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Spin entanglement in elastic electron scattering from lithium atoms

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In two recent papers (Phys. Rev. Lett. **116** (2016) 033201; Phys. Rev. A **94** (2016) 032331), the possibility of continuously varying the degree of entanglement between an elastically scattered electron and the valence electron of an alkali target was discussed. In order to estimate how well such a scheme may work in practice, we present results for elastic electron scattering from lithium in the energy regime of $1-5$ eV and the full range of scattering angles $0^\circ - 180^\circ$. The most promising regime for Bell-correlations in this particular collision system are energies between about 1.5 eV and 3.0 eV, in an angular range around $110^\circ \pm 10^\circ$. In addition to the relative exchange asymmetry parameter, we present the differential cross section that is important when estimating the count rate and hence the feasibility of experiments using this system.

In two recent publications, Blum and Lohmann [1] and Lohmann *et al.* [2] discussed a tunable entanglement in elastic electron collisions with atomic hydrogen or light alkali atoms, where explicitly spin-dependent interactions may be neglected and the process is completely described by two independent parameters, namely the absolute angle-differential cross section (DCS) and a spin-correlation parameter P, which (except for the opposite sign) is the exchange asymmetry $A_{\rm ex}$ that was measured by the Bielefeld [3, 4] and NIST [5] groups many years ago. Due to the available experimental data, Lohmann *et al.* [2] presented results for $P = -A_{\rm ex}$ from various close-coupling calculations for atomic hydrogen and sodium, but only for selected energies as a function of the scattering angle, and for lithium, but only at selected angles as a function of energy.

Entanglement is of interest in many areas of physics, but it has traditionally not been associated with either atomic or nuclear collision physics. In order to get a firm estimate whether such collision systems might be appropriate and also what the expected signal rate might be, it is highly desirable to have a comprehensive dataset on an energy-angle grid. Furthermore, a critical parameter for practical applications is the absolute angle-differential cross section, since it determines whether or not the signal rate is sufficient in an actual experiment.

The results reported below were obtained in a 5-state close-coupling model for e-Li collisions, including the $(1s^2 2s)^2S$, $(1s^2 2p)^2P^{\rm o}$, $(1s^2 3s)^2S$, $(1s^2 3p)^2P^{\rm o}$, and $(1s^2 3d)^2D$ states of Li in the close-coupling expansion. The $1s$ and $2s$ orbitals were taken from the tables by Clementi and Roetti [6], and the $2p$, $3s$, $3p$, and $3d$ orbitals were generated with the program `CIV3` of Hibbert [7]. Already without accounting for the small polarization of the $1s^2$ Li^+ core, the excitation energies and the ionization potential were accurate to about 1-2 % compared to the NIST-recommended values [8], and hence the structure calculation was judged to be of sufficient quality for the purpose of the present work.

For the collision energies of interest, such a simple model is sufficient, as we will demonstrate by comparing its predictions with the few experimental data that are currently available. In fact, tests showed that even a 2-state model, coupling just the $(1s^2 2s)^2S$ ground state and the $(1s^2 2p)^2P^o$ lowest excited state, would describe the main physics of the problem at hand. This is due to the fact that almost the entire electric dipole polarizability of the $(1s^2 2s)^2S$ state, which is very important for elastic scattering at low energies, originates from the coupling to the $(1s^2 2p)^2P^o$ state.

The close-coupling equations were solved with the Belfast R-matrix code [9], which has the advantage of being able to handle many collision energies very efficiently, once the inner-region problem has been solved by diagonalizing the hamiltonian matrices. Specifically, we set the R-matrix radius to 40 a_0, where $a_0 = 0.529^{-10}$ m is the Bohr radius. We calculated partial waves up to a total orbital angular momentum of $L = 15$ and employed 25 continuum orbitals to expand the R-matrix basis functions.

The essential point regarding spin entanglement is the following [1, 2]: After the collision, the projectile and the target valence electron are correlated. Depending on the collision energy and the scattering angle, the correlation can be classified by the value of [3]

$$P = -A_{\rm ex} = \frac{\sigma^{\uparrow\uparrow} - \sigma^{\uparrow\downarrow}}{\sigma^{\uparrow\uparrow} + \sigma^{\uparrow\downarrow}} = \frac{\sigma^t - \sigma^s}{3\,\sigma^t + \sigma^s} \qquad (1)$$

where $\sigma^{\uparrow\uparrow}\,(\sigma^{\uparrow\downarrow})$ and $\sigma^s\,(\sigma^t)$ are short-cut notations (instead of $d\sigma(E,\theta)/d\Omega$) for the angle-differential cross sections (DCSs) for parallel (anti-parallel) spin orientations of the projectile and target spins or triplet (singlet) scattering. The DCS for unpolarized projectile and target beams is given by

$$\sigma_u = \frac{1}{4}\sigma^s + \frac{3}{4}\sigma^t, \qquad (2)$$

and hence the limiting values for P are $+1/3$ for pure triplet and -1 for pure singlet scattering. The latter extreme case corresponds to the well-known situation of two spins forming a combined spin-0 system.

