J. Phys. B: At. Mol. Opt. Phys. **37** (2004) 2057–2066 PII: S0953-4075(04)73203-4

Influence of initial state distortion in ion–atom collisions

M F Ciappina[1], **W R Cravero**[1] **and C R Garibotti**[2]

[1] CONICET and Departamento de Física, Universidad Nacional del Sur, 8000 Bahía Blanca, Argentina
[2] CONICET and División Colisiones Atómicas, Centro Atómico Bariloche, 8400 Bariloche, Argentina

E-mail: ciappina@criba.edu.ar

Received 3 December 2003
Published 30 April 2004
Online at stacks.iop.org/JPhysB/37/2057
DOI: 10.1088/0953-4075/37/10/005

Abstract

We have studied the influence of initial state distortion in a single ionization by ion impact. We have taken a continuum distorted wave type distortion and by taking up to the first order in its asymptotic series expansion we build an eikonal-spherical distortion. In this way the influence of each term in the transition amplitude can be stated. This approximation can be considered an intermediate one between the eikonal initial state and the continuum distorted wave approaches for initial state distortion. We have computed doubly differential cross sections for helium ionization by protons and highly charged ions at high and intermediate impact energy. We have also discussed the contribution of the different terms in electron energy spectra, specially in the vicinity of ECC peak. Very good agreement is found with the available experimental data.

1. Introduction

The simplest model for single ionization process by ion impact involves a three particle system interacting through long range Coulomb potentials.

If intermediate to high energy ion–atom ionization is considered, the classical nature of the projectile and target nuclei can be safely assumed. This leaves us with the quantum motion of the active electron in the combined potential of two Coulomb centres in relative motion. The choice for the electron wavefunction associated with this motion is one of the main challenges for the evaluation of transition amplitudes at intermediate and high collision energies (McDowell and Coleman 1970).

Approximate wavefunctions for the continuum final state are usually obtained from the asymptotic condition in the Ω_0 region where the three particles are far away from one another. For three particles interacting through long range Coulomb potentials, the wavefunction is given as a product of plane waves and eikonal distortion factors (Rosenberg 1973). Distorted wave methods for collision processes make use of such wavefunctions so that the perturbation potential responsible for the electronic transition is a short range potential for which perturbative methods can be safely applied.

At intermediate and high energies, distorted wave theories have been used for the last 25 years. They provide a good overall picture for the ionization process in the presence of Coulomb potentials. Among these, continuum distorted wave (CDW) theory (Belkić 1978) and the continuum distorted wave–eikonal initial state (CDW-EIS) approximation (Crothers and McCann 1983) have probably been the most widely employed. In these models the Coulomb distortion in the electron–projectile coordinate is represented in the initial state by a Kummer type function and its asymptotic eikonal phase, respectively. In both cases, the final state wavefunction is written as the product of three two-body Coulomb wavefunctions, each corresponding to one interparticle relative position in the two-body energy shell.

Trying to describe the behaviour in the asymptotic regions Ω_{ij}, where two of the particles are close to one another and the third one is located far away, several authors have studied and analysed the effect of the distortion in the final state (Kunikeev 1998, 1999). In these works, three body wavefunctions have been proposed in which the electron–target nucleus relative momentum is dependent on the position (or momentum) of the impinging projectile. The calculation of transition amplitudes with these kinds of functions is not an easy task because it involves a six-dimensional coupled integral (Alt and Mukhamedzhanov 1993, Berakdar 1996). Moreover, if one has to evaluate doubly differential cross sections (DDCS), two additional integrals are needed, with the corresponding computational cost.

Our group has developed several approaches to take into account the correlation effects in the electronic final wavefunctions (Gasaneo *et al* 1997, Colavecchia *et al* 1998). When the same approach is used for the initial state, it leads to a picture in which the electronic state becomes metastable due to the presence of the incident projectile (Garibotti *et al* 2000, Ciappina *et al* 2002). We have also analysed the sensibility of the transition amplitude to the final and initial states for different versions (post and prior) finding that the post version is less sensitive to the final wavefunction (Ciappina *et al* 2003). Jones and Madison (2000) have studied the influence of the initial state wavefunctions for ionization of hydrogen atoms by fast electrons. They have demonstrated the importance of the initial *two centre effect* in the proper description of collision dynamics and proposed an initial *two centre* wavefunction that takes into account electron correlation effects.

