# Relativistic and Close-Coupling Effects in the Spin Polarization of Low-Energy Electrons Scattered Elastically from Cadmium

Christopher J. Bostock,* Michael J. Berrington,† Dmitry V. Fursa, and Igor Bray

*ARC Centre for Antimatter-Matter Studies, Curtin University, GPO Box U1987, Perth, WA 6845, Australia*

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The measurements of the Sherman function in elastic electron-cadmium scattering by Bartsch *et al.* [J. Phys. B **25**, 1511 (1992)] have been in serious disagreement with scattering theories for nearly two decades. The recently developed relativistic convergent close-coupling method is applied to the problem and found to be in excellent agreement with experiment over the complete energy range measured. The unusually rapid variation in the spin asymmetry parameter in the vicinity of 4 eV projectile energy is now explained in terms of unitarity of the close-coupling formalism.

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Understanding the role of spin in electron-atom interactions is a key component to progress in exciting research areas such as spintronics [1,2] and quantum information [3]. In addition, electron spin polarization measurements for elastic scattering are emerging as a tool to study spin entanglement [4,5]. Consequently, a quantitative understanding of spin-related phenomena will be of considerable benefit.

In this Letter, we report on a long-standing, and striking, discrepancy between theory and experiment for the spin asymmetry parameter (Sherman function) in the elastic scattering of electrons from cadmium ($Z = 48$) atoms. We resolve the discrepancy by utilizing the recently developed fully relativistic convergent close-coupling (RCCC) scattering theory, which is based on the Dirac equation and accounts for spin polarization effects in a completely *ab initio* manner. To indicate the extent of the discrepancies between experiment [6] and previous theories [7,8], Szmytkowski and Sienkiewicz [8] have highlighted: "...experiment and theory curves often differ significantly in magnitudes, locations of extrema, and sometimes even in shapes."

Spin polarization effects in electron scattering from atoms can be due to electron exchange, spin-orbit interactions, or their interference [9–14]. For the case of elastic electron scattering from a spin zero target such as the cadmium ground state, the spin polarization effects arise solely due to the spin-orbit interactions [15]. The exchange effects, while important in determining the magnitude of the cross section at low energies, do not give rise explicitly to any spin polarization in the scattering process. Conversely, even for low-energy electrons incident on a heavy target, the spin-orbit interaction can influence spin polarization effects in scattering because the electrons will accelerate significantly on approaching close to the nucleus. Thus the study of spin polarization effects in electron-cadmium scattering provides a sensitive test of the relativistic effects.

The RCCC method involves solving a set of relativistic Lippmann-Schwinger equations derived from the Dirac equation. Therefore the spin-orbit interaction is included *ab initio* in a consistent way between all electrons in the $e$-Cd collision system. Comprehensive details of the RCCC method for quasi-one- and -two-electron targets have recently been given [16]. RCCC results for scattering on quasi-two-electron targets such as Hg [17] and Yb [18] demonstrate that one advantage of the RCCC method is the ability to take into account coupling to the target continuum states. A very brief overview of the application of the RCCC method to the calculation of electron-cadmium spin polarization effects is as follows.

The cadmium atom is modeled as two active valence electrons above a frozen $[\mathrm{Kr}]4d^{10}$ Dirac-Fock core. The Dirac Hamiltonian for the active electrons above the $[\mathrm{Kr}]4d^{10}$ core is diagonalized by using a configuration interaction expansion based on a Dirac $L$-spinor basis [19]. The generated target states are then used to expand the total wave function of the electron-cadmium scattering system and formulate a set of relativistic Lippmann-Schwinger equations for the $T$ matrix elements. In this latter step, the relativistic Lippmann-Schwinger equations for the $T$ matrix elements have the following partial wave form:

$$T_{fi}^{\Pi J}(k_f\kappa_f, k_i\kappa_i) = V_{fi}^{\Pi J}(k_f\kappa_f, k_i\kappa_i) + \sum_n \sum_\kappa \oint dk \times \frac{V_{fn}^{\Pi J}(k_f\kappa_f, k\kappa) T_{ni}^{\Pi J}(k\kappa, k_i\kappa_i)}{E - \epsilon_n^N - \epsilon_{k'} + i0}. \quad (1)$$

The notation in Eq. (1), the matrix elements, and the method of solution using a hybrid OpenMP-MPI [20] parallelization suitable for high performance supercomputing architectures is given in Ref. [16]. Our target model consists of 55 bound states, and we found that adding extra continuum states in the scattering calculations did not change the $S_A$ parameter in the energy range considered. Therefore, the RCCC results presented are those of the 55-state calculation. Further details of the target structure and scattering calculation will be described elsewhere.

