Calculation of Electron Impact Total, Ionization, and Nonbreakup Cross Sections from the 3S and 3P States of Sodium

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We present convergent close-coupling calculations of the total, ionization, and nonbreakup cross sections for electron impact of Na 3S and 3P states. We show that the total and nonbreakup cross sections converge rapidly with increasing target orbital angular momentum $l_{\max}$ used in the close-coupling expansion. The total ionization cross section is less rapidly convergent, and typically has the largest partial contribution from ionization of the $l = l_{\max}$ states. The total cross sections and total ionization spin asymmetries are in excellent quantitative agreement with experiment. However, the total ionization cross section from the 3S state is approximately a factor of 2 lower.

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One of the more difficult aspects of electron scattering theory is the treatment of the target continuum. A fundamental test of the theory is provided by being able to calculate the total ionization cross section σ_i. Any close-coupling method that treats only the discrete spectrum yields identically zero for this cross section. Existence of accurate measurements allows us to test the quality of the treatment of the continuum. Availability of such data for hydrogenlike targets such as atomic hydrogen or the He^+ ion is very helpful to the theorist, as then the target wave functions are known analytically. Bray and Stelbovics [1] have demonstrated that the convergent close-coupling (CCC) method is able to reproduce the electron impact total ionization cross section of atomic hydrogen. Application of the method to the He^+ ion by Bray *et al.* [2] proved just as successful. Both of these works demonstrated that the σ_i may be obtained by treating the true continuum with a sufficiently large set of positive-energy square-integrable states. It was noted that convergence in the ionization cross section was readily obtained using target states with orbital angular momentum $l \leq 3$, but a detailed analysis of partial contributions σ_i^l to this cross section was not attempted.

The CCC method has been generalized to include targets that may be readily treated by the model of a single electron above a frozen Hartree-Fock core [3]. Application of the method to the calculation of many detailed spin-resolved measurements available for sodium has resulted in excellent quantitative agreement with experiment [3]. However, we found that the σ_i obtained from these calculations yielded a cross section that was around a factor of 2 less than the experiments performed in the sixties [4,5]. This we found surprising because we obtained excellent agreement with the measurements of the total, and many individual discrete cross sections, as well as the total ionization spin asymmetry. Furthermore, it was shown that the effect of the continuum in calculating the 3S-3P excitation observables was often very large, and treated very accurately using the CCC method.

The CCC method employs the close-coupling (CC) formalism where the coupled states have been obtained by diagonalizing the target Hamiltonian in a large one-electron Laguerre basis for hydrogenlike targets [3], or a two-electron basis in the case of helium [6]. These states are all square integrable with the positive-energy ones being a truncated discrete representation of the true target continuum. Upon solution of the coupled equations, the total ionization cross section σ_i is found by obtaining the total cross section σ_t and the total nonbreakup (elastic plus excitation) cross section $\sigma_{\rm nb}$, and then forming

$$\sigma_i = \sigma_t - \sigma_{\rm nb}. \tag{1}$$

The σ_t may be obtained by either summing the individual cross sections for each state used in the coupled equations or utilizing the unitarity of the CC formalism by using the optical theorem. The $\sigma_{\rm nb}$ is obtained by summing the cross sections for those states which have negative energy, multiplied by the projection of the state onto the true discrete subspace [1].

The cross sections $\sigma_{{\rm nb},i,t}$ are simply the sums of individual l-dependent contributions, i.e.,

$$\sigma_i^l = \sigma_t^l - \sigma_{\rm nb}^l, \tag{2}$$

with

$$\sigma_{{\rm nb},i,t} = \sum_{l=0}^{l_{\max}} \sigma_{{\rm nb},i,t}^l. \tag{3}$$

Given that previously convergence with increasing $l_{\max}$ had been obtained for all of the $\sigma_{{\rm nb},i,t}$, we would expect that $\sigma_{{\rm nb},i,t}^{l_{\max}} \approx 0$. We shall show that this is indeed true for $\sigma_{\rm nb}^{l_{\max}}$ and $\sigma_t^{l_{\max}}$, but not $\sigma_i^{l_{\max}}$.

