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LETTER TO THE EDITOR

Ultralow-energy electron scattering from alkaline-earth atoms: the scattering-length limit

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Abstract

We use the non-relativistic R-matrix method to treat ultralow-energy electron scattering from the alkaline-earth atoms Mg, Ca, and Sr. The sensitivity of the predictions for the scattering length is analysed by comparing results obtained from a variety of structure and collision models. We estimate the electron scattering lengths to be $-2.5\ a_0$ for e^-–Mg, $-12\ a_0$ for e^-–Ca, and $-18\ a_0$ for e^-–Sr, respectively.

Electron scattering has historically been a preferred tool for interrogating the structure and other properties of matter in gaseous or condensed phases. With the landmark confinement and manipulation of bosonic and fermionic matter at extremely low temperatures [1–5], new windows of opportunity have opened up for precision analysis of electron scattering from and photoionization of atoms in ultracold gases. Absolute measurements of electron collision and photoelectron cross sections in magneto-optical traps (MOTs) and Bose–Einstein condensates (BECs), leading to trap loss, have been performed for ground and excited states of alkali metals [6–12]. In addition, a strongly correlated ultracold neutral plasma of metastable xenon atoms has recently been created [13, 14], in which electron temperatures as low as $T_e \sim 100$ mK were achieved. By studying the plasma expansion, strong electron-correlation effects were verified in these experiments [15] and the formation of Rydberg atoms in electron–ion recombination in the expanding plasma gas was observed. Ultralow-energy electron scattering from ultracold bosonic and fermionic degenerate gases can also probe the different statistics obeyed by the trapped atomic species [16].

Recent predictions of the existence of an exotic class of highly excited molecular Rydberg states in collisions of neutral and Rydberg atoms in a MOT or a BEC—so-called trilobite and butterfly states [17, 18]—relied upon the Fermi pseudo-potential method [19] that treats the interaction of the Rydberg electron with a neutral atom in its ground state within the electron scattering-length limit. The scattering lengths for electron collisions with heavy

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alkali metal atoms have been calculated using a Dirac R-matrix method [20–22] for quasi-one-electron targets. To our knowledge, however, much less is known about ultralow-energy collisions of electrons with alkaline-earth atoms. Trapping of alkaline-earth atoms has advanced tremendously in the past few years [23, 24], driven by the interest in metrology and optical frequency standards. Alkaline-earth atoms are generally preferred to alkali atoms due to the lack of hyperfine interaction for the stable group II isotopes.

In this letter, we embark on the calculation of the electron scattering length in the collision of ultralow-energy ($T_e < 1$–10 K) electrons from the alkaline-earth atoms Mg, Ca, and Sr. We applied the non-relativistic R-matrix method [25] to calculate phaseshifts for electron collisions with these targets. Before describing the calculations in some detail, it is appropriate to address the strengths as well as the potential difficulties in applying this numerical model to treat such low-energy collisions.

One of the advantages of the R-matrix method is its foundation on a close-coupling plus correlation expansion. It is generally accepted that the treatment of low-energy electron collisions does not require to closely couple a large amount of target states. In fact, many calculations for elastic electron–noble-gas scattering have been performed with only two states in the close-coupling expansion, namely the ground state and a $^1P^o$ pseudo-state that is particularly designed to account for the dipole polarizability of the target due to the incident projectile [26]. Representing this dipole polarizability dynamically via the coupling to a closed channel instead of using a semi-empirical, often local and energy-independent, polarization potential, is certainly advantageous.

On the other hand, it is well known that multi-channel close-coupling calculations become numerically difficult, particularly when the projectile energy is in the vicinity of a threshold and when strongly closed channels are present. An additional complication in the case of the R-matrix method can arise from the basis-function expansion of the projectile wavefunction inside the R-matrix box. Here it is critical to avoid problems with less than perfect orthogonality of both the bound and continuum orbital sets, and to be careful about a potentially over-complete basis if pseudo-orbitals are used to improve the target description. Finally, the target description itself can become an issue. For example, the inclusion of core polarization and relaxation effects was shown to be important in the calculation of energy levels and oscillator strengths [27].

