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Fully differential cross sections in single ionization of helium by ion impact: Assessing the role of correlated wave functions

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Abstract

We study the effect of final state dynamic correlation in single ionization of atoms by ion impact analyzing fully differential cross sections (FDCS). We use a distorted wave model where the final state is represented by a Φ_2 type correlated function, solution of a non-separable three body continuum Hamiltonian. This final state wave function partially includes the correlation of electron–projectile and electron–recoil relative motion as coupling terms of the wave equation. A comparison of fully differential results using this model with other theories and experimental data reveals that inclusion of dynamic correlation effects have little influence on FDCS, and do not contribute to a better description of available data in the case of electronic emission out-of scattering plane.

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1. Introduction

One of the key points in any theory of single ionization by ion impact is the correct description of the final electronic state, in which the ionized electron moves in the long range Coulomb potential of two heavy ions. As with any three body problem, for which close solutions are not possible, it is important to look for approximated wave functions that fulfill known physical properties of the particular collision system. Back in the 80s, and based on the work of Belkic [2], Garibotti and Miraglia [3] developed one of the most widely used continuum wave functions to model final electronic states in single ionization: the so-called 2C wavefunction. This state complies with the *correct Coulomb asymptotic conditions* [4,5] and, at that time, represented an important advance in the field of atomic collisions. Shortly afterwards, the introduction of the continuum distorted wave–eikonal initial state (CDW–EIS) approximation by Crothers and McCann [6], using the 2C wavefunction in the final state, proved to be one of the most important approaches to deal with single ionization by ion impact (see e.g. [7,8] and references therein), then generalized to treat other processes such as capture (see e.g. [9]), excitation (see e.g. [10]) and transfer ionization (see e.g. [11] and references therein). The complexity of the calculations were eased by the fact that 2C wave functions were separable in the electron–projectile and electron–recoil relative coordinates. The price was to treat the non-separable terms of the Hamiltonian as a perturbation. Almost a decade ago, a final state correlated wave function was proposed by Gasaneo and coworkers [1], in order to deal with the *three body continuum* that results in single ionization of atoms by ion impact. The separability restriction was partially removed for the so-called Φ_2 wave function which takes into account part of the non-orthogonal kinetic energy from the full three body (3B) Hamiltonian. The analytical properties of the Φ_2 wave

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function have been thoroughly studied elsewhere [12]. It was also applied within distorted wave approximations in the calculation of doubly differential cross sections for ion impact ionization and it was demonstrated that the description of the low-energy region of the spectra, the so-called soft electron peak, is improved when this correlated theory is used [13,14].

The understanding of atomic and molecular processes has strongly benefited from the advent of the COLTRIMS (cold target recoil ion momentum spectroscopy) and reaction microscope techniques, which now allow simultaneous detection of the different particles that take part in the collision process (for a recent review see [15]). Thus, the complete kinematics of a considerable number of experiments can be determined by measuring the momenta of all fragments in coincidence. The results of these complete experiments represent a stringent test for the theoretical tools. Furthermore, it has been shown that even processes where perturbative approaches should to work, have still unexplained features [16,17].

Very recently, Olson and Fiol (see [18] and references therein) argued that fully differential cross sections (FDCS) can be very sensitive to the experimental conditions and uncertainties. In their calculations for single ionization by highly charged ions, they were able to reproduce the experimental results using a temperature of the target jet gas of 16 K. It has also been shown that, when convolution with experimental resolutions are added up to distorted wave theories, good agreement can be found between theory and experiments for events out-of the scattering plane (see [19] and references therein).

There is, however, a controversy regarding these conclusions. Very recently Schulz and coworkers [20] developed a method, based on quantum Monte Carlo events, to accurately account for both experimental resolution, and other effects such as target temperature and extracting electric fields. They concluded that a temperature of 16 K for the target jet gas is *unrealistic*, and that experimental resolution alone cannot account for electronic emission structures out-of the scattering plane.

One of the issues of the theoretical models used up to now within the framework of the distorted wave theories is the absence of correlation in the wave functions. The concept of correlation is a well-known idea in a wide range of physical processes that involve many bodies. However, this fact implies that its calculation is always based in some approximated model. Within atomic physics, correlation is a basic ingredient in the description of multielectronic atoms and ions. In electron impact ionization of neutral atomic targets correlation cannot be neglected, since in the final state of such process we have two light particles and the consequent exchange effects should to be addressed adequately.