Blum and Lohmann [1] analyzed in detail the spin density matrix of the combined (projectile + target electron) system after the collision. Specifics can be found in their paper. Note, however, that $A_{\rm ex}$ in Eq. (1) was defined solely with the collision experiments performed at the time in mind, i.e., comparing the count rates for parallel and anti-parallel spin polarizations of the initial projectile and target beams.

According to Blum and Lohmann, the combined projectile + target spin system can be classified as separable (S) if

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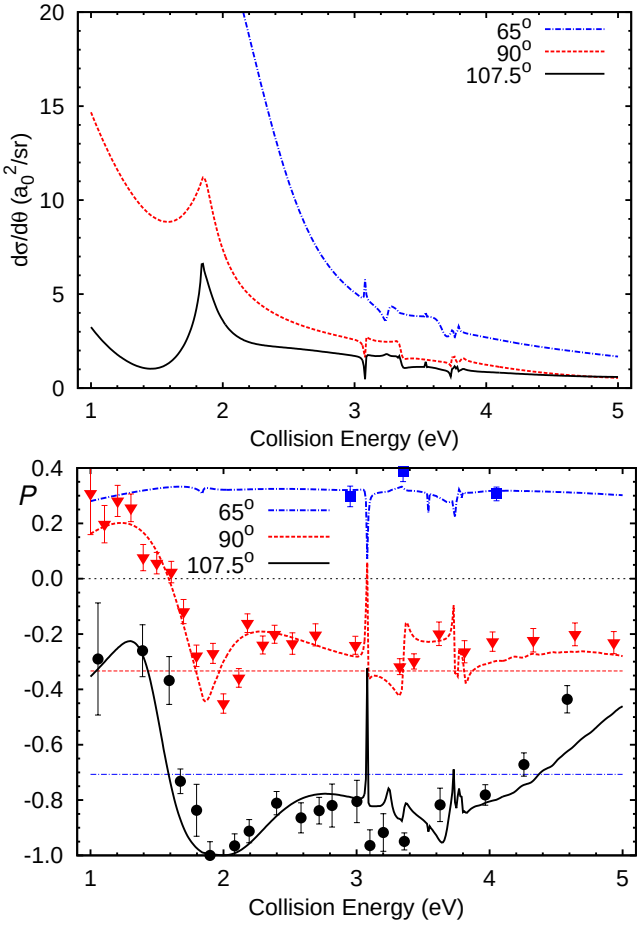

FIG. 1: Differential cross section (top) and spin correlation parameter P (bottom) for elastic electron scattering from Li atoms as a function of energy at scattering angles of $65°$, $90°$, and $107.5°$. The lines at $-1/3$ and $-1/\sqrt{2}$ in the panel for P mark the borders between separable and entangled as well as entangled and Bell-correlated regions, respectively. The experimental data for $P = -A_{\rm ex}$ are taken from Baum *et al.* [3].

$P > -1/3$, entangled (E) for $-1/3 > P > -1/\sqrt{2}$, or Bell-correlated (B) if $P < -1/\sqrt{2}$. These ranges of P are obtained by analyzing the eigenvalues of the combined spin density matrix and using the criteria introduced by Peres [10] and Horodecki *et al.* [11].

Hence, such systems may provide a knob to "dial in" the amount of correlation one would like. Note that it is not necessary for Bell correlations to have a pure singlet state.

Figure 1 shows that the present 5-state model is, indeed, sufficient for the problem at hand. The overall agreement with the available experimental in the energy range of $1 - 5$ eV is very satisfactory. Since Bell correlations appear to be only realizable in this energy regime, it is not necessary to include coupling to higher Rydberg states or even the ionization continuum. Note, however, the appearance of resonances in both the DCS and, even more pronounced, in P. Although these resonances would likely be washed out in practice due to the finite energy resolution (they are real, but not visible in Fig. 7 of [2], presumably due to the energy grid chosen in the calculations), it seems advisable to avoid the resonance regime from 3 eV up to the ionization threshold when choosing the energy.