In light of the above potential difficulties, considerable care must be taken to calculate reliable results at extremely low collision energies. In addition, electron collision data obtained with traditional experimental approaches are rare, and comparison with predictions from other theoretical methods, though important to recognize overall trends, is of limited value. Hence, we have performed some internal consistency checks among the results presented below and investigated the sensitivity of the predictions by comparing results obtained with a variety of structure and collision models.

Figure 1 shows results for the phaseshifts δ_ℓ ($\ell = 0, 1, 2$), the angle-integrated elastic (total) partial and summed cross sections, and the quantity $k \cot \delta_0$ for electron scattering from magnesium. The results were obtained by including only the ground state $(3s^2)^1S$ (1st), the lowest three states (3st), or the lowest nine states (9st) of Mg in the close-coupling plus correlation expansion of the scattering wavefunction. The 1s, 2s, 2p, 3s, and 3p orbitals were taken from the tables of Clementi and Roetti [28], while the valence orbitals were generated with the structure package `CIV3` or Hibbert [29].

As can be seen from figure 1, the low-energy collisions are dominated by a p-wave shape resonance leading to a cross-section maximum at an incident electron energy around 0.14 eV, in good agreement with experimental evidence of 0.15 ± 0.03 eV [30] and predictions from other calculations (0.165 eV by Robb [31] and 0.161 eV by Kim and Greene [32]). The position

