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Convergent close-coupling calculation of electron-sodium scattering

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We perform convergent close-coupling (CCC) calculations of electrons scattering on atomic sodium. We show that the results are in excellent quantitative agreement with the measurements of spin asymmetries and singlet and triplet $L_\perp$ at the two projectile energies considered of 10 and 20 eV. The CCC method is the only one that is able to achieve this to date, and demonstrates that the very large effects of the target continuum are very accurately treated using square-integrable states. The method is applicable to all hydrogenlike atoms or ions and all projectile energies.

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The calculation of electron-atom scattering is of both fundamental and practical interest to physicists. It is nontrivial for even the simplest of atomic species. To date there are still significant discrepancies between theory and experiment for angular correlation parameters in electron-hydrogen scattering (see Ref. [1] and references therein). As the discrepancies occur at projectile energies above the ionization threshold, it is necessary for theory to treat the target continuum. There has been a considerable effort from the theorists in developing ever more sophisticated calculations such as the intermediate-energy R-matrix method of Scholz *et al.* [2], the pseudostate methods of Callaway [3] and van Wyngaarden and Walters [4], the exact second-order method of Madison, Bray, and McCarthy [5], the coupled-channel optical (CCO) method of Bray, Konovalov, and McCarthy [6,7], and the convergent close-coupling (CCC) method of Bray and Stelbovics [1]. All of these treat the target continuum to various degrees of accuracy. None of these are able to explain the discrepancies with experiment, but are in good agreement with each other.

It was particularly disappointing to find that the latter of these also does not agree with experiment, as it solves the full e-H scattering problem to convergence. This is achieved by performing close-coupling (CC) calculations with target states, obtained by diagonalizing the target Hamiltonian in an ever increasing Laguerre basis, until convergence is obtained. We denote the converged close-coupling results by CCC. This is a general approach to electron-atom scattering that may be applied at all energies where the Born approximation is not valid. It has been tested [8] against the Poet-Temkin model [9,10], where only states of zero orbital angular momentum are treated. It was shown that the pseudoresonances associated with the use of square-integrable states diminished with increasing basis size, and that the results converged to the exact values of this model problem. This is a very important result, as it showed that the effect of the continuum may be treated by the use of square-integrable states directly, without encountering the usual pseudoresonance problems associated with the use of pseudostates [3].

Unfortunately, application of the CCC method to the calculation of the angular correlation parameters in the full e-H scattering problem did not resolve the discrepancies with experiment. However, an application of the method to the calculation of the total ionization cross section and asymmetry [11] resulted in remarkable quantitative agreement with experiment. The CCC method is the only general approach to electron-atom scattering

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calculations that is able to achieve this result to date. This confirms our belief that the treatment of the continuum via square-integrable states is justified in the full e-H scattering problem also.

It is quite clear that in order to calculate the total ionization cross section the effect of the continuum on the scattering must be taken into account. One would not expect this to be necessarily the case when observing scattering in just the elastic or the first inelastic channels. However, we found that when calculating electron-sodium scattering, the effect of the continuum on the elastic $3S$-$3S$ and the inelastic $3S$-$3P$ spin asymmetries (essentially ratios of triplet to singlet scattering) was very large at projectile energies of 10 and 20 eV, and brought about excellent agreement with experiment [12]. An earlier indication that this may be the case was found by McCarthy *et al.* [13], and later by Madison *et al.* [14]. Though these two theories do not achieve quantitative agreement with experiment, it is clear that their results are significantly improved by the treatment of the continuum states. The method of calculation we used was the CCO method, where the target states are eigenstates of the target Hamiltonian. The major approximation in this method is that of weak coupling in Q space, which contains the continuum. A full application of this method by Bray and McCarthy [15] showed that the effect of the continuum was particularly large when calculating spin asymmetries at projectile energies above the ionization threshold. It follows that inclusion of the continuum in the calculation has a significant effect on the scattering amplitudes, and so ideally should always be included irrespective of which observable is being calculated.

These results raise a few questions. Why is it that the continuum can have such a large effect on even the elastic channel? Does this mean that there is a very large interaction of the elastic channel with the continuum in the experiment? Furthermore, if the effect of the continuum is very large, why does the CCO method work so well, given that it calculates the continuum contributions subject to some approximations?

