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Cusp formation in classical trajectory Monte–Carlo calculations of single atomic ionization by the impact of neutral projectiles

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Abstract. The Classical-trajectory Monte-Carlo (CTMC) model provides an excellent description of the electron capture to the continuum (ECC) cusp in atomic ionization collisions whenever the electron-projectile interaction is of a Coulomb or even of a dipolar type. However, in this communication we show that this description fails for the case of a polarizability potential, such as in the one produced by a neutral He (2^1S) outgoing projectile. Actually the CTMC calculation predicts an ECC peak that is much broader and smaller than for a Coulomb interaction, a result that differs from experimental data and quantum-mechanical calculations.

1. Introduction

The velocity distribution of electrons emitted in atomic collisions often exhibits a peak centered at the velocity $\mathbf{v}_P$ of the incident projectile [1]. Classical-trajectory Monte-Carlo (CTMC) simulations provide an excellent description of this structure whenever the interaction between the electron and the outgoing projectile is of a Coulomb [2] or even of a dipolar type [3, 4]. However, serious doubts were recently cast over the general validity of any classical approach for the description of more general atom-atom ionization collisions [5]. These questionings are due to the visualization of the cusp as the result of a smooth continuation across the ionization limit of capture into highly excited electron-projectile bound states [6, 7]. By mimicking a bound spectrum accumulating at zero energy by a continuum, any classical description would succeed in describing the "electron capture to the continuum" (ECC) divergence observed whenever the electron-projectile interaction is of Coulomb or dipolar nature. But, if the electron-projectile interaction decreases faster than a dipole potential at large distances, the energy spectrum would not accumulate at zero energy, and a classical description would be bound to fail. Our purpose in this communication is to elucidate, through CTMC calculations [8], this limitation of the classical description of cusp formation. To this end we consider a He + Ar ionization collisions for the case of neutral He outgoing projectiles in the 2^1S metastable state, as first measured by the Debrecen group in 1989 [9]. Here the electron-projectile interaction is of a polarizability type, with a low-lying virtual state that is reported to produce a sharp distortion of the ECC structure [10, 11].

2. Theory

For the description of the ionization collision we apply the CTMC method [12]. This method is based on the numerical solution of Newton's classical equations of motion for a large number of trajectories under randomly chosen initial conditions. Details of the calculations of the electron cusp by means of the CTMC method can be found in our previous works (see, e.g., ref. [13] and references therein). Assuming the validity of the *independent particle* model, we used a three-body version of the CTMC approach, describing the target core by a model potential developed by Green *et al.* [14]. The parameters of the electron–argon potential were taken from Garvey [15].

For the electron–projectile potential we use a model polarization potential, with the correct long-range $-1/r^4$ behavior, and a short-range cutoff function. Many different cutoff functions have been employed in the literature (see, for instance, [16]). However, in a previous paper [17], we showed that the intricate polarization effects for the doublet scattering of electrons with a He atom in a 2^1S metastable state can be described fairly adequately by the simplest choice

$$V(r) = -\frac{\alpha e^2}{2R^4} + \left[\frac{\alpha e^2}{2R^4} - \frac{\alpha e^2}{2r^4}\right]\Theta(r-R)$$

that only depends on the range R and the polarizability α. Actually, as it is shown in Ref. [17], an excellent quantitative agreement between the exact s-wave distortion factor [18] and that obtained by the model potential is found. In fact, it would not be possible to distinguish both curves if they were shown together in figure 1.

