ELECTRONIC STRUCTURE OF MATERIALS CENTRE

Calculation of spin-dependent observables in electron-sodium scattering using the coupled-channel optical method.

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We present calculations of the 3^2S and 3^2P spin asymmetries and $L_\perp$ for singlet and triplet scattering for projectile energies of 10 and 20 eV. Together these observables give a most stringent test of any electron-atom scattering theory. We find excellent agreement between the results of our coupled-channel optical method and experiment, which for the spin asymmetries can only be obtained by a good description of the couplings between the lower-lying target states and the target continuum.

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Traditionally it is the electron-hydrogen scattering problem that has been used to test the validity of any general electron-atom scattering theory. This is because for theorists the hydrogen atom is ideal as a scattering target since it is the only atom for which the wavefunctions are known exactly. Unfortunately for experimentalists this is a rather difficult target to work with. Though a considerable amount of experimental data is available most of it is averaged over the singlet and triplet states. This loses a great deal of information which is of fundamental interest to the theorist.

The proper treatment of singlet and triplet scattering involves correct theoretical treatment of electron exchange using the Pauli exclusion principle. This is not a trivial task and there are some theories that treat exchange approximately in the hope that it won't effect the comparison with experiments, which are averaged over spin states.

In the close-coupling formalism (see Percival and Seaton [1] for example) the standard treatment of exchange is to symmetrize the wavefunction of the projectile and valence electrons explicitly via

$$\Psi^S(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{2}\sum_i \left(\phi_i(\mathbf{r}_2)F_i^S(\mathbf{r}_1) + (-1)^S\phi_i(\mathbf{r}_1)F_i^S(\mathbf{r}_2)\right), \tag{1}$$

where the $\phi_i(\mathbf{r})$ are the target electron wavefunctions (discrete and continuous) and the $F_i^S(\mathbf{r})$ are some spin dependent one electron functions which result from the solution of the full Schrödinger equation. However it is easily seen that for triplet scattering ($S = 1$) this expansion is not unique since for each particular i we can add $\lambda\phi_i(\mathbf{r})$ to $F_i^S(\mathbf{r})$ without effect on (1), for arbitrary constant λ. The general complete set of solution for $F_i^S(\mathbf{r})$ resulting from expansion (1) has been given by Bray and Stelbovics [2]. They also showed that in order to render the solutions $F_i^S(\mathbf{r})$ unique, they must satisfy

$$\langle\phi_j|F_k^S\rangle = (-1)^S\langle\phi_k|F_j^S\rangle. \tag{2}$$

To thoroughly test the treatment of exchange it is necessary to have measurements of spin dependent observables. An extensive set of such measurements have been carried out for electron-sodium scattering by McClelland *et al* [3], Scholten *et al* [4], and Kelley *et al* [5]. They measured the ratio of triplet to singlet scattering for the 3^2S and 3^2P channels as well as $L_\perp^S$ the angular moment im transferred to the atom perpendicular to the scattering plane for singlet ($S = 0$) and triplet ($S = 1$) scattering. In our view these measurements provide the most sensitive and extensive test of any electron-atom scattering theory to date.

The theory which we use for electron-atom scattering is based on the coupled-channel optical (CCO) method of Bray *et al* [6]. It has been extensively tested by achieving excellent agreement with measured observables summed over the spin states on atomic hydrogen [6, 7] and sodium [8, 9] for all projectile energies. This theory is based on the close-coupling formalism, but only treats a finite set of discrete states $|\phi_i\rangle$ (P space) in (1) explicitly as coupled channels with the remainder set of states (Q

space) being treated indirectly via a complex non-local polarization potential. This potential together with the first order potentials is known as the optical potential. It is calculated *ab initio* with the approximation of weak coupling in Q space. By this we mean that the effect of coupling between distinct Q-space states upon P space is ignored, but direct coupling between P and Q spaces is included. This approximation is readily tested for Q-space discrete states by observing the effect of having such a state in P space. We say that our results are internally consistent whenever we get similar corresponding results from nCCO and n'CCO calculations for $n > n'$, where n and n' are used to indicate the number of P-space states. The treatment of the continuum can only be tested by comparison with experiment.

