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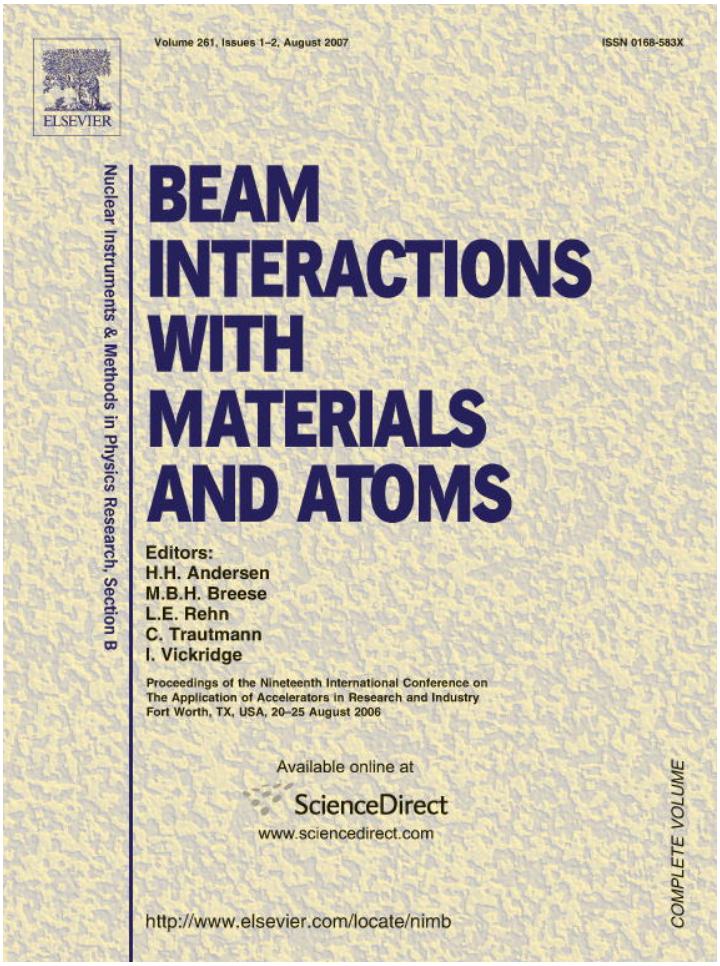

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CDW theoretical description of the single ionization of argon by positron and electron impact

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Abstract

In this work, we consider the single ionization of Ar by 200 eV positron and electron impact. The quantum mechanical continuum distorted wave (CDW) model is used in the one-active electron approximation. Parametrizations of Hartree–Fock potentials by Garvey et al. are used to represent the interaction of the light particles with the Ar^+ ion. The post collisional interaction (PCI) between the emitted electron and the receding projectile is naturally considered by the present model. Comparison with recent experimental data for very asymmetric geometries is made. The role of the PCI is studied by analyzing the differences in the angular distributions for positron and electron impact predicted by the CDW model and the first Born approximation.
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1. Introduction

Single ionization of atoms by light particle impact has been a topic subjected to wide interest from both the experimental and theoretical side. The first fully differential cross-sections (FDCS) were measured in 1969 [1] and considered the He target and very asymmetric collisions. Initial theoretical descriptions were based on perturbative methods like the first Born approximation (FBA) in which the projectile is assumed to have no influence neither on the bound electron in the initial state nor in the emitted electron trajectory in the final state. Further developments like the second-Born approximation or eikonal–Born series were developed in order to improve the FBA results (see [2] for a review on these methods).

During the 1980s, the experimental advances in the field pushed theoreticians to improve the available models. Besides FDCS measured for He, new data appeared for Ar targets [3,4]. A new theoretical description was developed by representing the three-body-final state of the collision by means of the product of three Coulomb waves. This wave function is usually referred in the literature as CDW, 3C or BBK [5,6] and being mass-independent has been widely used over the years in calculations also for ion–atom, electron–atom collisions and photo-double-ionization processes [5–8]. This wave function is an asymptotic solution to the three-body Hamiltonian and entirely considers the interparticle interactions. The main limitation of the model, in this sense, is that it neglects the non-orthogonal kinetic energy terms that take into account the influence of the third particle in the dynamics of each pair of particles. Initial studies were carried out by employing a Born initial state, resulting in a clear improvement over the FBA for intermediate collision energies [6]. For impact energies below 100 eV, the predictions of the Born-CDW depart from the experimental data due to the lack of initial state correlation.

