Relativistic *R* matrix with pseudostates calculations for electron scattering from cesium atoms

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The *R* matrix with pseudostates (RMPS) method was used with inclusion of relativistic effects to calculate differential cross sections and several spin asymmetries for elastic electron scattering from Cs atoms in the theoretically most difficult ''intermediate energy regime'' between one and five times the ionization threshold. Comparison of the RMPS predictions with experimental benchmark data for 7, 13, and 20 eV is satisfactory, thereby indicating the applicability of the method to collision systems involving heavy targets. Furthermore, justification for the apparent success of nonrelativistic calculations for the differential cross sections and the exchange asymmetry is given.

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Electron scattering from Cs atoms has provided a theoretical challenge for many years. After early attempts by Walker [1], Karule [2], and Burke and Mitchell [3], interest picked up substantially in recent years with the rapid increase of computational power [4–8]. However, all the calculations published so far neglected physical effects that are known to be important in order to obtain reliable results. In the ''intermediate energy regime'' of incident energies between approximately one and five times the ionization threshold (3.89 eV in Cs), these effects include a sophisticated target description, relativistic interactions both in the target and in the projectile-target interaction, and channel coupling between many discrete and continuum channels.

Based on early work of Norcross [9], an accurate, though still manageable (in a subsequent collision calculation) target description can be obtained by including a semiempirical core potential to describe the response of the target core to the outer target electron and the incident projectile. In fact, Thumm and Norcross [5] showed that correcting this potential even further, by including a dielectric term to account for the simultaneous effect of both outer electrons on the core, was essential at very low incident energies. Furthermore, calibrating the strength of the spin-orbit interaction in a perturbative treatment with nonrelativistic orbitals, using the experimentally known bound spectrum as a guide, provides results of comparable accuracy to what is typically obtained in *ab initio* full-relativistic structure calculations.

Regarding the treatment of the collision process, the aforementioned channel coupling is extremely important in the ''intermediate energy regime.'' A major step forward in the treatment of electron-atom collisions, later followed by applications to ionization by both photon and charged-particle impact, was the ''convergent close-coupling'' (CCC) approach of Bray and Stelbovics [10,11]. In this method, as well as in closely related treatments such as the ''*R* matrix with pseudostates'' (RMPS) approach [12,13], an attempt is made to account for the channel coupling effect, essentially to convergence, by including a sufficiently large number of physical and ''pseudostates'' in the close-coupling plus correlation expansion. The latter states approximate the coupling to both the high-lying discrete and the continuum states of the target that are not included explicitly. While CCC and RMPS have been extremely successful over the past five years, it is worth noting that neither method has yet been applied in a relativistic framework. Closest to this ultimate goal came nonrelativistic CCC calculations for electron scattering from barium atoms [14], in which relativistic effects in the target description were included *a posteriori* by adding nonrelativistic results weighted by the known intermediate-coupling coefficients.

Interestingly, the *nonrelativistic* CCC method was applied with some success also to elastic electron scattering from cesium atoms [7], the topic of interest for the present paper. Note, however, that relativistic effects are absolutely essential for generating a nontrivial result for several spin asymmetries constructed by adding or subtracting differential cross sections (DCS) for particular initial spin preparations of both the target and the projectile electron. Nevertheless, two observables that are nonzero without explicitly spin-dependent forces such as the spin-orbit interaction within the target or between the projectile electron and the target nucleus, namely, the differential cross section σ_0 for unpolarized incident beams and the ''exchange asymmetry'' A_{nn}, were predicted in quite satisfactory with experiment [15,16].

Recently, experimental and theoretical benchmark results for elastic *e*-Cs scattering were presented in a combined experimental and theoretical effort by Baum *et al.* [17] for a projectile energy of 3 eV. This energy was chosen since it was judged as presenting approximately an equal challenge to both experimentalists and theorists, with the former generally preferring higher energies due to the performance of electron optical elements and the latter preferring lower energies where the channel coupling is essentially restricted to a few strongly coupled states. (Very high energies, technically suitable for both experimentalists and theorists, were not chosen since several of the interesting asymmetry effects require exchange between the projectile and the target electrons to be important.) The overall conclusion of the 3 eV benchmark study was a generally good agreement between experiment and theoretical predictions from an eight-state semirelativistic Breit-Pauli *R*-matrix calculation [6] (labeled BP8 below). Predictions based on the corresponding full-relativistic eight-state Dirac-Breit *R*-matrix calculation [8] qualitatively agreed with experiment as well, but apparently suffered from deficiencies in the structure description of the target. Finally, the nonrelativistic CCC results agreed well