To approximate the structure of the sodium atom we use the self-consistent-field Hartree Fock model for the ground state of the atom, and the frozen-core Hartree-Fock model for the excited states, see [9] for more detail. As this is not an exact description of the sodium atom we do not expect to necessarily achieve complete quantitative agreement with experiment as we expect for hydrogen. Following the notation of [9] we solve the Lippmann-Schwinger equation for the total spin-dependent T matrix

$$\langle \mathbf{k}\phi_i \mid T^S \mid \phi_0\mathbf{k}_0\rangle = \langle \mathbf{k}\phi_i \mid V_Q^S(\theta) \mid \phi_0\mathbf{k}_0\rangle + \sum_{\phi_{i'}\in P}\int d^3k' \frac{\langle \mathbf{k}\phi_i \mid V_Q^S(\theta) \mid \phi_{i'}\mathbf{k}'\rangle}{(E^{(+)} - \epsilon_{i'} - k'^2/2)}\langle \mathbf{k}'\phi_{i'} \mid T^S \mid \phi_0\mathbf{k}_0\rangle, \qquad (3)$$

where the projectile with momentum $\mathbf{k}_0$ is incident on the target with the valence electron in the ground state $|\phi_0\rangle$ energy ϵ_0 above the frozen core, and where $E = \epsilon_0 + k_0^2/2$ is the on-shell energy. Writing the coordinate space-exchange operator as P_r the matrix elements of $V_Q^S(\theta)$ are given by

$$\begin{aligned}\langle \mathbf{k}\phi_i \mid V_Q^S \mid \phi_{i'}\mathbf{k}'\rangle = \langle \mathbf{k}\phi_i \mid v^{FC} + v_{12}(1 + (-1)^S P_r) \mid \phi_{i'}\mathbf{k}'\rangle \\ +(-1)^S(1-\theta)(\epsilon_i + \epsilon_{i'} - E)\langle \mathbf{k}|\phi_{i'}\rangle\langle\phi_i|\mathbf{k}'\rangle \\ +\delta_{ii'}\theta\sum_{\phi_n\in P}(\epsilon_i + \epsilon_n - E)\langle \mathbf{k}|\phi_n\rangle\langle\phi_n|\mathbf{k}'\rangle \\ -\delta_{ii'}\sum_{\psi_j\in C}\langle \mathbf{k}\psi_j \mid (2\varepsilon_j - E)P_r \mid \psi_j\mathbf{k}'\rangle \\ +\langle \mathbf{k}\phi_i \mid V_Q + (-1)^S V_Q P_r \mid \phi_{i'}\mathbf{k}'\rangle, \end{aligned} \qquad (4)$$

where v^{FC} is the projectile-core potential, v_{12} is the projectile-valence electron potential, $|\psi_j\rangle \in C$ are the frozen core wavefunctions, and V_Q is the polarization potential given in [6]. The constant θ above is arbitrary. Bray and Stelbovics [2] have shown that any non-zero θ imposes the symmetry condition (2) and leads to a unique answer for the T matrix independent of θ, both on and off the energy shell. In our previous work [6–9] we had in effect $\theta = 0$. Stelbovics [10] has shown that that for $\theta = 0$ only the on-shell T matrix is defined uniquely which explains why we achieved good results. However we have found as the number of P-space states is increased off-shell

instability effects the on-shell stability. This problem is eliminated for $\theta \neq 0$. In this work we take $\theta = 1$ for convenience.

We solve (3) for projectile energies of 10 and 20 eV in the 3^2S channel. The results for the spin asymmetries and $L_\perp^S$ (see ref [7] for relation to the T matrix elements) are in figures 1 and 2 respectively. We performed three calculations at each energy denoted by 6CCO, 6CCO$^-$, and 6CC. Each has P space containing the six 3^2S, 3^2P, 3^2D, 4^2S, 4^2P, and 4^2D states. The 6CCO calculation treats the complete set of discrete and continuum excited states to convergence via the polarization potential. The 6CCO$^-$ calculation only treats the discrete excited states. As our treatment of discrete excited states is internally consistent, it is equivalent to a multi-channel close-coupling calculation that uses the same set of states. The 6CC calculation is used as a basis to examine which effects are most significant. It treats only the P-space states.

