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Calculation of electron-Cs scattering at intermediate energies

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The convergent close-coupling method is applied to the calculation of electron scattering from cesium atoms at intermediate energies (7, 13.5, and 20 eV). Although we use a nonrelativistic model, good agreement is obtained with experimental data for the elastic differential cross section and the spin-exchange asymmetry. This rather surprising result indicates that relativistic effects are less important for these observables than a proper representation of the target continuum states. [S1050-2947(96)00608-7]

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Electron scattering from alkali-metal atoms has been of great interest for many years. These collision systems provide an ideal test ground for experiment and theory since, from an experimental point of view, the target is generally easier to prepare than atomic hydrogen while, from a theoretical point of view, the target structure is very much hydrogenlike. The latter point is important, since the experimentally known target structure is relatively easy to reproduce by using simple model potentials [1]. Consequently, the remaining uncertainty about the target structure is small, and it is very likely that any discrepancies between accurate experimental data and theoretical predictions are due to an insufficient theoretical model for the electron-atom collision process.

The usefulness of alkali-metal targets as a candidate for detailed testing of atomic collision theory was demonstrated in a very clear form by the comparison of experimental data for spin-polarized electron scattering from spin-polarized sodium atoms (measured by McClelland, Kelley, Celotta, Lorentz, and Scholten [2–4]) with various theoretical predictions based on perturbative, such as second-order Born [5], and nonperturbative close-coupling-type [6,7] methods. It was found, for example, that the experimental data for the elastic differential spin asymmetry

$$A^{\mathrm{ex}}=\frac{1}{P_A P_e}\,\frac{N_{\uparrow\downarrow}-N_{\uparrow\uparrow}}{N_{\uparrow\downarrow}+N_{\uparrow\uparrow}}=\frac{\sigma^{\mathrm{s}}-\sigma^{\mathrm{t}}}{\sigma^{\mathrm{s}}+3\sigma^{\mathrm{t}}} \qquad (1)$$

at intermediate energies could only be reproduced by the close-coupling methods that accurately treated the sodium target continuum [8,9]. The most accurate of these is the convergent close-coupling (CCC) method, introduced by Bray and Stelbovics [10], where full coupling between the discrete target states and the target continuum, represented through a large set of square-integrable pseudostates from a Laguerre basis, is included [7]. In Eq. (1), P_A and P_e are the spin polarizations of the target and electron beams, $N_{\uparrow\downarrow}$ and $N_{\uparrow\uparrow}$ are count rates for antiparallel and parallel orientations of the two polarization vectors, and σ^s and $\sigma^t$are the contributions to the differential cross section for unpolarized beams from the singlet and triplet total spin channels.

While the CCC method has been very successful in describing electron scattering from quasi-one-electron systems as well as helium [11], the applicability of the existing nonrelativistic code to electron collisions with heavy targets such as cesium is questionable, since relativistic effects are commonly thought to be important for this collision system. On the other hand, the degree of importance depends on the experimental observable of interest. Whereas a relativistic framework is definitely necessary to obtain a nonvanishing result for the spin polarization after scattering of unpolarized electrons from unpolarized target atoms, such an advanced theory may not be necessary to describe the total and differential cross sections for this case, or even the spin asymmetry (1). In fact, Breit-Pauli and Dirac R-matrix calculations at low energies [12,13] indicated that relativistic effects may indeed be of little importance for the spin-exchange asymmetry. This can be seen, for example, from Fig. 7 of Ref. [12]: If relativistic effects were dominant, one would expect a dependence of A^{ex} on the orientation of the beam polarizations relative to the scattering plane; however, the predicted results for $A_{\perp}^{\mathrm{ex}}$ and $A_{||}^{\mathrm{ex}}$ (perpendicular and parallel to the scattering plane) were nearly identical.

Consequently, we have applied the CCC method in its nonrelativistic form to the e-Cs collision problem. Below we present results for elastic scattering at 7, 13.5, and 20 eV, where relative differential cross sections have been measured by Gehenn and Reichert [14] and spin asymmetries have been published by Raith *et al.* [15,16]. We are not aware of any other theoretical attempt to calculate these parameters in this intermediate energy regime (between about two and five times the ionization threshold) which is very difficult to handle from a theoretical point of view. Further motivation for the present work was the availability of experimental data for total cross sections [17,18] and the total ionization spin asymmetry [19]. Note that the CCC method is an ideal approach to investigate the apparent problem of other close-coupling calculations with discrete states only which, according to Jaduszliwer and Chan [18], ''have yielded total cross sections which are consistently high [compared to experiment] over the covered energy range [up to 18 eV].''

