Ionization of helium by fast and highly charged ions

2007 J. Phys.: Conf. Ser. 58 259

(http://iopscience.iop.org/1742-6596/58/1/056)

IOP Publishing Journal of Physics: Conference Series **58** (2007) 259–262
doi:10.1088/1742-6596/58/1/056 13th International Conference on the Physics of Highly Charged Ions

Ionization of helium by fast and highly charged ions

P A Macri[1] **V D Rodríguez**[2] **and R O Barrachina**[3]

[1] Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad Nacional de Mar del Plata, Deán Funes 3350, 7600 Mar del Plata, Argentina.
[2] Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, 1428 Buenos Aires, Argentina.
[3] Centro Atómico Bariloche and Instituto Balseiro, 8400 S. C. de Bariloche, Río Negro, Argentina.

E-mail: `macri@mdp.edu.ar`

Abstract. We present CDW-EIS theoretical calculations for the projectile deflection in single ionization of Helium by heavy-ion impact as a function of ionized electron energies. These calculations account for the projectile-residual target ion interaction through a first order static potential and a second order polarization potential. The results are compared with recent experimental data by impact of 3.6 MeV/amu Au53+. A good agreement is found.

1. Introduction

It is only recently that multiple differential cross sections have been registered for Helium ionization by highly charged ions [1, 2]. Both double and triple differential cross sections have been measured in the perturbative regime for C^{6+} impact and in a strongly non-perturbative regime for Au^{53+} impact. Since these experiments provide a set of observations as a function of projectile deflection, the incorporation in the theoretical framework of a more detailed projectile - residual target ion interaction than the internuclear potential has become a pressing task. For many electrons atoms, the not ionized electrons screen the pure Coulombic interaction between the projectile and the target nuclei, making this task very involved. The simplest approach considers a pure Coulomb interaction where the target nuclear charge is replaced by a constant effective charge given by the binding energy of the active electron. This approach can not explain, however, the double hump structure found in the experiments [1, 2]. In [3], an alternative target ion charge depending on the projectile momentum transfer was proposed, which interpolating between the limits of total and zero screening attempted to explain the observed structures. In a recent work [4], the CDW-EIS has been applied incorporating a Hartree-Fock description for the target bound and continuum eigenfunctions and different static models for the projectile-residual target ion interaction. A first exploration for the contribution of passive electron excitation was also presented there. Nevertheless this ensemble of experimental data has still no full explanation from a first principles theory.

The aim of the present work is to compare these experimental data with a CDW-EIS calculation accounting for the effect of the passive electron on the total projectile-residual target ion interaction. We go beyond the first order static Hartree-Fock potential by considering a second order correction represented by the dynamic polarization potential [5]. The influence of the polarization potentials in the description of electron-atom scattering experiments is well known [6]. Although for target residual ions in their ground state the dipole polarizability α_1 is not expected to be large (for example, for He$^+$, $\alpha_1 = 9/32$ au), the full interaction must be scaled by a factor Z_P^2. For highly charged projectiles, as considered here, the effect introduced by the polarization potential could be therefore very important. In fact, the experiments above are useful to test the influence of polarization potential in heavy projectile scattering. In the next section we briefly review the general theory and describe in more detail the effect of the passive electrons in the projectile- residual target ion interaction. In Sec. 3 we present our principal findings. The main conclusions are drawn in Sec 4. Atomic units were used throughout except where explicitly otherwise stated.

2. General theory

Let us consider the following effective three-body problem: the ionization of an active electron initially bound to its ionic core by the collision of a heavy projectile of charge Z_P and impact energy E_P. In the framework of the impact parameter formalism, the post version of the CDW-EIS transition amplitude reads

$$A_{if}^{+}(\rho) = -i \, \exp\left(-i \int_{-\infty}^{\infty} dt \; V_{P-RTI}(R)\right) \; a_{ij}^{+}(\rho) \tag{1}$$

where a_{ij}^{+} represents the standard post CDW-EIS electronic amplitude, ρ is the impact parameter and V_{P-RTI} is the full electrostatic interaction between the projectile and the residual target ion.

