Superelastic electron scattering from laser-excited cesium atoms

D. S. Slaughter,[1] V. Karaganov,[1] M. J. Brunger,[1] P. J. O. Teubner,[1] I. Bray,[2] and K. Bartschat[3]
[1]*School of Chemistry, Physics and Earth Sciences, Flinders University, GPO Box 2100, Adelaide, 5001, Australia*
[2]*ARC Centre for Antimatter-Matter Studies, Curtin University, Perth, 6845, Australia*
[3]*Department of Physics and Astronomy, Drake University, Des Moines, Iowa 50311, USA*
(Received 29 March 2007; published 29 June 2007)

We present results from a joint experimental and theoretical investigation of superelastic electron scattering from laser-excited Cs atoms in the $(6p)^2P_{3/2}$ state. Comparison of the measured pseudo-Stokes parameters $\bar{P}_1$, $\bar{P}_2$, and $\bar{P}_3$ and the total degree of polarization P^+ for incident energies of 5.5 eV and 13.5 eV, respectively, with theoretical predictions based upon a nonrelativistic convergent close-coupling method and a 24-state semirelativistic Breit-Pauli *R*-matrix approach indicates that driving channel coupling to convergence for these observables is more important than accounting for relativistic effects.

DOI: 10.1103/PhysRevA.75.062717 PACS number(s): 34.80.Dp

I. INTRODUCTION

In recent times there has been enormous theoretical progress in describing electron-atom scattering phenomena. In particular, the convergent close-coupling (CCC) theory has been very successful for atomic targets that are well described by models of one electron or two electrons above an inert core; see Bray and Stelbovics [1] and Fursa and Bray [2], respectively. The same principal idea—namely, to treat the coupling of the target states of interest to the ionization continuum approximated by a large number of pseudostates—was subsequently implemented in the *R*-matrix with pseudostates (RMPS) method described by Bartschat *et al.* [3]. While more general, with respect to the complexity of the targets that can be handled and the possibility of accounting for relativistic effects through the most important terms of the Breit-Pauli Hamiltonian, the expansion of the continuum wave function in terms of an energy-independent basis set limits the number of states that can be coupled in this approach with currently available computational power. This is certainly the case when we compare to what is possible in the CCC method.

The present joint experimental and theoretical study of superelastic electron scattering from laser-excited cesium atoms in their $(6p)^2P_{3/2}$ state is a systematic extension of our earlier work on lithium [4] and potassium [5]. The move to the Cs target was motivated by two principal reasons: namely, to investigate whether a quasi-one-electron model, as used in the CCC [6] and RMPS [7] calculations for this problem, was still a good approximation or whether core effects would finally be visible (see Lukomski *et al.* [8] for a recent example in the ionization process) and also to test whether relativistic effects, currently neglected in the CCC model, would play a role in a heavy target such as Cs. In a recent paper, Andersen and Bartschat [9] suggested that this is not the case for the pseudo-Stokes parameters measured in the present experiment, but of course an experimental check is highly desirable.

A brief description of the experimental setup is given below, followed by a summary of the numerical methods. The results are presented and discussed in Sec. IV, and finally some conclusions are drawn.

II. EXPERIMENT

The apparatus and experimental techniques used in our series of superelastic experiments on cesium are described in detail by Karaganov *et al.* [4]. Several features essential for the present measurements are briefly outlined here, with the experimental configuration of the superelastic electron scattering experiment being shown in Fig. 1. In this case the pseudo Stokes parameters measured in the experiment are given by

$$\bar{P}_1 = \frac{1}{K}\frac{I_0 - I_{90}}{I_0 + I_{90}}, \quad \bar{P}_2 = \frac{1}{K}\frac{I_{45} - I_{135}}{I_{45} + I_{135}}, \quad \bar{P}_3 = \frac{1}{K'}\frac{I_{RHC} - I_{LHC}}{I_{RHC} + I_{LHC}}, \tag{1}$$

where I_ϕ is the count rate of the superelastically scattered electrons when the laser is linearly polarized at the angle of ϕ with respect to the direction of the scattered electrons or when the laser is right- and left-handed circularly polarized. K and K' denote superelastic depolarization factors associated with the linearly and circularly polarized optical pumping as defined by Farrell *et al.* [10]. The values of these coefficients can be determined when measuring the decay fluorescence from the interaction region [10,11]. In the case of cesium K was found to be 0.370 ± 0.010 for the present experimental conditions [4]; the depolarization factor for circularly polarized optical pumping K' was taken to be unity.