Figure 2 exhibits our results for a fixed energy of 3 eV as a function of the scattering angle. Here one can see how the negative values of the spin correlation parameter develop. Fortunately for a practical implementation, the DCS in the singlet spin channel assumes a local maximum around $110°$, while the DCS for triplet scattering assumes a deep minimum. This explains why Baum *et al.* [3] were able to carry out measurements with small error bars in this angular regime.

As mentioned above, we are now in a position to provide a comprehensive overview of the results that might be expected for the electron−lithium collision system. This is done in Fig. 3 for the spin correlation parameter and Fig. 4 for the DCS. In the latter, we limit the maximum DCS value in the plots to $10\,a_0^2$/sr in order to improve the visibility. There is virtually no chance to find P-values in the Bell-correlated regime when the DCS is too large.

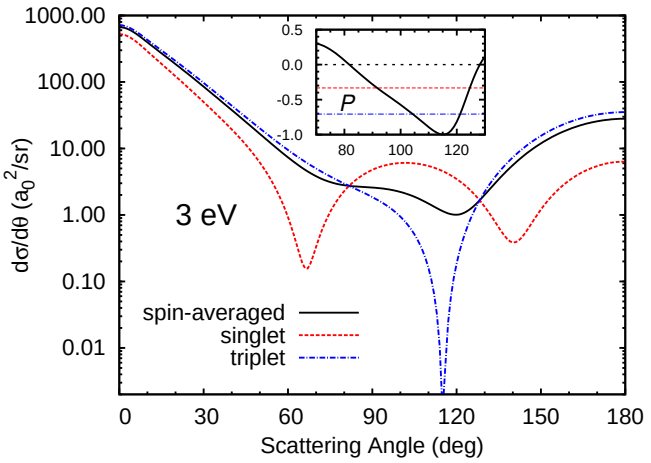

FIG. 2: Differential cross section as well as the individual contributions from the singlet and triplet total spin channels for elastic electron scattering from Li atoms at a collision energy of 3 eV. The insert shows the parameter P in the region $70° - 130°$. The lines at $-1/3$ and $-1/\sqrt{2}$ mark the borders between separable and entangled as well as entangled and Bell-correlated regions, respectively.

To summarize: We have carried out calculations for elastic electron scattering from lithium atoms in a simple, but sufficient model to accurately predict the spin correlation parameter and the angle-differential cross section. The most promising regime for Bell-correlations in this particular collision system are energies between about 1.5 eV and 3.0 eV, in an angular range around $110° \pm 10°$. While the cross sections are relatively small, the signal rate seems to be sufficient for a successful experimental implementation of the scheme. For higher energies than 3 eV, the results would first be affected by resonances. Subsequently, as for all scattering angles outside of the above range, triplet scattering is the dominant channel