While a detailed response to these questions we give elsewhere [16], the answers may be summarized as follows. It turns out that the very large effect of the continuum comes primarily from the imaginary part of the complex nonlocal polarization potential. It is this part that allows electron flux to escape into the ionization channels. A standard CC calculation that uses only discrete states confines all of electron flux to be within the discrete channels, and yields identically zero for the total ionization cross section. The fact that the real part of the complex polarization potential plays a small role indicates that intermediate interaction with the continuum is very small, as our intuition would suggest. The CCO method works well because it gives a reasonable reproduction of the total ionization cross section [6], though it does not model the ionization channels as well as the CCC method [11].

Since the effect of the continuum is so large it is not surprising that there remained a few small discrepancies between the CCO results [15] and experiment. One such discrepancy is for the singlet $L_\perp$ parameter (angular momentum transferred to the atom perpendicular to the scattering plane) at a projectile energy of 10 eV. In fact, we remarked in the earlier work that perhaps this parameter will serve as a test case of the accuracy of treating the target continuum. We will see that this does prove to be the case.

It must be mentioned that the detailed testing of theory has become possible due to the remarkable measurements of Celotta, Kelley, Lorentz, McClelland, and Scholten [17–21]. The experiments involve the measurement of ratios at each scattering angle and so are very accurate. Resolution of singlet and triplet scattering has given theorists the opportunity to thoroughly test the treatment of exchange, which is typically one of the more difficult aspects of the calculations. Furthermore, the measurements were performed at a number of projectile energies ranging from 1 to 54 eV, allowing for a comprehensive test of general electron-atom scattering theories.

In this Rapid Communication we present CCC calculations of spin asymmetries, and singlet and triplet $L_\perp$ at energies of 10 and 20 eV of electrons scattering on atomic sodium, and compare them with experiment and the previously best theory. The development of the CCC method for electron-hydrogen scattering to hydrogenlike atoms or ions is the natural progression of the work of Bray and Stelbovics [1,8,11] and Bray and McCarthy [15]. The former papers established the method for e-H scattering, whereas the latter showed that electron-alkali scattering may be treated similarly by replacing the local proton-electron potential of hydrogen with the nonlocal frozen-core Hartree-Fock potential of sodium. We make this adaptation to the CCC theory [1] as well as casting the method in the distorted-wave (or distorted-Coulomb-wave) formalism while still keeping essentially real arithmetic in the computation.

The use of Laguerre basis states has the effect of choosing a Gaussian-type quadrature rule for the integration over the continuum [22]. The Laguerre basis $\xi_{kl}(r)$ we use is

$$\xi_{kl}(r) = \left(\frac{\lambda_l (k-1)!}{(2l+1+k)!}\right)^{1/2} \times (\lambda_l r)^{l+1} \exp(-\lambda_l r/2) L_{k-1}^{2l+2}(\lambda_l r), \qquad (1)$$

where the $L_{k-1}^{2l+2}(\lambda_l r)$ are the associated Laguerre polynomials and k ranges from 1 to the basis size N_l. Upon diagonalization of the target Hamiltonian for partial-wave l we obtain N_l square-integrable states. The negative energy states converge pointwise to the discrete eigenstates as the basis size N_l is increased. Apart from a normalization factor, the positive energy states resemble the true continuum states until the exponential falloff dominates. The free parameter λ_l is typically set between 1 and 2. This results in the fastest rate of convergence with increasing N_l. It may be varied in addition to N_l to test that convergence has indeed been achieved. We find that the positive energy states that have energies which are sufficiently large for the corresponding channel to be closed may be left out of the calculation. This is consistent with the fact, found using the CCO model, that the effect of the continuum comes from allowance

of flux to go into the ionization channels. The 10-eV results presented here were generated using the lowest (in energy) $12s$ ($N_l = 35$), $10p$ ($N_l = 25$), and $9d$ ($N_l = 20$) states, all of which result in open channels. All of the remaining states, $23s$, $15p$, and $11d$ were omitted, as they generated closed channels. The 20-eV results were generated by taking the lowest $15s$, $15p$, and $15d$ states, with $N_l = 20$ for each l. All but five of these result in open channels. This is one of the largest [45 states, leading to $15 \times (1+2+3) = 90$ channels] calculations that we have performed thus far.