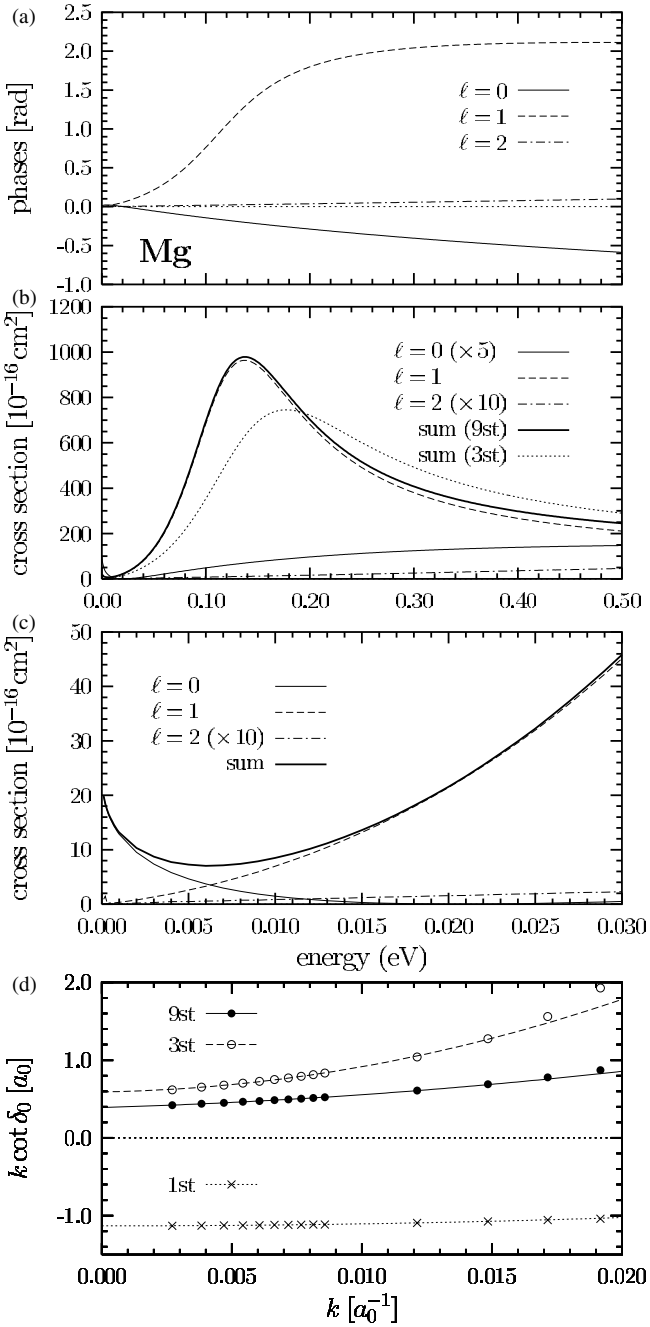

Figure 1. S-wave ($\ell = 0$), p-wave ($\ell = 1$), and d-wave ($\ell = 2$) phaseshifts, partial and summed angle-integrated cross sections, and results for $k \cot \delta_0$ for low-energy electron collisions with magnesium. If not indicated otherwise, (a)–(c) contain the results from the 9st close-coupling model. Some of the small cross sections have been multiplied by the factors listed. In (d), the numerical results are shown by the symbols, while the fit to a quadratic function of the momentum k is shown by the curves.

of this resonance, and the satisfactory agreement of the theoretical dipole polarizability of approximately 80 a_0^3 (obtained from the effective-range formula of O'Malley *et al* [33]) for the $\ell = 5$ wave) and the recommended value of 71.6 a_0^3 [34] gives us some confidence in the accuracy of our 9st model. The presence of the p-wave shape resonance should lead to the formation of molecular Rydberg 'butterfly' states in collisions of ultracold Mg ground-state and Rydberg atoms [18].

Most interesting for the present work, however, are the s-wave results which allow for the extraction of the scattering length. Figure 1(d) shows the actual results from the 1st, 3st, and 9st models, as well as fits to a quadratic function of the projectile linear-momentum magnitude k. The constant term of that expansion is the negative inverse of the scattering length [35]. The presumably best model (9st) yields a scattering length of $-2.5\ a_0$, while the 3st model predicts about $-1.5\ a_0$. On the other hand, the static-exchange approximation (1st), which does not include any polarization effects, actually yields a *positive* scattering length of approximately $+0.8\ a_0$. Hence, accounting for the distortion of the target charge cloud by the incident projectile is critical already for the prediction of the sign of the scattering length.

Figure 2 shows similar results for the calcium target. This collision system has also been investigated by Yuan and Zhang [36] and by Yuan and Fritsche [37], and extensive work has been done on the structure part alone (see, for example, [27] and references therein). For this system, we used the structure description given by Glass [38] to perform five-state (5st) and two-state (2st) calculations, including either the lowest five states or just the ground state and the $(4s4p)\,^1P^o$ state in the close-coupling expansion. We also used `CIV3` to generate our own target description, with and without pseudo-orbitals ($\bar{5}$s, $\bar{5}$p, $\bar{4}$d) to improve the representation of the target states. The 5st model with the Glass target description yields an effective dipole polarizability of approximately 180 a_0^3, very similar to that obtained in the 2st model and the value of 169 a_0^3 given by Miller and Bederson [34].

Since Ca^- forms a stable negative ion in the configuration $(4s^24p)\,^2P^o$, there is no longer a p-wave shape resonance. Instead, the p-wave phaseshift starts off positive but becomes negative at very low incident energy (approximately 0.02 eV). In this respect, our predictions agree well with those of Yuan and Zhang [36]. Nevertheless, there remain substantial differences in the phaseshifts for the s- and p-waves at higher energies. Fortunately, however, the predictions for the scattering length seem to be relatively insensitive to the details of the model, except that inclusion of the pseudo-orbitals is apparently important to obtain a sufficiently accurate target description. From figure 2(d), we estimate a value of approximately $-12\ a_0$ for the scattering length. Once again, the pure static-exchange model yields a qualitatively different result of about $+3\ a_0$.