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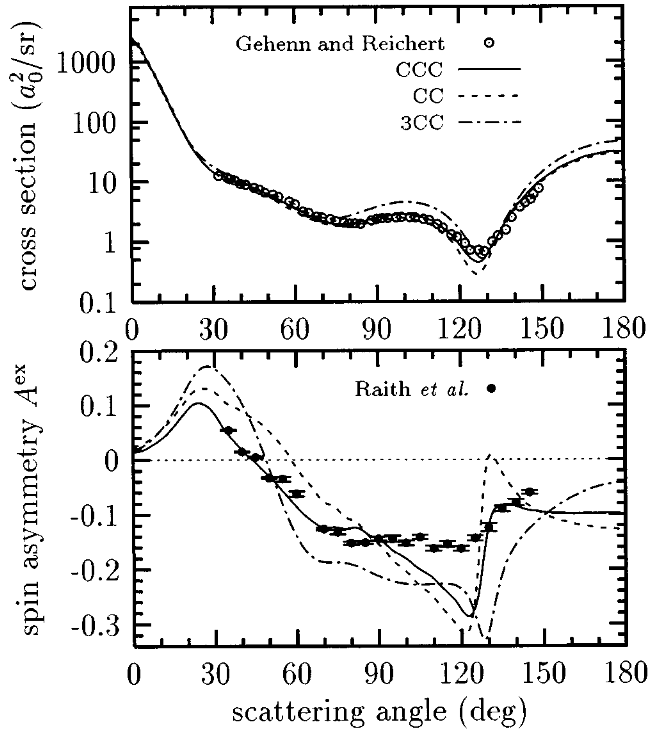

FIG. 1. Differential cross section (top) and spin-exchange asymmetry (bottom) for elastic *e*-Cs scattering at an incident electron energy of 7 eV. The relative cross section data of Gehenn and Reichert [14] were normalized to the CCC theory at small scattering angles. The asymmetry data are taken from Ref. [16]. See text for details of the theoretical models.

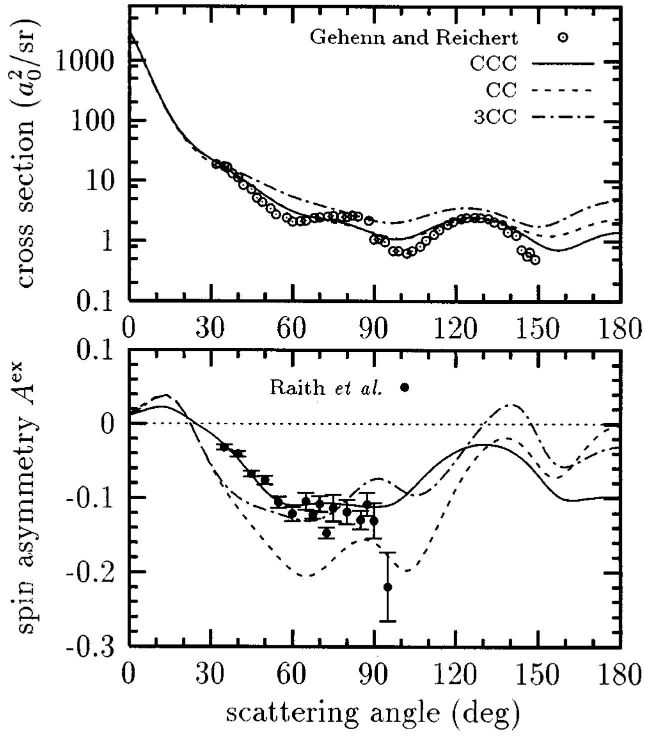

FIG. 2. Same as Fig. 1 except for an electron energy of 13.5 eV. The relative cross section data [14] are for 13.0 eV, and the asymmetry data are taken from Ref. [15].

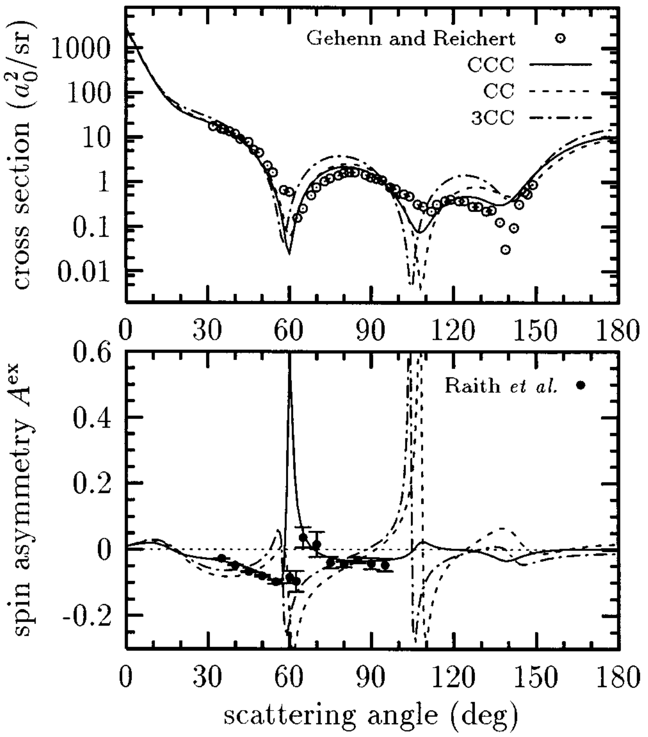

FIG. 3. Same as Fig. 2 except for an electron energy of 20.0 eV.

