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Fully differential cross sections for C^{6+} single ionization of helium: the role of nucleus–nucleus interaction

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Abstract

In this work, we present fully differential cross section (FDCS) calculations using distorted wave theories for helium single ionization by 2 MeV amu^{-1} C^{6+} ions. We study the influence of internuclear interaction on low-energy electron emission in the scattering plane. It is shown that by incorporating an internuclear effective charge which depends on the collision momentum transfer and taking into account its interplay with passive electron screening we obtain better agreement with experiments in most cases under consideration. Comparisons are made with absolute experimental measurements and with other theories. We found that for ejected-electron momentum similar to transferred momentum, internuclear potential effects have little contribution to FDCSs.

1. Introduction

The field of ionization by ion impact now has 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). As is already well known, with COLTRIMS the projectile's tiny scattering angle can be obtained indirectly by measuring the ionized electron and recoil ion momenta. Consequently, fully differential cross sections (FDCSs) for ion impact ionization can now be measured and constitute a challenging ground for existing theories (Foster *et al* 2004a). The first measurements of FDCSs, for various momentum transfers and ejected-electron energies, were reported in 2001 by Schulz *et al* for single ionization of helium by C^{6+} 100 MeV amu^{-1}.

Consequently, experiments using other projectiles and energy ranges have been performed. Fischer *et al* (2003) have reported absolute experimental measurements for C^{6+} 2 MeV amu^{-1} single ionization of helium in the scattering plane, defined by the plane containing the initial

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and final projectile momenta, for various momentum transfers and ejected-electron energies. Theoretical results reported in this work using a CDW–EIS model exhibited differences between experiment and theory on an absolute scale for emission in the scattering plane. Their calculations were made using the active electron approximation and hydrogenic wavefunctions for the initial and final states of the active electron (Fischer *et al* 2003). Indeed, the simplest description for the helium 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 (a) to reproduce the ionization energy or (b) so that the continuum wave is orthogonal to the initial state (Foster *et al* 2004a, Ciappina and Cravero 2006).

Of course, a more sophisticated way is to apply a Hartree–Fock (HF) description for both initial and final states of the active electron (Gulyás *et al* 1995, Gulyás and Fainstein 1998). HF wavefunctions, however, still do 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, might be necessary in that case.

The effects of the internuclear potential (N–N interaction) in ionization by ion impact within the framework of distorted wave theories are still a somewhat controversial topic. There have been several models to take into account N–N interaction, but none of them has been able to reproduce the experimental data in the whole range of parameters studied. It has been shown that high-energy projectiles can 'see' regions very close to the target nucleus and therefore the perturbative or Born series approach might not be adequate to describe this interaction (Madison *et al* 2003).

In the early computational days, a semi-classical approach was developed (McCarroll and Salin 1978) and various schemes based on it have been in use since then (Rodríguez 1996, Sánchez *et al* 2000).

Nowadays, due to the steady increase in computational power, all the interactions between pairs of particles in a single collision process can be put on 'equal footing'. One of the latest approaches developed in this direction is the so-called 3DW–EIS by Foster *et al* (2004a). In this model, the N–N interaction is taken into account by a Coulomb wavefunction for the final state and an eikonal phase for the initial one. The consequent FDCS is numerically calculated using quadratures. However, even this sophisticated theory is not able to completely reproduce the experimental data available (Foster *et al* 2004b).

Before COLTRIMS experiments (Moshammer *et al* 1994), the influence of the internuclear potential was usually overlooked since ionization double differential cross sections (DDCSs) in electron energy and angle do not depend (to the first order in $1/M_{T,P}$) on this interaction, as it incorporates only a phase to the transition amplitude (Fainstein *et al* 1991).

On the other hand, for other differential cross sections in terms of projectile scattering angle or recoil ion momentum, it has been shown that the N–N interaction has a relevant influence depending on the ejected-electron energies and momentum transfer values (Moshammer *et al* 2001, Sánchez *et al* 2000, Rodríguez and Barrachina 1998, Fainstein and Gulyás 2005).

