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Exchange asymmetry in elastic scattering of electrons by sodium atoms

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Calculations of the exchange asymmetry in elastic scattering of electrons by sodium atoms are reported at incident electron energies of 10 and 54.4 eV. The close-coupling calculations are performed with the four lowest target states of the sodium atom. At 10 eV, the present calculations predict nearly pure singlet-state scattering and nearly pure triplet-state scattering at certain angles. At 54.4 eV, the theoretical results are compared with recent measurements. Qualitative agreement is obtained, although some discrepancy remains.

Measurements of the scattering of spin-polarized electrons by spin-polarized sodium atoms have been recently reported by McClelland, Kelley, and Celotta.[1] Such studies reveal more detailed information about the scattering process than do investigations without spin-polarized projectiles and targets. Specifically, it is possible to examine electron exchange effects.

For the process of elastic scattering, one can define an asymmetry A by

$$A=\frac{(d\sigma/d\Omega)_{S=0}-(d\sigma/d\Omega)_{S=1}}{(d\sigma/d\Omega)_{S=0}+3(d\sigma/d\Omega)_{S=1}}\ , \quad (1)$$

in terms of the spin-dependent differential cross sections. We call it the exchange asymmetry. It may be expressed as

$$A=\frac{1-r}{1+3r}\ , \quad (2)$$

where r is the ratio of the triplet (total spin, $S=1$) to the singlet ($S=0$) scattering cross sections. In terms of the respective scattering amplitudes f_t and f_s, the ratio r is given by

$$r=\frac{|f_t|^2}{|f_s|^2}\ . \quad (3)$$

McClelland, Kelley, and Celotta have measured this exchange asymmetry in the elastic scattering cross section for scattering angles between 20° and 135° at an incident energy of 54.4 eV. They find a maximum exchange asymmetry of about 4%. In this Rapid Communication, I present theoretical results for the exchange asymmetry using a four-state close-coupling approximation. Calculations were performed at 54.4 eV for comparison with the experiment and at lower energies to investigate a regime where exchange effects are expected to be large. The exchange asymmetry is found to vary between its maximum and minimum allowable values between 8 and 12 eV. The results are reported here at 10 and 54.4 eV.

The close-coupling calculations are performed with the four lowest target states of the sodium atom.[2] The total wave function for the scattering electron and the valence electron of the sodium atom is antisymmetrized to permit the exchange of these two indistinguishable particles. I consider here the scattering of the electrons from the ground state, viz., the $3s$ state. It is most closely coupled to the $3p$ resonance state. Inclusion of the $3p$ state in the close-coupling expansion accounts for most of the polarizability of the sodium atom in its ground state. Therefore, the distortion in the scattering function, which is significantly affected by the energy-dependent polarization potential, particularly at lower incident energies, is accounted for. The $3d$ and the $4s$ states are also included in the expansion to account for partial loss of flux and because of their strong coupling to the $3p$ state.

The target states for the $3s$, $3p$, $3d$, and the $4s$ states used in this calculation are described by the frozen-core Hartree-Fock wave functions of Weiss.[3] For the sodium atom, the core is tightly bound with a single valence electron. It is for an atom like this that a single-configuration description would be fairly representative of the true wave function. An extensive configuration-interaction (CI) calculation[3] for the $3s$ and the $3p$ states reveals that the deviation of the leading coefficient for each of these states from unity is less than 2%. The relative energy differences between the four states and the dipole oscillator strengths between dipole-allowed states obtained by the single-configuration frozen-core Hartree-Fock functions used here are within a few percent of the experimental values.[4] The numerical solutions of the coupled integro-differential equations arising from the close-coupling approximation are obtained by employing the linear algebraic integral equation method.[5] The full details of these close-coupling calculations with additional results are presented elsewhere.[6] Here, I present only the exchange asymmetry for incident energies of 10 and 54.4 eV.

The exchange asymmetry at an incident electron energy of 10 eV is presented graphically in Fig. 1. The most remarkable point to note here is that the exchange asymmetry varies between its maximum possible value of 100% (pure singlet state scattering) and its minimum possible value of −33.33% (pure triplet state scattering) as a function of angle. Similar behavior is found[6] from about 8 to 12 eV (not shown here).