In 1998, Jones and Madison showed that the CDW-EIS approximation which includes the initial state correlation

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through the product of two eikonal functions provides a good description of electron hydrogen collisions for impact energies as low as 54 eV [9]. This model was initially developed by Crothers and McCaan for ion–atom collisions [10] and was successfully extended to the light particle impact case. For the intermediate impact energy range, (>150 eV), on the other hand, the CDW-EIS results were close to the Born-CDW results over the set of configurations measured by Ehrhardt et al. [11,12]. This showed that the initial state correlation only plays a role as the impact energy decreases.

As more data became available for the near-threshold region where perturbative methods are outside their validity range, non-perturbative theories were developed like the convergent close coupling (CCC) [13], and more recently the exterior complex scaling (ECS) [14] and the time dependent close coupling (TDCC) [15]. These powerful numerical methods reached an unprecedented level of agreement with available experimental data. However, they have been mainly applied for the hydrogen target and only recently have been extended to other light targets and molecules [16,17].

Multielectronic targets like those represented by the noble gases have been so far tackled by means of the distorted wave Born approximation (DWBA) and the DWBA + R-matrix [18,19] model. The multielectronic targets represent a completely different challenge since besides the wave functions employed, an additional problem is the choice of the effective potentials in the one-active electron representation and how the exchange terms are treated. In many cases, the agreement of these theoretical models with available experimental data and between themselves has only been qualitative (for Ar see [19–21]).

In this paper, we present theoretical results obtained with a Born-CDW model for 200 eV positron and electron single ionization of Ar(3p) under very asymmetric geometries. We compare these theoretical results with recent experimental data and we discuss the role of the projectile charge sign in the FDCS. To represent the interaction between the projectile as well as the emitted electron with the parent ion, we have chosen the Garvey parametrization [22] which mainly consists in fits of Hartree–Fock potentials. These potentials are supposed to include or model the exchange terms up to a certain extent.

The influence of the post collisional interaction (PCI) on the FDCS is discussed by examining the ratios of the FDCS to those provided by the FBA. Finally, conclusions are drawn and possible extensions of the present work summarized. Atomic units are used throughout this work unless explicitly stated.

2. Theory and results

The FDCS for positron impact (and electron impact if asymmetric geometries are considered and the exchange between the projectile and the emitted electron can be neglected) is given by,

$$\frac{\mathrm{d}^5\sigma}{\mathrm{d}E_1\mathrm{d}\Omega_1\mathrm{d}\Omega_2} = (2\pi)^4\frac{k_1k_2}{k_0}\left|\left\langle \Psi_\mathrm{f}^-\middle|W_\mathrm{i}\middle|\Phi_\mathrm{i}\right\rangle\right|^2.$$

Here, $k_{0,1,2}$ denote the incident momentum, the projectile final momentum and the emitted electron momentum, respectively. In our case, we use a Born initial state and we consider $\mathbf{r}_{1,2}$ the coordinates of the projectile and the emitted electron with respect to the nucleus. The initial and final states as well as the perturbation are given by

$$W_\mathrm{i} = V(r_1) \pm \frac{1}{r_{12}},$$
$$\langle \mathbf{r}_1\mathbf{r}_2|\Phi_\mathrm{i}\rangle = (2\pi)^{-3/2}\mathrm{e}^{\mathrm{i}\mathbf{k}_0\cdot\mathbf{r}_1}\varphi_\mathrm{i}(\mathbf{r}_2),$$
$$\left\langle \mathbf{r}_1\mathbf{r}_2\middle|\Psi_\mathrm{f}^-\right\rangle = \chi_{\mathbf{k}_1}(\mathbf{r}_1)\chi_{\mathbf{k}_2}(\mathbf{r}_2)N_{C^1}^-F_1[\mathrm{i}\alpha_{12}, 1, -\mathrm{i}k_{12}r_{12} - \mathrm{i}\mathbf{k}_{12}\cdot\mathbf{r}_{12}].$$

The χ wave functions are two-body problem solutions for Garvey central potentials and the Kummer function represents the projectile-emitted electron interaction which is Coulomb attractive or repulsive according to the projectile nature. To evaluate the transition amplitude we use the Fourier transform technique [23], which leads to a 3D numerical integration. In the evaluation of the continuum–continuum transition we have used a cutoff factor $z_\mathrm{c} = 0.005$ a.u. and we have considered the infinite partial waves for the projectile–Ar^+ interaction by correcting Nordsieck-type integrals in the required number of partial waves until convergence to the Coulomb case was achieved.

In Fig. 1, we show the ratio of the FDCS calculated by the BCDW to that obtained within the FBA, for 200 eV positron and electron impact for different emission energies. The scattering angle has been set at 3.5° and we only include in the present analysis emission from the 3p shell.