The $T$ matrix elements obtained from the solution of Eq. (1) are used to determine the scattering amplitudes

 

[16], which in turn are used to calculate the spin asymmetry parameter $S_A$. For scattering of unpolarized spin 1/2 electrons on an unpolarized target, this is given by Scott *et al.* [21]:

$$S_A = \frac{-2}{\sigma_u(2J_0+1)} \mathrm{Im}\left\{ \sum_{M_1 M_0} f\left(M_1 \tfrac{1}{2}; M_0 - \tfrac{1}{2}\right) f^*\left(M_1 \tfrac{1}{2}; M_0 \tfrac{1}{2}\right) \right\}, \quad (2)$$

where Im{} denotes the imaginary part and where the cross section $\sigma_u$ is

$$\sigma_u = \frac{1}{2(2J_0+1)} \sum_{M_1 M_0 m_1 m_0} |f(M_1 m_1; M_0 m_0)|^2. \quad (3)$$

The scattering amplitude $f(M_1 m_1; M_0 m_0)$ describes the transition from a target state with total angular momentum $J_0$ and spin projection $M_0$ to a target state with $J_1$ and $M_1$. The initial and final spin projections of the scattered electron are $m_0$ and $m_1$, respectively. For elastic scattering of unpolarized electrons on an unpolarized spin zero target, the $S_A$ parameter is equivalent to the Sherman function [22]. Note that the nonrelativistic CCC method has a zero spin-flip amplitude [$f(0\tfrac{1}{2}; 0 - \tfrac{1}{2}) = 0$] due to the absence of spin-orbit coupling in the formalism, and therefore Eq. (2) yields identically zero for $S_A$. The review article by Gay [12] gives a lucid explanation of the physical meaning of the spin asymmetry function $S_A$:

$$\frac{I(+\theta) - I(-\theta)}{I(+\theta) + I(-\theta)} = S_A P_e, \quad (4)$$

where $I(\theta)$ is the scattering intensity at a given angle, and the electron polarization specified perpendicular to the reaction plane is