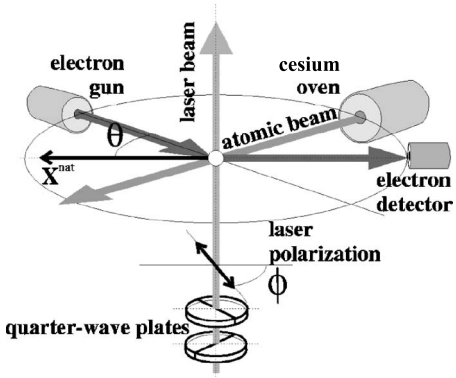

FIG. 1. Schematic diagram of the experimental geometry.

A traditional set of parameters $L_\perp$, $\bar{P}_\ell$, and γ, which characterize the shape of the post-collisional electron charge cloud, and a coherence parameter P^+ can also be deduced. While we do not present our data in terms of all these parameters, for completeness we note that they are related to the Stokes parameters we measure by [12,13]

$$L_\perp = -\bar{P}_3, \quad \bar{P}_\ell = \sqrt{\bar{P}_1^2 + \bar{P}_2^2}, \quad \gamma = \frac{1}{2}\arg(\bar{P}_1 + i\bar{P}_2), \quad (2)$$

$$P^+ = \sqrt{\bar{P}_1^2 + \bar{P}_2^2 + \bar{P}_3^2}. \quad (3)$$

A beam of Cs atoms was produced in a resistively heated oven. The oven operated at a typical temperature of 120 °C, which resulted in an atomic density of about 4×10^9 cm^{-3} at the interaction region. A multistage electron gun produced electron currents between 0.2 μA and 0.5 μA over an energy range between 5.5 eV and 13.5 eV. The superelastically scattered electrons that gained an energy of 1.5 eV were selected by a retarding field electron analyzer and detected by a channel electron multiplier. The energy resolution of the system ($\approx$0.3 eV) was largely due to the Maxwellian thermal energy distribution of the incident electrons.

A single-frequency tunable diode laser (Tuioptics DL100) was tuned to 852.346 nm to optically pump the $(6s)^2S_{1/2} \rightarrow (6p)^2P_{3/2}$ transition in Cs. The laser intensity in the interaction region was normally 5 mW/mm^2. Laser frequency stabilization was achieved by a standard saturated absorption technique [14]. This technique has significant advantages over that which we have previously used [4,5]. Six different polarization states of the laser radiation required for the superelastic experiment were obtained using a polarization rotator consisting of two quarter-wave plates. All three Stokes parameters were measured during the same run without changing the polarizing optics.

The issue of experimental uncertainties including those due to imperfect laser polarization, finite angular resolution, and electron energy variation is addressed in more detail by Karaganov *et al.* [4]. The errors bars given in the figures below are statistical and represent one standard deviation. Care was taken when analyzing the experimental results at scattering angles of about zero degrees. The effects of the finite angular resolution of the measuring system were simulated by performing the convolution transform of the theoretical data and the Gaussian function which characterizes the instrumental effects. The target density was chosen so that the results were demonstrably free of resonance absorption effects.

III. THEORY

The numerical calculations have been described in several recent publications and therefore these descriptions will not be repeated here. Details can be found, for example, in Baum *et al.* [15] and references therein. Briefly, any collision calculation for targets other than hydrogenlike atoms or ions requires first a description of the target structure. This alone can be a significant challenge, in particular if an additional electron has to be coupled in to form the projectile-target complex. Specifically for low-incident-energy electron collisions with the valence electron of cesium, it is well known that a core-potential approach—i.e., obtaining orbitals for the target valence electrons and subsequently performing a quasi two-electron collision calculation by treating the inner 54 electrons by a core potential—is very advantageous, as long as inner-shell excitation processes can be neglected. In the present work, we adopted this strategy and performed semirelativistic Breit-Pauli RMPS calculations using a local static plus exchange potential, as well as nonrelativistic CCC calculations using the Hartree-Fock core potential [16]. In both models, core-polarization effects were simulated by adding a semiempirical long-range polarization potential, whose adjustable parameters were determined by comparing the calculated valence spectrum with experimental data.