In the case of single ionization by ion impact, we deal with a broader definition of correlation, that can be understood as an absence of separability between relative motions which translates into the non separability of the associated wavefunctions, even when a one electron system is considered, i.e, the motion of the electron–projectile subsystem is no longer independent of the electron–recoil-ion-target motion. One of the simplest system in which this correlation can be studied is the three body Coulomb problem (3BCP). Single ionization by ion impact can be modeled as a 3BCP and offers the opportunity to investigate the full continuum state that describes the final state of the collision, as well as the distorted bound state of the initial channel.

In the present work we aim to assess how correlation contributes to the structure of the emission pattern both in the scattering plane and out-of the scattering plane. Atomic units are used throughout unless stated otherwise.

2. Theoretical framework

We treat helium single ionization as a single electron process assuming that in the final state the *active* target electron moves in the combined Coulomb field of the incoming projectile and the residual-target core with a given effective charge. This charge takes into account the partial screening due to the passive helium electron. Within correlated continuum wave–eikonal initial state (CCW–EIS) theories, the electronic final state is represented by a correlated non-separable wave function. Like in the CDW–EIS approximation, electron–projectile interaction in the initial channel is taken into account by an eikonal phase (see e.g. [7,8]).

Throughout the work we use non-orthogonal Jacobi coordinates $(\mathbf{r}_\mathrm{P}, \mathbf{r}_\mathrm{T})$ to describe the collision process [21]. These coordinates represent the position of the active electron with respect to the projectile $(\mathbf{r}_\mathrm{P})$ and the target ion $(\mathbf{r}_\mathrm{T})$, respectively. $\mathbf{R}_\mathrm{T}(\mathbf{R}_\mathrm{P})$ is also needed, representing the position of the projectile (target) with respect to the center of mass (c.m.) of the e–T (e–P) subsystem. If we neglect terms of order $1/M_\mathrm{T}$ and $1/M_\mathrm{P}$, where M_T is the mass of the target ion nucleus and M_P is the corresponding to the incident heavy ion, we get $\mathbf{R}_\mathrm{P} = \mathbf{R}_\mathrm{T} \approx \mathbf{r}_\mathrm{T} - \mathbf{r}_\mathrm{P}$ [21].

In the (c.m.) frame, the FDCS in electron energy and ejection angle, and direction of the outgoing projectile is given by [22–24]

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}E_k \mathrm{d}\Omega_k \mathrm{d}\Omega_K} = N_e (2\pi)^4 \mu^2 k \frac{K_\mathrm{f}}{K_\mathrm{i}} |T_\mathrm{fi}|^2 \delta(E_\mathrm{f} - E_\mathrm{i}), \tag{1}$$

where N_e is the number of electrons in the atomic shell, $K_\mathrm{i}(K_\mathrm{f})$ is the magnitude of the incident particle initial (final) momentum and μ is the reduced mass of the projectile–target subsystem. The ejected-electron's energy and momentum are given by E_k and k, respectively. The solid angles $\mathrm{d}\Omega_K$ and $\mathrm{d}\Omega_k$ represent the direction of scattering of the projectile and the ionized electron, respectively. We also note that the solid angle subtended by the projectile $\mathrm{d}\Omega_K = \sin\theta_K \mathrm{d}\theta_K \mathrm{d}\phi_K$ can be expressed in terms of the momentum transfer q via the relations $q \approx K_\mathrm{i} \sin\theta_K$ and

$K_i \approx K_f$, fulfilled for heavy ions projectiles, i.e. small scattering angles [7].

The main quantity in (1) is the transition matrix T_{fi}, that in the prior version can be written as

$$T_{fi} = \langle \Psi_f^{(-)} | V_i | \Psi_i^{(+)} \rangle, \tag{2}$$

where the initial (final) state wave $\Psi_i^{(+)}(\Psi_f^{(-)})$ is an approximation to the initial (final) state which satisfies outgoing-wave (+) (incoming-wave (−)) conditions and V_i the perturbation. For these initial and final states there exist several alternatives, corresponding to different proposed approximations. In expression (2), the interaction between the projectile and the target nucleus, the so-called N–N interaction, must be included (see e.g. [25] and references therein). The case of heavy ion impact ionization is easier to treat when is compared with, e.g. ionization by electron impact, since the projectile can be considered classically and we do not have to deal with exchange effects in the final electronic state. Consequently, in our scheme we incorporate the N–N interaction *exactly* in a semiclassical way [26].