A clue to why such large exchange asymmetry exists at 10 eV can be found by examining individual partial-wave contributions to the scattering amplitude.

$$f_S(\theta)=\frac{i}{2k}\sum_{L=0}^{\infty}(2L+1)T^{L,S}_{3s,3s}P_L(\cos\theta)\ . \quad (4)$$

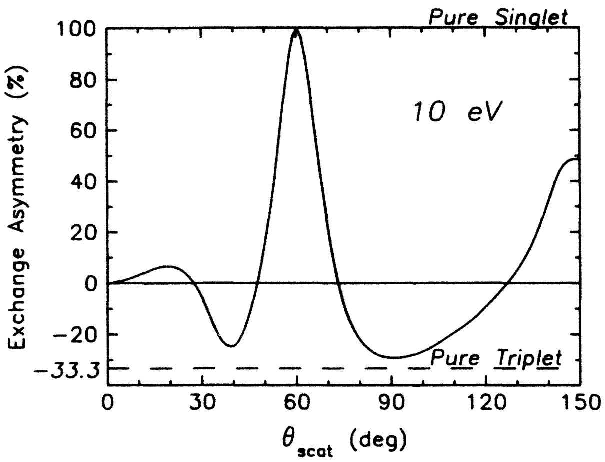

FIG. 1. Calculated exchange asymmetry (solid) as a function of scattering angle at an incident energy of 10 eV. The limiting cases of pure triplet-state scattering (dashes) and pure singlet-state scattering (top border) are indicated.

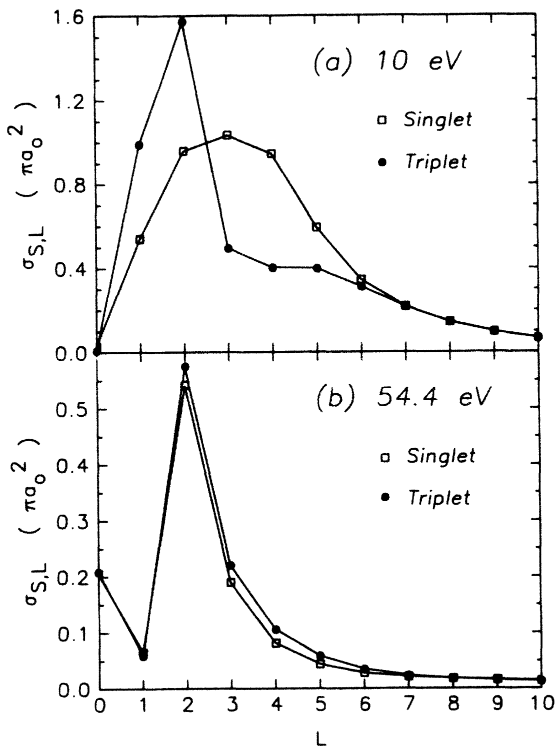

FIG. 2. Partial-wave cross sections $\sigma_{S,L}$ vs L at (a) 10 eV and at (b) 54.4 eV for the singlet state (open squares) and the triplet state (filled circles). The vertical scales for the two energies are different. The difference between the singlet and the triplet cross sections indicates the effect of exchange between the scattering and the target valence electrons.

The symbol S labels the spin for the scattering amplitude, L is the angular momentum of the partial wave, k is the momentum of the electron, T is the transition-matrix element, and P_L is the Legendre polynomial (atomic units are used). An estimate of the relative importance of various transition-matrix elements can be deduced from the partial-wave cross sections,

$$\sigma_{S,L} = \frac{\pi}{4k^2}(2L+1)\,|T^{L,S}_{3s,3s}|^2(a_0^2) \ . \qquad (5)$$

The partial-wave cross sections for the singlet spin state and the triplet spin state as a function of L are displayed in Fig. 2. Note that the spin-weighting factor of $(2S+1)$ is not included. At an incident energy of 10 eV, one observes that the triplet cross sections are dominated by the $L=2$ partial wave. On account of the nodes in the Legendre polynomials, this dominant partial wave would vanish at $\theta=55°$ and 125°. Therefore, it is no surprise that the exchange asymmetry (Fig. 1) implies that all scattering occurs in the singlet state near 55°. Of course, the effect of the other partial waves is constructive in the forward direction (the value of the Legendre function at $\theta=0°$ is 1 for all L) and displaces the exact angle of this prediction slightly as seen in Fig. 1. On the other hand, the effect of various partial waves is destructive in the backward direction (the value of the Legendre function at $\theta=180°$ is $+1$ for even L and -1 for odd L leading to a sensitive cancellation). This destructive interference makes it very difficult to predict the angular positions of the positive and negative peaks in the exchange asymmetry in the backward direction (90°–180°). It also reduces the accuracy of the calculations near 180° somewhat. Therefore the results are presented here only up to 150°.

The analysis of the singlet cross sections is not as straightforward. The singlet cross sections have the largest contribution from the $L=3$ partial wave with the $L=2$ and $L=4$ partial waves contributing in comparable magnitudes. The $L=3$ partial wave vanishes at $\theta=39°$, 90°, and 141°. The $L=2$ and $L=4$ partial waves have contributions of opposite signs from the Legendre functions at $\theta=39°$ and 90°, and so cancel each other to some extent. This cancellation effect of singlet cross sections for the $L=2$, 3, and 4 partial waves at $\theta=39°$ and 90° results in almost pure triplet scattering near 39° and 90° as reflected in Fig. 1. Since the cancellation is not total, one does not have an exchange asymmetry of $-\frac{1}{3}$ at these angles. The destructive interference in the backward direction prevents us from a meaningful analysis.