Our collision calculations are based upon the close-coupling expansion. Using a large number of physical discrete as well as finite-range pseudostates, an attempt is made to account for all important channel-coupling effects, ideally to convergence, by comparing the results generated with different numbers of pseudostates. Specifically, we will show below results from a CCC model with up to 72 *LS*-coupled states and from a 24-state Breit-Pauli RMPS model (BPRM-24) corresponding to 12 *LS*-coupled states. It will be seen that the latter calculation is, indeed, apparently not converged with the number of states retained in the close-coupling expansion. Increasing the number of *LS*-coupled states to 23, thereby forming a 40-state Breit-Pauli RMPS model, changed the results but did not yield any further improvement in the agreement between theory and experiment. Unfortunately, the much larger number of coupled channels in a relativistic compared to a nonrelativistic angular-momentum-coupling scheme did not allow us to push the RMPS model to convergence with the available computational resources for this project.

IV. RESULTS AND DISCUSSION

Figure 2 exhibits the pseudo-Stokes parameters $\bar{P}_1$, $\bar{P}_2$, and $\bar{P}_3$ and the total degree of polarization P^+ for superelastic e-Cs collisions at an incident energy of 5.5 eV, corresponding to 7.0 eV for the inelastic $(6s)^2S_{1/2} \rightarrow (6p)^2P_{3/2}$ transition. We notice excellent agreement between the experimental data and the predictions from the nonrelativistic CCC model. The overall agreement with the BPRM-24 results is good, but not excellent. The minimum in $\bar{P}_2$ for scattering angles around 100° is better reproduced by the CCC calculation, while the RMPS model reproduces the minimum around 40°. The BPRM-24 results for the circular light polarization $\bar{P}_3$ do not reach the values measured in the $\approx 100° - 120°$ regime. Both calculations predict $\bar{P}_1$ very well, as well as the total degree of polarization P^+. In any nonrelativistic model, a deviation of P^+ from unity indicates the importance of exchange effects between the projectile and the active target electron. The largest such effects apparently appear at scattering angles around 125°, as well as in the near-forward direction. In the latter case, however, the observed deviation of P^+ from unity is due to experimental

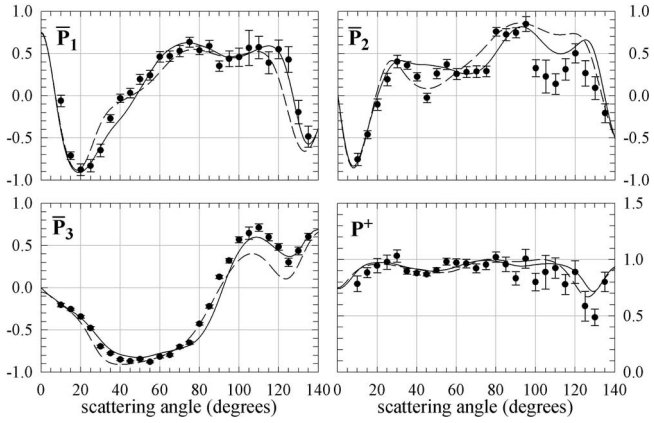

FIG. 2. Pseudo-Stokes parameters $\bar{P}_1$, $\bar{P}_2$, and $\bar{P}_3$ and total degree of polarization P^+ for superelastic e-Cs collisions. The incident electron energy of 5.5 eV is equivalent to 7.0 eV for the corresponding inelastic $(6s)^2S_{1/2} \rightarrow (6p)^2P_{3/2}$ transition. The present experimental data (●) are compared with theoretical predictions from a nonrelativistic CCC (solid lines) and a semirelativistic BPRM-24 (dashed lines) approach. The theoretical results have been convoluted with the experimental angular resolution.

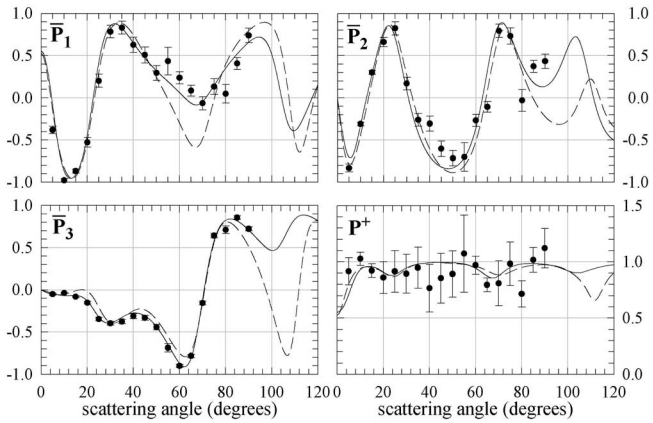

FIG. 3. Pseudo-Stokes parameters $\bar{P}_1$, $\bar{P}_2$, and $\bar{P}_3$ and total degree of polarization P^+ for superelastic e-Cs collisions. The incident electron energy of 13.5 eV is equivalent to 15.0 eV for the corresponding inelastic $(6s)^2S_{1/2} \rightarrow (6p)^2P_{3/2}$ transition. The present experimental data (●) are compared with theoretical predictions from a nonrelativistic CCC (solid lines) and a semirelativistic BPRM-24 (dashed lines) approach. The theoretical results have been convoluted with the experimental angular resolution.

convolution rather than exchange effects. Note, however, that P^+ being close to unity does not mean exchange is not important.