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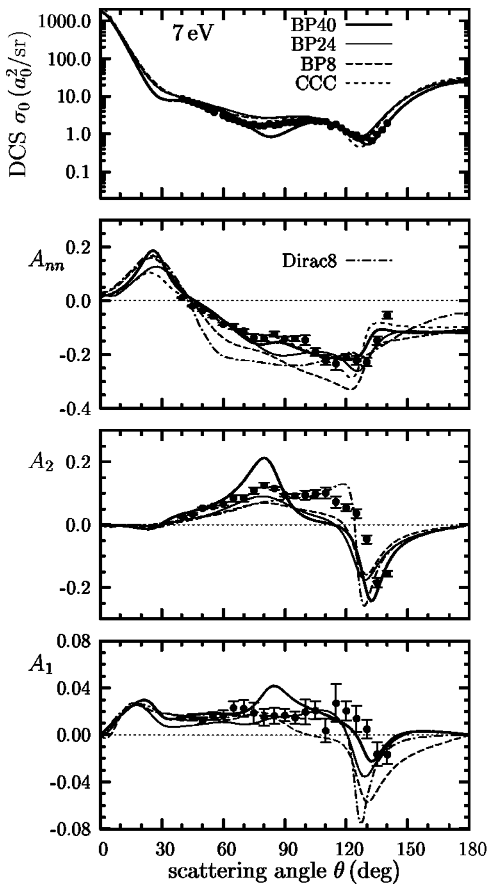

FIG. 1. Differential cross section σ_0 and spin asymmetries A_{nn}, A_2, and A_1 for elastic electron scattering from cesium atoms at an energy of 7 eV. The experimental results of the Bielefeld group [17] are compared with theoretical predictions described in the text.

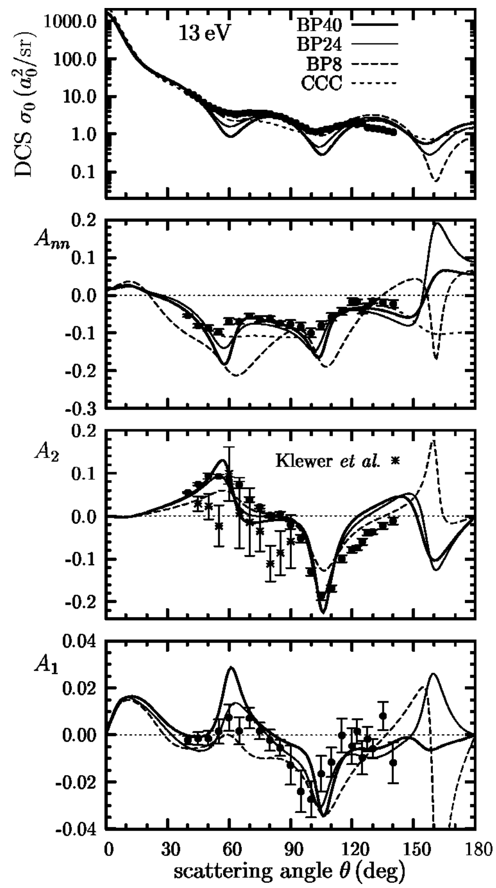

FIG. 2. Same as Fig. 1 for an energy of 13 eV. Also shown are the A_2 results of Klewer *et al.* [19].

with experiment and the BP8 results for the DCS and the exchange asymmetry, but would predict exactly zero for two other spin asymmetries that, experimentally, were found to be nonzero over a wide range of scattering angles.

In this paper, we report results of a semirelativistic Breit-Pauli *R*-matrix calculation in the theoretically most difficult ''intermediate energy regime.'' The atomic structure, relativistic effects, and channel coupling were finally treated on an equal footing, thereby allowing for the accurate prediction of the DCS and all three spin asymmetries measured by the Bielefeld group at incident energies of 7, 13, and 20 eV. In detail, the observables of interest are

$$\sigma_0=\frac{1}{4}[\sigma(\uparrow\uparrow)+\sigma(\downarrow\uparrow)+\sigma(\uparrow\downarrow)+\sigma(\downarrow\downarrow)], \qquad (1)$$

$$A_{nn}=[\sigma(\uparrow\downarrow)+\sigma(\downarrow\uparrow)-\sigma(\uparrow\uparrow)-\sigma(\downarrow\downarrow)]/4\sigma_0, \qquad (2)$$

$$A_1=[\sigma(\uparrow\uparrow)+\sigma(\uparrow\downarrow)-\sigma(\downarrow\uparrow)-\sigma(\downarrow\downarrow)]/4\sigma_0, \qquad (3)$$

$$A_2=[\sigma(\uparrow\uparrow)+\sigma(\downarrow\uparrow)-\sigma(\uparrow\downarrow)-\sigma(\downarrow\downarrow)]/4\sigma_0, \qquad (4)$$

where $\sigma(\uparrow\downarrow)$ corresponds, for example, to the differential cross section obtained with the initial target spin up and the projectile spin down relative to the scattering plane.