The CDW approximation is known to give better results for highly charged ions than CDW-EIS (Gulyás and Fainstein 1998). However, the lack of proper normalization associated with CDW initial state leads to a large overestimation of experimental data at intermediate energies and large projectile charge (Crothers 1982), and in this approximation it is not easy to identify the different physical mechanisms implicit in the full CDW distortion. In this paper, we analyse the entrance channel distortion by expanding it in an asymptotic series expansion. Our aim is to understand the physical picture provided by the different series terms. In this way it may be possible to suggest a way to improve the distortion, in particular, for highly charged projectiles. The paper is organized as follows: in section 2 we describe the theoretical framework. In section 3, we calculate DDCS using this approximation and compare the obtained results with other distorted wave methods and the experimental data. Finally we state our main conclusions. We use atomic units unless otherwise stated.

2. Theory

DDCSs for ionization are defined in the impact parameter approximation by

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}E\,\mathrm{d}\Omega} = \int |a_{i,f}(b)|^2\,\mathrm{d}b \tag{1}$$

where b is the projectile impact parameter. The transition amplitude $a_{i,f}(b)$ is given in the post version by

$$a_{i,f}(b) = -\mathrm{i}\int_{-\infty}^{+\infty}\mathrm{d}t\big\langle\Phi_f^-\big|\left(H_{\mathrm{el}} - \mathrm{i}\frac{\partial}{\partial t}\right)^{\dagger}\big|\Psi_i^+\big\rangle \tag{2}$$

where Ψ_i^+ represents the exact solution wavefunction for H_{el} with initial conditions

$$\lim_{t\to-\infty}\Psi_i^+ = \Phi_i^+. \tag{3}$$

In the same way, we define the prior transition amplitude as

$$a_{i,f}(b) = -\mathrm{i}\int_{-\infty}^{+\infty}\mathrm{d}t\big\langle\Psi_f^-\big|\left(H_{\mathrm{el}} - \mathrm{i}\frac{\partial}{\partial t}\right)\big|\Phi_i^+\big\rangle \tag{4}$$

with Ψ_f^- being the exact solution wavefunction for H_{el} with final conditions

$$\lim_{t\to+\infty}\Psi_f^- = \Phi_f^-. \tag{5}$$

As for the electronic Hamiltonian H_{el} , it reads

$$H_{\mathrm{el}} = -\frac{1}{2}\nabla_r^2 + V_T(r_T) - \frac{Z_P}{r_P} + \frac{Z_P Z_T}{R}. \tag{6}$$

For hydrogenic targets we have

$$V_T = -\frac{Z_T}{r_T} \tag{7}$$

whereas for multielectronic targets we have to use model potentials (HF) or Coulomb potentials with effective charges to take into account the passive electron screening. In using distorted wave methods, we use the long range distortion potential to solve a part of the total Hamiltonian exactly, so that the potential we left as perturbation is a short range potential where a rapid convergence of the perturbative approach can be achieved (Dodd and Greider 1966).

The usual procedure is to define distortion potentials U_i and U_f, such that

$$H_{\mathrm{el}} = H_i + U_i + W_i \tag{8}$$

and

$$H_{\mathrm{el}} = H_f + U_f + W_f \tag{9}$$

and find *distorted* wavefunctions that verify

$$\left(H_i + U_i - \mathrm{i}\frac{\partial}{\partial t}\right)\chi_{\mathrm{i}}^+ = 0 \tag{10}$$

and

$$\left(H_f + U_f - \mathrm{i}\frac{\partial}{\partial t}\right)\chi_f^- = 0 \tag{11}$$

respectively. Then we find the transition amplitudes in the distorted wave approximation (DW), in its post

$$a_{i,f}^{+\mathrm{DW}}(b) = -\mathrm{i}\int_{-\infty}^{+\infty}\mathrm{d}t\big\langle\chi_f^-\big|W_f^{\dagger}\big|\Psi_i^+\big\rangle \tag{12}$$

and prior versions

$$a_{i,f}^{-\mathrm{DW}}(b) = -\mathrm{i}\int_{-\infty}^{+\infty} \mathrm{d}t \langle \Psi_f^- | W_i | \chi_i^+ \rangle. \tag{13}$$

Selecting different wavefunctions and distortion potentials several approximations are obtained for the transition amplitude.

