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Post–prior discrepancies in CDW–EIS calculations for ion impact ionization fully differential cross sections

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Abstract
In this work we present fully differential cross sections (FDCSs) calculations using post and prior versions of CDW–EIS theory for helium single ionization by 100 MeV C^{6+} amu^{-1} and 3.6 MeV amu^{-1} Au^{24+} and Au^{53+} ions. We performed our calculations for different momentum transfer and ejected electron energies. The influence of internuclear potential on the ejected electron spectra is taken into account in all cases. We compare our calculations with absolute experimental measurements. It is shown that prior version calculations give better agreement with experiments in almost all studied cases.

1. Introduction

The study of electron emission spectra in ion–atom collisions has been a field of intense activity for years (Stolterfoht *et al* 1997). For intermediate to high-energy single ionization there has been considerable theoretical effort focused in the so-called two-centre electron emission (TCEE) (Fainstein *et al* 1991, Pedersen *et al* 1990). Improvement in the description of the ionized electron moving in the presence of both residual target and projectile fields after the collision (final state) has been the key for the correct description of experimental data (Gulyás *et al* 1995).

Within distorted wave approximations, it has been shown that, at least for high impact energy and multiply charged projectiles, CDW theory of Belkić (1978), used together with an appropriate description of the initial bound and final continuum electron states, yields best results for doubly differential cross sections (DDCSs) (Gulyás and Fainstein 1998, Ciappina *et al* 2003). However, when the projectile impact velocity decreases, the CDW–EIS theory of Crothers and McCann (1983) gives better results, its only difference being the choice of the initial state. Moreover, the CDW–EIS approximation is formally free of criticisms regarding the initial state proper normalization, and the transition amplitudes have not the divergent behaviour that CDW exhibits (Crothers 1982) (although it has been demonstrated that CDW amplitudes are integrable and its DDCSs are well behaved) (Dubé and Dewangan 1995).

The field has experienced a renewed interest as a result of the development of the experimental technique known as COLTRIMS (cold-target recoil-ion momentum spectroscopy) (Moshammer *et al* 1994). With COLTRIMS, the projectile's tiny scattering angle can be obtained indirectly by measuring the ionized electron and recoil ion momenta. Fully differential cross sections (FDCS) for ion impact ionization can be measured now and this constitutes a challenging ground for existing theories (Foster *et al* 2004).

The first measurements of the FDCS, for various momentum transfers and ejected-electron energies, were reported in 2001 by Schulz *et al* for single ionization of helium by 100 MeV amu^{-1} C^{6+}. Theoretical results for this process were made later by Madison *et al* (2002), using several approximation schemes. They obtained reasonable good agreement between experiment and theory in the scattering plane for intermediate momentum transfer, but the theories used were not able to reproduce the measurements for large values of momentum transfer and out of scattering plane.

Subsequently, experiments with other projectiles and energy ranges have been performed. Fischer *et al* (2003) have reported absolute experimental measurements for 2 MeV amu^{-1} C^{6+} single ionization of helium in the scattering plane for various momentum transfers and ejected-electron energies. Foster *et al* (2004) have presented 3DW–EIS results for the single ionization of helium by 3.6 MeV amu^{-1} Au^{24+} and Au^{53+} ions. The 3DW–EIS model is a modified version of the CDW–EIS approximation. A fully quantum mechanical treatment is carried on for the internuclear interaction by explicitly including the corresponding nuclear–nuclear Coulomb distortion in the exit channel, while in the standard CDW–EIS model only an asymptotic eikonal phase is retained for the internuclear distortion in both channels, which is equivalent to an impact parameter treatment of the internuclear motion.

Although the authors found good agreement for 3DW–EIS with 2 MeV amu^{-1} C^{6+} data, the theory did not yield a significant improvement for higher charged ions. Theoretical results calculated by Fischer *et al* (2003) using a CDW–EIS model exhibited differences between experiment and theory on an absolute scale for emission in the scattering plane, defined by the plane containing the initial and final projectile momenta. Their calculations were made using a post version of the CDW–EIS theory and an active electron approximation with hydrogenic wave functions for the initial and final electron states. Indeed, the simplest description for the He bound initial state is to assume that it has one 'active' and one 'passive' electron and that the 'active' electron can be described as moving in the effective Coulomb field of the atomic core with an effective charge chosen either: (a) to reproduce the ionization energy or (b) so that the continuum wave is orthogonal to the initial state.