The results of our CCC calculations of electron-sodium scattering are given in Figs. 1 and 2 for projectile energies of 10 and 20 eV, respectively. At each energy we present three calculations denoted by CCC, CCO, and CC. The former treats a large number of Laguerre basis states directly via the close-coupling formalism as specified above. The CCO and CC calculations are taken from Ref. [15], with the latter treating only the discrete target states to convergence (first 15 discrete states), and so by comparison with CCC and CCO, the effect of the inclusion of the target continuum may be readily observed.

In Fig. 1 we see that the continuum plays a significant role in calculating both the elastic and inelastic spin asymmetries. Both the CCC and CCO methods yield very similar results and are in excellent agreement with experiment. This agreement is very encouraging, given that the electron-sodium system is treated as a three-body problem of an inert core (though exchange allowed) and two electrons. In calculating the sodium target states we take the electron-core potential to be essentially the frozen-core Hartree-Fock potential. We also add a small local phenomenological polarization potential to slightly improve the one-electron energies [15], but this has little effect at the projectile energies considered here. The result for the singlet $L_\perp$ is particularly pleasing. Of all the measured $L_\perp$ parameters, this is the only one with which the CCO theory [15] had a major discrepancy. We see that the CCC theory is in complete agreement with experiment and indicates the importance of treating the continuum accurately. By contrast to the singlet $L_\perp$ we see that the triplet $L_\perp$ is totally insensitive to the continuum, and all three theories are in perfect agreement.

The fact that coupling within the continuum is important to reproduce the singlet $L_\perp$ is quite remarkable. For many years it was believed that just the inclusion of the $3s$ and $3p$ target states was sufficient to reproduce e-Na scattering data. This belief was due to the fact that most of the polarization is due to the $3p$ state. Good agreement with differential cross sections, particularly at forward angles, supported this belief. Now we have seen that for the simple hydrogenlike system like sodium the effect of the continuum is large and requires very accurate treatment. Fortunately, the projectile energy range where this is the case is restricted to the intermediate region.

The largest effect of the continuum on the spin asymmetries can be seen in Fig. 2 for a projectile energy of 20 eV. Here we see that the CCC and CCO theories are in excellent agreement with experiment, with the former being a small improvement on the latter for the inelas-

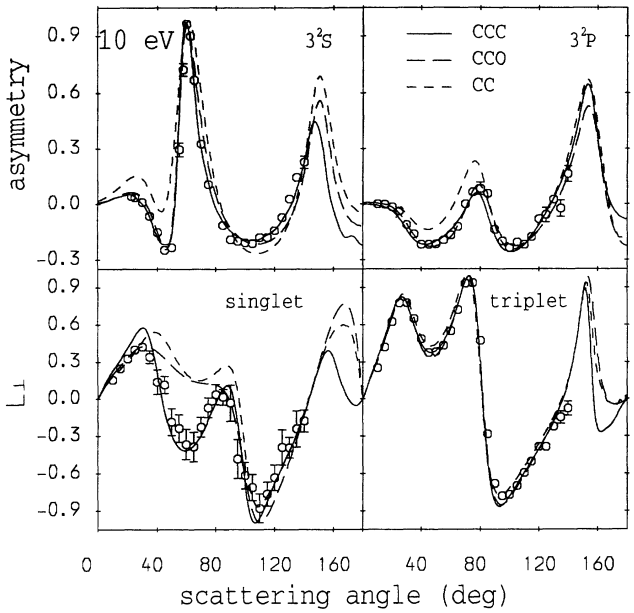

FIG. 1. Elastic and inelastic spin asymmetry, singlet and triplet $L_\perp$ for electron scattering on sodium at 10 eV. The convergent close-coupling (CCC) calculation couples $12s$, $10p$, and $9d$ Laguerre basis states (see text for details). The coupled-channel optical (CCO) method [15] couples the first 15 ($3 \le n \le 6$ and $0 \le l \le 3$) discrete eigenstates, with the effect of continuum states with $l \le 5$ included via a complex polarization potential. The CC calculation denotes a standard close-coupling calculation that truncates the multichannel expansion after convergence in the use of just the discrete target eigenstates has been obtained. These are the same 15 states used in the CCO calculation [15]. The measurements are due to Kelley et al. [20], with the error bars only shown if they are bigger than the size of the symbol denoting the experiment.