For the final state we will use the CDW approximation

$$\chi_f^{-\mathrm{CDW}} = {}^{B1}\Phi_f^- \times L_f^{-\mathrm{CDW}} \tag{14}$$

with distortion

$$L_f^{-\mathrm{CDW}} = \exp\left(-\mathrm{i}\frac{Z_P Z_T}{v_P} \ln\left(v_P R + v_P^2 t\right)\right) N^*(\zeta)\, {}_1F_1(-\mathrm{i}\zeta; 1; -\mathrm{i}k_P r_P - \mathrm{i}\mathbf{k}_P \mathbf{r}_P) \tag{15}$$

whereas for the final perturbation potential we have

$$W_f^{\mathrm{CDW}} \chi_f^{\mathrm{CDW}} = {}^{B1}\Phi_f^- \left(\vec{\nabla}_{\mathbf{r}_T} \ln {}_1F_1(-\mathrm{i}\xi; 1; -\mathrm{i}k_T r_T - \mathbf{k}_T \mathbf{r}_T) \cdot \vec{\nabla}_{\mathbf{r}_P} L_f^{-\mathrm{CDW}}\right).$$

${}^{B1}\Phi_i^+$ and ${}^{B1}\Phi_f^-$ are the usual first Born approximation (FBA) wavefunctions for the initial and final states, respectively, with $\zeta = \frac{Z_P}{k_P}$ and $\xi = \frac{Z_T}{k_T}$ being the Sommerfeld parameters.

For the initial state, CDW approximation is defined by

$$\chi_i^{+\mathrm{CDW}} = {}^{B1}\Phi_i^+ \times L_i^{+\mathrm{CDW}} \tag{16}$$

with

$$L_i^{+\mathrm{CDW}} = N(\nu)\, {}_1F_1(\mathrm{i}\nu; 1; \mathrm{i}v_P r_P + \mathrm{i}\mathbf{v}_P \mathbf{r}_P) \tag{17}$$

$$\nu = \frac{Z_P}{v_P} \tag{18}$$

where the perturbation potential is defined by

$$W_i^{\mathrm{CDW}} \chi_i^{+\mathrm{CDW}} = {}^{B1}\Phi_i^+ \left(\vec{\nabla}_{\mathbf{r}_T} \ln \varphi(r_T) \cdot \vec{\nabla}_{\mathbf{r}_P} L_i^{+\mathrm{CDW}}\right). \tag{19}$$

Let us rewrite the distortion using parabolic coordinates

$$\eta_P = r_P + \widehat{\mathbf{v}}_P \cdot \mathbf{r}_P.$$

So that the initial distortion can be written as

$$L_i^{+\mathrm{CDW}} = N(\nu)\, {}_1F_1(\mathrm{i}\nu; 1; \mathrm{i}v_P\, \eta_P) \tag{20}$$

where ${}_1F_1$ is the usual confluent hypergeometric function (Abramowitz and Stegun 1965). Now if we take its asymptotic series expansion and keep up to first order, we get

$$L_i^{+\mathrm{SEIS}} = \mathrm{e}^{(-\mathrm{i}\nu \ln v_P \eta_P)} - \mathrm{i}\frac{\Gamma(1-\mathrm{i}\nu)}{\Gamma(\mathrm{i}\nu)}\, \mathrm{e}^{(\mathrm{i}v_P \eta_P)}\, \mathrm{e}^{(-(1-\mathrm{i}\nu)\ln v_P \eta_P)}. \tag{21}$$

Here we see that the electron projectile distortion in this approximation amounts to a no-scattering eikonal term (the same distortion used in the CDW-EIS approximation) plus a spherical wave term which takes into account a single Coulomb scattering event. In the next section, we will use this eikonal spherical wave distortion within a CDW-type approximation for the calculation of helium ionization by ion impact.