The dominant partial waves for the singlet and triplet states are similar to 10 eV energy from about 8 to 12 eV. At higher energies, the dominant partial waves have the same L value for the triplet and the singlet spin states, only their magnitudes differ [e.g., see Fig. 2(b)]. This brings about a qualitatively different behavior on the dependence of the exchange asymmetry on the scattering angle. As the energy of the impinging electron increases, the peak values of the exchange asymmetries gradually decrease, indicating a reduction of exchange effects as expected. At 20 eV and at incident energies above it, the exchange asymmetry is negative for most of the angular range with the peak value of about −28% at 20 eV and −10% at 30 eV. The partial wave cross sections at 54.4 eV are shown in Fig. 2(b). The small difference between the singlet and the triplet cross sections implies a small exchange effect. The exchange asymmetry at this energy is discussed below.

The present results of the four-state close-coupling calculations are compared with the experimentally measured values of exchange asymmetry at an energy of 54.4 eV in Fig. 3. The overall agreement is at best qualitative; quantitatively, there are obvious differences. The differential cross section has a minimum at 108°. The structure in the theoretical exchange asymmetry at this angle arises from the difference between the singlet and the triplet differential cross sections; both have a minimum at this angle. The theoretical results imply triplet scattering dominating singlet scattering at all angles. The theoretical results have a shallow dip at about 15°, the measurements have a shallow dip of about the same magnitude at about 40°. Possible causes for the discrepancy are suggested below.

It must be remarked that the present calculations do not include the spin-orbit effects and the experimentally measured[1] asymmetry corresponding to the spin-orbit interaction is nonzero (although it is small). The quantitative differences between the present theoretical results and the experimental ones could arise due to the neglect of the spin-orbit interaction in the calculation.

Another possible cause for the differences in Fig. 3 could be an incomplete expansion in the close-coupling scheme. Specifically, the loss of flux of channels corresponding to excitations of higher states or of the continuum channels is not accounted for in the present calculations. In regard to the latter point, it is interesting to note that the inclusion of the $3d$ and the $4s$ states does not make a significant change from the two-state calculation[7] reported earlier in Ref. 1 (see Fig. 3). The two-state calculation reported in Ref. 1 was performed in momentum space representation. The present two-state close-coupling calculations performed in coordinate space (not reported here) obtain the same results.

A third possible cause for the difference could be the assumption that the sodium atom core is inert; the core electrons only affect the determination of the wave function of the valence electron, but are not explicitly involved in excitations or exchange with the scattering electron.

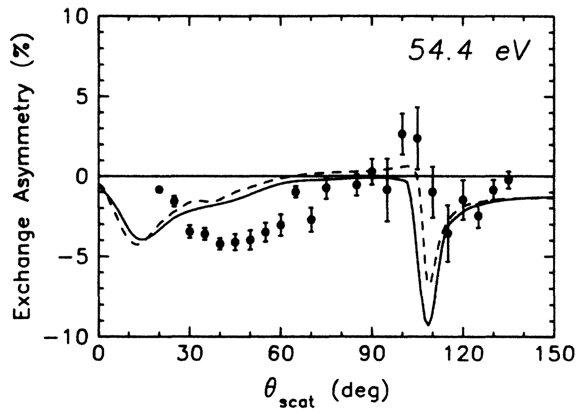

FIG. 3. Comparison of the theoretically calculated exchange asymmetry from the present four-state close-coupling calculations (solid) and the two-state close-coupling calculations of Ref. 7 (dashes) with the experimentally measured values (circles with error bars) from Ref. 1 at an incident energy of 54.4 eV.

Since a discrepancy exists between the theoretical results and the experiment at 54.4 eV, theoretical investigations which incorporate the three above-mentioned physical effects either separately or cumulatively would be very useful towards a better understanding of the dynamics of the scattering phenomenon at this energy.

The three likely possibilities, mentioned here as sources of difference between the theory and experiment at 54.4 eV, would have quite different influence on the scattering process at lower energies (~10 eV). At an electron energy of 10 eV, the spin exchange asymmetries are quite large, and hence it would be interesting to see if the future experiments confirm this prediction.

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[2]For a review article on close-coupling approximation and other approximations of prevalent use in theoretical calculations of electron scattering by atoms, see J. Callaway, Adv. Phys. **29**, 771 (1980).

[3]A. W. Weiss (private communication).

[4]A recent and rather precise lifetime measurement by A. Gaupp, P. Kuske, and H. J. Andra [Phys. Rev. A **26**, 3351 (1982)] indicated a value of 0.95 for the oscillator strength of the $3s$-$3p$ transition compared to the previously accepted value of 0.98. The geometric mean of the length and velocity forms of the oscillator strength determined from the target-state wave functions used here is 0.98.

[5]D. H. Oza and J. Callaway, J. Comput. Phys. **68**, 89 (1987).

[6]D. H. Oza (unpublished).

[7]J. Mitroy, I. E. McCarthy, and A. T. Stelbovics (private communication).