A more sophisticated description involves the use of full numerical Hartree–Fock wave functions for both initial and final states of the active electron (Gulyás *et al* 1995, Gulyás and Fainstein 1998, Foster *et al* 2004). Hartree–Fock (HF) description, however, does not include proper angular correlations in the initial state, and for large perturbations, there might be the chance that the projectile interacts with more than one electron in a single event. An explicit two-electron description, i.e., a full-blown four-body theory for the collision process might be necessary in that case. Fischer *et al* (2003) concluded that calculating FDCSs for large perturbations and including both the internuclear interaction and numerical HF wave functions is not practical. On the other hand, we have shown that by using the prior version of CDW–EIS together with an appropriate Roothan–Hartree–Fock (RHF) description of the initial state and an effective charge Coulomb wave function for the target-electron continuum, we get similar results to those obtained by using numerical HF wave functions in both channels (Ciappina *et al* 2004), for ion impact helium ionization DDCSs. The reason for this behaviour is that the initial bound states in these calculations (RHF) are qualitatively better wave functions than final electron target continuum ones (effective charge coulomb waves). We have found that the prior version shows 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. We have reported (Ciappina *et al* 2003) that large discrepancies between using HF and Coulomb wave treatment for the final state can instead be found in post CDW–EIS. Large discrepancies can also arise in other theories, in particular in Born-type theories, at the DDCS or FDCS level, and some have been reported (see for example, Madison *et al* 2002). However, we think that our finding at the DDCS level, i.e., that prior CDW–EIS with Coulomb wave functions gives similar results to CDW–EIS with HF numerical wave functions on both channels, deserves to be tested at the FDCS level. Consequently, we will present post and prior CDW–EIS calculations with internuclear interaction between the projectile and the target (N–N interaction) taken into account for helium ion single ionization FDCSs at different perturbation regimes. Atomic units are used throughout unless otherwise stated.

2. Theories

We regard He single ionization as a single electron process and assume that (i) the initial state for the 'active' electron is described by a semi-analytical Rothan–Hartree–Fock scheme using a 5 parameters wave function (Clemente and Roetti 1974) and (ii) in the final state the 'active' target electron moves in the combined Coulomb field of the target core with an effective charge $Z_{\mathrm{eff}} = 1.6875$. The electron–projectile relative motion are represented in a CDW–EIS approach, i.e. one eikonal phase in the entrance channel and a pure Coulomb distortion in the final one. N–N interaction is treated as a pure Coulomb interaction between the projectile with a charge Z_P and the true target core charge, $Z_T = 1$.

N–N interaction is taken into account in the transition amplitude $a_{if}(\boldsymbol{\rho})$, in the usual semi-classical or eikonal approximation, through its multiplication by a phase factor (McCarroll and Salin 1978), which for pure coulomb internuclear interaction results in (Crothers and McCann 1983)

$$a'_{if}(\boldsymbol{\rho}) = \mathrm{i}(\rho v)^{2\mathrm{i}\nu} a_{if}(\boldsymbol{\rho}) \tag{1}$$

where $\nu = Z_P Z_T / v$, v is the velocity of the impinging projectile and ρ is the impact parameter $(\boldsymbol{\rho} \cdot \mathbf{v} = 0)$. $a_{if}(\boldsymbol{\rho})$ $(a'_{if}(\boldsymbol{\rho}))$ is the transition amplitude with (without) internuclear interaction. Using two-dimensional Fourier transforms for the transition amplitude elements, the CDW–EIS transition matrix can be written alternatively as a function of the momentum transfer:

$$T'_{if}(\boldsymbol{\eta}') = \frac{\mathrm{i}v^{2\mathrm{i}\nu}}{(2\pi)^2} \int \mathrm{d}\boldsymbol{\eta}\, T_{if}(\boldsymbol{\eta}) \int \mathrm{d}\boldsymbol{\rho}\, \rho^{2\mathrm{i}\nu} e^{\mathrm{i}(\boldsymbol{\eta}-\boldsymbol{\eta}')\cdot\boldsymbol{\rho}} a_{if}(\boldsymbol{\rho}). \tag{2}$$