Our aim is to explore the role of internuclear interaction in FDCSs for highly charged ion impact electron emission. We will incorporate this interaction in a semi-classical way, using a dynamical effective charge to model the interaction between the projectile and the residual ion core. In the following section, we briefly describe the dynamic effective charge for the N–N interaction. We will use this model together with prior CDW–EIS theory (Ciappina *et al* 2003) to perform calculations for C^{6+} 2 MeV amu^{-1} ion single ionization of helium. Atomic units are used throughout unless otherwise stated.

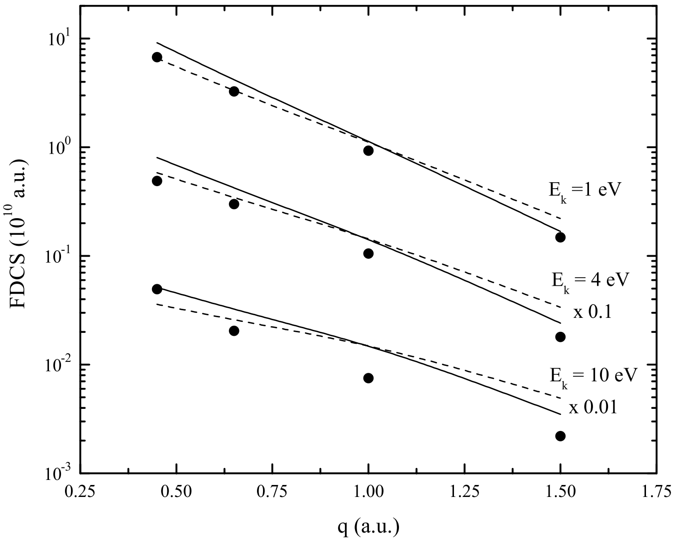

Figure 1. FDCS for C^{6+} 2 MeV amu^{-1} single ionization of helium as a function of q for different emitted electron energies in the binary peak direction. Solid line: prior CDW–EIS with 'static' N–N interaction; dashed line: prior CDW–EIS without N–N interaction.

2. Theories

We regard helium single ionization as a single electron process and assume that in the final state the 'active' target electron moves in the combined Coulomb field of the impinging projectile and the residual target core with a given effective charge that takes into account the partial screening due to the other helium electron as considered within the prior CDW–EIS approach. Within it, electron–projectile interaction is represented by a pure Coulomb distortion in the final state and by an eikonal phase in the entrance channel (Crothers and McCann 1983). N–N interaction is usually treated as a pure Coulomb interaction between a projectile with charge Z_P and the 'true' target core charge, $Z_T = 1$. This approximation is fairly good for low charge projectiles. However, multicharged ions may induce large polarizations in the target, modifying the screening due to passive electrons (and potentially also the active one). This effect will naturally depend on the projectile impact parameter.

In figures 1 and 2 we present FDCS calculations for C^{6+} 2 MeV amu^{-1} made in prior CDW–EIS approximation as a function of the projectile momentum transfer $q(\mathbf{q} = \mathbf{K}_i - \mathbf{K}_f, \mathbf{K}_i$ $(\mathbf{K}_f)$ being the initial (final) momentum of the incident particle) with and without the usual N–N interaction taken into account, and for electron emission corresponding to binary and recoil peaks, respectively. We see that for low emission energy and small momentum transfer, experimental data are better described by the theory without N–N interaction. As momentum transfer increases, experiment is better described if N–N interaction is accounted for in the prior CDW–EIS model.

At least for low-energy emission, it looks as if the internuclear interaction is gradually switched on as momentum transfer increases. This behaviour suggests that for large impact parameters both target electrons participate in the screening and the projectile does not 'see' the target nucleus. Large momentum transfer on the other hand corresponds to smaller impact parameters; the target electrons screening (particularly the ejected-electron screening) is not so effective in this case and the N–N interaction becomes increasingly important.