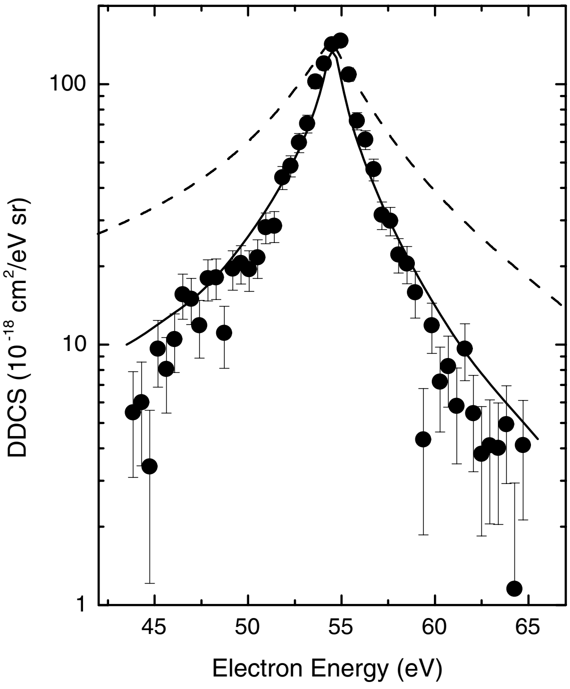

Figure 1. Double differential cross section (DDCS) in the forward direction for ionization of Ar atoms by the impact of 400 keV He, in coincidence with neutral outgoing projectiles in the 2^1S metastable state. The experimental (●) [11] and theoretical (——) [18] results are compared with those for a He^{2+} projectile (– – –). The theoretical curves were renormalized in order to fit the measured cusps on an absolute scale.

Concerning the choice of the random initial parameters, we followed the procedure proposed by Reinhold and Falcón [19] for non-Coulombic interaction. We used the experimental ionization potential of Ar for the calculation of the initial Kepler orbits. Our CTMC code was checked by comparing the results of our total cross-section calculations for 100-keV protons on He collisions with those of Reinhold and Falcón [19], as is discussed in ref. [13].

3. Results

As figure 1 shows, the cusp in both the experimental data and the quantum-mechanical calculations is much sharper than the one produced by He^{2+} projectiles [11]. This phenomenon was attributed to a low-lying virtual state on the electron-projectile system [10], an effect that no classical description can reproduce. Actually, as figure 2 shows, the CTMC calculation produces a peak that is much broader and smaller than for a Coulomb interaction.

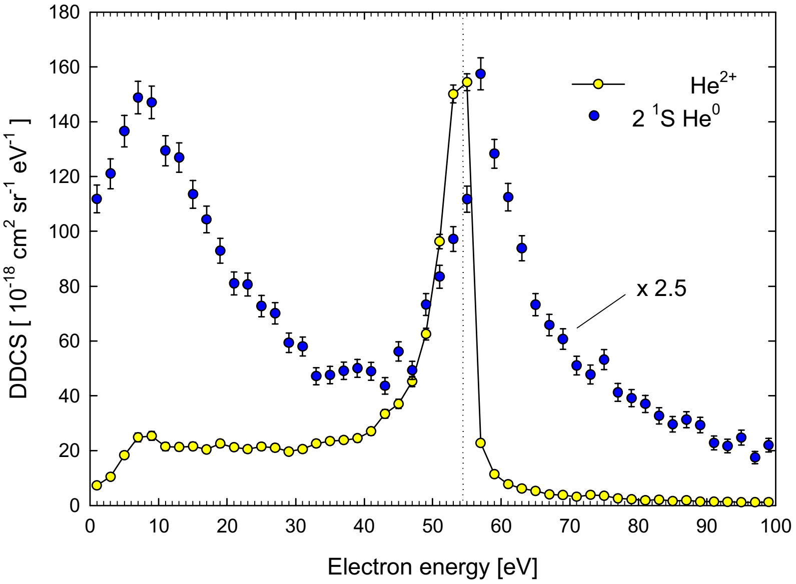

Figure 2. CTMC calculation of the double differential cross section (DDCS) in the forward direction for ionization of Ar atoms by the impact of 400 keV He, in coincidence with neutral outgoing projectiles in the 2^1S metastable state. The result for He^{2+} projectiles is also shown for comparison. The acceptance angle is 1 deg. These results were obtained by integrating 0.36×10^9 trajectories.

4. Conclusions

By mimicking a bound spectrum accumulating at zero energy by a continuum, the CTMC method succeeds in describing the ECC cusp whenever the electron-projectile interaction is of Coulomb or dipolar nature. However, when this interaction decreases faster than a dipole potential at large distances, as it is the case for the He (2^1S) outgoing projectile analized here, the results depicted in figure 2 show that this classical theory fails in providing a correct description of the ECC cusp. This result clearly testifies against any supposedly classical origin of the ECC phenomenon.

Acknowledgments

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