$$P_e = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}, \quad (5)$$

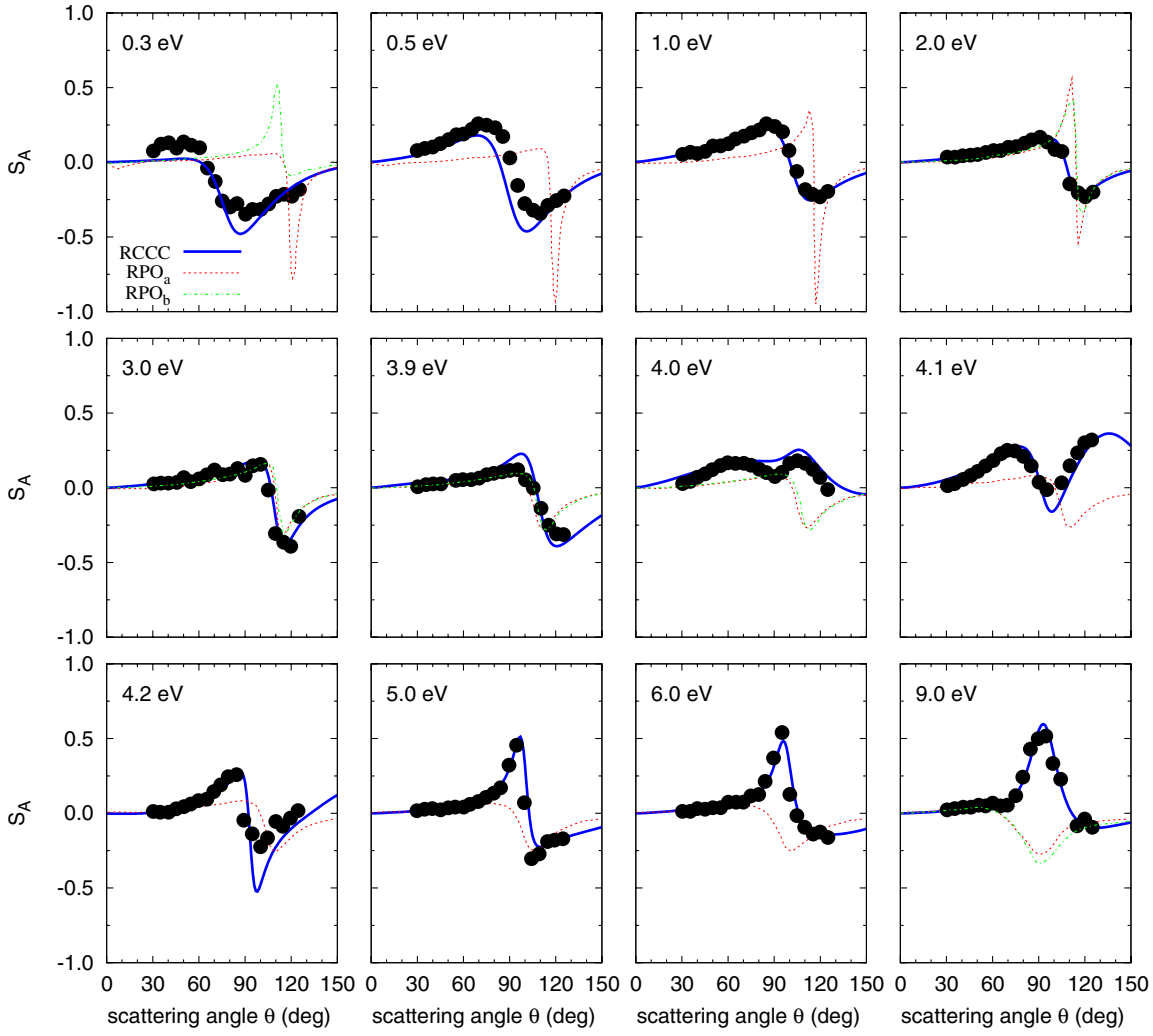


FIG. 1 (color online). Spin asymmetry parameter $S_A$ at a range of energies and angles for elastic electron scattering on cadmium. Measurements of Bartsch *et al.* [6] are presented. RCCC calculations are described in the text. Relativistic polarized orbital calculations of McEachran and Stauffer [7] and Szmytkowski and Sienkiewicz [8] are denoted by RPO$_a$ and RPO$_b$, respectively.

TABLE I. RCCC energy levels for Cd compared with experimental levels listed by the NIST Atomic Spectra Database [23].

| Configuration | Term | $J$ | Parity | RCCC (eV) | Experiment (eV) |
|---|---|---|---|---|---|
| $5s^2$ | $^1S_0$ | 0.0 | 1 | 0.000 | 0.000 |
| $5s5p$ | $^3P_0^o$ | 0.0 | −1 | 3.748 | 3.734 |
| $5s5p$ | $^3P_1^o$ | 1.0 | −1 | 3.826 | 3.801 |
| $5s5p$ | $^3P_2^o$ | 2.0 | −1 | 4.003 | 3.946 |
| Ionization limit | | | | 8.996 | 8.994 |

with $N_{\uparrow(\downarrow)}$ specifying the number of electrons in the scattered beam with spin up (down). From the measured number of electrons, $I(+\theta)$ and $I(-\theta)$, scattered through the angle $\theta$ to the left and right of the nucleus, respectively, the spin asymmetry $S_A$ can be calculated.

