Dirac *R*-Matrix Modeling of Spin-Induced Asymmetry in the Scattering of Polarized Electrons from Polarized Cesium Atoms

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Recent experiments by Baum, Raith, and co-workers to measure the spin-induced asymmetries in electron scattering from cesium have stimulated theoretical work to interpret these measurements. We present Dirac R-matrix calculations of the interference asymmetry function, and of the spin-orbit and spin-exchange asymmetries, for comparison with experimental data at 7 and 13.5 eV and with nonrelativistic predictions of the spin-exchange asymmetry from the convergent close coupling method. We find that a simple relativistic target model provides a basis for the understanding and analysis of ongoing experiments. [S0031-9007(97)04271-3]

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Spin polarization effects in elastic electron-atom scattering can be attributed to several different causes. Exchange polarization arises because electrons are indistinguishable; we have no way of knowing if the scattered electron is the same as the incident electron or was initially bound in the target, making the cross section dependent on the relative spin orientations of the incoming and target electrons. Relativistic dynamics, approximated nonrelativistically by the spin-orbit interaction, also makes the scattering cross section spin dependent. Following an analysis by Burke and Mitchell [1], Farago [2] suggested that the interference between the exchange and spin-orbit scattering amplitudes might be detectable. Atomic cesium was proposed as an ideal target with which to investigate this possibility, as it is easy to prepare experimentally and its atomic number, $Z = 55$, is large enough for appreciable spin-orbit effects. A preliminary calculation of elastic scattering from the Cs $6s$ ground state by Walker [3] suggested that the interference effect should be observable below about 15 eV in the vicinity of a diffraction minimum in the differential cross section.

The differential cross section for scattering of polarized electrons from polarized target atoms depends upon the polarization vectors $\mathbf{P}_e$ and $\mathbf{P}_t$ of the incident and target electrons, respectively, through the formula [4]

$$\sigma(\theta) = \sigma_u(\theta)[1 - A_{\rm ex}(\theta)\mathbf{P}_e \cdot \mathbf{P}_t + A_{\rm s.o.}(\theta)\mathbf{P}_e \cdot \mathbf{n} + A_{{\rm int}(\theta)}\mathbf{P}_t \cdot \mathbf{n}],$$

Here $\mathbf{n}$ is normal to the scattering plane containing the tracks of the incident and scattered electrons, and $\sigma_u(\theta)$ is the differential cross section for the scattering of unpolarized electrons. The asymmetry functions $A_{\rm ex}(\theta)$, $A_{\rm s.o.}(\theta)$, and $A_{\rm int}(\theta)$ can thus be obtained by combining cross sections for four different polarization settings of the target and the incident electron relative to $\mathbf{n}$ [4]. While this does not constitute a "perfect scattering experiment" in the sense of Bederson [5], which would require the measurement of 11 parameters [1], the measurement of these asymmetry functions alone constitutes a stringent test of our understanding of the underlying physics [6,7].

More than twenty years after Farago's suggestion [2], it has become possible to measure the interference effect in electron scattering from polarized Cs targets, and so to make an experimental verification of this essentially relativistic phenomenon. Gehenn and Reichert [8] had shown that the differential cross section for elastic scattering from cesium in the energy range 20 down to 0.8 eV has at least one deep diffraction minimum in the angular range $32° < \theta < 143°$. Klewer *et al.* [9] measured $A_{\rm s.o.}(\theta)$ between 13 and 25 eV, and Raith *et al.* [4] estimated that $A_{\rm int}(\theta)$ might be observable in the range from 10 to 20 eV. Their first results for the interference asymmetry, [4], show that $A_{\rm int}(\theta)$ is close to zero at 13.5 eV but is definitely nonzero at 7 eV. These results disagree with the predictions made by Walker [3] at 5 and 13.6 eV so that a better calculation than his is needed to explain the observations successfully.