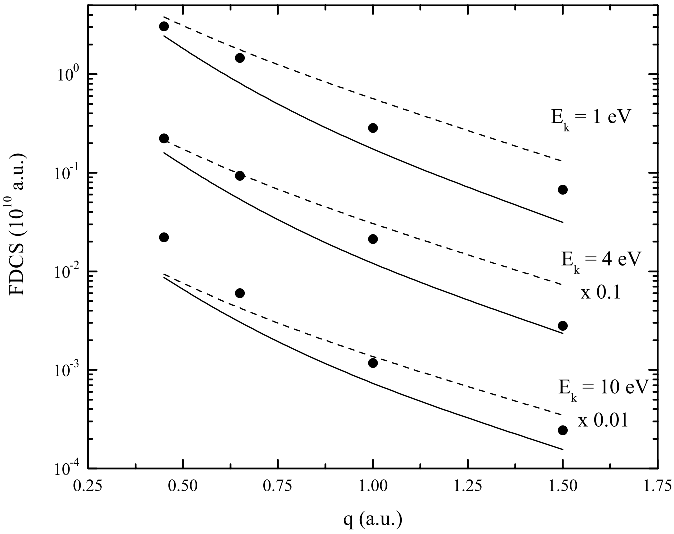

Figure 2. FDCS for C^{6+} 2 MeV amu^{-1} single ionization of helium as a function of q for different emitted electron energies in the recoil peak direction. Solid line: prior CDW–EIS with 'static' N–N interaction; dashed line: prior CDW–EIS without N–N interaction.

We will thus choose to treat N–N interaction as a pure Coulomb potential between the projectile with charge Z_P and a target core charge Z_T which depends on the magnitude of the perpendicular momentum transfer η. For high-energy ion–atom collisions $\mathbf{q}$ can be written using two suitable orthogonal coordinates, i.e. $\mathbf{q} \approx \boldsymbol{\eta} + \frac{\Delta\epsilon}{v^2}\hat{\mathbf{v}}$, with $\Delta\epsilon = k_T^2/2 - \epsilon_i$ being the ionized electron energy difference and v and $\hat{\mathbf{v}}$ the magnitude and direction of the projectile velocity, respectively. Note that $\boldsymbol{\eta}\cdot\hat{\mathbf{v}} = 0$. To some extent we can say that this charge is a function of the impact parameter through the projectile scattering angle, since for small angles we can write $\theta_s \approx \eta/M_P v$, with M_P being the projectile mass (Stolterfoht *et al* 1997).

As we are interested in soft electron emission by swift projectiles, the internuclear screening is not only due to the passive electron but also by the active one, which ends in a low lying continuum. This effective charge is obtained within the first Born approximation and can be written (Bransden and Joachain 2003, Rodríguez 2003) as

$$Z_T(\eta) = Z_{\mathrm{eff}}^T - 16\frac{Z_{\mathrm{eff}}^{T\,4}}{\left[4Z_{\mathrm{eff}}^{T\,2} + \eta^2\right]^2} \tag{1}$$

where Z_{eff}^T is the target ion effective charge that takes into account the presence of the passive electron. In figure 3 we can see the behaviour of $Z_T(\eta)$ as a function of η. We use different values of Z_{eff}^T to model the electronic screening. If we analyse the limits of $Z_T(\eta)$ we can observe that for small values of η the projectile 'sees' a small charge due to the partial screening by the two electrons and feels the usual effective charge when the deflection angle is large, i.e. for large values of η.

N–N interaction is then included in the transition amplitude $a_{if}(\boldsymbol{\rho})$, in the 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, Stolterfoht *et al* 1997)