In this work, we approximate the full interaction V_{P-RTI} between the projectile and the residual target interaction by an effective second order two-body potential. More specifically, we consider that during the process, the projectile scatters elastically off the potential $V_{P-RTI} = V_{P-RTI}^{(1)} + V_{P-RTI}^{(2)}$ where the first order static potential is given by [7]

$$V_{P-RTI}^{(1)} = \frac{Z_P Z_T}{R} - \frac{Z_P}{R}\left[1 - (1 + Z_T R)\exp\left(-2 Z_T R\right)\right], \tag{2}$$

and the second order polarization potential is represented by [6]

$$V_{P-RTI}^{(2)} = -\frac{\alpha_1 Z_P^2}{2} \frac{R^2}{\left(R^2 + d^2\right)^2} - \frac{\alpha_2 Z_P^2}{2} \frac{R^3}{\left(R^2 + d^2\right)^5}. \tag{3}$$

The expression for $V_{P-RTI}^{(1)}$ is obtained with a hydrogenic orbital of charge Z_T and has the expected short-range and long-range Coulomb charges $Z_P Z_T$, $Z_P(Z_T - 1)$, respectively. On the other hand, in $V_{P-RTI}^{(2)}$, α_1 and α_2 are *statical* dipole and quadrupole polarizabilities, and d represents an effective distance beyond which the potential takes its long-range behavior $V_{P-RTI}^{(2)} \rightarrow -\alpha_1 Z_P^2/2R^4 - \alpha_2 Z_P^2/2R^6$. A formula for d was obtained in [6, 5] as $d = 3v/8\Delta$, where Δ is the mean excitation energy of the residual target ion. In [8], Δ was obtained in such a way that total inelastic cross sections are given exactly in the Born approximation up to orders v^{-4}. A model polarization potential like (3) was used in the past to describe intermediate and high energy elastic collisions between electrons and atoms [6]. However, we have to observe that the main contribution of the polarization potential to elastic electron-atom scattering goes to the small deflection angles, where the transfer momentum of the electron is also very small. In that situation it is reasonable to consider the static values for the dipole and the quadrupole polarizabilities and for the mean excitation energy. But in collisions by heavy ions such as Au^{53+}, the relevant deflection angles may involve a momentum transfer as large as a few atomic units. Therefore, it is necessary to find proper *dynamical* values for α_1, α_2 and Δ depending on the modulus of the momentum transfer q. We can accomplish this by formulating a generalization for the mean excitation energy as

$$\Delta(q) = \exp\left[L(-1,q)/S(-1,q)\right]/2, \tag{4}$$

where $L(-1,q), S(-1,q)$ are the generalized oscillator and optical strengths given by Inokuti [9] for Hydrogen atoms. Following [5], we express α_1, α_2 as derived quantities of $\Delta(q)$ as $\alpha_1 = 2/Z_T^2\Delta(q)$, $\alpha_2 = 6\ d^2\alpha_1$.

3. Results

We consider the helium single ionization experimental results that have been recently reported in a strongly non-perturbative regime at $Z_P/v = 4.4$ corresponding to 3.6 MeV/amu Au^{53+} ions impact [1]. In figure 1 we compare the experimental DDCS with the CDW-EIS theories which take into account the effects of the passive electron through different projectile-residual target ion potentials. In solid line, we show the CDW-EIS theory with first order static and second order polarization potential $V^{(1)}_{P-RTI} + V^{(2)}_{P-RTI}$. In dashed line, the CDW-EIS theory with static $V^{(1)}_{P-RTI}$ first order potential, and in dotted line the CDW-EIS theory with a ionic Coulomb