Examining the two figures we find agreement of our 6CCO results with experiment to be quite remarkable. We see that in general the 6CC calculation gives a good qualitative agreement with experiment. The 6CCO$^-$ improves the agreement, and finally the addition of the continuum states achieves excellent quantitative agreement. It is very interesting to see the considerable effect that the continuum states have upon the asymmetries at both energies, particularly around 40 degrees for the 3^2P channel. This indicates that a simple CC calculation using only excited discrete states can never get correct asymmetries at these energies (see [4] for comparison with some other theories). In fact it would only approximate our 6CCO$^-$ results which are not even in qualitative agreement with the asymmetry measurements at 20 eV.

These results give the best indication yet that our CCO treatment of the continuum is very good. They also confirm that exchange is being treated correctly. We will now apply our theory to more energies where such extensive measurements exist and attempt a more detailed study of the present discrepancies with experiment, in particular around 60 degrees for the 10 eV singlet $L_\perp$ and around 40 degrees for the 20 eV elastic asymmetry. Given the very large effect of the continuum, which we are unable to treat exactly, and the structure approximations we are not perturbed by the remaining small discrepancies.

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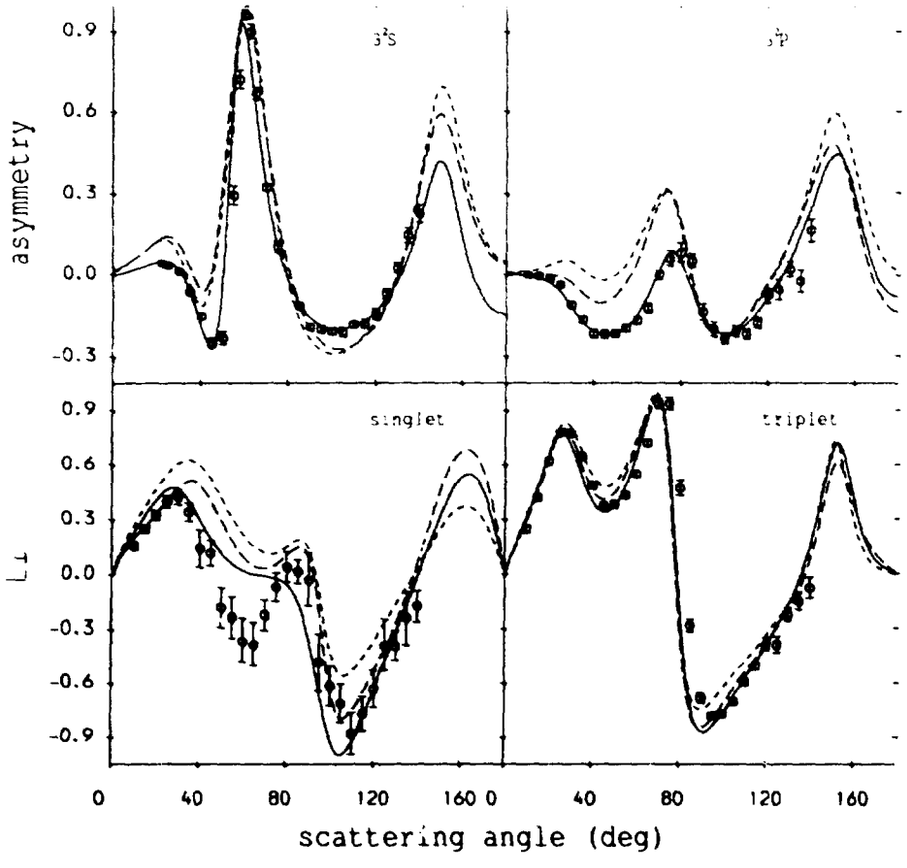
FIGURES

FIG. 1. Spin asymmetries and $L_\perp$ for electron-sodium scattering at 10 eV. The elastic measurements are due to Kelley *et al* [5] and the inelastic due to Scholten *et al* [4]. The solid line denotes the 6CCO theory which treats the complete set of excited target states, discrete and continuous. The long-dashed line denotes the 6CCO$^-$ theory which only treats the excited discrete states. The short-dashed line treats only the six P-space states: 3^2S, 3^2P, 3^2D, 4^2S, 4^2P, and 4^2D.