3. Cross sections

Let us incorporate the distortion derived in the previous section in a CDW-type theory in its post version, i.e.,

$$T_{if}^{\mathrm{SEIS}} = \left\langle \chi_f^- \middle| V_f^{\mathrm{CDW}} \middle| \chi_i^{+\mathrm{SEIS}} \right\rangle \tag{22}$$

where V_f^{CDW} is the usual non-orthogonal electronic kinetic energy, and

$$\chi_i^{+\mathrm{SEIS}} = {}^{B1}\Phi_i^+ \times L_i^{+\mathrm{SEIS}}. \tag{23}$$

After the usual factorization, one ends with the product of an integral in the electron–target coordinate, which is identical to the corresponding one in the CDW-EIS approximation, and an integral in the electron–projectile coordinate, i.e.

$$T_{if} = \mathbf{J}^T \cdot \mathbf{J}^P$$

with

$$\mathbf{J}^T = \langle \chi_T | \nabla_{r_T} | \varphi_i \rangle \qquad \mathbf{J}^P = \langle \chi_P | \nabla_{r_P} | \mathcal{E}\mathbf{v}_P \rangle + \langle \chi_P | \nabla_{r_P} | \mathcal{E}'\mathbf{v}_P \rangle$$

where

$$\mathcal{E}\mathbf{v}_P(\mathbf{r}_P) = \mathrm{e}^{(-\mathrm{i}\nu \ln v_P \eta_P)} \qquad \mathcal{E}'\mathbf{v}_P(\mathbf{r}_P) = \mathrm{e}^{(-(1-\mathrm{i}\nu) \ln v_P \eta_P)}.$$

DDCSs in the electron energy and emission angle are as usual given by

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}E\,\mathrm{d}\Omega} = (2\pi)^4 \frac{k_T}{v} \int |T_{if}|^2 \,\mathrm{d}\Omega_P.$$

As we are interested in looking for different contributions to the cross section due to each part of the electron–projectile distortion, we write $|T_{if}|^2$ as

$$|T_{if}|^2 = \left|T_{if}^{\mathrm{EIS}}\right|^2 + \left|T_{if}^{\mathrm{SPH}}\right|^2 + 2\,\mathrm{Re}\, T_{if}^{\mathrm{EIS}} \cdot \left(T_{if}^{\mathrm{SPH}}\right)^*.$$

So basically we get this new approximation by adding to the CDW-EIS transition amplitude a term that corresponds to the eikonal spherical wave distortion, i.e. T_{if}^{SPH}. We name this theory CDW-SEIS (continuum distorted wave–spherical eikonal initial state). In the next section we show the results obtained for ion-impact ionization of helium using this approximation.

4. Results

We have performed DDCS calculations for helium single ionization with the theory outlined in the previous sections. In all our calculations we have employed Roothan–Hartree–Fock wavefunctions for the helium target initial bound state (Clemente and Roetti 1974). In figure 1, results for helium ionization by 1 MeV amu^{-1} H^+ and F^{9+} impact are displayed (Lee *et al* 1990). Very good agreement is found for the CDW-SEIS approximation, particularly for the highly charged F^{9+} projectile. Since CDW-SEIS can be thought of as an intermediate approximation between CDW and CDW-EIS, this behaviour could be expected, since pure CDW calculations also show a generally better behaviour as the projectile charge increases (Gulyás and Fainstein 1998). These results may suggest that a two-term expansion for the CDW distortion could be enough to retain its behaviour. Figure 2 shows similar calculations at intermediate energy, also showing a very good agreement (Bernardi *et al* 1989). Angular calculations (figures 3 and 4) (Stolterfoht *et al* 1995) also show an overall better agreement with experiments than CDW-EIS.

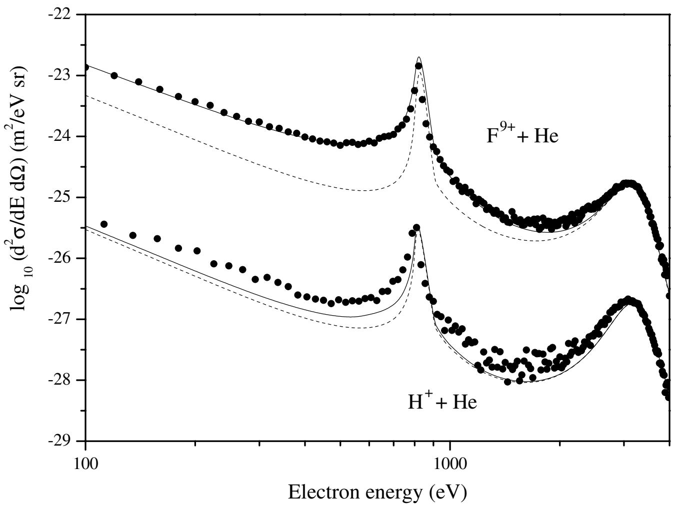

Figure 1. DDCS for single ionization of helium by 1.5 MeV amu^{-1} H^+ and F^{+9} impact in the forward direction. CDW-SEIS, full curve; CDW-EIS, dashed curve; experimental data (Lee *et al* 1990), solid circles.