Finally, figure 3 shows our results for the strontium target. In this case, we performed two 5st calculations, using either `CIV3` or the `SUPERSTRUCTURE` (SS) [39] package to generate the target orbitals. The results obtained with the `CIV3` orbitals agree very well with those given by Yuan and Zhang [36]. In addition, the energy spectrum was predicted in better agreement with experiment by `CIV3` than by `SUPERSTRUCTURE`. However, this is essentially an effect of the optimization procedure rather than the quality of the structure package. The theoretical dipole polarizabilities in the two models were approximately 190 a_0^3 (`CIV3`) and 310 a_0^3 (SS), to be compared with the value of 186 a_0^3 given in [34]. We show the SS results mainly to indicate the sensitivity of theoretical predictions to such details, but believe that the more accurate result is a scattering length of approximately $-18\ a_0$.

In summary, we have performed a number of calculations to obtain the scattering length for ultralow-energy electron collisions with the alkali-earth targets Mg, Ca, and Sr. These results are of potential interest for analysing collisions between ultracold neutral ground-state and Rydberg alkaline-earth atoms, as well as for electron scattering in a MOT. At these very

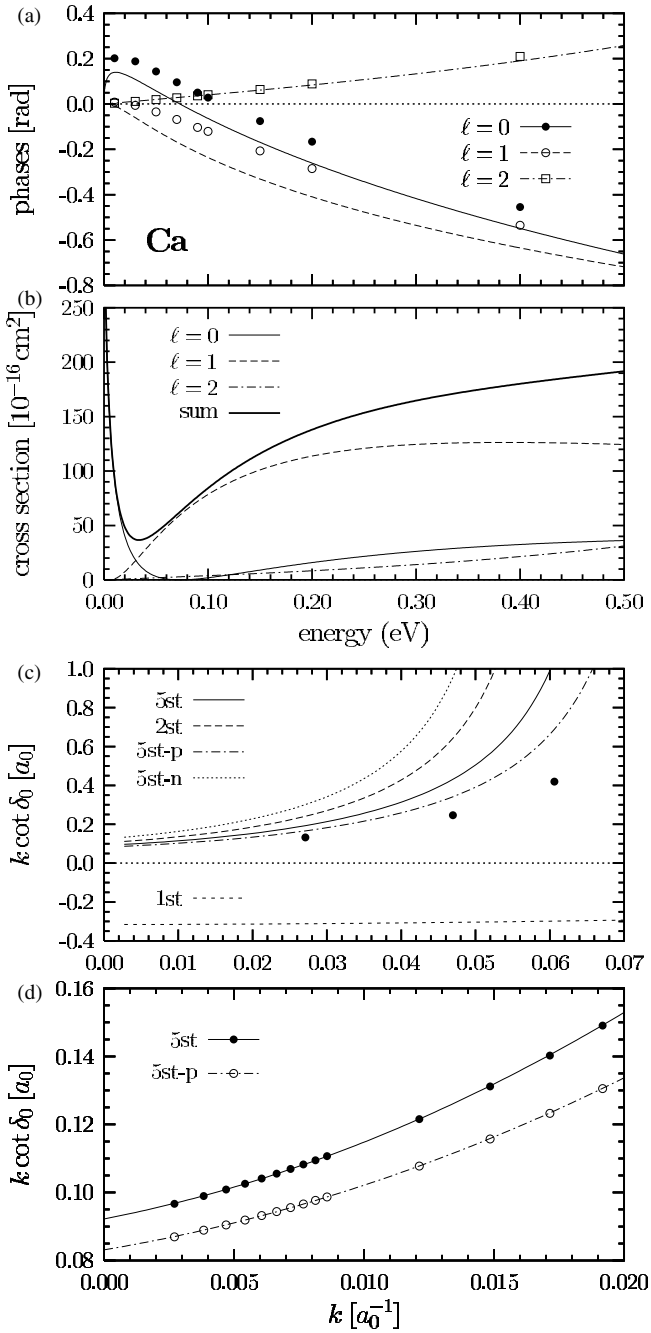

Figure 2. Same as figure 1 for electron collisions with calcium. The results shown in (a) and (b) were obtained in a 5st calculation with the target description given by Glass [38]. The curves labelled 5st-p and 5st-n correspond to 5st calculations using `CIV3` orbitals with (p) and without (n) pseudo-orbitals. The symbols in (a) and (c) represent the results of Yuan and Zhang [36]. In (d) the symbols are the numerical results from the model indicated while the curves are the fit to a quadratic function of k.