The accuracy of the RCCC method in the calculation of the $S_A$ parameter is illustrated in Fig. 1. Here, the spin asymmetry parameter is calculated across a wide range of energies and angles and compared with the measurements of Bartsch *et al.* [6] and the previous relativistic polarized orbital theories of McEachran and Stauffer [7] and Szmytkowski and Sienkiewicz [8]. The detector has an angular resolution of 3.5°, and this is incorporated by convolution of the RCCC results. Note in Fig. 1 that there is a rapid variation in the measurements of the spin asymmetry parameter in the vicinity of 3.9–4.0 eV. This rapid variation of the Sherman function is a signature of the elastic channel coupling to the $(5s5p)^3P_{0,1,2}$ states which begin to open in this energy region; see Table I, where the lowest energy states generated in the RCCC method are compared with the experimental values. The completeness of the underlying Dirac $L$-spinor basis [19] generates a sufficiently accurate set of states that span the Hilbert space of the target. The unitarity of the close-coupling formalism accounts for the influence of excited states on the elastic channel spin asymmetry [24]. There is a significant change in the shape, magnitude, and sign of the experimental results, and these changes are reproduced by the RCCC calculations but not by previous theories. It is interesting to note that even well away from this region at the largest incident projectile energy of 9.0 eV the measurements and RCCC results are in excellent agreement and have a large positive sign for $S_A$ in the vicinity of 90°, whereas both the relativistic polarized orbital theories disagree with the measurements and predict a negative sign. Similarly, at the smallest energy of 0.3 eV, there is excellent agreement between the measurements and the RCCC results; however, the relativistic polarized orbital calculations of McEachran and Stauffer [7] and Szmytkowski and Sienkiewicz [8] have significant differences in the spin asymmetry shape and location of extrema. We found that the RCCC results for the spin asymmetry $S_A$ are extremely stable against variation in the number of states used in the calculation and also against variation in the internal parameters used in obtaining the target structure. We estimate the uncertainty in the calculation of $S_A$ to be within 5% at most scattering angles.

In Fig. 2, we present the results of RCCC calculations for the spin asymmetry parameter $S_A$ as a function of incident projectile energy. The detector is placed at $\theta = 110°$, and its angular resolution of 3.5° is accounted for by convolution of the RCCC results. The energy spread of the electron beam is between 0.13 and 0.15 eV (FWHM). The presence of the rapid variation in the spin asymmetry parameter is illustrated in a conspicuous manner in both the measurements and the RCCC calculations, which are in excellent agreement with each other. Once again, the unitarity of the RCCC method accounts for the elastic channel coupling to the $(5s5p)^3P_{0,1,2}$ excited states, and this produces the rapid variation in the calculated spin asymmetry parameter in the region between 3.8 and 4.2 eV.

We conclude by emphasizing that an accurate treatment of spin-orbit interaction requires a theory that incorporates the relativistic spin-orbit term in a consistent manner for the target and projectile electrons. Furthermore, an account of the rapid variation in the behavior in the Sherman function requires a unitary theory. The excellent comparison with experiment presented here indicates that the

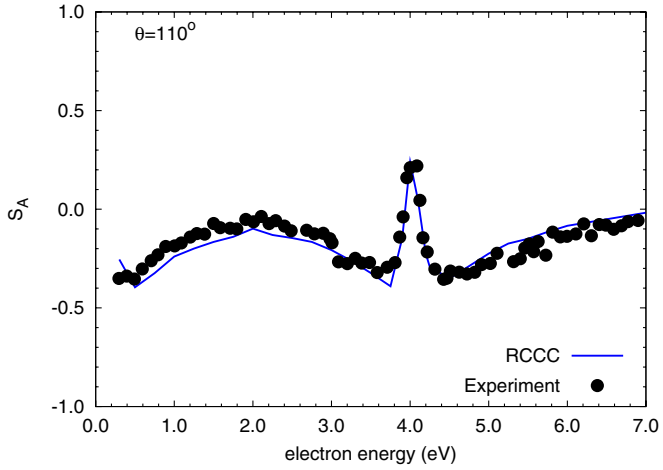


FIG. 2 (color online). Spin asymmetry parameter $S_A$ as a function of energy for elastic electron scattering on cadmium. The detector is located at $\theta = 110°$. Measurements of Bartsch *et al.* [6] are compared with the results of the RCCC calculations described in the text.

RCCC method is an ideal tool for quantitative studies of spin-related phenomena.

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*c.bostock@curtin.edu.au
†Deceased.

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