Details of the experimental determination of these asymmetries were given by Baum *et al.* [17]. Regarding the physical meaning of the spin asymmetries, A_1 and A_2 correspond to ''spin up-down'' (with respect to the reaction plane) asymmetries in the DCS for scattering of unpolarized electrons from polarized atoms (A_1) or polarized electrons from unpolarized atoms (A_2), while A_{nn} represents an ''antiparallel-parallel'' asymmetry. In contrast to the nonrelativistic case, however, not only the relative orientation of the projectile and target spins is relevant for this ''exchange asymmetry,'' but also their orientation with respect to the reaction plane [3]. Finally, as pointed out by Farago [18], nonvanishing values of A_1 require the *simultaneous* importance of spin-orbit and exchange effects. Hence, this parameter is often called the ''interference asymmetry.'' It is generally the smallest (in magnitude) of the three asymmetries and provides the greatest theoretical (and experimental) challenge.

Several calculations were performed during the present work. Starting with the BP8 model described in detail by Bartschat [6], with the target description based upon a model potential for the inner 54 core electrons and a set of physical orbitals ($6s,6p,5d,7s,7p$), we generated an additional physical $6d$ orbital through optimization of the corresponding ionization potential. Then, pseudo-orbitals ($\overline{8}s-\overline{11}s$, $\overline{8}p-\overline{11}p$, $\overline{7}p-\overline{10}d$, $\overline{4}f-\overline{8}f$) were constructed as the

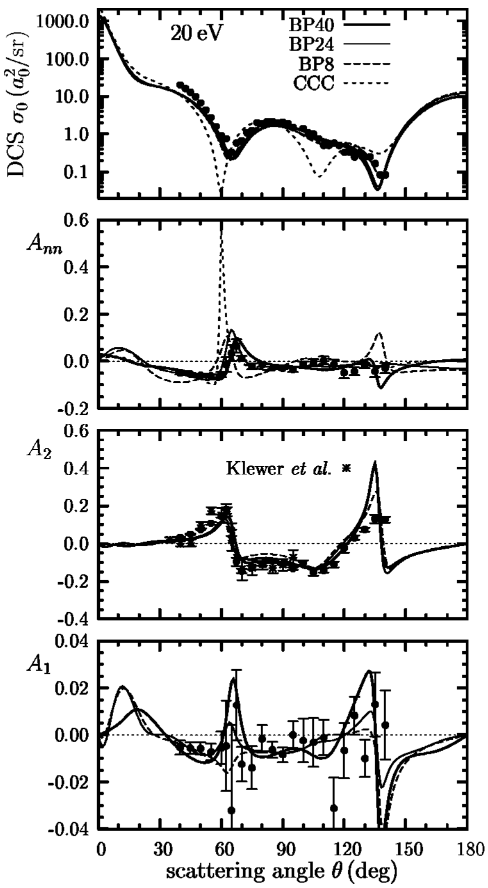

FIG. 3. Same as Fig. 1 for an energy of 20 eV. Also shown are the A_2 results of Klewer *et al.* [19].

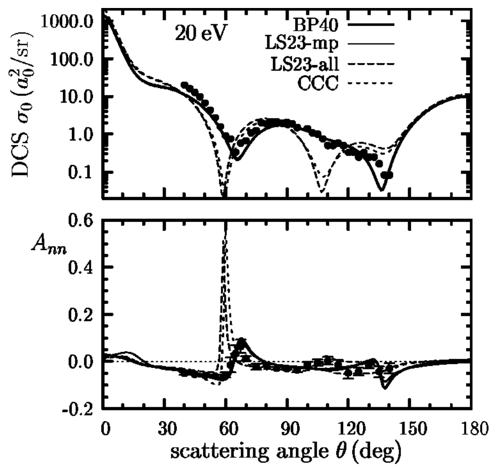

FIG. 4. Differential cross section σ_0 and spin asymmetry A_{nn} for elastic electron scattering from cesium atoms at an energy of 20 eV. The comparison of the various theoretical results indicates the sensitivity on the target model and on the inclusion of relativistic effects.

minimum Sturmian basis $P_{nl}(r)=\Sigma_i a_i r_i^{l+1+i}\exp(-\alpha_l r)$ for which the orbitals were normalized and orthogonal to all orbitals with lower *n* for the same angular momentum *l*. The range parameters $\alpha_s=0.8$, $\alpha_p=0.7$, $\alpha_d=0.65$, and $\alpha_f=0.9$ were chosen in such a way that the lowest pseudostate for each angular momentum was still below the ionization threshold while the others lay in the target continuum. Experience shows [13] that this choice is advantageous for fast convergence with the number of pseudostates in the close-coupling expansion.

