Total cross sections for transfer ionization in fast ion–helium collisions

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Abstract

The effects of electron correlation and second-order terms on theoretical total cross sections of transfer ionization in collisions of the helium atom with fast H^+, He^{2+} and Li^{3+} ions are studied and reported. The total cross sections are calculated using highly correlated wavefunctions with expansion of the transition amplitude in the Born series through the second order. The results of these calculations are in sensible agreement with experimental data.

1. Introduction

Since the 1980s, double-electron transitions have been one of the top research areas in atomic physics. The quest for the nature of electron correlation motivated extensive experimental and theoretical research on the two-electron transitions in collisions of atoms with photons, electrons and ions (McGuire 1997). Mechanisms of the two-electron transitions, interplay of electron correlation and collision dynamics, alternative formulation for the many-body perturbation theory were also of much interest. It is thought that such research could potentially lead to solving the few-body problem.

The two-electron helium atom, being the simplest correlated atomic system, is the most studied target in both symmetric and asymmetric two-electron transitions, such as excitation ionization, transfer ionization, transfer excitation, double ionization, double excitation and double transfer. Highly sensitive and sophisticated experimental techniques have been used for measurements of the two-electron transition cross sections. COLTRIMS, 'a reaction microscope,' is one of the newest experimental methods that provide an exceptional insight into the physics of reaction dynamics (Dörner *et al* 2000). On the theoretical side, however, little progress has been made in past perturbative methods. Nevertheless, theoretical studies

have shed light on mechanisms of these transitions. It is apparent that any realistic theoretical model for double electron transitions must employ electron correlation as an integral part of the model.

Studies of the two-electron transitions have also stimulated research on electron correlation in the time domain, i.e. time ordering (Stolterfoht 1993, Nagy *et al* 1997). Time ordering provides a causal-like constraint on the sequencing of the interactions, $V(t)$, between the particles involved in a transition. In this model, transitions of electrons are interconnected or correlated with time. Time ordering forces the scattering process off the energy shell and on a practical side, time ordering becomes essential for accurate second-Born calculations (Godunov *et al* 2001, McGuire and Godunov 2003). Calculations with time ordering take a lot of computer time, but just ignoring it, or approximating it, is risky.

While multiple differential cross sections provide detailed information about collision processes, total cross sections give insights into global trends. Except for the widely studied case of double ionization (McGuire *et al* 1995), total cross sections for other two-electron transitions have not been extensively explored. Furthermore, transfer ionization is one of the least understood two-electron transitions, which is not surprising since even single charge transfer has always challenged theory. Experimental observations of the Thomas peak (Horsdal-Pedersen *et al* 1983) demonstrated the importance of the double-scattering mechanisms of single transfer at high velocities. For this reason, one may expect that perturbative models lacking the third- or higher-order terms will not provide a good description of the transfer ionization process. However, roles of electron correlation in transfer ionization in comparison to the higher-order terms remain unclear. The transfer ionization by H^+ impact is clearly preferable for theoretical studies because there is no three-body Coulomb interaction in the final state, the final state simply has a neutral hydrogen atom and only two charged particles, namely, an ionized electron and a recoil atom.

Initial systematic measurements for total cross sections of transfer ionization of He by fast H^+, He^{2+} and Li^{3+} ions were done by Shah and Gilbody (1985). Later Mergel *et al* (1997) and very recently Schmidt *et al* (2005) measured total cross sections of transfer ionization in H^++He collisions. Using the COLTRIMS technique they succeeded in relating the contribution from the Thomas p–e–e mechanism to transfer ionization. Woitke *et al* (1998) measured total cross sections of transfer ionization for Li^{3+} + He collisions but for energy higher compared to Shah and Gilbody (1985). Several research groups have presented theoretical calculations of the total cross sections for transfer ionization. The semiclassical calculations of Dunseath and Crothers (1991) in the independent-event model were considerably larger than those of experiment. The coupled channel semiclassical impact parameter model employing the independent electron approximation (Shingal and Lin 1991) overestimated the cross sections and exposed the inadequacy of simple uncorrelated models to describe this process. The four-body continuum distorted-wave CDW-4B approximation by Belkic *et al* (1997) did agree satisfactorily with the experiment for He^{2+}+He collision.

In an attempt to understand the mechanisms of the transfer ionization process, the Frankfurt group of Schmidt-Böcking measured multiple differential cross sections for

$$H^+ + He \rightarrow H^0 + He^{2+} + e^-,$$
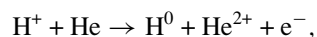
using the COLTRIMS technique (Mergel *et al* 2001, Schmidt-Böcking *et al* 2003a). These experiments revealed numerous aspects that defied explanation. Schmidt-Böcking suggested that the effect of electron correlation, namely a contribution from non-s^2 terms to the initial state wavefunction of helium (Schmidt-Böcking *et al* 2003b) accounted for the aberrant results. However, this explanation was met with skepticism by many. In contrast, recent joint experimental and theoretical papers (Godunov *et al* 2004, 2005, Schöffler *et al* 2005)

demonstrated that a relatively simple perturbative model which included proper electron correlation did closely agree with measured multiple differential cross sections.