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

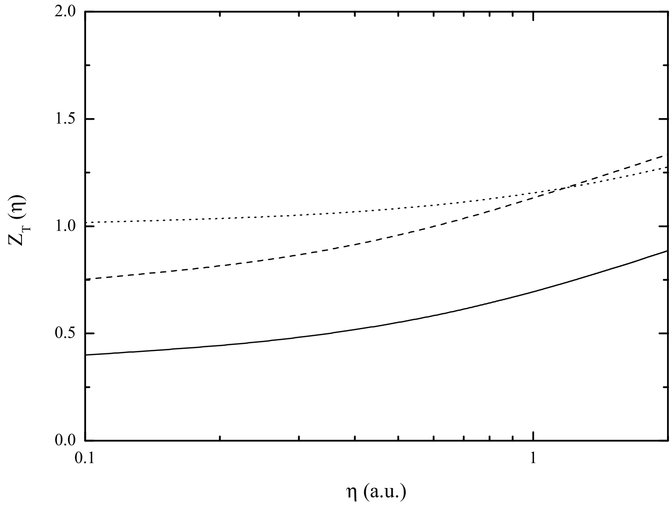

Figure 3. Dynamic screened charge $Z_T(\eta)$ of the target in the interaction with the projectile, for different values of $Z_{\rm eff}^T$. Solid line: $Z_{\rm eff}^T = 1.3549$; dashed line: $Z_{\rm eff}^T = 1.6875$; dotted line: $Z_{\rm eff}^T = 2$.

where $\nu = Z_P Z_T(\eta)/v$, $Z_T(\eta)$ is calculated from (1) and $\boldsymbol{\rho}$ defines 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 transition matrix can be written alternatively as a function of the perpendicular momentum transfer $\boldsymbol{\eta}$:

$$T_{if}(\boldsymbol{\eta}) = \frac{\mathrm{i}v^{2\mathrm{i}\nu}}{2\pi}\int \mathrm{d}\boldsymbol{\rho}\,\rho^{2\mathrm{i}\nu}\,\mathrm{e}^{\mathrm{i}\boldsymbol{\eta}\cdot\boldsymbol{\rho}} a'_{if}(\boldsymbol{\rho}), \tag{3}$$

$$T'_{if}(\boldsymbol{\eta}) = \frac{1}{2\pi}\int \mathrm{d}\boldsymbol{\rho}\,\mathrm{e}^{\mathrm{i}\boldsymbol{\eta}\cdot\boldsymbol{\rho}} a'_{if}(\boldsymbol{\rho}). \tag{4}$$

Applying the inverse Fourier transform of (4) and replacing in (3), we have

$$T_{if}(\boldsymbol{\eta}) = \frac{\mathrm{i}v^{2\mathrm{i}\nu}}{(2\pi)^2}\int \mathrm{d}\,\boldsymbol{\eta}'\,T'_{if}(\boldsymbol{\eta}')\int \mathrm{d}\boldsymbol{\rho}\,\rho^{2\mathrm{i}\nu}\,\mathrm{e}^{\mathrm{i}(\boldsymbol{\eta}-\boldsymbol{\eta}')\cdot\boldsymbol{\rho}}. \tag{5}$$

The integral over impact parameter can be done analytically to obtain (Sánchez *et al* 2000)

$$T_{if}(\boldsymbol{\eta}) = \nu\frac{\mathrm{i}v^{2\mathrm{i}\nu}(2\pi)^{-\mathrm{i}\nu}}{2^4\pi^3}\int \mathrm{d}\boldsymbol{\eta}'\,T'_{if}(\boldsymbol{\eta}')|\boldsymbol{\eta}-\boldsymbol{\eta}'|^{-2(1+\mathrm{i}\nu)}. \tag{6}$$

The remaining integral in (6) is evaluated numerically with an adaptive integration scheme when the parameter ν is larger than some limit value $\nu_{\rm max}$. 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.

In the centre of mass (CM) frame, the FDCS in energy and ejection angle of the electron, and direction of the outgoing projectile is given by (Bethe 1930, Inokuti 1971, Berakdar *et al* 1993)

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}E_k\,\mathrm{d}\Omega_k\,\mathrm{d}\Omega_K} = N_e(2\pi)^4\mu^2 k_T\frac{K_f}{K_i}|T_{if}|^2\delta(E_f - E_i) \tag{7}$$

