Post–prior discrepancies in the continuum distorted wave–eikonal initial state approximation for ion–helium ionization

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Abstract
We have explored post–prior discrepancies within continuum distorted wave–eikonal initial state theory for ion–atom ionization. Although there are no post–prior discrepancies when electron–target initial and final states are exact solutions of the respective Hamiltonians, discrepancies do arise for multielectronic targets, when a hydrogenic continuum with effective charge is used for the final electron–residual target wavefunction. We have found that the prior version calculations give better results than the post version, particularly for highly charged projectiles. We have explored the reasons for this behaviour and found that the prior version shows less sensitivity to the choice of the final state. The fact that the perturbation potentials operate upon the initial state suggests that the selection of the initial bound state is relatively more important than the final continuum state for the prior version.

1. Introduction

Ionization in ion–atom collisions has been a very active field of research for years. There has been a comprehensive effort towards an understanding of the various processes that lead to the emission of one or several electrons from a neutral atom by ion impact. In recent years, advances in experimental techniques have made possible measurements of a large variety of processes, in different energy regimes, for different targets and projectile charge states (for a review, see, for example, Stolterfoht *et al* (1997)).

From the theoretical point of view, the simplest model for the ionization process involves a three-particle system interacting through long range Coulomb potentials. At intermediate and high energies distorted wave theories have been used for the last 25 years (Belkic 1978). They provide a good overall picture for the ionization process in the presence of Coulomb potentials.

Among these, the continuum distorted wave–eikonal initial state (CDW-EIS) approximation has probably been the most widely employed (Crothers and McCann 1983).

When dealing with multielectronic targets, initial and final target states become a source of concern, as exact wavefunctions are not available in this case. Slater orbital expansions of Roothaan–Hartree–Fock wavefunctions are usually employed for the initial bound state (Clementi and Roetti 1974). In order to circumvent this problem in the final continuum, the system is reduced to that of one active electron in a model potential. In that scheme the remaining target electrons provide a partial screening of the nuclear charge. The simplest approach is to represent the continuum by hydrogenic wavefunctions with an effective nuclear charge accounting for the screening effects. In this way we can obtain an analytical expression for both the wavefunction and the transition amplitude.

It is well known that theoretical models for ionization are sensitive to the quality of the target states. Following Madison (1973), Gulyás *et al* (1995) have extended the CDW–EIS model to include both initial and final numerically calculated wavefunctions.

However, it is still desirable to explore further improvements to a simple and successful approximation such as CDW–EIS which still allow us to get an analytical expression for the transition amplitude.

Gulyás *et al* (1995) used the prior version of the CDW–EIS for their calculations. While it is true that no post–prior discrepancies arise if both initial and final target wavefunctions are exact (as is the case for hydrogen) or at least good enough (as it is for numerical wavefunctions for multielectronic atoms), this is not the case when effective charges are used for the final target continuum state.

The aim of this paper is to explore the post–prior discrepancies for CDW–EIS in ion–helium single ionization, and to assess the sensitivity of both versions to the quality of the initial and final states.

This paper is organized as follows: in the next section the required transition amplitudes and wavefunctions are reviewed. In section 3, the prior version is compared to the post version, the numerical CDW–EIS calculation and experimental data where available. Impact energy and projectile charge dependences are also shown. In section 4, a test for the sensitivity of both post and prior versions to variations of the initial and final states are performed and the results discussed. Finally we state our main conclusions. We use atomic units unless otherwise stated.

2. Theory

The doubly differential cross section for ionization is defined in the impact parameter approximation by

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

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

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

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

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

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 gives

$$H_{\mathrm{el}} = -\frac{1}{2}\nabla_r^2 + V_{\mathrm{T}}(r_{\mathrm{T}}) - \frac{Z_{\mathrm{P}}}{r_{\mathrm{P}}} + \frac{Z_{\mathrm{P}} Z_{\mathrm{T}}}{R}. \tag{6}$$

For hydrogenic targets we have

$$V_{\mathrm{T}} = -\frac{Z_{\mathrm{T}}}{r_{\mathrm{T}}}. \tag{7}$$

For multielectronic targets we have to use model potentials (HF) or Coulomb potentials with effective charges to take account of passive electron screening.

When using distorted wave methods we insert the long range distortion in the part of the total Hamiltonian we resolve exactly, so that the potential we left as perturbation is a short range potential and 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

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

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, in its post

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

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, different approximations are obtained for the transition amplitude.