We solve the integral over impact parameter analytically to obtain

$$T'_{if}(\boldsymbol{\eta}) = \nu \frac{\mathrm{i}v^{2\mathrm{i}\nu}(2\pi)^{-\mathrm{i}\nu}}{2^4\pi^3} \int \mathrm{d}\boldsymbol{\eta}'\, T_{if}(\boldsymbol{\eta}')|\boldsymbol{\eta} - \boldsymbol{\eta}'|^{-2(1+\mathrm{i}\nu)}. \tag{3}$$

The remaining integral in (3) is evaluated numerically with an adaptive integration scheme. This approximation is valid as long as (i) the projectile suffers very small deflections in the collision and (ii) the velocity of the recoil ion remains small compared to that of the emitted electron.

Within CDW–EIS, the transition amplitude can be computed as

$$T_{if}^{+\mathrm{CDW-EIS}} = \langle \chi_f^{-\mathrm{CDW}} | W_f^{\dagger} | \chi_i^{+\mathrm{EIS}} \rangle \tag{4}$$

in its post version or

$$T_{if}^{-\mathrm{CDW-EIS}} = \langle \chi_f^{-\mathrm{CDW}} | W_i | \chi_i^{+\mathrm{EIS}} \rangle \tag{5}$$

in the prior version, where the initial (final) state distorted wave χ_i^+ (χ_f^-) is an approximation to the initial (final) state which satisfies outgoing-wave (+) (incoming-wave (−)) conditions.

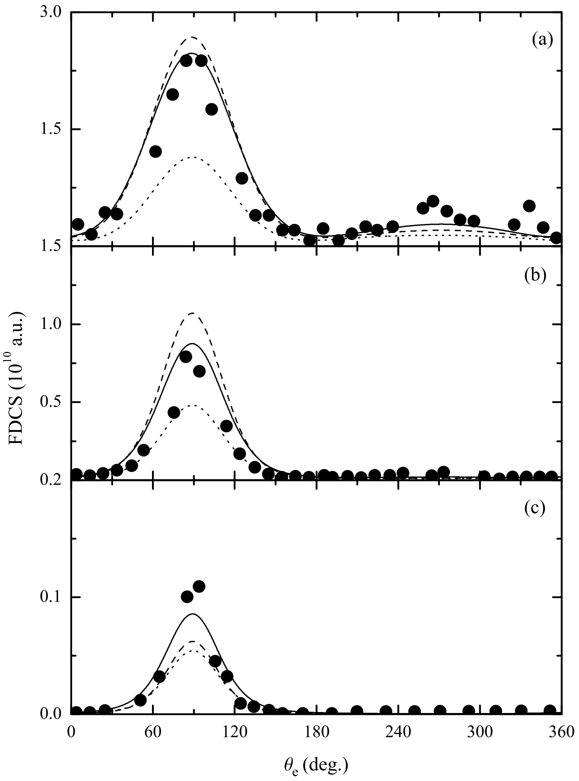

Figure 1. FDCS for 100 MeV amu^{-1} C^{6+} single ionization of helium calculated in prior CDW–EIS: solid line; post CDW–EIS: dashed line; FBA: dotted line; experimental data, (Schulz *et al* 2001) solid circles. (a) $E_e = 6.5$ eV, $|q| = 0.88$ au (b) $E_e = 17.5$ eV, $|q| = 1.43$ au (c) $E_e = 37.5$ eV, $|q| = 2.65$ au.

