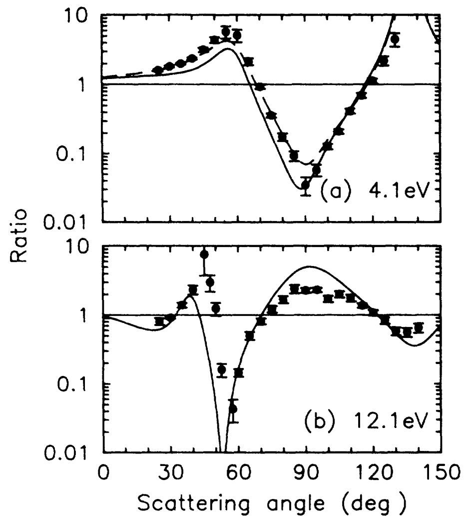

FIG. 1. Triplet-to-singlet ratio r for elastic electron scattering from sodium vs scattering angle. (a) 4.1-eV incident energy; (b) 12.1-eV incident energy. Error bars represent one standard deviation derived from counting statistics. Solid line: 9-state close-coupling calculation of Bray *et al.* [19]. Dashed line: 10-state close-coupling calculation of Zhou [20].

show the scattering to be predominantly triplet below about 70°, and mostly singlet above 70°. At 12.1 eV, the ratio has a good deal more structure, including a very deep triplet minimum at about 55°. The magnitude of the ratio at both impact energies indicates that exchange effects are quite substantial in this energy regime.

Also shown in Fig. 1 are two state-of-the-art close-coupling calculations: the 9-state work of Bray *et al.* [19], and the 10-state work of Zhou [20] (at 4.1 eV only). Generally, the comparison between theory and experiment is good, though at 4.1 eV, the 10-state theory appears to match the experiment more closely than the 9-state at smaller scattering angles, and at 12.1 eV, some discrepancies still exist around 45°–50°.

Figure 2 shows the singlet and triplet scattering amplitudes derived from the ratios in Fig. 1 and the differential cross sections measured by Gehenn and Reichert [11] at 4.0 and 12.0 eV. In the original work, these cross sections were measured on a relative scale, and the 4-eV data were normalized to the theory of Moores and Norcross [21]. For the present work each data set was renormalized (or normalized) at a single point (90°) to the corresponding 9-state close-coupling theory. The measured ratios were then used to generate the amplitudes via Eqs. (2)–(3). For the purpose of this derivation, we consider the slight difference in energy between the data sets to be negligible. No error estimates are shown in Fig. 2. Estimates of the uncertainty contribution from the ratio measurements were calculated, but these are much smaller than the plotting symbols. We believe the dominant uncertainty in these curves most likely arises from the cross-section measurements, although quantitative uncertainty estimates are unavailable.

The 9-state and 10-state close-coupling theories are also shown in Fig. 2. Most remarkable is the excellent

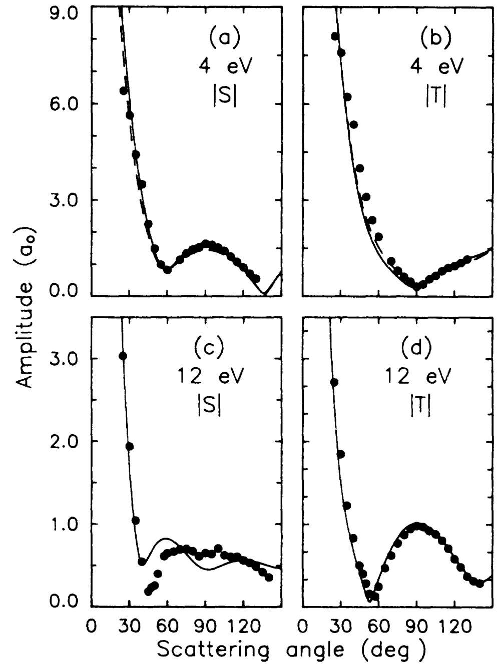

FIG. 2. Scattering amplitude magnitudes for elastic electron scattering from sodium vs scattering angle. (a) Singlet amplitude $|S|$ at 4-eV incident energy, (b) triplet amplitude $|T|$ at 4-eV incident energy, (c) singlet amplitude $|S|$ at 12-eV incident energy, (d) triplet amplitude $|T|$ at 12-eV incident energy. Solid line: 9-state close-coupling calculation of Bray *et al.* [19]. Dashed line: 10-state close-coupling calculation of Zhou [20].