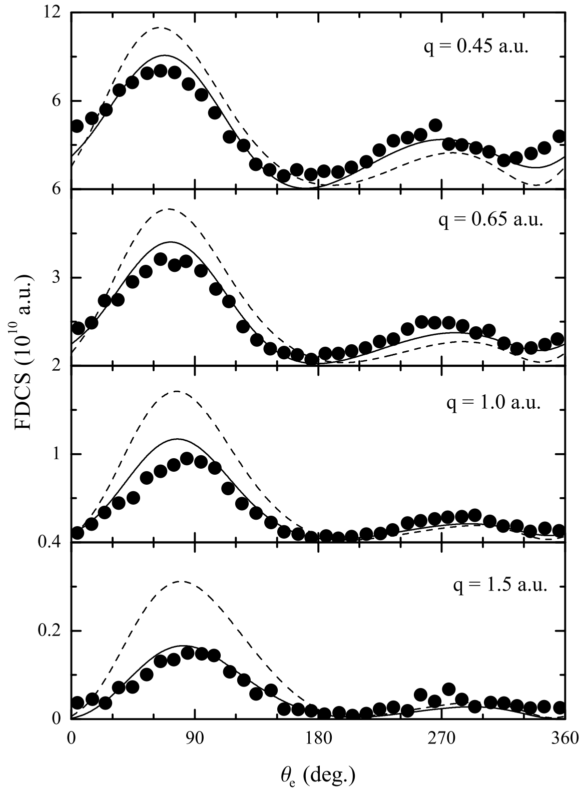

Figure 4. FDCS for C^{6+} 2 MeV amu^{-1} single ionization of helium calculated for $E_k = 1$ eV. Solid line: prior CDW–EIS using the dynamic charge (1); dashed line: prior CDW–EIS using a 'static' charge $Z_T = 1$; solid circles: experimental data (Fischer *et al* 2003).

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_T respectively. The solid angles $d\Omega_K$ and $d\Omega_k$ 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 describe the collision process. These coordinates represent the position of the active electron with respect to the projectile $(\mathbf{r}_P)$ and the target ion $(\mathbf{r}_T)$ respectively. $\mathbf{R}_T$ is also needed, representing the position of the incoming projectile with respect to the CM 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 that of the incident heavy ion, we can write $\mathbf{R}_T = \mathbf{r}_T - \mathbf{r}_P$.

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

$$T_{if}^{-\text{CDW}-\text{EIS}} = \left\langle \chi_f^{-\text{CDW}} \middle| W_i \middle| \chi_i^{+\text{EIS}} \right\rangle \tag{8}$$

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. 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 wavefunction (Clementi and Roetti 1974)

$$\chi_i^{+\text{EIS}} = (2\pi)^{-3/2} \exp(\text{i}\mathbf{K}_i \cdot \mathbf{R}_T)\, \psi_{1s}(\mathbf{r}_T)\mathcal{E}_v^+(\mathbf{r}_P) \tag{9}$$

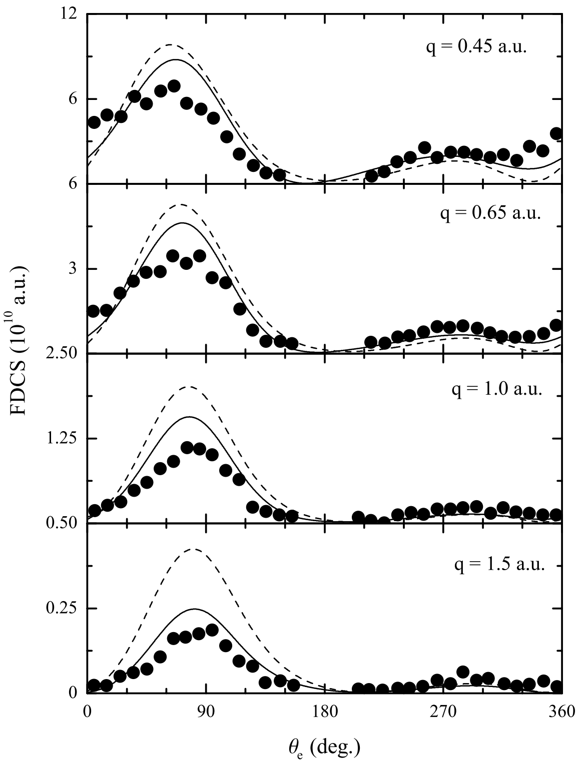

Figure 5. Same as in figure 4 for $E_k = 4$ eV.