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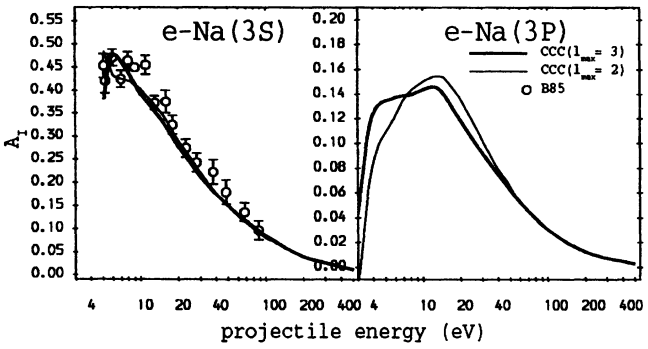

FIG. 1. Total ionization spin asymmetry A_l for electron impact ionization of Na($3S$) and Na($3P$) states. The calculation denoted by the thick line couples around 40 states with the maximum orbital target angular momentum $l_{max} = 3$. At each energy the number of states for each l is taken to be sufficiently large so that convergence is obtained. The thin line corresponds to similar calculations except that $l_{max} = 2$, and the required number of states is around 30. The measurements are due to Baum *et al.* [8].

Further motivation for this work is provided by the fact that there has been a recent study of the ionization of sodium by electron impact [7]. In this experiment the target may be prepared in the $3P$ state, and so we present the cross sections for the sodium target being in the excited $3P$ state as well.

In order to demonstrate our point we need to present some rather detailed information. We introduce the notation by starting with a simple figure. In Fig. 1 we present CCC results for the total ionization spin asymmetry A_l for the two cases of $l_{max} = 2$ (thin line) and $l_{max} = 3$ (thick line). Both are convergent with increasing basis size $N_l \gtrsim 10$ for $0 \leq l \leq l_{max}$. We see that both calculations are almost identical, indicating convergence with increasing l_{max}. Agreement with the available experiment [8], where the target is in the ground state, is excellent. This is a very encouraging result as it means that the ratio of singlet to triplet ionization is correctly reproduced by the theory.

Now we turn to the absolute cross sections, which are shown in Fig. 2. Once again we use the thickness of the line to indicate to which of the two calculations the cross section $\sigma_{nb,i,t}$ belongs. This time we have also presented the partial contributions $\sigma^l_{nb,i,t}$ for each l. The solid lines correspond to the cross sections obtained by summing over all l. The broken lines are the partial contributions. The shorter the dashes the larger the l in the $\sigma^l_{nb,i,t}$ contribution. Turning first to the total and the nonbreakup cross sections we see, by comparison of the thick and thin corresponding lines, that we have good convergence as a function of l_{max}. The summed cross sections are clearly converged, and the convergence within the individual contributions is best for the smallest l, where they are the largest. We also see that the smallest