For the initial state the asymptotic form of the Coulomb distortion (eikonal phase) is used in the electron–projectile interaction together with a semi-analytical Rothan–Hartree–Fock description for the initial bound-state wave function (Clementi and Roetti 1974)

$$\chi_i^{+\mathrm{EIS}} = (2\pi)^{-3/2} \exp(\mathrm{i}\mathbf{K}_i \cdot \mathbf{R}_T)\psi_{1s}(\mathbf{r}_T)\mathcal{E}_v^+(\mathbf{r}_P) \tag{6}$$

where $\mathcal{E}_v^+(\mathbf{r}_P)$ is

$$\mathcal{E}_v^+(\mathbf{r}_P) = \exp\left(-\mathrm{i}\frac{Z_P}{v}\ln(vr_P - \mathbf{v}\cdot\mathbf{r}_P)\right). \tag{7}$$

The final state wave function is collected into the form (Rosenberg 1973, Garibotti and Miraglia 1980, Crothers and McCann 1983)

$$\chi_f^{-\mathrm{CDW}} = (2\pi)^{-3/2} \exp(\mathrm{i}\mathbf{K}_f \cdot \mathbf{R}_T)\chi_T^-(\mathbf{r}_T)C_P^-(\mathbf{r}_P) \tag{8}$$

where C_P^- represents the Coulomb distortion of the ejected electron wave function due to the projectile coulomb potential.

$$C_P^-(\mathbf{r}_P) = N(\nu_P)\,{}_1F_1(-\mathrm{i}\nu_P, 1, -\mathrm{i}k_P r_P - \mathrm{i}\mathbf{k}_P \cdot \mathbf{r}_P) \tag{9}$$

being $\nu_P = \frac{Z_P}{k_P}$ the Sommerfeld parameter, and $\mathbf{k}_P$ is the relative momentum of the e-P subsystem. The ${}_1F_1$ is the Kummer function and $N(\nu_P)$ is the usual normalization factor

$$N(\nu_P) = \Gamma(1 - \mathrm{i}\nu_P)\exp(\pi\nu_P/2) \tag{10}$$

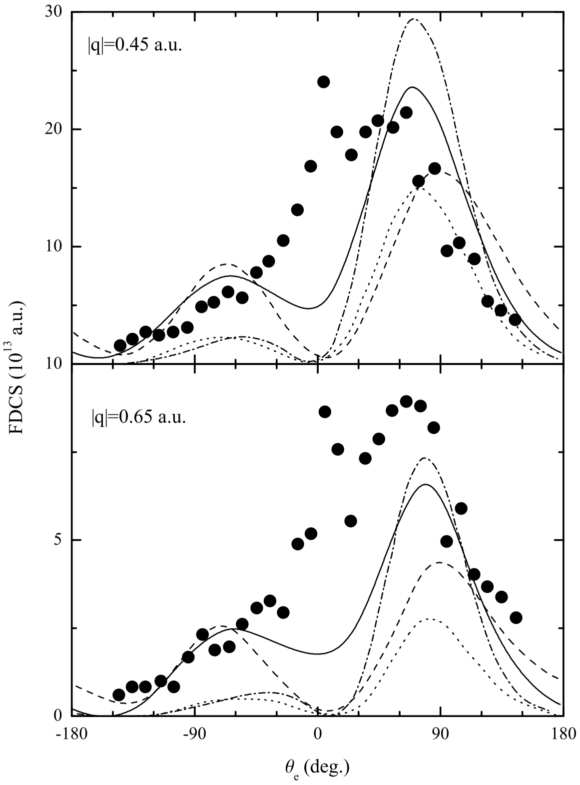

Figure 2. FDCS for 3.6 MeV amu^{-1} Au^{24+} single ionization of helium for $E_e = 4$ eV. Prior CDW–EIS: solid line; post CDW–EIS: dashed line; CDW–EIS (Fischer *et al* 2003): dash-dotted line; 3DW–EIS (Foster *et al* 2004): dotted line; experimental data (Fischer *et al* 2003): solid circles. Note that the angle of electron emission has been changed with respect to the other figures and now is measured in a range of $-180°$ to $+180°$, 0° being the direction of the incoming projectile.