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

$$\mathcal{E}_v^+(\mathbf{r}_P) = \exp\left(-\mathrm{i}\frac{Z_P}{v}\ln\left(vr_P - \mathbf{v}\cdot\mathbf{r}_P\right)\right). \tag{10}$$

The final state wavefunction is cast into the form (Rosenberg 1973, Garibotti and Miraglia 1980, Crothers and McCann 1983)

$$\chi_f^{-\mathrm{CDW}} = (2\pi)^{-3/2}\exp(\mathrm{i}\mathbf{K}_f\cdot\mathbf{R}_T)\chi_T^-(\mathbf{r}_T)C_P^-(\mathbf{r}_P) \tag{11}$$

where C_P^- represents the Coulomb distortion of the ejected-electron wavefunction due to the projectile,

$$C_P^-(\mathbf{r}_P) = N(\nu_P)\ {}_1F_1\left(-\mathrm{i}\nu_P, 1, -\mathrm{i}k_Pr_P - \mathrm{i}\mathbf{k}_P\cdot\mathbf{r}_P\right) \tag{12}$$

with $\nu_P = \frac{Z_P}{k_P}$ being the Sommerfeld parameter, $\mathbf{k}_P$ is the relative momentum of the e–P subsystem and $N(\nu_P)$ is the usual Coulomb factor

$$N(\nu_P) = \Gamma(1-\mathrm{i}\nu_P)\exp(\pi\nu_P/2). \tag{13}$$

On the other hand $\chi_T^-(\mathbf{r}_T)$ is the wavefunction for the ejected electron in the field of the target residual ion,

$$\chi_T^-(\mathbf{r}_T) = (2\pi)^{-3/2}\exp\left(\mathrm{i}\mathbf{k}_T\cdot\mathbf{r}_T\right)N(\nu_T)_1F_1\left(-\mathrm{i}\nu_T, 1, -\mathrm{i}k_Tr_T - \mathrm{i}\mathbf{k}_T\cdot\mathbf{r}_T\right) \tag{14}$$

with $\nu_T = \frac{Z_T}{k_T}$ and where $\mathbf{k}_T$ is the relative momentum of the e–T subsystem.

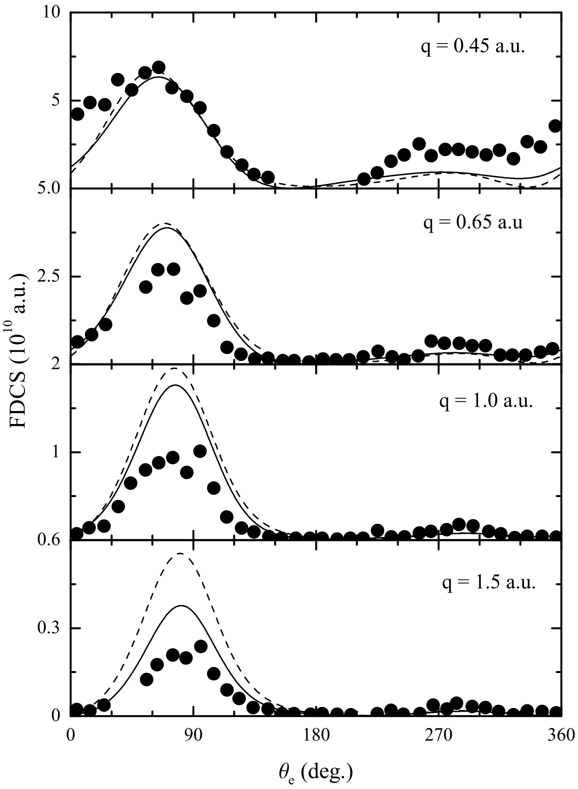

Figure 6. Same as in figure 4 for $E_k = 10$ eV.