Walker's relativistic distorted wave calculations [3] represented the Cs core by a model potential incorporating core polarization. There have been a number of calculations since then. Scott *et al.* [10] used a 5-state Breit-Pauli semirelativistic R-matrix model (BPRM) including only the $6s_{1/2}$, $6p_{1/2}$, $6p_{3/2}$, $5d_{3/2}$, and $5d_{5/2}$ target states. Bartschat [6] added $7s_{1/2}$, $7p_{1/2}$, and $7p_{3/2}$ to give an 8-state target model, revealing some consistency problems in the earlier 5-state calculations. Thumm *et al.* [7,11] employed an equivalent 5-state Dirac (relativistic) model in which the effect of the noble-gas-like core was represented by a model potential which was carefully optimized to reproduce observed target levels. Bartschat and Bray [12] have recently made calculations with the (nonrelativistic) CCC ("convergent close coupling") method, which pays particular attention to target state completeness. Since it pays no regard to spin-orbit coupling, it is able to predict only $\sigma_u(\theta)$ and $A_{\text{ex}}(\theta)$ but not the other asymmetry parameters. The differential cross section is well represented by both the recent BPRM and CCC models at low scattering energies, but there are significant discrepancies for large scattering angles with the Dirac R-matrix results. The asymmetry functions on which we focus in this paper are more sensitive to the choice of model and have so far been less well investigated.

A calculation which treats both the electrons of the target atom and the dynamics of the scattering process in a relativistically consistent manner is clearly the most desirable way to interpret the experiments. Our development of the DARC Dirac R-matrix code [13,14] was intended to facilitate such investigations. DARC incorporates the widely used GRASP2 relativistic atomic structure package [15] for target state calculation, and uses fully compatible computational methods. DARC has been available for some years to study electron scattering from atoms and ions [13,16], and we have now extended it to evaluate angular distributions and polarization-asymmetry observables. We here report our first results for the interpretation of the electron polarization experiments at 7 and 13.5 eV.

DARC calculations.—The Cs target is described by a closed core and eight one-electron orbitals: $6s_{1/2}$, $6p_{1/2}, 6p_{3/2}, 5d_{3/2}, 5d_{5/2}, 7s_{1/2}, 7p_{1/2}, 7p_{3/2}$. These are determined by an extended average level (EAL) self-consistent field GRASP2 calculation (see [15] for details). This method of generating target wave functions is simple and cheap, but neglect of core polarization and other correlation effects will limit its accuracy. The N-electron target states determine a static potential for the R-matrix continuum pseudostates which DARC uses in the scattering calculation. In this energy region, a large number of partial waves are needed for satisfactory convergence. We included all relativistic quantum numbers $\kappa = \mp 1, \mp 2, \ldots, \mp 43$ and constructed the Dirac Hamiltonian of the $(N + 1)$-electron system inside the R-matrix sphere for each of the symmetries $J^\pi = 0^\mp, 1^\mp, \ldots, 40^\mp$. All possible jj-coupled channels were included and use was made of the Buttle correction [17] to compensate for the incompleteness of the target state description. DARC constructs the K matrices from which the scattering amplitudes and all derived quantities—the cross sections and asymmetry functions—can be calculated. Small contributions from high partial waves not treated explicitly can be approximated with the effective range formula of [18]

$$K_{ij} = \frac{\pi \alpha_d k_i^2}{(2l_i + 3)(2l_i + 1)(2l_i - 1)} \delta_{ij},$$

where k_i and l_i are, respectively, the linear momentum and the orbital angular momentum of the continuum electron in channel i and α_d is the dipole polarizability. Up to 400 symmetries can thus be included, sufficient to give reasonable convergence provided the matching is done at a suitable value of J.

Our aim in this Letter is to see whether this relatively simple model based on a consistent relativistic approach gives a reasonable description of the observed spin polarization data, particularly the asymmetries $A_{\text{s.o.}}(\theta)$ and $A_{\text{int}}(\theta)$ which can be predicted only by a relativistic theory. As the cesium states in question are weakly bound, we expect to obtain very similar results to an equivalent BPRM calculation, although we are not in a position to demonstrate this in the present paper.

