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A hybrid distorted wave model: a (almost) *complete-post* version of the CDW model for single ionization

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Abstract. A hybrid CDW–CDW-EIS model is developed in order to include the dynamic screening in the *post* CDW approximation for single ionization. Doubly differential cross sections for single ionization of water molecules are calculated and comparison with available experimental data and other theories are shown.

1. Introduction and Theory

The distorted wave models are perturbative methods that were introduced in order to accelerate the convergence of the Born series and to avoid the presence of disconnected diagrams that may originate divergent Born sub-series. Among the distorted wave models, there are two that merit to be cited: the Continuum Distorted Wave (CDW) [1] and the Continuum Distorted Wave-Eikonal Initial State (CDW-EIS) [2]. These models were initially formulated to describe single ionization of monoelectronic targets by bare ion impact. Later on,they were extended to study single ionization of multielectron targets [3]. Since then, they have been widely used to calculate cross sections for single ionization involving a large collection of projectiles, such as heavy bare ions, antiprotons, and more recently highly-charged dressed ions, and also a variety of targets as simple atomic systems to large biological molecules (see [4, 5, 6, 7]).

Recently, an extension of these two distorted wave models was developed by Monti *et al.* for the case of single ionization of atomic targets by swift dressed-ion impact [8].

Here, we study the case of bare projectiles and multielectronic targets within an independent electron model following the procedure given in [4]. By assuming only one active electron, the multielectronic Hamiltonian can be reduced to:

$$H_{el} = -\frac{1}{2}\nabla^2 + V_T(\boldsymbol{x}) + V_P(\boldsymbol{s}) + V_s(\boldsymbol{R}) \tag{1}$$

where $\boldsymbol{x}$ and $\boldsymbol{s}$ give the active electron position in the target and projectile reference frames, respectively. $V_T(\boldsymbol{x})$ is a potential which takes into account the interaction of this electron with the rest of the target, $V_P(\boldsymbol{s}) = -Z_P/s$ is the interaction between the bare projectile and the active electron, and $V_s(\boldsymbol{R})$ the interaction the projectile with the target nucleus and the passive electrons. This potential depends only on the internuclear coordinate $\boldsymbol{R}$ and thus, within the straight-line version of the impact-parameter approximation, gives place to a phase factor which,

in our calculations, does not affect the electron dynamics. Within a distorted wave formalism, the initial and final distorted-waves are given by:

$$\chi_i^+(\boldsymbol{x},t) = \Phi_i(\boldsymbol{x},t)\,\mathcal{L}_i^+(\boldsymbol{s}) \quad (2)$$

$$\chi_f^-(\boldsymbol{x},t) = \Phi_f(\boldsymbol{x},t)\,\mathcal{L}_f^-(\boldsymbol{s})\,. \quad (3)$$

Here $\Phi_i(\boldsymbol{x},t) = \phi_i(\boldsymbol{x})\exp(\mathrm{i}\varepsilon_i t)$ and $\Phi_f(\boldsymbol{x},t) = \phi_f(\boldsymbol{x})\exp(\mathrm{i}\varepsilon_f t)$ are the initial-bound and final-continuum states solution of the time-dependent Schrödinger equation. We considered a RHF initial wavefunction and an effective Coulomb target potential $V_T(\boldsymbol{x})$ in the final state. ε_i and ε_f are the electron energies in the initial and final states, respectively.
In particular, considering the CDW approximation, the initial distortion in (2) is proposed as:

$$\mathcal{L}_i^{+CDW}(\boldsymbol{s}) = N(\nu)\ {}_1F_1(\mathrm{i}\nu;1;\mathrm{i}vs+\mathrm{i}\boldsymbol{v}\cdot\boldsymbol{s}) \quad (4)$$

whereas the final distortion in (3) is chosen as:

$$\mathcal{L}_f^{-CDW}(\boldsymbol{s}) = N^*(\zeta)\ {}_1F_1(-\mathrm{i}\zeta;1;-\mathrm{i}ps-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{s}) \quad (5)$$