The perturbation potential W_i in (8) is defined by

$$(H_i - E_i)\chi_i^+ = W_i \chi_i^+ \tag{15}$$

where H_i is the full electronic initial Hamiltonian (neglecting the total CM motion) and E_i is the total initial energy of the system in the CM frame. W_i consists of two differential operators that can be written as (Crothers and Dubé 1992)

$$W_i = \frac{1}{2}\nabla^2_{\mathbf{r}_P} - \nabla_{\mathbf{r}_T} \cdot \nabla_{\mathbf{r}_P}. \tag{16}$$

We compute the FDCS, equation (7) for single ionization of helium, using the prior CDW–EIS scheme (8) together with the dynamical model for the internuclear charge, equation (1) in the semi-classical approach.

3. Results

Among the numerous experimental data available we have chosen one experiment taking into account (a) the validity range of the CDW–EIS theory and (b) where does the usual 'static' scheme fail. In this sense, we apply our model for C^{6+} 2 MeV amu^{-1} single ionization of helium.

In figure 4 we present results for C^{6+} 2 MeV amu^{-1} single ionization of helium calculated in prior CDW–EIS, for ejected electrons emitted into the scattering plane with energy $E_k = 1$ eV and various values of momentum transfer q (Fischer *et al* 2003).

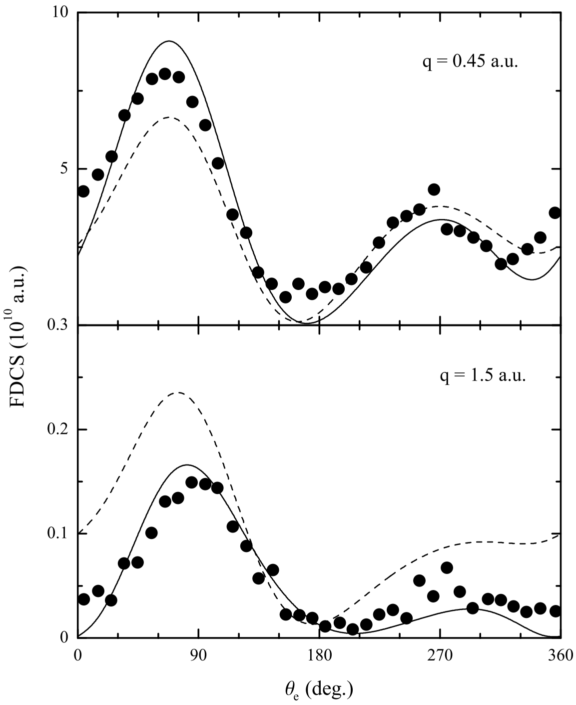

Figure 7. FDCS for C^{6+} 2 MeV amu^{-1} single ionization of helium calculated for $E_k = 1$ eV. Solid line: prior CDW–EIS using the dynamic charge (1); dashed line: prior CDW–EIS without N–N interaction; solid circles: experimental data (Fischer *et al* 2003).

The experimental data show the usual structures for these processes: a large binary peak near the **q** direction, and the smaller recoil peak in the vicinity of −**q** direction, produced by a double scattering mechanism, i.e. the electron first collides with the projectile and afterwards it is scattered off the target nucleus. We observe that our model reproduces very well these two structures in contrast with the static one, which does not account for the magnitude of the peaks in all cases. We can say that to some extent the internuclear charge seems ‘overestimated’ in the static model.

We performed calculations for the same process but for electron emission energy $E_k = 4$ eV. The results are displayed in figure 5. The behaviour of the theories is similar to the first case, and our screened model reproduces reasonably well the FDCS and its structures for the whole range of q values considered. We note that difference between our model and the standard N–N is smaller here for low q and increases with q.

In figure 6 we show calculations for $E_k = 10$ eV. The trend of the theories is comparable to the former cases considered, but here our screened model does not behave as well as for a smaller emission energy. A larger energy of the ejected electron needs to be taken into account here.