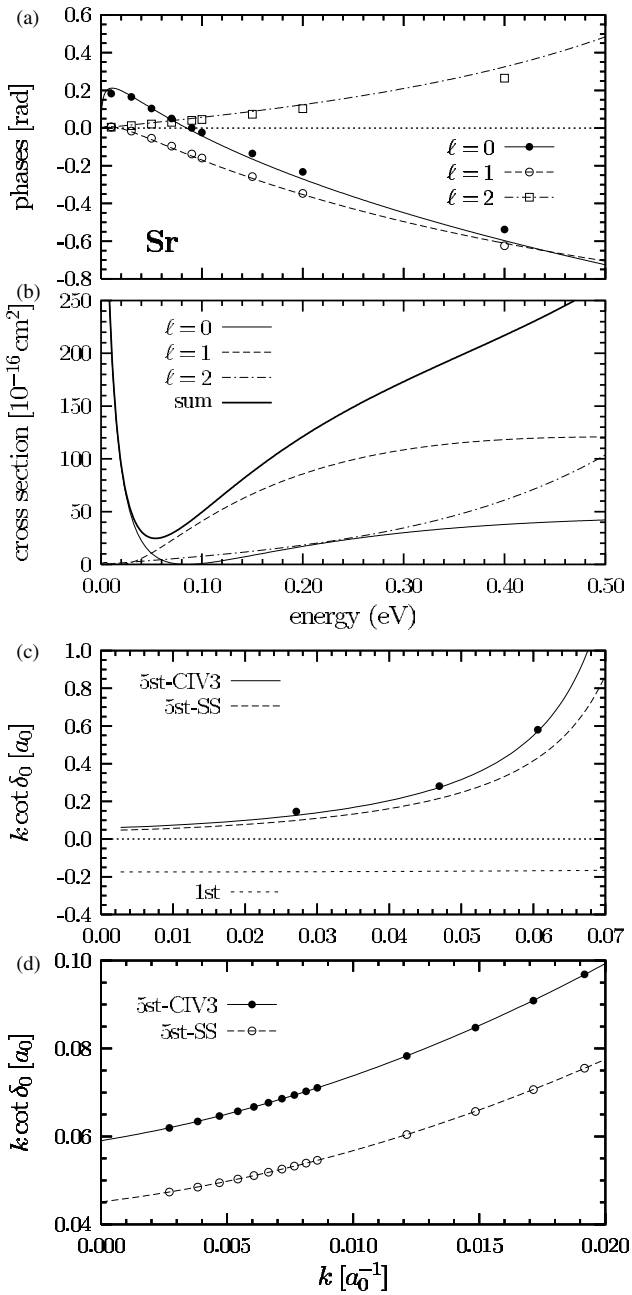

Figure 3. Same as figure 1 for electron collisions with strontium. The results shown in (a) and (b) were obtained in a 5st calculation with the target description obtained with the `CIV3` orbitals. The curves labelled 5st-SS correspond to a 5st calculation using `SUPERSTRUCTURE` orbitals. The symbols in (a) and (c) represent the results of Yuan and Zhang [36]. In (d), the symbols are the numerical results from the model indicated while the curves are the fit to a quadratic function of k.

low energies, the numerical calculations are by no means trivial and hence we regard these numbers as preliminary. It is, however, very likely that the values of the scattering length in all three systems are negative, with increasing magnitudes when going from Mg to Sr. The

principal reason for the predicted negative values is the inclusion of the charge-cloud distortion in the numerical model, which is achieved through the coupling of the $^1S^e$ ground state to closed channels associated with a $^1P^o$ excited state.

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