where $\boldsymbol{v}$ is the projectile velocity, $\nu = Z_P/v$, $\zeta = Z_P/p$, $\boldsymbol{p} = \boldsymbol{k} - \boldsymbol{v}$ is the ejected electron momentum in the projectile reference frame, $\boldsymbol{k}$ is the ejected electron momentum in the target reference frame, and ${}_1F_1$ is the confluent hypergeometric function, and N its normalization factor.
It is well known that within the distorted wave framework, the transition matrix may be written either in its *prior*- or *post*-version (or *complete-post*, see [9]), depending on whether the perturbation operators act over the initial of final distorted waves, respectively. It was shown [10] that the *prior*-version of the CDW transition amplitude for single ionization has an intrinsic logarithmic divergence near the binary encounter peak. This prevents us from using this form of the transition amplitude to calculate ionization cross sections. Therefore the *post*-version of the CDW approximation, which does not contain such divergence, was used to calculate ionization cross sections.
Recently the *post*-version of the CDW-EIS model was revisited by Monti *et al.* [9] showing that approximating the target potential V_T by an effective-Coulomb one neglects a part of the *dynamic-screening*, leading to the omission of a term in the transition amplitude, causing the well known post-prior discrepancies [11, 12]. Properly including the term containing the dynamic-screening in the *post*-version of the CDW-EIS model, therefore obtaining a *complete*-post-version, almost vanishes the post-prior discrepancies. The same approximation to the V_T potential is made in the CDW approximation. Hence the usual *post*-version of the CDW approximation also lacks the dynamic screening contribution.
The *complete-post*-version of the CDW transition amplitude consists of two terms:

$$\mathcal{A}^{+CDW} = \mathcal{A}^{+CDW(a)} + \mathcal{A}^{+CDW(b)} \quad (6)$$

where the firs term is the usual *post*-version (see [1, 5, 6]) and the second one is the term related to the dynamic screening:

$$\mathcal{A}^{+CDW(b)}(\rho) = -i\int_{-\infty}^{+\infty} dt\ e^{i\Delta\varepsilon\, t}\int d\boldsymbol{x}\ V_T(\boldsymbol{x})\phi_f^*(\boldsymbol{x})\mathcal{L}^{*-CDW}_f(\boldsymbol{s})\phi_i(\boldsymbol{x})\mathcal{L}_i^{+CDW}(\boldsymbol{s}) \quad (7)$$

Unfortunately, this term also contains the logarithmic divergences that are found in the *prior*-version. Therefore, in order to include this term avoiding any divergences, we replace, only in the dynamic-screening term, the $\mathcal{L}_i^{+CDW}$ distortion by its asymptotic approximation, I.E. an eikonal phase,

$$\mathcal{L}_i^{+CDW}(\boldsymbol{s}) \approx \mathcal{L}_i^{+EIS}(\boldsymbol{s}) = \exp\left(-\mathrm{i}\nu\ln(vs+\boldsymbol{v}\cdot\boldsymbol{s})\right), \quad (8)$$

obtaining

$$\mathcal{A}^{+EIS(b)}(\rho) = -i \int_{-\infty}^{+\infty} dt\ e^{i\Delta\varepsilon\, t} \int d\boldsymbol{x}\ V_T(\boldsymbol{x})\phi_f^*(\boldsymbol{x})\mathcal{L}_f^{*-CDW}(\boldsymbol{s})\phi_i(\boldsymbol{x})\mathcal{L}_i^{+EIS}(\boldsymbol{s}) \tag{9}$$