In the present CCC theory we treat Cs as a hydrogenlike target with one active electron outside a frozen core [7]. The core potential is a combination of the frozen-core Hartree-Fock part and a local ℓ-dependent core-polarization term. With this model we are able to describe the target structure with similar accuracy as in previous close-coupling calculations [12,20]. Using a single exponential fall-off factor λ_ℓ in the Laguerre basis, we have to diagonalize the target Hamiltonian with as many as 50 basis functions. We thus obtain a sufficient number of discrete states and a predominance of positive-energy pseudostates. As in the *e*-Na case [7], we may drop the closed channels at energies substantially above the ionization threshold. At the energies considered here, this results in a total of around 40 states in the close-coupling expansion, approximately ten states for each $\ell=0,1,2,3$.

Our results for the differential cross section and the spin-exchange asymmetry are shown in Figs. 1–3 for elastic *e*-Cs scattering at incident electron energies of 7, 13.5, and 20 eV. We present results from a three-state (3CC) calculation with only the $(6s)^2S$, $(6p)^2P^o$, and $(6d)^2D$ states included in the close-coupling expansion, a 19-state (CC) calculation with only discrete states included that has converged within this subspace, and a CCC calculation which has converged (in the discrete and continuum subspaces) to better than 10% at most scattering angles. Note that this convergence is within the nonrelativistic framework and the approximations made in the target description. Our results are compared with the relative cross section data of Gehenn and Reichert [14] (normalized to the CCC results at small scattering angles) and with the asymmetry measurements of Raith *et al.* [15,16].

As one might have expected from the corresponding results on *e*-Na scattering, the effect of the continuum states is very important for the spin-exchange asymmetry, and its im-

TABLE I. Angle-integrated elastic σ_{6s}, excitation σ_{6p} and σ_{5d}, ionization σ_i, and total σ_t cross sections (in units of πa_0^2) and ionization spin asymmetry A_i for e-Cs scattering obtained from a nonrelativistic CCC calculation. The numbers presented in the columns labeled ''expt.'' have been estimated at the calculated energies from the available experimental data in the given reference.

Energy (eV)	σ_{6s}	σ_{6p}	σ_{5d}	σ_i	σ_t	Expt. [18]	A_i	Expt. [19]
7.0	66.8	67.0	16.1	7.11	169	131 ± 10	0.213	0.30 ± 0.002
13.5	53.9	67.2	10.3	9.51	153	102 ± 10	0.200	0.23 ± 0.005
20.0	37.2	59.3	7.5	8.36	126	91 ± 10	0.136	0.15 ± 0.006

portance increases with increasing collision energy. Very satisfactory agreement is obtained at 13.5, 20, and mostly at 7 eV, though for the latter energy the predicted minimum near 120° scattering angle is apparently not confirmed by experiment. Oddly enough, at the lowest energy the agreement between theory and the shape of the experimental results is excellent for the differential cross section, while some discrepancies remain at 13.5 eV (the experimental data are actually for 13 eV) and 20 eV. We also note that some evidence for the sharp peak in the spin-exchange asymmetry for 20 eV near 60° is visible in the experiment. In fact, it seems very interesting to repeat the measurement in this angular range with a very high angular resolution.

Finally, we present in Table I our results for the angle-integrated cross sections in the elastic channel, excitation to the $(6p)^2P^o$ and $(6d)^2D$ states, direct (no core excitation or ionization) total ionization (σ_i) and its spin asymmetry (A_i), as well as the total collision cross section (summed over all discrete and continuum channels). The agreement with the experimental data for the ionization asymmetry is not perfect but certainly satisfactory in light of the complexity of the problem and the neglect of ionization-excitation as well as core ionization contributions to the ionization cross section at the higher energies (cf. Ref. [19], Fig. 2). We are somewhat surprised, however, by the fact that our results, too, lie clearly above the experimental data of Jaduszliwer and Chan [18]. Calculations at energies below 4 eV yielded good agreement with other theoretical predictions [12,20], thereby indicating that the discrepancies between these predictions and the existing experimental data [17,18] persist but are not due to the neglect of the continuum channels in the earlier calculations. We note, in passing, that our Born cross sections for elastic scattering are in excess of an order of magnitude larger than the CCC results at the considered energies. It would be very helpful to have total cross-section data available at high energies where the Born approximation is valid. It may be that our structure approximations, and those of other calculations [12,20], lead to a systematic exaggeration of the elastic and hence total cross section.

In conclusion, we have applied the CCC method in its nonrelativistic form to calculate elastic differential cross sections and spin asymmetries, as well as angle-integrated ionization asymmetries for e-Cs collisions at 7, 13.5, and 20 eV. For these observables, proper accounting of the effects due to the target continuum states appears to be more important than the inclusion of relativistic effects. It will be very interesting to study this problem in more detail with the CCC method extended to a relativistic framework. Such development is planned for the near future.

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