It can be seen that the PCI provides different and well defined signatures on the FDCS depending on the projectile nature. For positron (electron) impact, the intensity in the vicinity of the momentum transfer vector is more (less) intense than that provided by the FBA. This is the region where a maximum is obtained in the FDCS and is usually called "binary peak" by analogy with the observations on hydrogen targets (binary collision between the projectile and the emitted electron). This would mean that for positrons as projectiles, the electronic emission in binary-like collisions is more likely than for electrons.

On the other hand, in the quasi-opposite direction to the momentum transfer vector the opposite behavior turns evident. This region which is dominated by the so called "recoil peak" (which for hydrogen target is usually associated to a second collision of the emitted electron with its parent ion) shows an increase (decrease) of intensity compared to the FBA for electron (positron) impact. Being repelled (attracted) by the projectile, the emitted electron maximizes (minimizes) the interaction with the parent ion compared to the FBA. The same trends seem to be present in the three cases under consideration.

In Fig. 2, we present the binary to recoil peak ratio as a function of the emission energy. The BCDW results for

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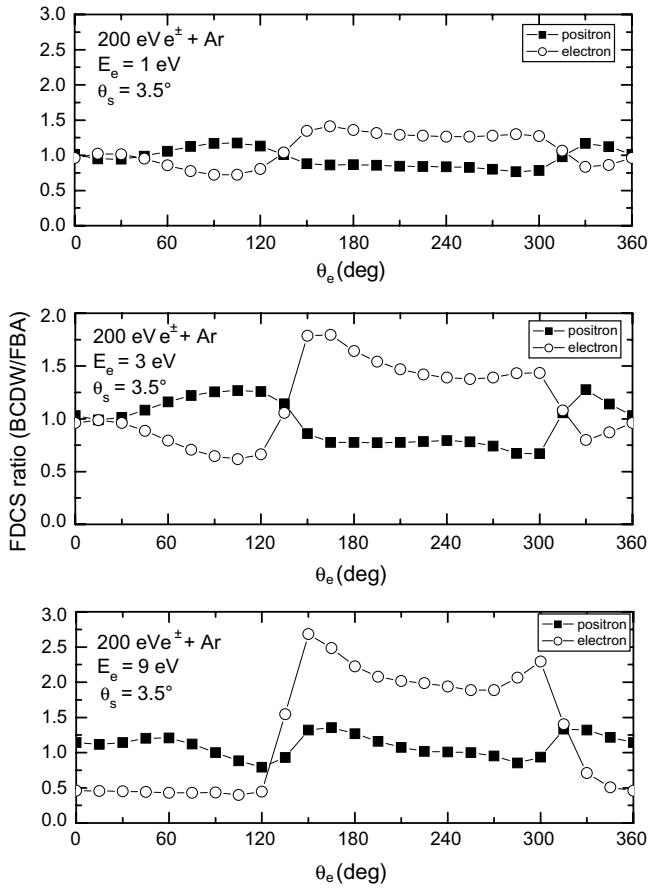

Fig. 1. FDCS ratios (BCDW/FBA) as a function of the emission angle θ_e for three different emission energies: 1 eV, 3 eV and 9 eV. The scattering angle of the projectile is in all cases 3.5°.

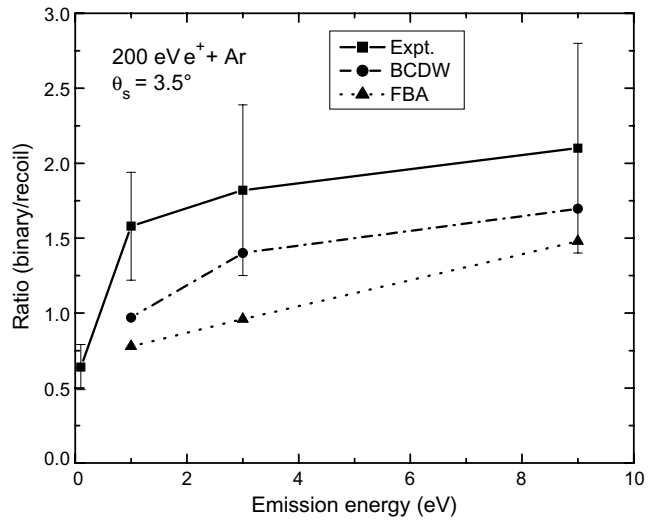

Fig. 2. Binary to recoil peak ratio for the emission energies here considered. The experimental data corresponds to de Lucio et al. [24].

positron impact as well as the FBA results are compared to the recent experimental data of de Lucio et al. [24,25]. Due to the large computation times, the theoretical data have not been convoluted over the reported experimental uncertainties [24]. It can be seen that for low emission energies (<1 eV) the experiment predicts the recoil peak to be more intense. As the emission energy increases, this situation reverses and in the considered energy range the binary is 1.5–2 times larger than the recoil peak. The BCDW theory lies within the error bars between the 3 eV and 9 eV cases but predicts a ratio of nearly unity at 1 eV, where the experiment lower limit is of about 1.2. The FBA on the other hand, lies outside the experimental error bars with the exception of the 9 eV case. This clearly shows the role that the PCI plays in the FDCS. Data for electron impact have not been presented yet for this particular configuration, but would be extremely useful to discern on the role the projectile charge sign plays in the binary to recoil ratio.