Results at 7.0 and 13.5 eV.—Figures 1 and 2 display our results for all three asymmetry functions at scattering energies of 7.0 and 13.5 eV, respectively, (solid lines) for comparison with data communicated by the Bielefeld

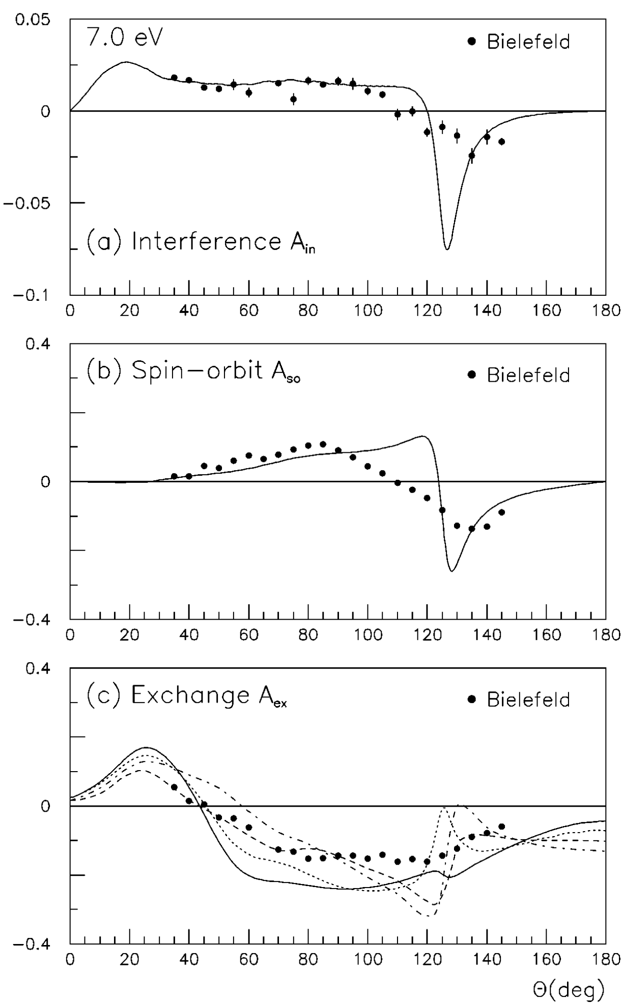

FIG. 1. Asymmetry functions for electron scattering from Cesium at 7.0 eV. The DARC results (solid lines) are compared with data supplied by Dr. Tondera of the Bielefeld group [19]. Other theoretical results due to Bray and Bartschat [12] are shown in (c): 19-state CC calculation (chain curve); full CCC calculation (dashed curve). The effect of using experimental rather than theoretical thresholds in the DARC calculations is shown as the line of short dashes.

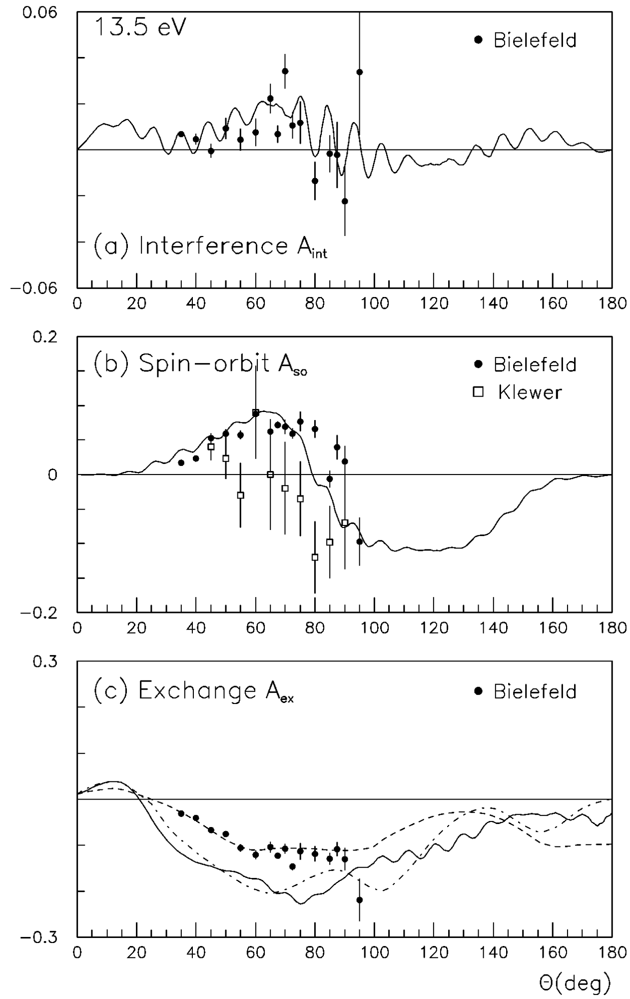

FIG. 2. Asymmetry functions for electron scattering from cesium at 13.5 eV. Bielefeld data [4] are shown as filled circles and the data of Klewer *et al.* [8] as open squares. Otherwise the symbols are the same as in Fig. 1.