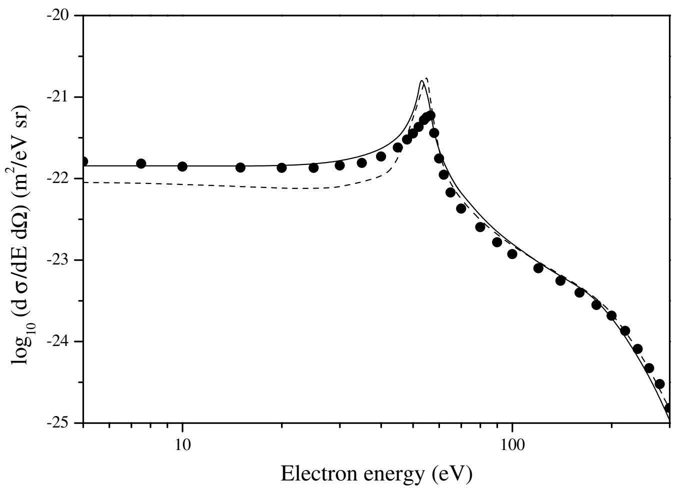

Figure 2. DDCS for single ionization of helium by 100 keV amu^{-1} H^+ impact in the forward direction. CDW-SEIS, full curve; CDW-EIS, dashed curve; experimental data (Bernardi *et al* 1989), circles.

Unlike pure CDW calculations, with CDW-SEIS the influence of the different terms in the distortion expansion can be studied. Figures 5 and 6 show the different contributions to the cross section from the different terms. It can be seen that the relative contributions change rather abruptly at the projectile velocity for forward emission. At emission velocities greater than v_P, CDW-EIS calculations (i.e. the first term in our expansion) seem to be enough to describe the experimental data. In fact, the simple Coulomb Born approximation is also a good approximation here, which is reasonable given that the binary encounter (BE) and the electron capture to continuum (ECC) mechanisms are essentially independent. However, the so-called

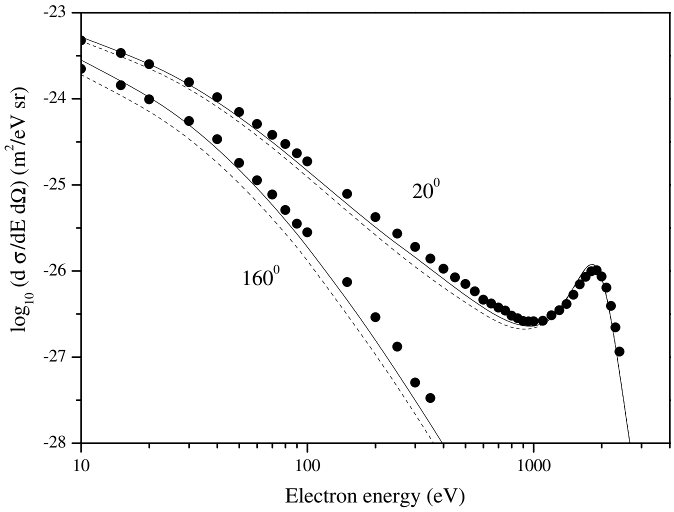

Figure 3. DDCS for single ionization of helium by 1 MeV amu^{-1} H^+ impact, for 20° and 160° emission angle. CDW-SEIS, full curve; CDW-EIS, dashed curve; experimental data (Stolterfoht *et al* 1995), circles.

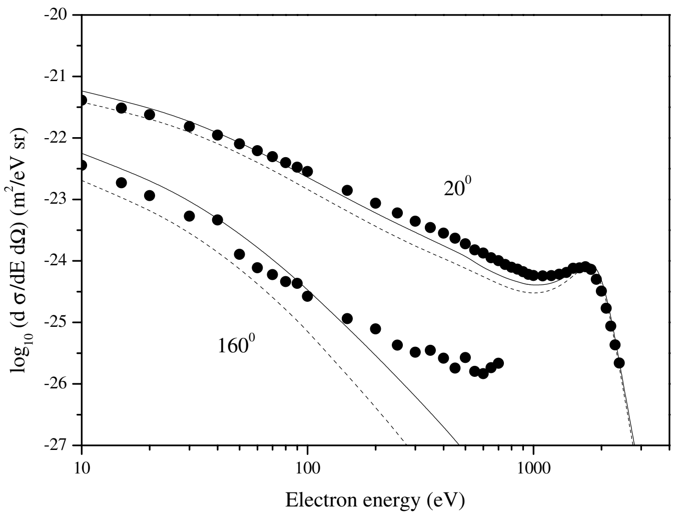

Figure 4. Same as in figure 3, for 1 MeV amu^{-1} O^{8+}.