Here, we will use the CDW–EIS approximation (Crothers and McCann 1983). For the initial state we have

$$\chi_i^{+\mathrm{EIS}} = {}^{B1}\Phi_i^+ \times L_i^{+\mathrm{EIS}} \tag{14}$$

where the distortion is explicitly

$$L_i^{+\mathrm{EIS}} = \exp\left(\mathrm{i}\frac{Z_{\mathrm{P}} Z_{\mathrm{T}}}{v_{\mathrm{P}}} \ln(v_{\mathrm{P}} R + v_{\mathrm{P}}^2 t) - \mathrm{i}v \ln(v_{\mathrm{P}} r_{\mathrm{P}} + \mathbf{v}_{\mathrm{P}} \mathbf{r}_{\mathrm{P}}) \right) \tag{15}$$

and the perturbation potential is

$$W_i^{\text{EIS}} \chi_i^{+\text{EIS}} = {}^{B1}\Phi_i^+ (\tfrac{1}{2}\nabla_{r_P}^2 L_i^{+\text{EIS}} + \vec{\nabla}_{\mathbf{r}_T} \ln \varphi(r_T) \cdot \vec{\nabla}_{\mathbf{r}_P} L_i^{+\text{CDW}}). \tag{16}$$

For the final state we have

$$\chi_f^{-\text{CDW}} = {}^{B1}\Phi_f^- \times L_f^{-\text{CDW}} \tag{17}$$

with distortion

$$L_f^{-\text{CDW}} = \exp\left(-\mathrm{i}\frac{Z_P Z_T}{v_P}\ln(v_P R + v_P^2 t)\right) N^*(\zeta) {}_1F_1(-\mathrm{i}\zeta; 1; -\mathrm{i}k_P r_P - \mathrm{i}\mathbf{k}_P \mathbf{r}_P). \tag{18}$$

For the final perturbation potential we have

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

where ${}^{B1}\Phi_i^+$ and ${}^{B1}\Phi_f^-$ are the usual unperturbed wavefunctions for the initial and final state, respectively.

When dealing with multielectronic targets, the usual approach is that of one active electron plus a frozen core. The influence of the passive electrons is to add a short range potential to the long range Coulomb potential given by the electron–residual ion interaction. One simple approach is to consider a pure Coulomb potential with an effective charge. There are several recipes as to how the effective charge should be chosen (McDowell and Coleman 1970, Belkic 1978). In this way, a multielectronic target is cast into a hydrogenic one, and closed form solutions are possible for the wavefunctions and the transition amplitudes. The other approach is to numerically calculate the final state for the total target potential (Cravero 1995, Gulyás and Fainstein 1998). The drawback of this approach is that no closed forms are possible for the wavefunctions or the transition amplitudes. On the other hand, it is possible to get initial and final states that are completely orthogonal, yielding no post–prior discrepancies.

There is an issue to explore here, still. CDW–EIS calculations using effective charge hydrogenic wavefunctions have invariably been calculated in the post version, while CDW–EIS calculations using final numerical target wavefunctions have been calculated in the prior version. While it is true that the latter, in principle, shows no post–prior discrepancies, the same is not true for the former. In the next section we will show calculations using CDW–EIS in both versions and check for discrepancies.

3. Post versus prior

In figure 1 we show the forward electron emission spectrum for helium ionization by 1.5 MeV F^{9+} impact (Lee *et al* 1990). So-called binary electron (BE), electron capture to the continuum (ECC) and soft electron (SE) peaks are the well known features of this spectrum (Stolterfoht *et al* 1997). It can be seen that CDW–EIS with hydrogenic final state in the prior version closely agrees with the numerical CDW–EIS version, while the much used post version gives poorer results. Agreement is especially good for the energy region between the ECC and the binary peak. Removing the ECC divergence, it can be seen that the discrepancy remains essentially constant in that region (figure 2).

In figures 3 and 4 we show results for other projectiles and impact energies, with similar Sommerfeld parameters $\frac{Z_P}{v_P}$.