group [4,19] and with earlier calculations. At 7 eV, we found only small differences between 5-state and 8-state calculations at the level of a few percent, and we have therefore plotted only 8-state results. Similar differences appear when the transition to the effective range formula is made at $J = 32$ or 36 rather than at $J = 40$. If the transition is made at too low a value of J, the asymmetries oscillate about a stable smooth curve, which is well enough represented at this energy by making the change at $J = 40$. We estimate that the overall error of our results at 7 eV is in the region 5%–10%. Resources have not permitted us to increase the largest value of J at the transition point to be greater than 40.

The exchange asymmetry $A_{\rm ex}(\theta)$ is essentially nonrelativistic, and in Fig. 1 we compare our results at 7 eV (solid lines) with experimental data from Bielefeld and from the paper of Klewer *et al.* [8]. In Fig. 1(c) we also include CCC results of Bartschat and Bray [12]. They used a model potential based on a frozen-core Hartree-Fock calculation augmented with a local l-dependent core polarization potential chosen to fit several low-lying Cs levels. The target Hamiltonian for this potential was diagonalized in a Sturmian basis to give a pseudostate representation of the excited states and the continuum, and its eigenstates were then used to solve the Lippman-Schwinger equations. The chain curve shows 19-state results from [12] claimed to be converged in the discrete subspace and the dashed curve includes also continuum contributions which are said to be converged to about 10%. These agree better with experiment than the DARC results, probably because they included a core polarization potential which improves the agreement between observed and computed atomic levels and slightly changes the wave functions. The short dashes show an attempt to correct the DARC results partially for core polarization by shifting the predicted levels to the experimental positions. This improves the fit to experiment below 90°, and moves the curve closer to the CCC curves. None of the theoretical calculations agree very well with experiment at larger angles.

The observables $A_{\rm s.o.}(\theta)$ and $A_{\rm int}(\theta)$, Fig. 1(a) and 1(b), can be predicted only by a relativistic or semirelativistic theory which includes spin-orbit coupling, and we have only our own theoretical results. Again, theory and experiment diverge for $\theta > 100°$, and there are prominent features in the theoretical curves at around 120° which are not reproduced by experiment. The differences at large angles need further investigation.

The comparisons at 13.5 eV in Fig. 2 show the same general trends, although the oscillations of the theoretical curves reveal that the transition to the effective range formula should be made at a higher value of J to obtain a smooth result. This problem is likely to become worse at higher energies. Our results for $A_{\rm s.o.}(\theta)$ at 13.5 eV support the Bielefeld data [4] rather than the older data of Klewer *et al.* [8]. No experimental data are available at this energy at angles greater than about 95°.

Discussion.—We have compared polarization asymmetry functions computed with our relativistic DARC code with experiment and with predictions made by the nonrelativistic CCC model. Both theoretical models agree reasonably well with experiment for the exchange asymmetry at 7 eV and at angles below about 100°. The agreement is not good when $\theta > 100°$, and improvements in the target wave function representation and careful attention to the convergence of the partial wave expansion will be needed to do better. While the CCC method goes some way towards achieving these aims for the essentially nonrelativistic observables $\sigma_u(\theta)$ and $A_{\rm ex}(\theta)$, the disagreement between theory and experiment at large angles suggests that more needs to be done. It would be desirable to make a more direct comparison of DARC, BPRM, and CCC models for all measurable quantities in the future using the same choice of target states and the same core polarization potential. The CCC work suggests that the inclusion of more continuum pseudostates in the R-matrix calculations, as, for example, in Bartschat *et al.* [20], would improve the agreement with experiment at 13.5 eV, and one might hope that a relativistic version of CCC could be devised to do the same thing. This is entirely feasible.

Investment in more elaborate relativistic calculations based on the Dirac Hamiltonian to interpret scattering of polarized electrons from polarized atoms is now justifiable.

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