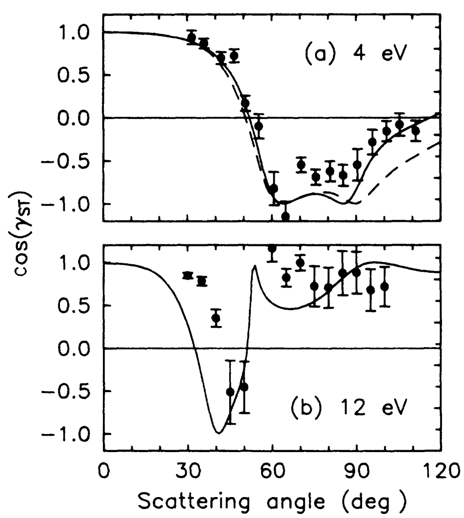

FIG. 3. Cosine of the phase difference γ_{ST} between singlet and triplet scattering amplitudes for elastic electron scattering from sodium vs scattering angle. (a) 4-eV incident energy; (b) 12-eV incident energy. Error bars represent one standard deviation derived from counting statistics. Solid line: 9-state close-coupling calculation of Bray *et al.* [19]. Dashed line: 10-state close-coupling calculation of Zhou [20].

agreement between experiment and theory seen in all cases, with the notable exception of the singlet amplitude at 12 eV. It is interesting to compare the results shown here with the disagreements seen in Fig. 1. At 4 eV, we see that the difference in the ratio between experiment and the 9-state calculation can be attributed exclusively to the triplet channel. This is not an artifact of the normalization, because at 90°, both the singlet and triplet amplitudes agree well with the theory. On the other hand, at 12 eV, the theory clearly does not do well in the singlet channel, but accurately reproduces the experimental triplet amplitude.

In Fig. 3 we show the values of $\cos\gamma_{ST}$ derived from our measurements of r and the measurements of P'/P by Hegemann *et al.* [9]. Once again, we have ignored the small differences in energy between the data sets. The uncertainty estimates for $\cos\gamma_{ST}$ were obtained by propagating the estimates for the r data and the P'/P data, assuming all to be one standard deviation.

Also shown in Fig. 3 are the 9-state and 10-state close-coupling calculations of Bray *et al.* [19] and Zhou [20]. Again, good qualitative agreement between experiment and theory is generally seen. We note, however, that at 4 eV, the 9-state calculation matches the experiment more closely than the 10-state, which is contrary to what was observed in the ratio measurement.

In summary, we have presented determinations of the magnitudes and phase-angle differences for the triplet and singlet scattering amplitudes T and S in low-energy elastic electron scattering from an alkali-metal atom. These measurements represent an unprecedented level of detail in an electron-atom scattering experiment. With the exception of a determination of the overall sign of γ_{ST}, they comprise a complete characterization of the complex scattering amplitudes. The comparison of these results with theoretical calculations has shown remarkable agreements in some cases, and disagreements in others. As a result, theoretical approaches can now be modified to better predict electron-atom scattering phenomena.

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[1] B. Bederson, Comm. At. Mol. Phys. **1**, 41 (1969).

[2] O. Berger and J. Kessler, J. Phys. B **19**, 3639 (1986); H. A. Silim *et al.*, Phys. Rev. A **35** 4454 (1987).

[3] W. Lichten and S. Schultz, Phys. Rev. **116**, 1132 (1959); W. Jitschin *et al.*, J. Phys. B **17**, 1899 (1984); N. Ludwig *et al.*, Z. Phys. D **4**, 177 (1986); X. L. Han *et al.*, Phys. Rev. A **42**, 1245 (1990).

[4] R. E. Collins *et al.*, Phys. Rev. A **3**, 1978 (1971).

[5] D. Hils *et al.*, Phys. Rev. Lett. **29**, 398 (1972).

[6] G. D. Fletcher *et al.*, Phys. Rev. Lett. **48**, 1671 (1982).

[7] G. Baum *et al.*, Phys. Rev. Lett. **57**, 1855 (1986).

[8] J. J. McClelland *et al.*, Phys. Rev. Lett. **58**, 2198 (1987).

[9] T. Hegemann *et al.*, Phys. Rev. Lett. **66**, 2968 (1991).

[10] S. R. Lorentz *et al.*, Phys. Rev. Lett. **67**, 3761 (1991).

[11] W. Gehenn and E. Reichert, Z. Phys. **254**, 28 (1972).

[12] P. G. Burke and H. M. Schey, Phys. Rev. **126**, 163 (1962).

[13] J. Kessler, *Polarized Electrons*, 2nd ed. (Springer-Verlag, Berlin, 1985).

[14] J. Kessler, Adv. Atom. Mol. Opt. Phys. **27**, 81 (1991).

[15] J. J. McClelland *et al.*, Phys. Rev. A **40**, 2321 (1989).

[16] D. T. Pierce *et al.*, Rev. Sci. Instrum. **51**, 478 (1980).

[17] J. J. McClelland and M. H. Kelley, Phys. Rev. A **31**, 3704 (1985).

[18] P. R. Bevington, *Data Reduction and Error Analysis for the Physical Sciences* (McGraw-Hill, New York, 1969).

[19] I. Bray *et al.*, Phys. Rev. A **44**, 7179 (1991); **44**, 7830 (1991); and private communication.

[20] H.-L. Zhou, Ph.D. thesis, University of Colorado, 1991 (unpublished).

[21] D. L. Moores and D. W. Norcross, J. Phys. B **5**, 1482 (1972).