two centre ridge between the ECC and the soft electron (SE) peaks is not so easy to describe, suggesting a complicated mechanism of emission (Pedersen *et al* 1990). Miraglia and Macek (1991) also got good agreement in this region with the impulse approximation (IA) by changing the initial projectile–electron distortion. On the other hand, it is symptomatic that by refining the final state (Colavecchia *et al* 1998) no equivalent improvement has been achieved. Within the CDW-SEIS approximation, it is in this region that the spherical eikonal term becomes more important. As projectile charge increases, the spherical eikonal term becomes almost dominant and explains the agreement between CDW-SEIS and data for emission velocities lower than v_P. While the physical picture is far from complete, the obtained results suggest,

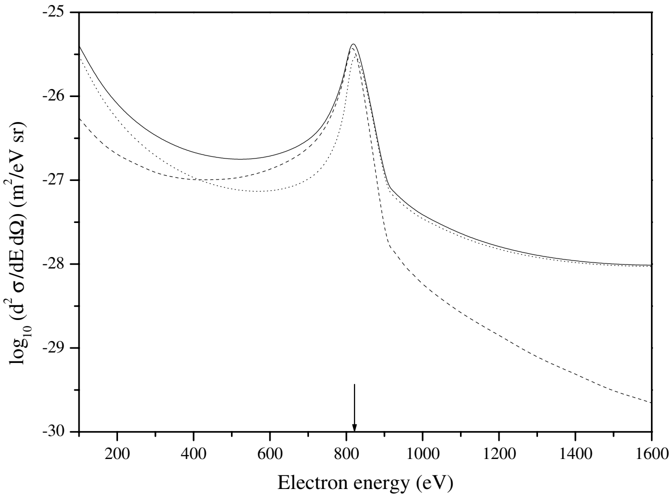

Figure 5. Contribution to DDCS for the different terms of CDW-SEIS theory for 1.5 MeV amu^{-1} H^+ impinging over He in the forward direction. CDW-SEIS (all terms), full curve; CDW-EIS term, dotted curve; spherical wave term, dashed curve. The arrow indicates the position of the ECC divergence.

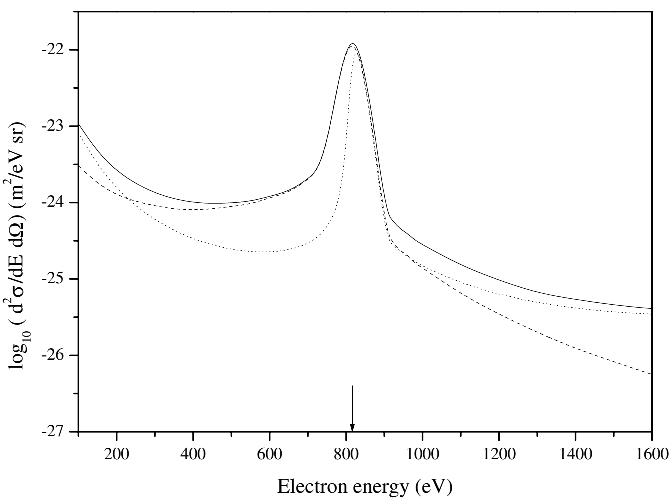

Figure 6. Same as in figure 5, for 1.5 MeV amu^{-1} F^{9+}.

in our opinion, that a different mechanism for the emission of the ionized electron may be important for that lower energy region.