In figures 5 and 6 we show the dependence of the discrepancy as a function of projectile charge and ion impact velocity. A detailed study would require the assessment for different regions of the emission spectrum. However, the trend we found for forward emission $v/2$ electrons is likely to be typical. The origin of the discrepancy is related to the electron–target wavefunctions. However, the relative importance of the discrepancy should decrease as impact
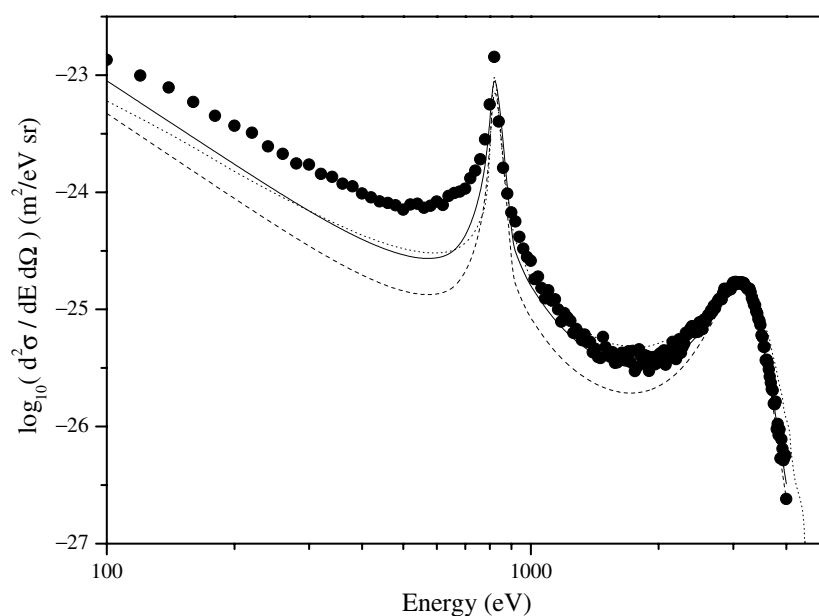
Figure 1. Doubly differential cross section for single ionization of helium by 1.5 MeV amu^{-1} F^{9+} impact in the forward direction. Prior CDW–EIS: full curve; post CDW–EIS: broken curve; Gulyás and Fainstein (1998): dotted curve; experimental data (Lee *et al* 1990): circles.
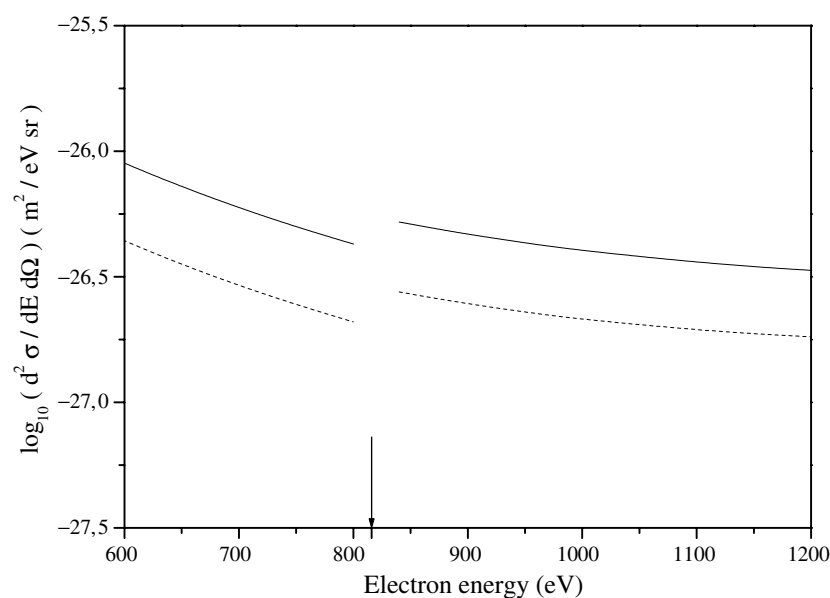

Figure 2. As for figure 1, showing the ECC region, after removing the Coulomb divergence. The arrow indicates the position of the ECC divergence. Prior CDW–EIS: full curve; post CDW–EIS: broken curve.