Γ being the gamma function. On the other hand $\chi_T^-(\mathbf{r}_T)$ is the wave function for the ejected electron in the field of the target residual ion.

$$\chi_T^-(\mathbf{r}_T) = (2\pi)^{-3/2}\exp(\mathrm{i}\mathbf{k}_T\cdot\mathbf{r}_T)N(\nu_T)\,{}_1F_1(-\mathrm{i}\nu_T, 1, -\mathrm{i}k_T r_T - \mathrm{i}\mathbf{k}_T\cdot\mathbf{r}_T) \tag{11}$$

being $\nu_T = \frac{Z_T}{k_T}$ and now $\mathbf{k}_T$ is the relative momentum of the e-T subsystem. We use $Z_T = Z_{\mathrm{eff}} = 1.6875$ to model the screened target residual ion as a pure Coulomb potential.

The perturbation potentials W_f in equation (4) and W_i in (5) are defined by

$$(H_f - E_f)\chi_f^- = W_f\chi_f^- \tag{12}$$

and

$$(H_i - E_i)\chi_i^+ = W_i\chi_i^+ \tag{13}$$

where H_f (H_i) are the full electronic final (initial) Hamiltonian (neglecting the total centre-of-mass motion) and E_f (E_i) are the total final (initial) energy of the system in the cm frame, respectively.

The explicit forms of these operators can be written (Crothers and Dubé 1992)as

$$W_f = -\nabla_{\mathbf{r}_T}\cdot\nabla_{\mathbf{r}_P} \tag{14}$$

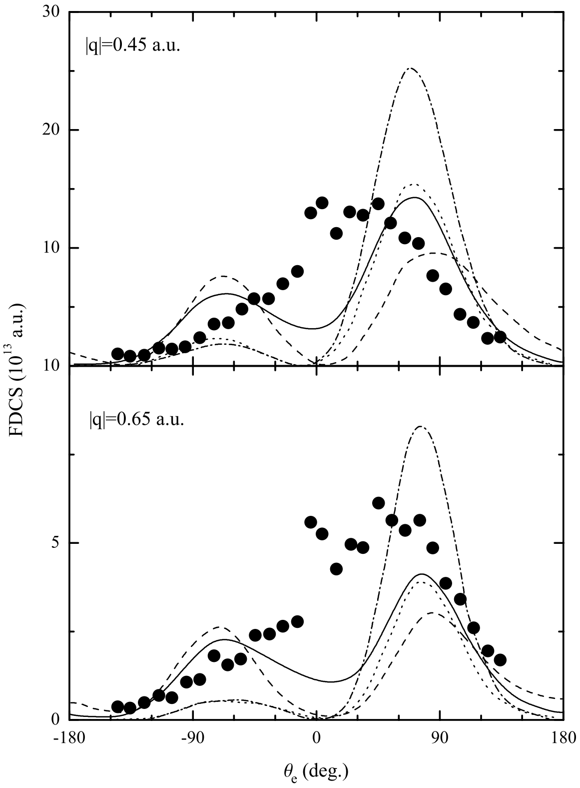

Figure 3. Same as in figure 3 for $E_e = 10$ eV.

and

$$W_i = \tfrac{1}{2}\nabla^2_{\mathbf{r}_P} - \nabla_{\mathbf{r}_T} \cdot \nabla_{\mathbf{r}_P}. \tag{15}$$

In the centre-of-mass frame, the FDCS in energy and ejection angle of the electron and direction of the outgoing projectile is given by (Berakdar *et al* 1989, Inokuti 1971, Bethe 1930)

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}E_k\,\mathrm{d}\Omega_k\,\mathrm{d}\Omega_K} = N_e(2\pi)^4\mu^2 k\frac{K_f}{K_i}|T_{if}|^2\delta(E_f - E_i) \tag{16}$$

where N_e is the number of electrons in the atomic shell, μ is the reduced mass of the projectile-target subsystem, $K_i(K_f)$ is the magnitude of the incident particle initial (final) momentum. 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 use non-orthogonal Jacobi coordinates $(\mathbf{r}_P, \mathbf{r}_T)$ to outline the collision process. These coordinates are the position of the active electron with respect to the projectile $(\mathbf{r}_P)$ and to the target ion $(\mathbf{r}_T)$ respectively. Also the coordinate $\mathbf{R}_T$ is needed, that represents the position of the incoming projectile with respect to the centre of mass of the subsystem e-T. If we neglect terms of order $1/M_T$ and $1/M_P$, where M_T is the mass of the target ion nucleus and M_P is the corresponding to the incident heavy ion, we can write $\mathbf{R}_T = \mathbf{r}_T - \mathbf{r}_P$.