A hybrid CDW–CDW-EIS model is then obtained, in which the transition matrix is given by the sum of the usual CDW *post*-version and the dynamic screening term as described in the CDW-EIS approximation:

$$\mathcal{A}^{+CDW} = \mathcal{A}^{+CDW(a)} + \mathcal{A}^{+EIS(b)}. \tag{10}$$

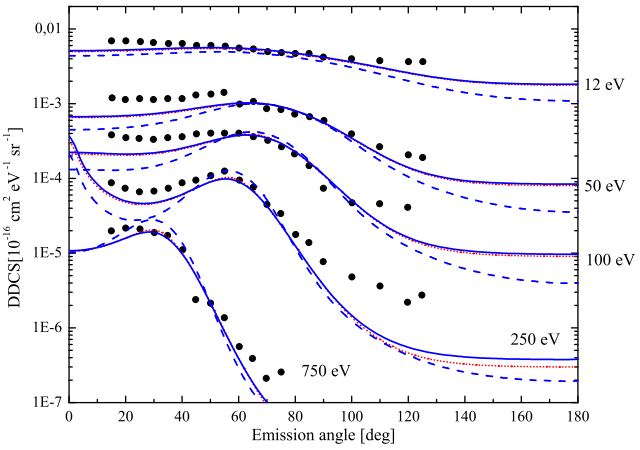

Figure 1. DDCS for single ionization of water molecules by 500 keV proton impact as a function of the ejection angle for 12 eV, 50 eV, 100 eV, 250 eV and 750 eV fixed emission energies. ——Present hybrid model calculations; - - - -*post* CDW calculations; · · · · · ·*prior* CDW-EIS calculations. ● experimental results from [13].

2. Results

In figures 1 and 2, we show doubly differential cross sections (DDCS) for single ionization of a single isolated water molecule by 500 keV H^+ and 6 MeV/u C^{6+} impact, respectively, as a function of the ejection angle for several fixed emission energies. Calculations performed with the *post*-version CDW model and the hybrid model are shown and compared with *prior*-version CDW-EIS calculations and experimental results. The contribution of the dynamic screening can be directly observed by comparing the *post* CDW calculations and the *hybrid* model. Its inclusion leads to a better agreement with the experimental results for forward and backward emission angles, though underestimation of the experiments is still found. Also, for the 500 keV H^+ impact and 250 keV and 750 keV emission energies, it can be seen that considering the dynamic screening leads to a better description of the binary-encounter peak. In the 6 MeV/u case, a large overestimation in the binary encounter region is found for the 192 ev and 384 eV emission energies case for all theories.

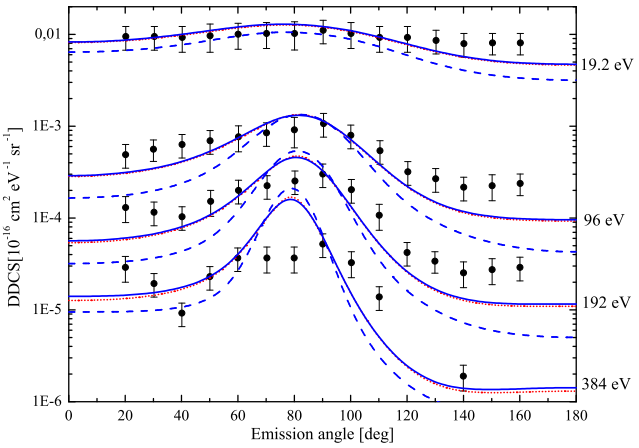

Figure 2. DDCS for single ionization of water molecules by 6 MeV/u C^{6+} impact as a function of the ejection angle for 19.2 eV, 96 eV, 192 eV, and 384 eV fixedemission energies. ——Present hybrid model calculations; - - - -*post* CDW calculations; ·····*prior* CDW-EIS calculations. ● experimental results from [14].

3. Conclusions

In order to avoid the logarithmic divergences present in the *prior* CDW model and in its *post*-version dynamic-screening term, a hybrid CDW–CDW-EIS model is presented in which the dynamic screening is considered through an eikonal approximation. It is shown that its inclusion leads to a major improvement of the previous *post* CDW calculations and a better agreement with experimental results.

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