3. Conclusions

In this work, we have presented theoretical results concerning the single ionization of Ar(3p) by 200 eV light particle impact. By analyzing ratios of FDCS we have identified the main trends associated to the PCI according to the projectile nature.

Furthermore, we have compared recent measurements of the binary to recoil peaks ratio showing that the present BCDW theory is capable to predict the proper relative intensities between peaks in the energy range considered.

In this one-active electron representation, the interactions of the light particles with the Ar^+ ions have been represented by means of the Garvey parametrization which consists in fits of Hartree–Fock potentials and is supposed to include some information on the electronic exchange.

The validity of the present results to a more precise representation of the electronic exchange for the emitted electron with the other Ar electrons remains an open issue.

It would also be interesting to implement a more sophisticated theory, like the CDW-EIS approximation. That would help elucidate on the role played by the initial state correlation when considering multielectronic targets.

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References

[1] H. Ehrhardt, M. Schulz, T. Tekaat, K. Willmann, Phys. Rev. Lett. 22 (1969) 89.
[2] F.W. Byron Jr., C.J. Joachain, Phys. Rep. 179 (1989) 211.
[3] K. Jung, R. Muller-Fiedler, P. Schlemmer, H. Ehrhardt, H. Klar, J. Phys. B: At. Mol. Opt. Phys. 18 (1985) 2955.
[4] A. Lahmam-Bennani, H.F. Wellenstein, A. Duguetand, A. Daoud, Phys. Rev. A 30 (1984) 1511.
[5] C.R. Garibotti, J.E. Miraglia, Phys. Rev. A 21 (1980) 572.
[6] M. Brauner, J.S. Briggs, H. Klar, J. Phys. B: At. Mol. Opt. Phys. 22 (1989) 2265.

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[7] M. Brauner, J.S. Briggs, J.T. Broad, J. Phys. B: At. Mol. Opt. Phys. 24 (1981) 287.
[8] F. Maulbetsch, J.S. Briggs, J. Phys. B: At. Mol. Opt. Phys. 26 (1993) L647.
[9] S. Jones, D.H. Madison, Phys. Rev. Lett. 81 (1998) 2886.
[10] D.S.F. Crothers, J.F. MacCaan, J. Phys. B: At. Mol. Opt. Phys. 16 (1983) 3229.
[11] H. Ehrhardt, J. Röder, in: C.T. Whelan, H.R.J. Walters (Eds.), Coincidence Studies of Electron and Photon Impact Ionization, Plenum, New York, 1997, p. 1.
[12] H. Klar, A.C. Roy, P. Schlemmer, K. Jung, H. Ehrhardt, J. Phys. B: At. Mol. Opt. Phys. 20 (1987) 821.
[13] I. Bray, Phys. Rev. Lett. 89 (2002) 273201.
[14] T.N. Rescigno, M. Baertschy, W.A. Isaacs, X. Li, C.W. McCurdy, Science. 286 (1999) 2474.
[15] J. Colgan, M.S. Pindzola, F.J. Robicheaux, D.C. Griffin, M. Baertschy, Phys. Rev. A 65 (2002) 042721.
[16] M.S. Pindzola, F. Robicheaux, J. Colgan, J. Phys. B: At. Mol. Opt. Phys. 39 (2006) L127.
[17] S. Pindzola, F. Robicheaux, S.D. Loch, J. Colgan, Phys. Rev. A 73 (2006) 052706.
[18] J. Rasch, C.T. Whelan, R.J. Allan, S.P. Lucey, H.R.J. Walters, Phys. Rev. A 56 (1997) 1379.
[19] A. Prideaux, D.H. Madison, K. Bartschat, Phys. Rev. A 72 (2005) 032702.
[20] M.A. Haynes, B. Lohmann, Phys. Rev. A 64 (2001) 044701.
[21] M.A. Stevenson, B. Lohamnn, Phys. Rev. A 73 (2006) 020701, R.
[22] R.H. Garvey, C.H. Jackman, A.E.S. Green, Phys. Rev. A 12 (1975) 1144.
[23] M.A. Kornberg, J.E. Miraglia, Phys. Rev. A 48 (1993) 3714.
[24] O.G. de Lucio, J. Gavin, R.D. DuBois, Phys. Rev. Lett. 97 (2006) 243201.
[25] O. de Lucio et al., private communication.

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