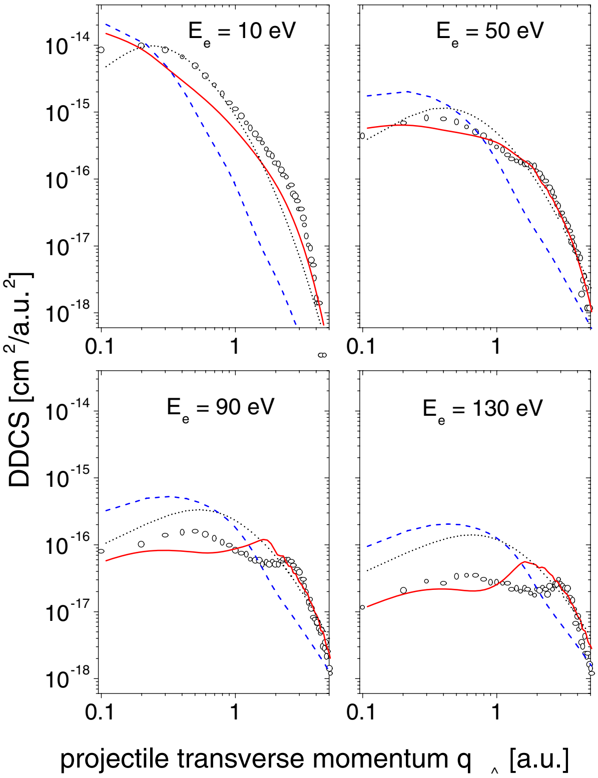

Figure 1. DDCS as a function of the transverse projectile momentum transfer$q_\perp$ at fixed electron energies for single ionization of He by 3.6 MeV/amu Au^{53+} ions. Symbols, experimental data from [1]. Solid line, CDW-EIS theory with $V^{(1)}_{P-RTI} + V^{(2)}_{P-RTI}$. Dashed line, CDW-EIS theory with $V^{(1)}_{P-RTI}$. Dotted line, CDW-EIS theory with effective charge $Z_T = 1.35$.

effective charge $Z_T = 1.35$. The doubly differential cross sections (DDCS) $\mathrm{d}^2\sigma/(\mathrm{d}q_\perp \mathrm{d}E_e)$ are displayed as a function of the projectile transverse momentum transfer $q_\perp$ and for specific electron energies E_e. The data show a clear transition from the distant ionizing collision (photon like) for low electron energies towards the binary encounter for higher electron energies. In fact, for the latter the DDCS exhibit a characteristic peak at a transverse momentum transfer equal to the momentum of the ejected electron $q_\perp \sim \sqrt{2E_e}$. We observe that although the simplest model where the full projectile-residual target ion interaction is represented by an effective two-body Coulomb potential of charge $Z_T = 1.35$ does not describe the binary peak, it gives an overall reasonable agreement with the experimental data scale except for high electron energies and low to intermediate projectile transverse momentum transfer where the theoretical calculations overestimate the experiments in almost one order of magnitude. Surprisingly, the more sophisticated first order static potential $V^{(1)}_{P-RTI}$ gives a worse agreement with the data than the effective charge model. It overestimates the DDCS at low momentum transfer and underestimates it at high momentum transfer. The first defect is increased, while the second one is reduced for higher electron energies. As noted in [4], the first order static potential gives an almost identical DDCS than the obtained with an effective charge $Z_T = 1$ (not shown in the figure) suggesting that the DDCS is influenced mostly by the long-range part of the interaction. Finally, we consider the contribution of both the first order static plus the second order polarization potential $V^{(1)}_{P-RTI}+V^{(2)}_{P-RTI}$. Our preliminary results show that the inclusion of $V^{(2)}_{P-RTI}$ improves the comparison with the experiments at low and intermediate $q_\perp$ and show the bump at higher transverse momentum transfer reproducing the double hump observed structure.

4. Conclusions

In this paper, a theoretical attempt to account for the influence of the non-active electron on projectile scattering related cross sections is presented. This has been accomplished by considering both a first order static potential and a second order polarization potential. For highly charged ions the second order potential scales as Z_P^2 and therefore its influence could be noticeable. The comparison of our results with the experiments gives a better agreement than with others models for the interaction between the projectile and residual target, given support to the explanation of the observed cross section by second order effects in the projectile scattering.

Acknowledgments

This work has been partially supported by the Consejo Nacional de Investigaciones Científicas y Técnicas CONICET (Grants PIP 583, 595, and 5831), and the Agencia Nacional de Promoción Científica y Tecnológicas ANPCYT (Grants 03-12567, 03-20548 and 04-26356), Argentina.

References

[1] Moshammer R, Perumal A N, Schulz M, Rodríguez V D, Kollmus H, Mann R, Hagman S and Ullrich J 2001 *Phys. Rev. Lett.* **87** 223201
[2] Schulz M, Moshammer R, Perumal A N and Ullrich J 2002 *J. Phys.* B **35** L161
[3] Rodríguez 2003 V D *Nuc. Instrum. Methods* B **205** 498
[4] Fainstein P D and Gulás L 2005 *J. Phys.* B **38** 317
[5] Byron F W, Joachain C J 1974, *Phys. Rev.* A **9** 2559
[6] Jhanwar B L, Khare S P and Kumar Jr A 1978 *J. Phys.* B **11** 887
[7] Rivarola R D, Piacentini R D, Salin A and Dz Belkic 1980 *J. Phys.* B **13** 2601
[8] Bonham R A 1974 *Phys. Rev.* A **9** 2559
[9] Inokuti M 1971 *Rev. Mod. Phys.* **43** 297