FIG. 2. Spin asymmetries and $L_\perp$ for electron-sodium scattering at 20 eV. The elastic measurements are due to Kelley *et al* [5] and the inelastic due to McClelland *et al* [3]. The solid line denotes the 6CCO theory which treats the complete set of excited target states, discrete and continuous. The long-dashed line denotes the 6CCO$^-$ theory which only treats the excited discrete states. The short-dashed line treats only the six P-space states: 3^2S, 3^2P, 3^2D, 4^2S, 4^2P, and 4^2D.



10 eV

Fig.1

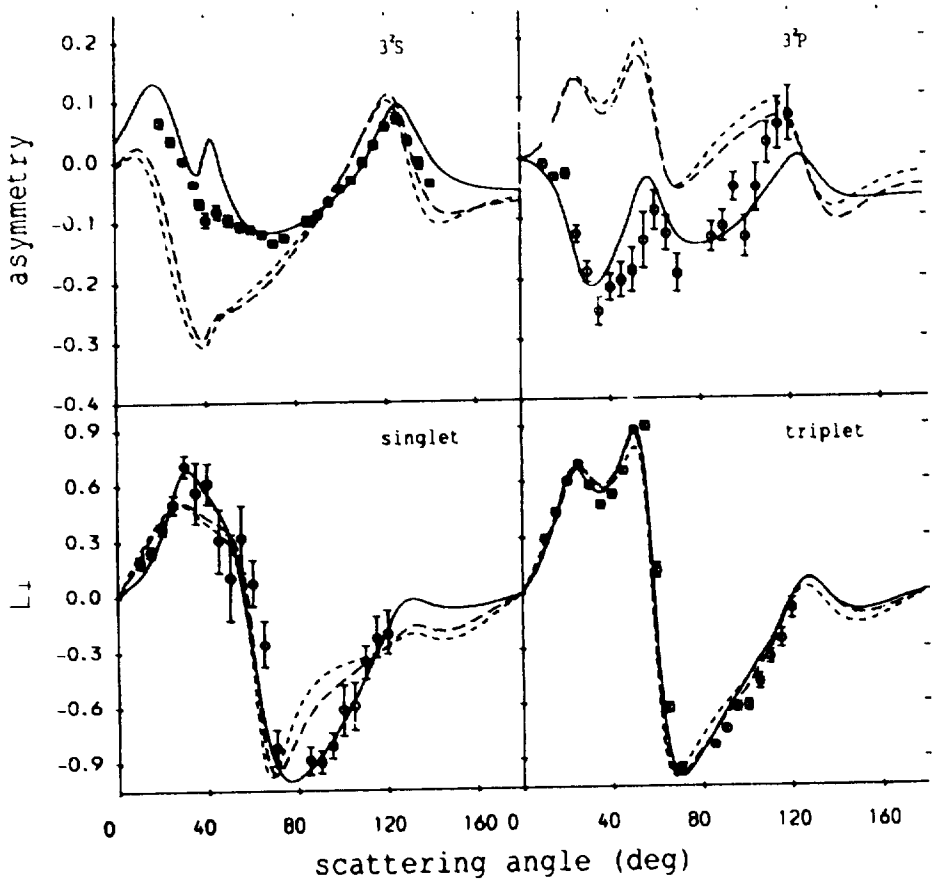
——— 6CCO

– – – – 6CCO⁻

····· 6CC

20 eV

Fig.2



20 eV

Fig.2

——— 6CCO

- - - - 6CCO⁻

------ 6CC