In the initial state the asymptotic form of the Coulomb distortion, the so-called eikonal phase, is used in the electron–projectile interaction together with a semi analytical Rothan–Hartree–Fock description for the initial bound state wavefunction $\psi_i(\mathbf{r}_T)$, i.e.

$$\Psi_i^{EIS,(+)} = (2\pi)^{-3/2} \exp(i\mathbf{K}_i \cdot \mathbf{R}_T) \psi_i(\mathbf{r}_T) \mathscr{E}_v(\mathbf{r}_P), \tag{3}$$

where $\mathscr{E}_v(\mathbf{r}_P)$ is

$$\mathscr{E}_v(\mathbf{r}_P) = \exp\left(-i\frac{Z_P}{v}\ln(vr_P - \mathbf{v}\cdot\mathbf{r}_P)\right), \tag{4}$$

$\mathbf{v}$ being the incoming projectile velocity and Z_P its charge. Also we have modeled the incoming projectile by a plane wave of momentum $\mathbf{K}_i$.

For the final state we propose a non-separable wave function, known as Φ_2 [2]. This distorted wave function introduces part of the so-called non-orthogonal kinetic energy, present in the full 3B Hamiltonian. The Φ_2 is a two-variable hypergeometric function, solution of a differential equation involving mixed derivatives [1,27]. Consequently, we can write the final state as

$$\Psi_f^{\Phi_2,(-)} = N_{\Phi_2}(2\pi)^{-3} \exp(i\mathbf{k}_T \cdot \mathbf{r}_T + i\mathbf{K}_f \cdot \mathbf{R}_P) \times \Phi_2[-i\alpha_T, -i\alpha_P, 1, -ik_T\xi_T, -ik_P\xi_P], \tag{5}$$

where $\mathbf{k}_T(\mathbf{k}_P)$ is the relative momentum of the e–T (e–P) subsystem and $\alpha_T = \frac{Z_T}{k_T}\left(\alpha_P = \frac{Z_P}{k_P}\right)$ is the two-body e–T (e–P) Sommerfeld parameter. Here the outgoing projectile is considered also as a plane wave, but now with momentum $\mathbf{K}_f$. The coordinates $\xi_j = r_j + \hat{\mathbf{k}} \cdot \mathbf{r}_j$ with $j = T$ or P are the well-known parabolic coordinates for incoming boundary conditions.

The asymptotic behavior of the wavefunction (5) fulfills the *correct asymptotic Coulomb conditions* [4,5]. Furthermore, it introduces a correlation in the wavefunction that modifies the behavior of the function for all distances among the particles. In fact, analyzing the normalization factor N_{Φ_2} we observe that it is a non-separable function depending on the sum of the Sommerfeld parameters of each relevant interaction α_T and α_P [28].

The $\Psi_f^{\Phi_2,(-)}$ function can be expanded as

$$\Psi_f^{\Phi_2,(-)} = N_{\Phi_2}(2\pi)^{-3} \exp(i\mathbf{k}_T \cdot \mathbf{r}_T + i\mathbf{K}_f \cdot \mathbf{R}_P) \times \sum_{m=0}^{+\infty} a_m \mathscr{F}_m^T(\xi_T) \mathscr{F}_m^P(\xi_P), \tag{6}$$

with

$$a_m = \frac{(-i\alpha_T)_m(-i\alpha_P)_m}{m!(m)_m(1)_{2m}}, \tag{7}$$

$(\alpha)_m$ being the Pochammer symbols and

$$\mathscr{F}_m^j(\xi_j) = (-ik_j\xi_j)^m {}_1F_1[-i\alpha_j + m, 1 + 2m, -ik_j\xi_j], \tag{8}$$

with $j = T$ or P. This series can be considered as an expansion of the $\Psi_f^{\Phi_2,(-)}$ function in terms of target-centered and projectile-centered two-body functions. It is worth noting that, besides the normalization factor, the lowest order of this series, i.e. $m = 0$, is the well-known 2C function and coupling is included in higher orders of the series expansion. We can generalize Eq. (6) by taking the a_m coefficients as parameters and finding them by solving the 3BCP Schrödinger equation according to restrictions and other physical properties such as Kato cusp conditions or asymptotic behavior [29]. From a computational point of view, the most important feature of the wavefunction (6) is that the transition matrices for single ionization within a distorted wave framework can be obtained analytically.