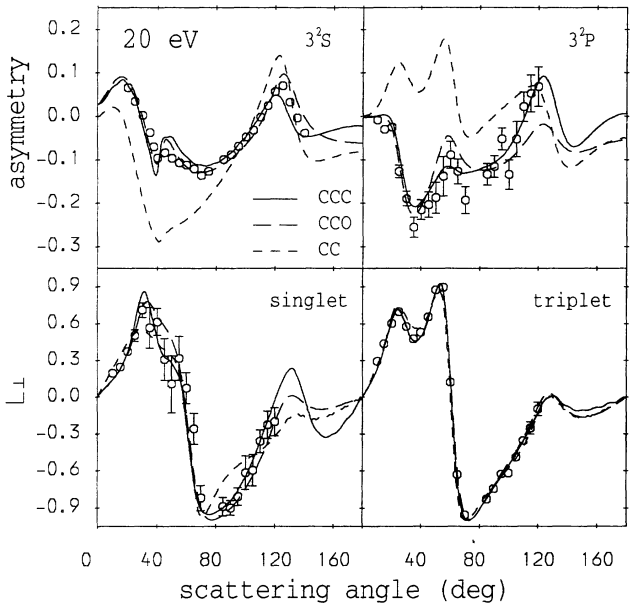

FIG. 2. Elastic and inelastic spin asymmetry, singlet and triplet $L_\perp$ for electron scattering on sodium at 20 eV. The CCC results have been generated using $15s$, $15p$, and $15d$ Laguerre basis states (see text for details). The CCO and CC theories as well as experiment are as in Fig.1.

tic asymmetry at the backward angles. By contrast, the CC calculation predicts very different spin asymmetries, indicating the effect of the continuum whether treated by positive energy square-integrable states or a complex polarization potential generated from true continuum states.

We would like to emphasize the significance of the similarity of the CCC and CCO results. In the former case all negative and positive energy states are square integrable; the potentials are real and are fast to calculate. Most of the calculation time goes into solving the resulting coupled equations which form a linear set of equations of order 5000. In this method we are only able to treat target states up to orbital angular momentum $l = 3$ as the size of the linear equations becomes prohibitively large for our computational resources. Furthermore, ill conditioning of the linear equations increases linearly with the order of the equations. In the CCO method, the target states are eigenstates of the target Hamiltonian. The true continuum states are used to form a complex nonlocal polarization potential subject to approximation, which is then added to the first-order potential generated from the discrete states. The resulting linear equations have complex elements, but are of order 500. Most of the calculation time goes into making the polarization potential matrix elements. These may contain contributions from target states with arbitrary l, and we typically have up to $l = 5$. Thus, the two calculations are very different. If they agree with each other, then this gives a very strong indication of the reliability of the results. If they differ, then by performing CCO with target states up to $l = 3$ only, as in CCC, we can establish whether the discrepancy is due to the more accurate treatment of the continuum in CCC or due to the higher target partial waves treated in CCO.

In conclusion, we have demonstrated that the target continuum needs to be treated accurately when calculating spin asymmetries and the singlet $L_\perp$ in the intermediate energy range. In other words, the underlying results of collision theory, the scattering amplitudes, are significantly affected by the accuracy in the treatment of the continuum. We find that the effect of the continuum is taken into account quite well by the CCC method using only open channels. This reinforces our belief that the effect of the continuum on the lowest-lying channels comes about primarily from electron flux being allowed to escape to all open channels. We have shown that the most accurate way to date of treating the target continuum is provided by the CCC formalism. This is not only the case at the intermediate energy range, but also at the low and high energies, where the number of coupled states necessary for convergence is considerably reduced. As such, we believe that we are in a unique position to provide very accurate electron-hydrogenlike target scattering amplitudes for any transition (including ionization), at all projectile energies, for neutral targets of H, Li, Na, and K, as well as ions He^+, Li^{2+}, Ar^{7+}, to name a few. The targets may be in the ground state or any excited state. We will follow this paper with a comprehensive description of the CCC method for electron-hydrogenlike target scattering, and apply it to the wide range of energies where many more observables have been measured.

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