Figure 3 presents our results for an incident energy of 13.5 eV, corresponding to 15.0 eV for the inelastic transition. Once again, the CCC model yields excellent agreement with experiment, while BPRM-24 predicts too deep a minimum in $\bar{P}_1$ in the angular range $\approx 50° - 70°$.

The results embodied in Figs. 2 and 3, specifically the level of agreement between the two theories and between them and the present experimental data, clearly indicate that the pseudo-Stokes parameters we have determined are not sensitive to core or relativistic effects. Of more importance here in obtaining accurate numerical results is correctly accounting for the channel coupling.

V. CONCLUSIONS

In conclusion, we performed benchmark experiments for electron collisions with laser-excited cesium atoms. Comparison of the measured pseudo-Stokes parameters $\bar{P}_1$, $\bar{P}_2$, and $\bar{P}_3$ and the total degree of polarization P^+ for incident energies of 5.5 eV and 13.5 eV, respectively, showed excellent agreement with predictions from a nonrelativistic convergent close-coupling model treating the Cs target as an effective one-electron system through a core potential for the inner 54 electrons. The agreement between experiment and a calculation with less coupled states but accounting for relativistic effects was also good but not excellent. These findings suggest that the pseudo-Stokes parameters studied in the present experiment are neither sensitive to core nor to relativistic effects, while accounting for channel coupling is very important to obtain an accurate numerical answer.

ACKNOWLEDGMENTS

This work was supported by the Australian Research Council and by the U.S. National Science Foundation under Grant No. PHY-0244470 (K.B.). D.S. thanks the Ferry Trust for financial support. I.B. acknowledges the support of the Australian Partnership for Advanced Computing and its Western Australian node iVEC.

[1] I. Bray and A. T. Stelbovics, Adv. At., Mol., Opt. Phys. **35**, 209 (1995).
[2] D. V. Fursa and I. Bray, J. Phys. B **30**, 757 (1997).
[3] K. Bartschat, E. T. Hudson, M. P. Scott, P. G. Burke, and V. M. Burke, J. Phys. B **29**, 115 (1996).
[4] V. Karaganov, I. Bray, and P. J. O. Teubner, Phys. Rev. A **59**, 4407 (1999).
[5] K. A. Stockman, V. Karaganov, I. Bray, and P. J. O. Teubner, J. Phys. B **34**, 1105 (2001).
[6] K. Bartschat and I. Bray, Phys. Rev. A **54**, 1723 (1996).
[7] K. Bartschat and Y. Fang, Phys. Rev. A **62**, 052719 (2000).
[8] M. Lukomski, S. Sutton, W. Kedzierski, T. J. Reddish, K. Bartschat, P. L. Bartlett, I. Bray, A. T. Stelbovics, and J. W. McConkey, Phys. Rev. A **74**, 032708 (2006).
[9] N. Andersen and K. Bartschat, J. Phys. B **35**, 4507 (2002).
[10] P. M. Farrell, W. R. MacGillivray, and M. C. Standage, Phys. Rev. A **44**, 1828 (1991).
[11] X. K. Meng, W. R. MacGillivray, and M. C. Standage, Phys.

Rev. A **45**, 1767 (1992).
[12] N. Andersen, J. W. Gallagher, and I. V. Hertel, Phys. Rep. **165**, 1 (1988).
[13] N. Andersen and K. Bartschat, *Polarization, Alignment, and Orientation in Atomic Collisions* (Springer, New York, 2001).
[14] W. Demtröder, *Laser Spectroscopy: Basic Concepts and Instrumentation*, 2nd enlarged ed. (Springer, Berlin, 1996).
[15] G. Baum, N. Pavlovic, B. Roth, K. Bartschat, Y. Fang, and I. Bray, Phys. Rev. A **66**, 022705 (2002).
[16] I. Bray, Phys. Rev. A **49**, 1066 (1994).