If we see the collision event from the projectile reference frame, we can see the target active electron impinging the incident projectile. The long range nature of the projectile–electron potential implies an infinite number of collisions off the projectile. Even when there is not a one-to-one relation between these scattering events and the different terms in the distortion expansion, certainly the spherical-eikonal term takes into account at least one of these scattering events. When the transition amplitude is calculated, the term corresponding to the spherical eikonal term is to be added to the no-scattering one (CDW-EIS). Small impact parameters with higher momentum transfer collisions dominate for electrons ejected with velocities higher than the projectile, and therefore single binary encounter mechanisms prevail. In this region, the term corresponding to no-scattering in the initial state (CDW-EIS) suffices to explain the experimental results. On the other hand, the spherical-eikonal term is expected to become increasingly important for a large impact parameter and a low momentum transfer. This is the case for electrons ejected in the forward direction with velocities lower than the projectile's.

5. Conclusions

We have studied the influence of initial state distortion in a single ionization by ion impact. We have considered a continuum distorted wave type distortion and by taking a first order in its series expansion we have built an eikonal-spherical distortion. In this way the influence of each term can be stated. This approximation can be considered as an intermediate one between CDW-EIS and the pure CDW approaches for initial state distortion. We have computed DDCSs for helium ionization by protons and highly charged ions at high and intermediate impact energy. Very good agreement is found with the available experimental data. By writing the distortion as an asymptotic expansion, it was possible to establish the relative importance of the different terms. While it is necessary to carry out more detailed analysis on the role that various emission mechanisms play in the different expansion terms, it certainly looks as if a two term expansion is enough to retain much of the full CDW distortion behaviour. We have found that zero scattering and single scattering orders contribute differently in different emission regimes. The single scattering term is particularly important for low energy and the forward direction.

Acknowledgments

This work has been partially supported by ANPCyT Argentina under PICT99/03/06249 and Universidad Nacional del Sur, Argentina, under PGI 24/F026 and 24/F027.

References

Abramowitz M and Stegun I A 1965 *Handbook of Mathematical Functions* (New York: Dover)
Alt E O and Mukhamedzhanov A M 1993 *Phys. Rev.* A **47** 2004
Belkić Dž 1978 *J. Phys. B: At. Mol. Phys.* **11** 3529
Berakdar J 1996 *Phys. Rev.* A **53** 2314
Bernardi G C, Suárez S, Fainstein P D, Garibotti C R, Meckbach W and Focke P 1989 *Phys. Rev.* A **40** 6863
Ciappina M F, Cravero W R and Garibotti C R 2003 *J. Phys. B: At. Mol. Opt. Phys.* **36** 3775
Ciappina M F, Otranto S and Garibotti C R 2002 *Phys. Rev.* A **62** 052711
Clemente E and Roetti C 1974 *At. Data. Nucl. Data Tables* **14** 177
Colavecchia F D, Gasaneo G and Garibotti C R 1998 *Phys. Rev.* A **58** 2926
Crothers D S F 1982 *J. Phys. B: At. Mol. Phys.* **15** 2061
Crothers D S F and McCann J F 1983 *J. Phys. B: At. Mol. Phys.* **16** 3229
Dodd L D and Greider K R 1966 *Phys. Rev.* **146** 657
Garibotti C R, Gasaneo G and Colavecchia F D 2000 *Phys. Rev.* A **62** 022710
Gasaneo G, Colavecchia F D, Garibotti C R, Macri P and Miraglia J E 1997 *Phys. Rev.* A **55** 2809
Gulyás L and Fainstein P D 1998 *J. Phys. B: At. Mol. Opt. Phys.* **31** 3297
Jones S and Madison D H 2000 *Phys. Rev.* A **62** 042701
Kunikeev Sh D 1998 *J. Phys. B: At. Mol. Opt. Phys.* **31** 2649
Kunikeev Sh D 1999 *J. Phys. A: Math. Gen.* **32** 677
Lee D H, Richard P, Zouros T J M, Sanders J M, Shinpaugh J L and Hidmi H 1990 *Phys. Rev.* A **41** 4816

McDowell M R C and Coleman J P 1970 *Introduction to the Theory of Ion–Atom Collisions* (Amsterdam: North-Holland)
Miraglia J E and Macek J 1991 *Phys. Rev.* A **43** 5919
Pedersen J O, Hvelplund P, Petersen A G and Fainstein P D 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** L597
Rosenberg L 1973 *Phys. Rev.* D **8** 1833
Stolterfoht N, DuBois R D and Rivarola R D 1997 *Electron Emission in Heavy Ion–Atom Collisions* (Berlin: Springer)
Stolterfoht N, Platten H, Schiwietz G, Schneider D, Gulyás, Fainstein P D and Salin A 1995 *Phys. Rev.* A **52** 3796