In figures 7 and 8 we compare our theory with prior CDW–EIS calculations without N–N interaction. We observe that CDW–EIS calculation without N–N interaction gives better results for those momentum transfers that correspond, or are close to, ‘binary encounter’ conditions, i.e., where the electron is ejected with a momentum close to that transferred by the projectile. For 1 eV emission energy, this corresponds to a $k_T \approx 0.27$ au, so the condition

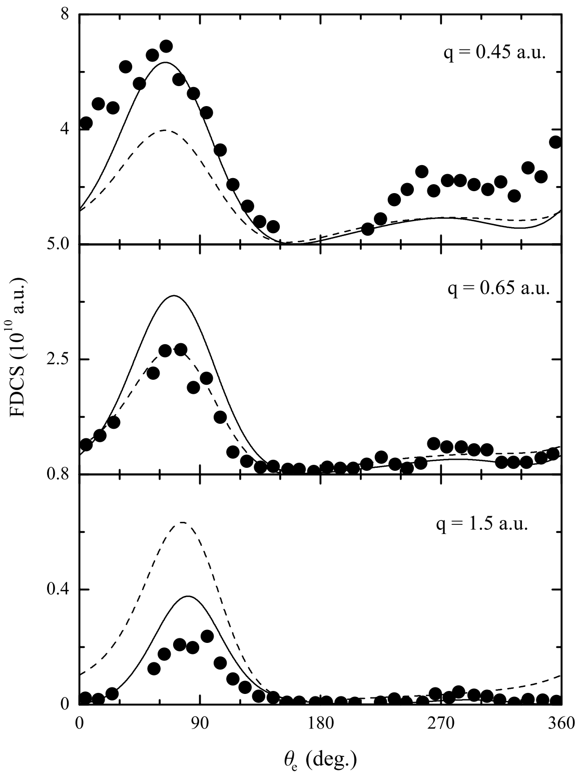

Figure 8. Same as in figure 7 for $E_k = 10$ eV.

is better fulfilled in figure 7 for $q = 0.45$ au. In figure 8 emission energy corresponds to $k_T \approx 0.85$ au and the nearer set is $q = 0.65$ au, where again calculations without N–N interaction give very good agreement. In that condition, the recoil ion's role is minimum and the internuclear potential role is also minimum. N–N interaction is of course not necessary to have a true three-body interaction during the collision process. The interaction of the outgoing electron with the residual target is taken into account in standard CDW–EIS calculations (even in FBA calculations, as long as Coulomb wavefunctions are used for the ejected electron). Two-step scattering processes where all three partners play a role are accounted for, where the electron is first scattered by the incoming projectile and then bounces off the He^+ residual target ion. However, internuclear potential inclusion opens a second 'two-step' process in which part of the momentum is transferred to the active electron and then (or before) the projectile is scattered off the target nucleus. We realize that this is a semi-classical picture probably more suitable for a higher electron emission energy, and of course other purely quantum mechanisms do play an important role here. As projectile velocities are high and ejected-electron velocity is low, electrons may be screening N–N interaction so their inclusion should be more important for close collisions, or large momentum transfer, as it seems to be the case.

Calculations show, however, that for emission energy above 10 eV and small enough momentum transfer, internuclear potential plays again an important role and cannot be neglected, as can be seen in figure 8 for $q = 0.45$ au. We note that this would be in line with reports for DDCSs (Fainstein and Gulyás 2005).

4. Conclusions

We have shown that taking into account a simple dynamical model for the internuclear effective charge in the eikonal model, given by equation (1), we were able to reproduce with good agreement FDCSs for C^{6+} 2 MeV amu^{-1} single ionization of helium. This scheme has the advantage of being simpler and less computer intensive than other approaches.

A charge that dynamically varies by the presence of the passive and active electron, together with the semi-classical approach, seems to be a suitable scheme for soft electron emission, in the cases where the usual static approach fails but the CDW–EIS approach should still be valid. We have found that for ejected-electron momentum similar to transferred momentum, internuclear potential effects have little contribution to FDCSs in the scattering plane.

The next step in this direction will be (a) to refine the dependence of the internuclear interaction on the ejected-electron energy and (b) to develop some scheme where we can model the initial and final internuclear interaction separately, so as to separate the influence of entrance channel polarization in internuclear interaction from post-collision effects.

Acknowledgments

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