energy increases, because mechanisms well described by the first Born approximation (FBA) become dominant. Conversely, it should increase with projectile charge, as other emission mechanisms become relatively more important.
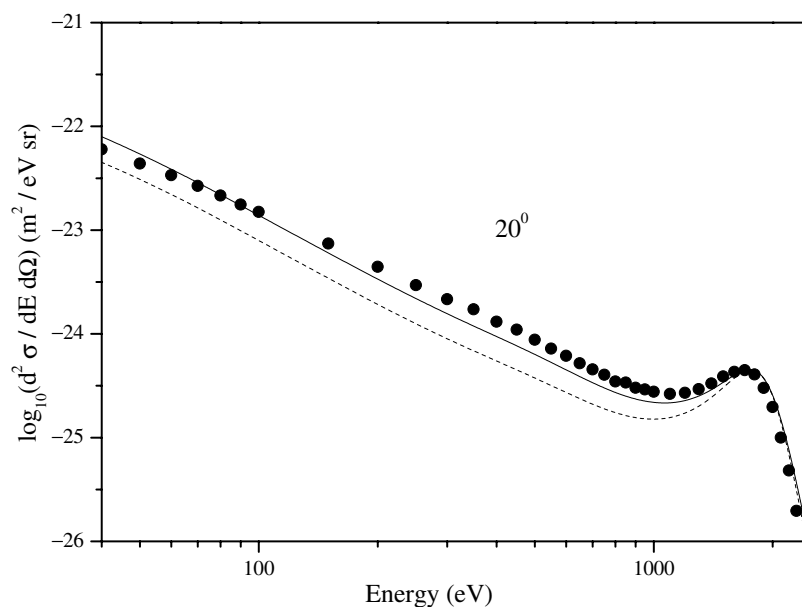
Figure 3. Doubly differential cross section for single ionization of helium by 1 MeV amu^{-1} C^{6+} impact for 20° emission angle. Prior CDW–EIS: full curve; post CDW–EIS: broken curve; experimental data (Pedersen *et al* 1990): circles.

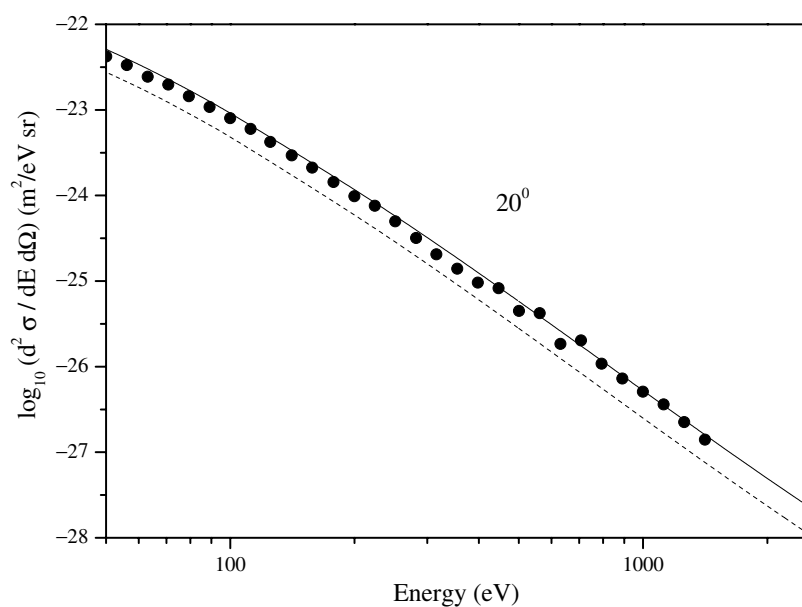**Figure 4.** Doubly differential cross section for single ionization of helium by 25 MeV amu^{-1} Mo^{40+} impact for 20° emission angle. Prior CDW–EIS: full curve; post CDW–EIS: broken curve; experimental data (Stolterfoht *et al* 1987): circles.