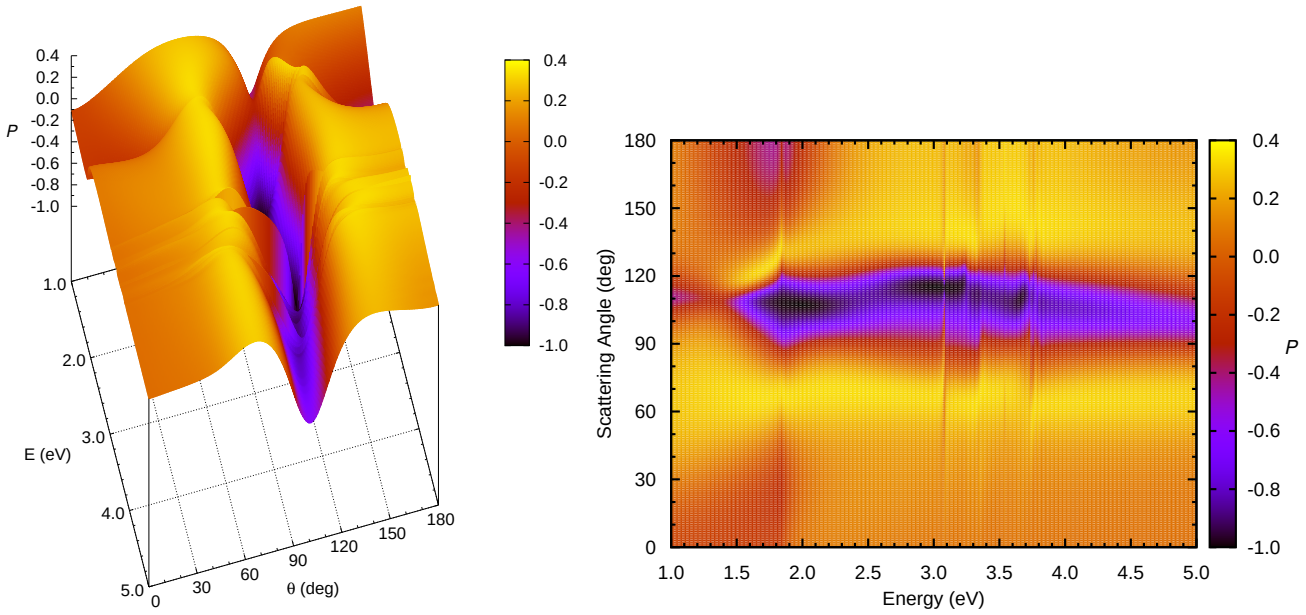

FIG. 3: Spin correlation parameter P for elastic electron scattering from lithium atoms, as 3D figure (left) and as contour plot (right).

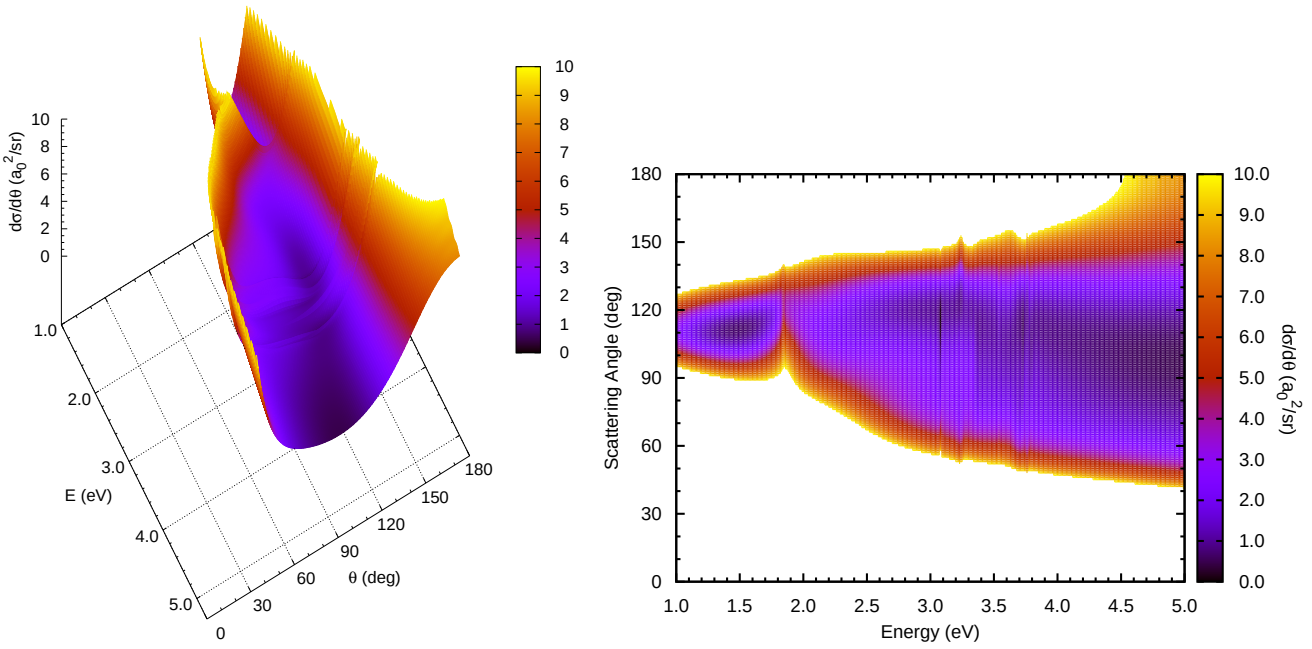

FIG. 4: Differential cross section for elastic electron scattering from lithium atoms, as 3D figure (left) and as contour plot (right). In the white areas of the contour plot, the DCS is larger than $10\,a_0^2$/sr.

everywhere and hence P-values in the Bell-correlated regime will not be achievable. In the future, we plan to carry out similar calculations for atomic hydrogen and other alkali targets. Such efforts seem well justified in order to determine the most promising collision system. It would also be interesting to investigate heavy targets such as Cs, in order to study potential modifications due to relativistic effects.

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