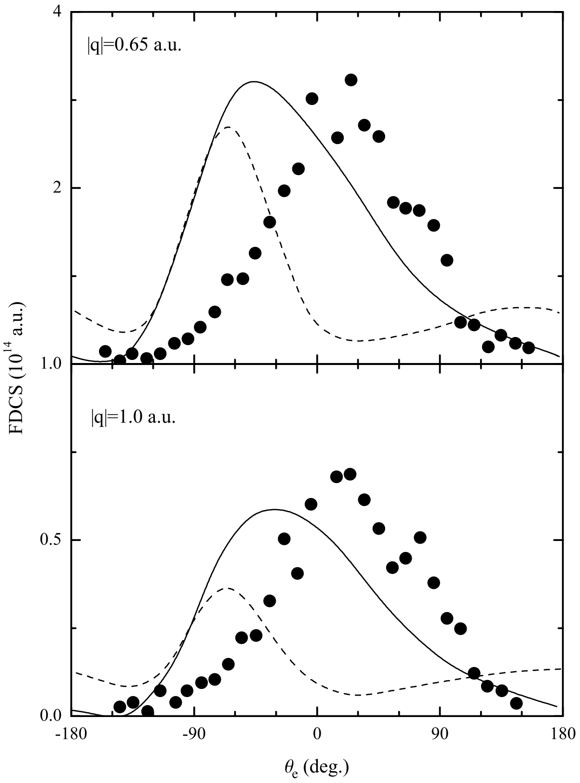

Figure 4. FDCS for 3.6 MeV amu^{-1} Au^{53+} single ionization of helium for $E_e = 4$ eV. Prior CDW–EIS: solid line; post CDW–EIS: dashed line; experimental data: (Fischer *et al* 2003) solid circles.

We have replaced the transition matrix in the post and prior schemes (equations (4) and (5)) in the definition of FDCS (16) and we have applied it to several single ionization processes.

3. Results

We have performed calculations for different projectiles, spanning a large range of perturbation strengths as measured by charge to velocity ratio $\eta = Z_P/v$. In figure 1 we present results for 100 MeV amu^{-1} C^{6+} (Schulz *et al* 2001) single ionization of helium calculated in prior and post CDW–EIS and also using for comparison FBA approximation, for different values of electron emission energy (E_e) and momentum transfer ($\mathbf{q} = \mathbf{K}_i - \mathbf{K}_f$). We see that prior CDW–EIS gives the best results in all cases studied here. Even when $\eta = 0.1$ both FBA and post CDW–EIS fail to accurately describe the experimental results, although they broadly reproduce the angular distribution.

Figures 2 and 3 show results for 3.6 MeV amu^{-1} Au^{24+} impact ionization of He (Fischer *et al* 2003), calculated in prior and post CDW–EIS. For $E_e = 4.0$ eV, results for the prior version are in reasonable agreement with experiment. However, both theories fail to correctly reproduce the strong forward emission peak. As was pointed out by Foster *et al* 2004, the electron–projectile interaction is taken into account in CDW–EIS at all orders, and so the strong projectile–electron post collisional interaction should account for the forward peak, and still