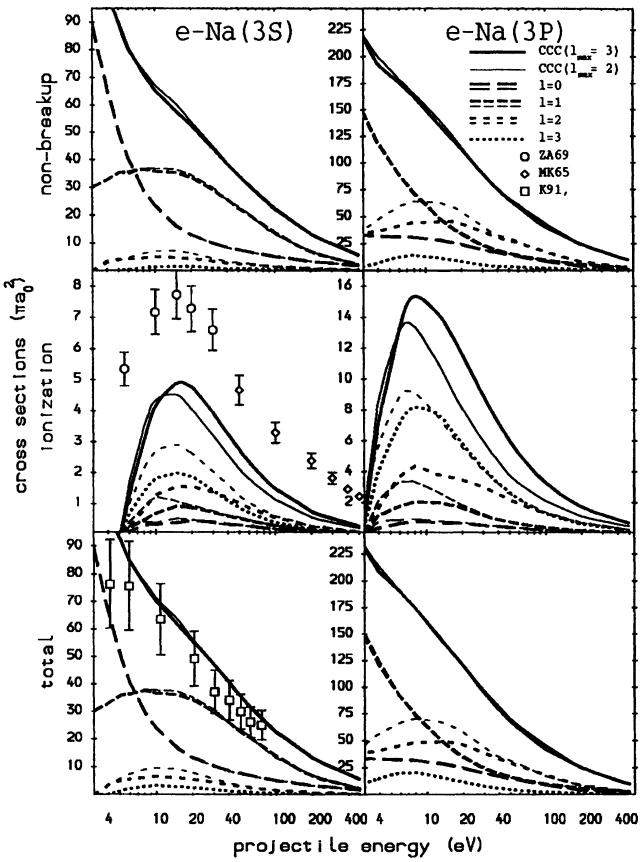

FIG. 2. The total σ_t, nonbreakup σ_{nb}, and total ionization σ_i cross sections calculated using the CCC method. As in Fig. 1 the thick and thin lines correspond to calculations having target states with maximum orbital angular momentum $l_{max} = 3$ and $l_{max} = 2$, respectively. The solid lines are the results of adding the partial contributions $\sigma^l_{nb,i,t}$, which are denoted by the broken lines. The shorter dashes denote the larger l contributions. Note that unlike the case of σ_t and σ_{nb} cross sections, the largest contribution to σ_i comes from $\sigma_i^{l_{max}}$. See text for more detail. The measurements denoted by ZA69, MK65, and K91 are from Refs. [4,5,10], respectively. Quantitative results may be obtained by sending a request to the author.

contribution to the summed cross section comes from the largest l. This is what might be expected.

However, when we look at the total ionization cross section the situation is reversed. Here we see that the contribution of the largest l, in either calculation, is often by far the largest. Yet the summed cross sections (solid lines) are relatively close to each other. Concentrating in the energy region of 10 to 20 eV where σ_i is at a maximum, we have that $\sigma_i^{l_{max}=2}$ is the largest. Addition of an extra l to the calculation leads to $\sigma_i^{l_{max}=3}$ being the largest contribution to σ_i, and yet σ_i has remained relatively stable. So how is it possible to obtain a relatively convergent σ_i when the individual contributions σ_i^l are clearly not convergent?

The nonbreakup cross section has to converge rapidly with increasing l_{max} because it is dominated by the cross sections of states with small l; see Ref. [3] for some individual contributions. The total cross section must also rapidly converge with increasing l_{max} because it may be obtained from the imaginary part of the elastic forward scattering amplitude via the optical theorem, and elastic scattering amplitudes converge rapidly with increasing l_{max}. Note that convergence for σ_i is better for the case where the target is in the ground $3S$ state. Together, these facts guarantee convergence in σ_i with relatively small l_{max}, but say nothing about the distribution of flux within the continuum. It is the unitarity of the CC formalism that allows us to extract convergent total ionization cross sections σ_i without requiring convergent partial contributions σ_i^l. This interesting behavior of σ_i^l may also be the reason why we encountered considerable difficulties when applying the CCC method to calculating $(e,2e)$ differential cross sections at low energies, though this does not seem to be a problem at high energies [9].

The mechanism of the scattering is such that for the l_{max} considered here, the larger l contributions are dominant. As we typically have at least 10 states within each l, increasing l_{max} rapidly increases the size of the calculations. Careful analysis of the partial contributions σ_i^l in Fig. 2 for both values of l_{max} suggests that should it be possible to perform calculations with larger l_{max} then the individual contributions would indeed converge, and begin to diminish for the larger l. This appears to be the case at the higher energies.

Convergence in σ_i has not been demonstrated to the same accuracy at the higher energies as for σ_{nb} or σ_t. The same was the case for the H and He^+ targets [1,2], where we found that for the larger energies it was necessary to take larger l_{max} to obtain excellent quantitative agreement with experiment.

We now turn to the comparison with experiment. Good agreement with the measurements of the total cross section [10] is very encouraging, but due to the size of the error bars and the magnitudes of the cross sections, this does not help us to resolve the factor of 2 discrepancy with the measurements of the total ionization cross section [4,5]. For the reasons discussed above, we do not believe that any larger calculations than those presented here will give significantly different results. Interestingly, though the Born based approximations for ionization are often higher than experiment [1], the Born results of McGuire [11] are also considerably below the experiment, but are in good agreement with our calculations.

Perhaps the development of experimental techniques since the sixties may be able to assist us to resolve the discrepancies with the current measurements of the total ionization cross sections. We hope that the recent work of Tan *et al.* [7] may provide some resolution of the current discrepancy between theory and experiment. Preliminary investigation shows excellent agreement for the ratio of the ionization cross sections from the $3P$ and $3S$ states. For our part, we shall apply the CCC method systematically to the ions in the sodium sequence, Mg^+ to Ar^{7+}, where, for example, initial application to electron impact ionization of the Mg^+ ion has yielded excellent quantitative agreement with experiment. As the techniques in treating electron scattering on sodium and sodiumlike Mg^+ are the same, we believe that the results of the CCC calculations should be equally reliable for both targets.

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