When relativistic effects were included explicitly, the 23 nonrelativistic *LS* states constructed from the above orbitals resulted in a total of 40 fine-structure states. In light of the additional possibilities for channel coupling, the computational effort for the resulting BP40 model was more than an order of magnitude larger than that required for the LS23 approach. With 30 continuum orbitals per angular momentum chosen to expand the projectile wave function inside the *R*-matrix box of radius $58a_0$, Hamiltonian matrices of dimensions up to 6000 had to be diagonalized for each partial-wave symmetry with total (target + projectile) electronic angular momentum *J* and parity π. Partial waves up to $J=13$ were calculated numerically, and partial-wave convergence was achieved by extrapolating the $\mathcal{T}$ matrices smoothly toward higher angular momenta. The extrapolation procedure was carefully checked by replacing a different number of numerically calculated $\mathcal{T}$ matrices by the extrapolated ones. We also performed a smaller BP24 calculation by dropping two pseudo-orbitals for each angular momentum and a second nonrelativistic LS23 calculation in which exchange with the core electrons was treated explicitly. These calculations allowed us to assess (i) the importance of channel coupling, (ii) the importance of including relativistic effects explicitly in the calculation of σ_0 and A_{nn}, and (iii) the effect of a different target description.

Figures 1–3 show our results at incident energies of 7, 13, and 20 eV for the elastic differential cross section σ_0 and the asymmetries A_{nn}, A_2, and A_1. Since the experimental DCS data are relative, they were normalized to the BP40 calculation to provide a good visual fit. The experimental data plotted in the graphs are slightly different from those published earlier [15,16], because of recent improvements in the experimental procedure [17]. The data are compared with predictions from the BP8, BP24, and BP40 calculations, the full-relativistic Dirac eight-state *R*-matrix model (only at 7 eV), and nonrelativistic CCC results (for σ_0 and A_{nn} only).

Overall, we note satisfactory agreement between our BP40 predictions and the experimental data, particularly in light of the remaining scatter in the latter data. Also, for 13 eV incident energy, our results support the recent Bielefeld data compared to the older measurements of Klewer *et al.* [19]. Furthermore, we see a clear tendency toward convergence with the number of states included in the close-coupling expansion, indicating that accounting for additional channel coupling with just a few pseudostates goes a long way toward a converged result.

The predictions from the various models are more similar at 20 than at 7 eV, indicating that channel coupling may lose importance relative to the details of the target description. This indication is supported in Fig. 4 that shows substantial differences between the LS23 results obtained in an all-electron calculation relative to those obtained in a model-potential approach for an energy of 20 eV. The position and

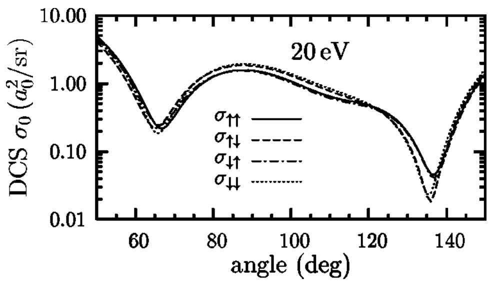

FIG. 5. BP40 results for the differential cross sections $\sigma(\uparrow\uparrow)$, $\sigma(\uparrow\downarrow)$, $\sigma(\downarrow\uparrow)$, and $\sigma(\downarrow\downarrow)$ for elastic electron scattering from cesium atoms at an energy of 20 eV.

the value of the minima in the differential cross section start to depend very strongly on the structure model, and the predictions for spin asymmetries such as A_{nn} reflect this sensitivity. Interestingly, Fig. 4 shows almost identical results for σ_0 and A_{nn} in the BP40 and LS23 (model-potential) calculations. This similarity explains the success of the nonrelativistic CCC model for these two parameters, which can apparently be calculated accurately with complete negligence of relativistic effects.

Finally, Fig. 5 gives an impression of the difficulty faced by both experimentalists and theorists in the accurate determination of the spin asymmetries. The figure shows the individual cross sections $\sigma(\uparrow\uparrow)$, $\sigma(\uparrow\downarrow)$, $\sigma(\downarrow\uparrow)$, and $\sigma(\downarrow\downarrow)$ for an energy of 20 eV, as predicted by the BP40 model. The similarity of all four cross sections indicates the strong possibility of cancellation errors in the asymmetries, a problem that does not exist for σ_0.

In conclusion, we have presented results of *R* matrix with pseudostates calculations for elastic electron scattering from cesium atoms at intermediate energies, in which an accurate target description, explicitly spin-dependent forces, and electron exchange were accounted for. The satisfactory agreement between the RMPS predictions and recent experimental data of the Bielefeld group provides confidence in this method to extend the calculations to inelastic and superelastic collisions, particularly the $6s\leftrightarrow 6p$ transition. Joined experimental and theoretical efforts in this direction are in progress.

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