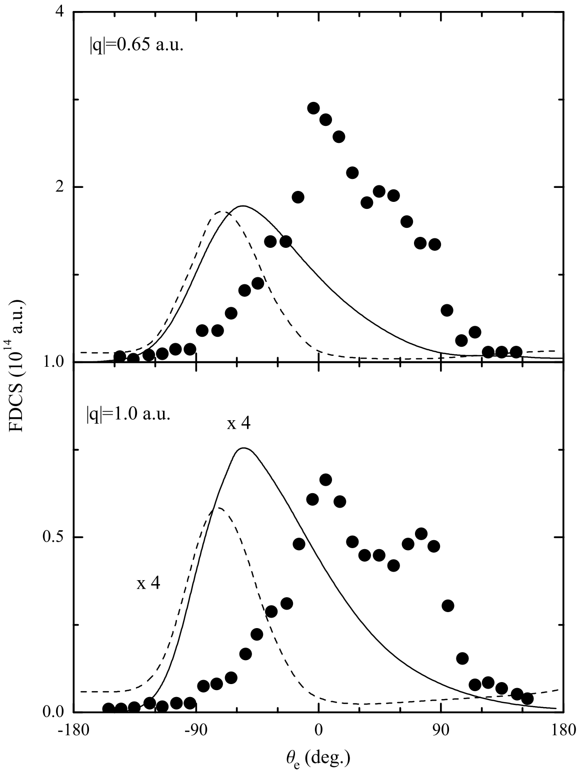

Figure 5. Same as in figure 5 for $E_e = 10$ eV.

does not. However, it should be stressed that first order distorted wave theories are not in this case within their validity range. In fact it is surprising that they still yield reasonable results. Two possible explanations for the lack of the forward peak are that higher order distorted wave theories are needed (due to the high perturbation that multicharged projectile implies) or that polarization of the target (which should be large) needs to be considered in the entrance channel. Trend is similar for $E_e = 10.0$ eV, (figure 3) where we see a better performance in prior version calculations, in particular in the prediction of the direct peak position. Note that no renormalization factor is included in these calculations. For comparison we also show CDW–EIS calculations by Fischer *et al* 2003, and 3DW–EIS calculations by Foster *et al* (2004). Discrepancies between CDW–EIS calculations are evident. However, while our calculations are made with RHF wave functions for the helium ground state, those reported by Fischer have hydrogenic wave functions both for initial and final electron states.

In figures 4 and 5 we show prior and post CDW–EIS calculations for 3.6 MeV amu^{-1} Au^{53+} impact ionization of He. Even when we are stretching the validity range of the perturbative treatment ($\eta \approx 2, 4.4$ for Au^{24+} and Au^{53+} projectiles respectively), angular structure with only one strong peak is correctly predicted in the prior version while the post version of the theory predicts two distinct direct and recoil peaks. However, the angular position of the peak given by the prior version does not agree with the experimental data, probably due to the same causes as in the previous case. Both versions including N–N interaction fail to yield the correct order of magnitude of experimental data. Large projectile charges are likely to induce quite a large polarization in the target. Effective charges both for residual target–electron and

N–N interactions are probably not the same than for lower charged projectiles, and it is indeed very probable that the effective charge approach is not a good approximation here. Model potentials taking into account polarization effects need to be considered for the target, at least in the exit channel, but most probably in both initial and final states.

4. Conclusions

We have performed FDCSs calculations for highly charged ion impact ionization of helium. We employed prior and post versions of CDW–EIS theories taken into account N–N interaction but otherwise using as simple an approach for electronic wave functions as possible. Indeed, the use of prior version helps us to avoid the need of more precise wave functions for the initial or final electronic state. We found reasonably good agreement with experimental data, even for projectile charges for which the system is arguably outside the range of validity of a perturbative theory.

We see that for emission in the collision plane, three-body dynamics seems to be enough to explain most of the structures observed for low energy emission and low projectile charge. For Au^{24+} and Au^{53+} projectiles the larger emission in the forward direction is not well reproduced by the theory but, as said before, those cases are outside the range where perturbative treatments are known to be valid. However, if the effect of target polarization in the entrance channel and the inclusion of higher orders in the exit channel distortions are taken into account, perturbation based calculations could probably be brought closer to experimental results. As expected, we found that large post–prior discrepancies arise in FDCSs for CDW–EIS theory if different approaches are used for initial and final wave functions.

Acknowledgments

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