Finally, the transition matrix T_{fi} can be calculated using the series expansion (6) in the following way

$$T_{fi} = \sum_{m=0}^{\infty} a_m \langle \mathscr{F}_m^P | V_i^P | \mathscr{E}_v \rangle \langle \mathscr{F}_m^T | V_i^T | \psi_i \rangle, \tag{9}$$

where we have divided the perturbation V_i in its e–T and e–P parts. Using hydrogenic wave functions, T_{fi} can be calculated analytically to all orders. The resulting expressions are in terms of the two-variable non-confluent hypergeometric F_1 of Appell and Kampé de Feriet and there exists numerical routines to calculate it [30,31]. It was shown that the series expansion (9) has an excellent numerical convergence [28,13].

3. Results and discussion

The present CCW–EIS results are compared with those of the CDW–EIS theory and the first born approximation (FBA). Nowadays there exists a huge amount of experimental results for single ionization by ion impact and it would seem too restrictive to analyze one case only, but our goal is to chose a set of parameters for which the theories predict results comparable with experiments. To this end in Fig. 1–3 we show results for 100 MeV amu^{-1} C^{6+} single ionization of helium and for different electron

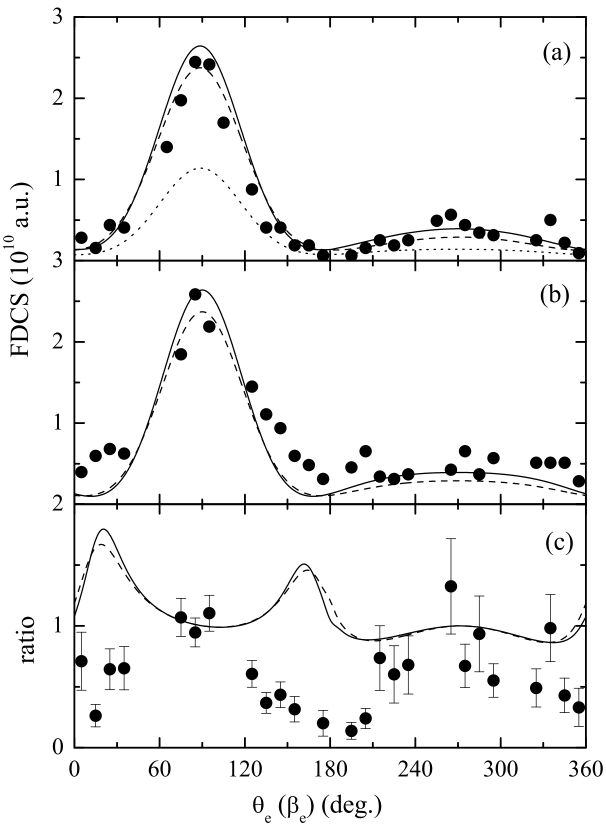

Fig. 1. Comparison of in-plane and out-of-plane FDCS in the laboratory frame for 100 MeV amu^{-1} for C^{6+} single ionization of helium. The energy of the ejected electron is $E_e = 6.5$ eV and the momentum transfer of the projectile is $q = 0.88$ a.u. Panel (a) corresponds to the in-plane FDCS, panel (b) corresponds to the plane perpendicular to the incident beam direction, containing the momentum transfer **q**. Panel (c) corresponds to the ratio of the in-plane (panel (a)) and out-of-plane (panel (b)) results. Solid line: CCW–EIS, dashed line: CDW–EIS, dotted line: FBA; circles: experimental data [32].