We see that the prior CDW-EIS yields very good results outperforming post CDW-EIS calculations. Figures 7–9 show a comparison for electron angular emission for 5 MeV
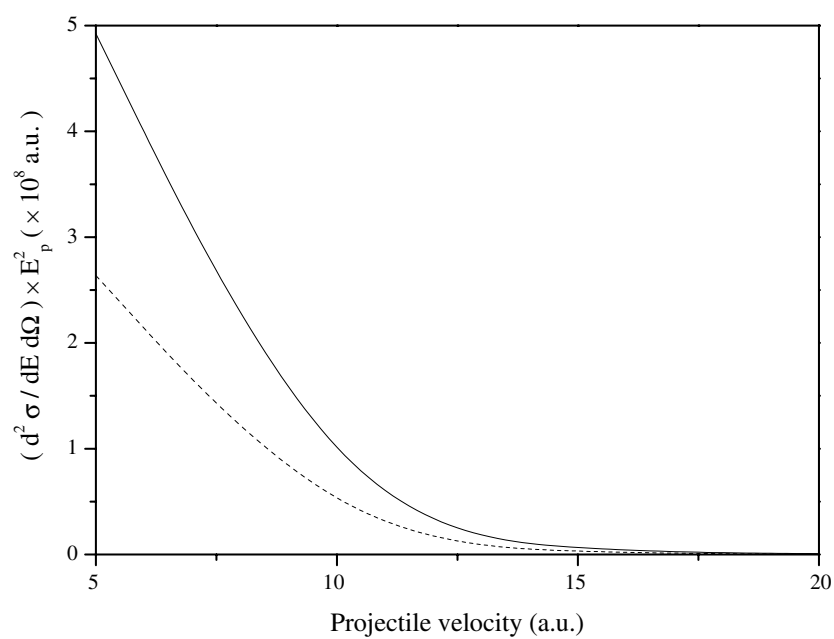
Figure 5. Doubly differential cross section for forward $v/2$ electron emission in helium ionization by F^{9+} impact as a function of projectile velocity. Prior CDW–EIS: full curve; post CDW–EIS: broken curve.
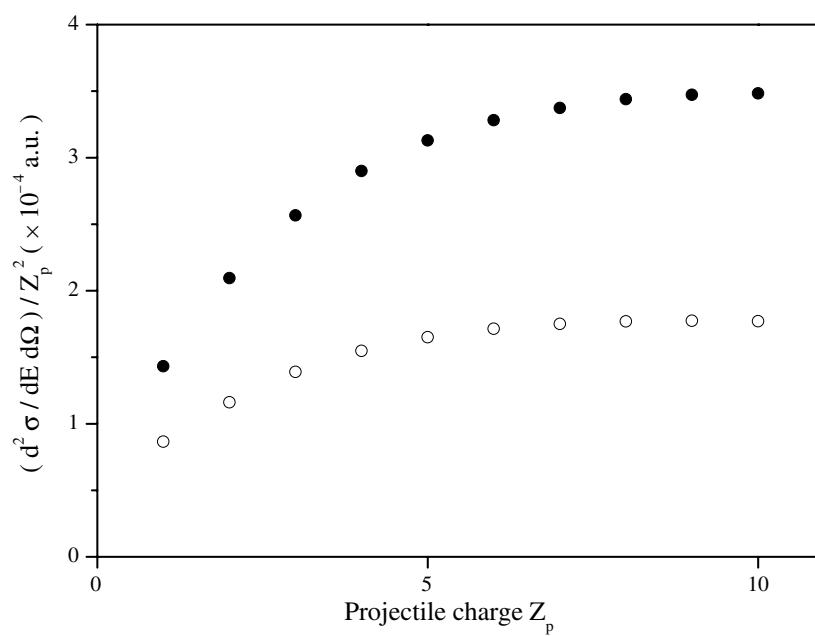

Figure 6. Doubly differential cross section for forward $v/2$ electron emission in helium ionization for 1.5 MeV amu^{-1} ion impact as a function of projectile charge state. Prior CDW–EIS: full circles; post CDW–EIS: open circles.
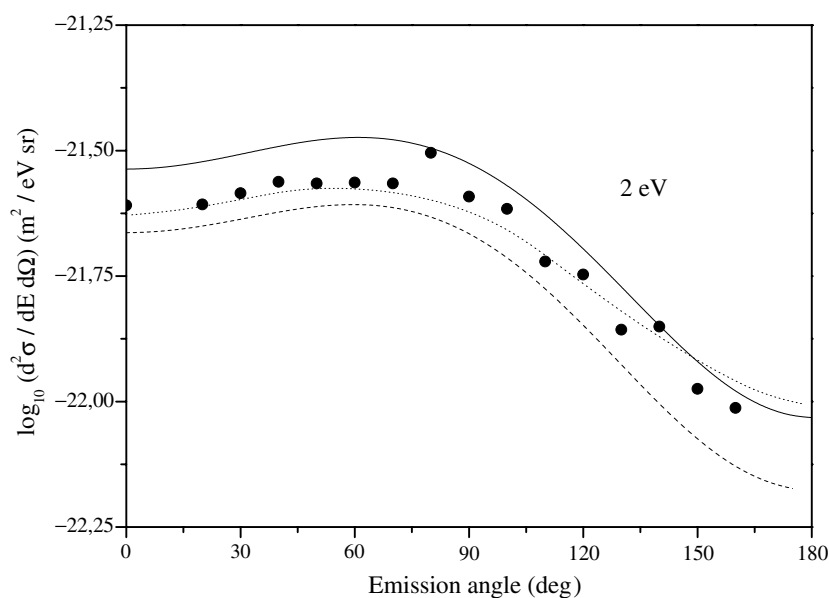
Figure 7. Doubly differential cross section for single ionization of helium by 5 MeV amu^{-1} Ne^{10+} impact as a function of ejection angle for 2 eV emission energy. Prior CDW–EIS: full curve; post CDW–EIS: broken curve; Gulyás and Fainstein (1998): dotted curve; experimental data (Stolterfoht *et al* 1995): circles.

Ne^{10+} $\longrightarrow$ He for 2, 15 and 150 eV, respectively. The prior version gives better results than the post version, lying closer to the numerical CDW–EIS for 15 and 150 eV, particularly for forward and backward directions. As the electron energy is lowered, however, agreement both with experimental data and numerical CDW–EIS worsens, although it has to be pointed out that experimental data at 2 eV have uncertainties of around 50% (Stolterfoht *et al* 1995).

4. Discussion

Why does the prior version yield results closer to the numerical CDW–EIS? In both the prior and post version calculations we have employed Roothan–Hartree–Fock wavefunctions for the initial bound states (Clementi and Roetti 1974). So we can regard the initial target wavefunctions as very good ones. As we discussed before, the same is not true for the final continuum. So it looks as if the prior version is less sensitive to the 'not-so-good' target final state than the post version is. Mathematically, it makes sense, since in the prior version the perturbation potentials, which are differential operators within the CDW–EIS approximation, operate upon the initial state, while in the post version they operate upon the final state. If that final state is not a good approximation, its derivative will be an even worse one. That is, the differential nature of the perturbation potentials makes the prior (post) version more sensitive to the quality of the initial (final) states, upon which they respectively operate.

We tested this ansatz by calculating the CDW–EIS approximation using initial and final hydrogenic wavefunctions in both versions and varying the initial and final effective charge.

We present those calculations in figures 10–12. In figures 10 and 11 we show calculations for the prior version, varying the initial and final effective charge, respectively. It is evident that this version is more sensitive to variations of the initial states. The final state effective charge has a remarkably small influence. That could explain why prior calculations give better results
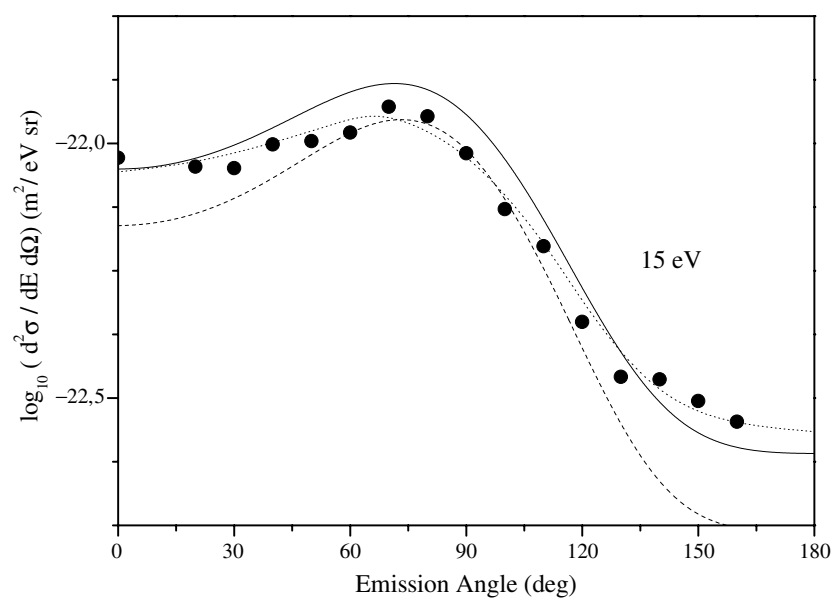
Figure 8. As figure 7 for 15 eV emission energy.
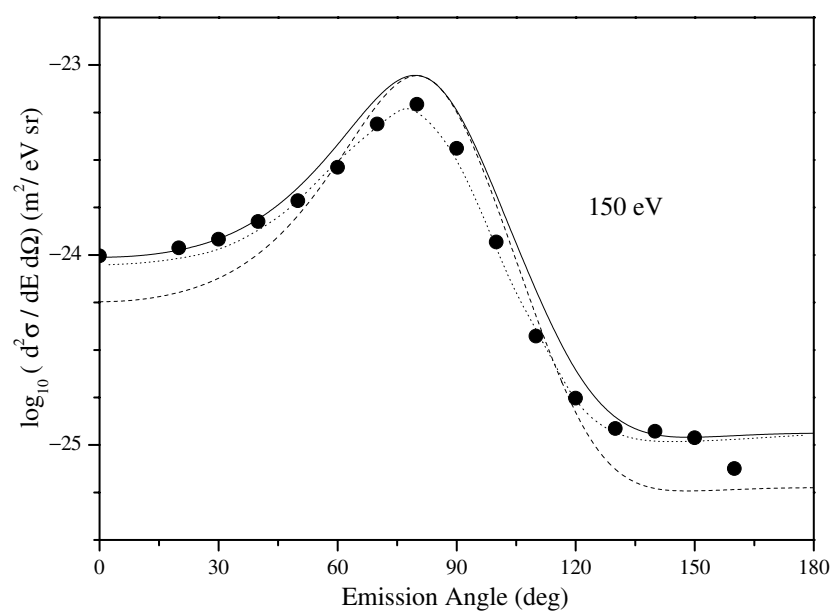