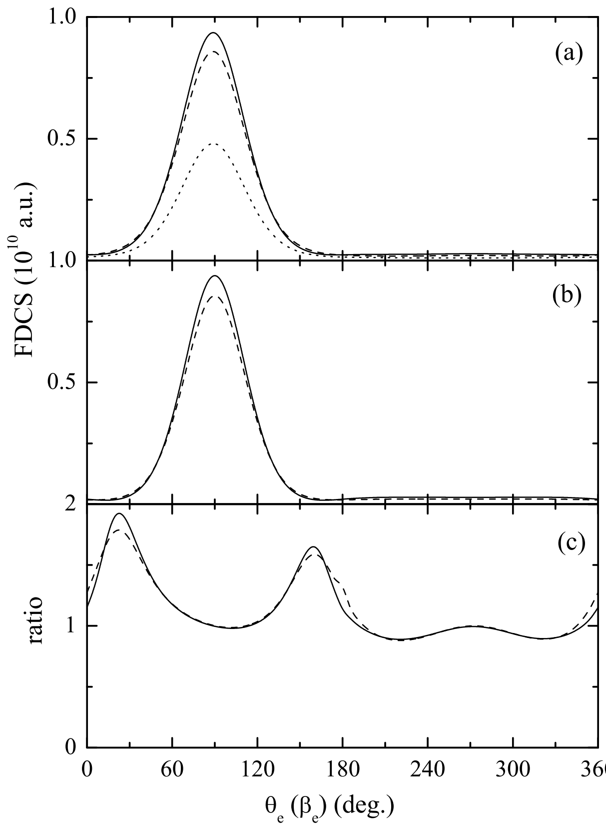

Fig. 2. As in Fig. 1, but using for an energy of the ejected electron $E_e = 17.5$ eV and the momentum transfer of the projectile $q = 1.43$ a.u.

energies and projectile parameters, based in the experimental data reported in [32]. This process is particularly striking, since it has been analyzed in detail using different formalisms, and there are still open questions concerning to the failures of first order perturbation theories and distorted wave approaches.

In panels (a) we show experimental data and theoretical predictions ionization events within the scattering plane (for details about the collision geometry see, e.g. [16]). To plot all the results in a single graph, we define the scattering plane x–z using θ_e from 0° to 360° which corresponds first to the $\phi_e = \pi$ half-plane ($0° \leqslant \theta_e \leqslant 180°$) followed by the $\phi_e = 0$ half-plane ($180° \leqslant \theta_e \leqslant 360°$) with the angles being measured continuously clockwise relative to the beam direction.

In panels (b), on the other hand, the experimental data and theoretical results for events out-of the scattering plane are displayed. Here, as in [16], and in order to make a direct comparison with the in-plane results, we have defined a new azimuthal angle $\beta_e = \phi_e - \pi/2$ for the ionized electron.

Finally, in panels (c) the ratio between the in-plane results and the out-of-plane events, is shown. Furthermore, following experimental requirements, the cross sections in all the figures are presented in the laboratory system. The conversion from c.m system to the laboratory system is given by a constant factor of 16 for the present FDCS.

From the panels (a) of Figs. 1–3, we observe that both experiment and theories have the same characteristic shape as one would expect from electron impact scattering with a binary peak (larger peak at $\theta_e \approx 90°$) and recoil peak (smaller peak at $\theta_e \approx 270°$). The binary peak results from a single two-particle projectile–electron collision and is located in the direction of the momentum transfer vector **q**. The recoil peak is due to a double scattering mechanism in which the projectile first collides with the electron and then the electron back-scatters off the atomic nucleus. To correctly describe these second order events it is necessary to incorporate *on equal footing* all the interactions present in the ionization process. As it can be seen from our results, the recoil peak decreases rapidly with increasing momentum transfer, i.e. larger projectile scattering angles. Both CCW–EIS and CDW–EIS results are in reasonable agreement with the absolute data for all the parameters presented where experimental data exist. On the other hand, the FBA reproduces correctly only the shape of the FDCS and is about a factor of 2 smaller than the data. For electron impact, the FBA and CDW–EIS results would be essentially identical for projectile–electron energies above about 1 keV (speed of about 10 a.u.). Considering that

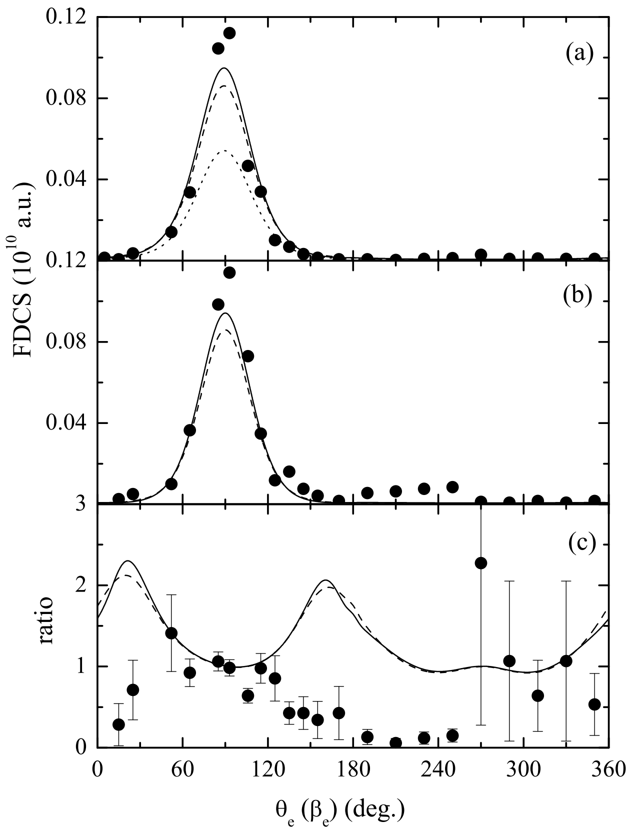

Fig. 3. As in Fig. 1, but using for an energy of the ejected electron $E_e = 37.5$ eV and the momentum transfer of the projectile $q = 2.65$ a.u.

the velocity of the 100 MeV amu^{-1} C^{6+} projectiles is about 60 a.u., the discrepancy between FBA and CDW–EIS predictions in this case is a bit surprising. The differences present for the lower ejected-electron energies and smaller momentum transfers could be consequently attributable to the larger charge of the projectile.

It is argued that events out-of the scattering plane, i.e. the FDCS data of panels (b) of Figs. 1–3, appear as a result of higher-order contributions to the ionization collision process. Distorted wave-type theories, as CDW–EIS and CCW–EIS, include to some extent these higher order events, since all the interactions, i.e. the e–T and e–P Coulomb potentials and eventually N–N interaction, are contained to all orders in the initial and final wave functions. The comparison between our theoretical results and the experimental data, however, shows that none of the theories is able to reproduce the FDCS data in the full angular range. The same trend has been already observed by other authors using full numerical schemes [16].

Analyzing the ratios, i.e. panels (c) of Figs. 1–3, it is possible to observe the strong discrepancies between theory and experiments. While in the experiments these ratios are between 0 and 2, both the respective values for CDW–EIS and CCW–EIS are around 1 and 2, but the tendency is in the opposite direction. Similar behavior was also observed in another more elaborated theories [16]. From this analysis we could conclude that (i) the correlation incorporated in the CCW–EIS is not sufficient to reproduce adequately the asymmetry between events out of the scattering plane and the in-plane ones or (ii) dynamical correlation is not an important feature in out-of-plane events.

4. Conclusions and perspectives

We have carried out calculations of FCDS for single ionization of Helium by 100 MeV amu^{-1} C^{6+} projectiles using a correlated distorted wave theory. We have assessed the contribution of dynamic correlation taken into account in CCW–EIS theory comparing it with the usual CDW–EIS calculations. Both approaches have the advantage to be computationally simpler and far less time consuming than full numerical models. CCW–EIS theory shows results very close to those yielded by CDW–EIS calculations, both in the scattering plane and out-of the scattering plane. We conclude that the effect of dynamic correlation is very small and does not explain the experimental results. These results favor then the hypotheses that ionization events out-of the scattering plane are dominated by higher-order processes that are not accurately described even by this correlated CCW–EIS theory. However, we were able to elucidate some global conclusions about the importance of correlation in single ionization by ion impact. There still exists some room within distorted wave formalisms to overcome the unexplained discrepancies. For example, it should be necessary to include, at the FDCSs level, all the interactions, including the nuclear–nuclear one, on an *equal footing*, e.g. by incorporating distorted Coulomb waves for the initial and/or final channels within a distorted wave approach. In this line, the role of the nuclear–nuclear interaction within the CCW–EIS framework, deserves to be analyzed in detail. It is worth to mention that more elaborated numerical approaches have been applied to this process already, but such complex models have shown only marginally better results when compared with simpler ones, at the expense of more problematic analysis and computational effort.

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