Figure 9. As figure 7 for 150 eV emission energy.

even when target final state wavefunctions are a relatively crude approximation compared to a full numerical continuum. This will be true provided good initial target bound states are used, since this version shows a substantial dependence on the quality of the initial state (figure 10).

In figure 12 we perform a similar calculation using the post version, in which the final state effective charge is varied.
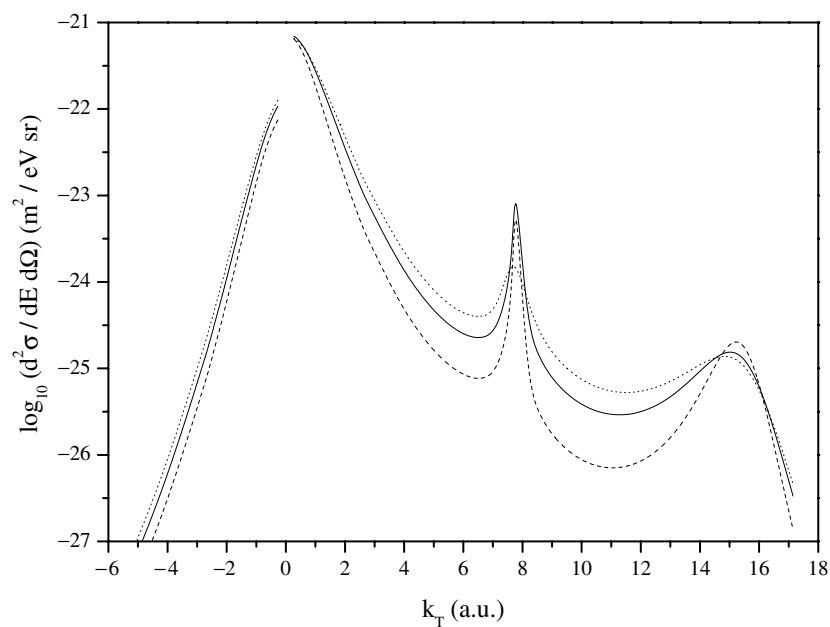
Figure 10. Doubly differential cross section for single ionization of helium by 1.5 MeV amu^{-1} F^{9+} impact in the forward and backward directions, calculated in prior CDW–EIS, varying the initial state effective charge. $Z_i = 1.6875$: full curve; $Z_i = 1.2$: broken curve; $Z_i = 2.0$: dotted curve.
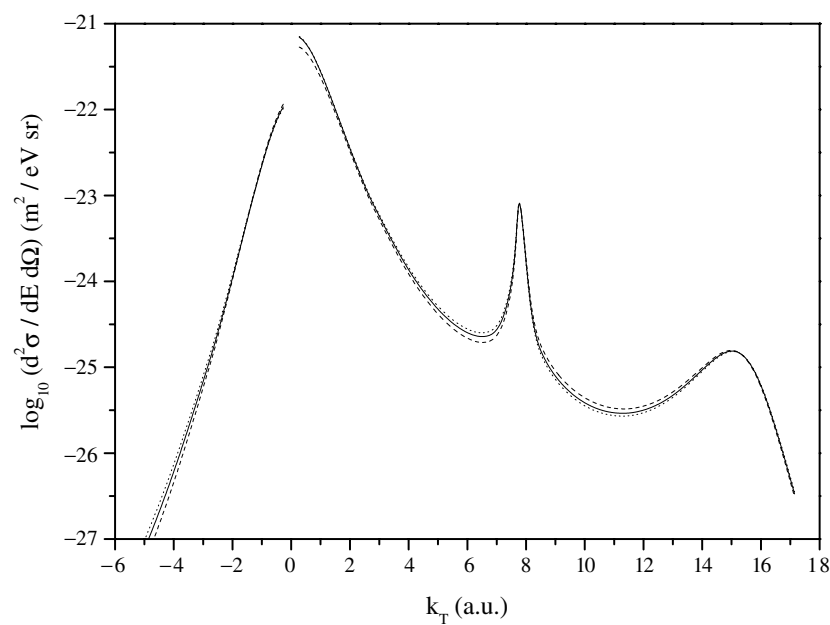

Figure 11. As figure 10, varying the final state effective charge. $Z_f = 1.6875$: full curve; $Z_f = 1.2$: broken curve; $Z_f = 2.0$: dotted curve.
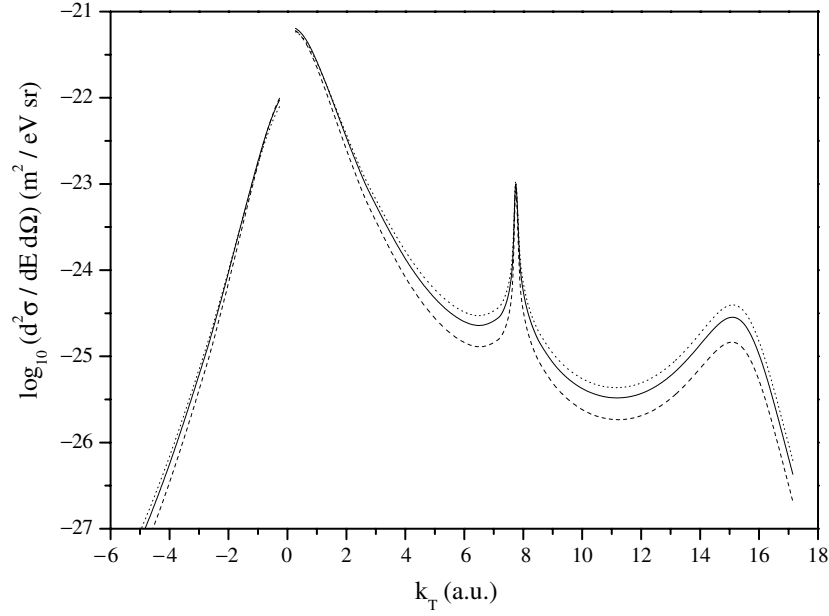
Figure 12. Doubly differential cross section for single ionization of helium by 1.5 MeV amu^{-1} F^{9+} impact in the forward and backward directions, calculated in post CDW–EIS, varying the final state effective charge. $Z_f = 1.6875$: full curve; $Z_f = 1.2$: broken curve; $Z_f = 2.0$: dotted curve.

In this case the final state effective charge does change the result. If the initial effective charge is varied, results similar to figure 10 are obtained. This means that the post version is sensitive to both initial and final wavefunctions. Anyway, good bound states are easily available and they can be easily introduced in CDW–EIS calculations by way of Slater orbital expansions, so that analytical expressions can still be obtained for the transition amplitudes. Unfortunately the same is not true for final continuum states.

5. Conclusions

We have explored post–prior discrepancies within the CDW–EIS theory for ionization. We found that there are no post–prior discrepancies as long as the electron–target initial and final state are exact wavefunctions, such as in ion–hydrogen collisions. The same is true if good numerical wavefunctions are used for multielectronic targets. However, post–prior discrepancies do arise for multielectronic targets, when a hydrogenic continuum with effective charge is used for the final electron–residual target state.

We have found that prior version calculations give generally better results than post version calculations. We think the reason for this behaviour is that the initial bound states in these calculations are qualitatively better wavefunctions than final electron target continuum ones. While post version results rely on the quality of both channels' wavefunctions, we have found that the prior version shows surprisingly little sensitivity to the choice of the final state effective charge. The fact that in this case the perturbation potentials operate upon the initial state suggests that the selection of the initial bound state is relatively more important than the final state for the prior version. Having said that, we acknowledge that there are some regions of the emission spectra which may be particularly sensitive to the final state, such as the low energy emission region, where there is little or no improvement by using the prior version.

Acknowledgments

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