In the present paper we extend the perturbative model of Godunov *et al* (2004, 2005) through second-order terms. We calculated total cross sections of transfer ionization in fast H^+ + He, He^{2+} + He and Li^{3+} + He collisions. Our goal is to determine (a) the usefulness and reliability of the perturbative model with correlation for total cross sections of transfer ionization (b) the importance of correlation for transfer ionization and (c) the theoretical v^{-b} dependence of total cross sections.

2. Theoretical model for the transfer ionization

2.1. The first Born amplitude

We consider a structureless projectile incident upon a two-electron target in the ground state $\Phi_i(\mathbf{r}_1, \mathbf{r}_2)$. The first-Born amplitude for the transfer ionization can be written as (Godunov *et al* 2004)

$$f^{B1} = -(2\pi)^2 \sqrt{\mu_i \mu_f} \langle \Psi_f | V_i | \Psi_i \rangle, \tag{1}$$

where the initial channel wavefunction Ψ_i is

$$\Psi_i = \frac{1}{(2\pi)^{3/2}} \exp(i\mathbf{K}_i \mathbf{R}_i) \Phi_i(\mathbf{r}_1, \mathbf{r}_2), \tag{2}$$

and the wavefunction Ψ_f in the final channel is

$$\Psi_f = \frac{1}{(2\pi)^{3/2}} \exp(i\mathbf{K}_f \mathbf{R}_f) \left[\varphi_{nl}(\mathbf{r}_1 - \mathbf{R}) \psi_{\mathbf{k}_2}^{(-)}(\mathbf{r}_2) \right], \tag{3}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the position vectors for the electrons relative to the target nucleus, the vectors $\mathbf{R}_i$ and $\mathbf{R}_f$ describe the position of the centre of mass of the projectile system relative to that of the target system before and after the collision, while $\mathbf{K}_i$ and $\mathbf{K}_f$ are the associated relative momenta, and μ_i and μ_f are the corresponding reduced masses defined as

$$\mu_i = \frac{M_p(M_t + 2)}{M_p + M_t + 2}, \qquad \mu_f = \frac{(M_p + 1)(M_t + 1)}{M_p + M_t + 2}, \tag{4}$$

where M_p is the mass of the projectile and M_t is the mass of the target nucleus. In equation (3) $\varphi_{nl}(\mathbf{r}_1 - \mathbf{R})$ is the hydrogen-like wavefunction of the captured electron, $\psi_{\mathbf{k}_2}^{(-)}(\mathbf{r}_2)$ is the Coulomb wavefunction for the ionized electron with momentum $\mathbf{k}_2$ in the field of the target nucleus (normalized as $\langle \psi_{\mathbf{k}} | \psi_{\mathbf{k}'} \rangle = \delta(\mathbf{k} - \mathbf{k}')$). The interaction potential V_i between the projectile of charge Z_p and a two-electron atomic system with nuclear charge Z_t is given by

$$V_i = -\frac{Z_p}{|\mathbf{r}_1 - \mathbf{R}|} - \frac{Z_p}{|\mathbf{r}_2 - \mathbf{R}|} + \frac{Z_p Z_t}{R}, \tag{5}$$

where $\mathbf{R}$ is the coordinate of the projectile respective to the target nucleus.

In our actual calculations we properly include symmetrization over space coordinates, however it is conceptually useful to present the theory as if the particles were distinguishable. We use index 1 for the 'transferred' electron and index 2 for the 'ionized' electron. The transition amplitude (1) contains three terms arising from the three terms in the potential V_i. The first term may be considered as one electron of the target being captured by the interaction with the projectile and the second is ejected because of correlation ('transfer first' transition). The second term describes the picture when one electron is initially ionized and then the second is captured due to correlation ('ionization first' transition). The last term in (5) takes into account the heavy particle interaction in ion–atom collision.

In order to evaluate the first-Born amplitude (1), it is instructive to introduce the Fourier transform of the hydrogenic wavefunction $\varphi_{nl}(\mathbf{r})$,

$$
\begin{aligned}
\varphi_{nl}^{\mathrm{F}}(\mathbf{s}) &= \int \exp(+i\mathbf{s}(\mathbf{r}_1 - \mathbf{R}))\varphi_{nl}(\mathbf{r}_1 - \mathbf{R})\, d(\mathbf{r}_1 - \mathbf{R}) \\
\varphi_{nl}(\mathbf{r}_1 - \mathbf{R}) &= \frac{1}{(2\pi)^3} \int \exp(-i\mathbf{s}(\mathbf{r}_1 - \mathbf{R}))\varphi_{nl}^{\mathrm{F}}(\mathbf{s})\, d\mathbf{s}.
\end{aligned}
\tag{6}
$$

Then the integration over the internuclear coordinate $\mathbf{R}$ in the first-Born amplitude can be easily performed to yield the following form for the 'transfer first' amplitude:

$$
f_{\mathrm{tr}} = -\frac{\sqrt{\mu_i \mu_f}}{(2\pi)^4} \int d\mathbf{s}\, \frac{-4\pi Z_{\mathrm{p}}}{|\mathbf{s} - \mathbf{K}|^2} \varphi_{nl}^{\mathrm{F}*}(\mathbf{s}) T(\mathbf{k}_2; \mathbf{Q}, -\mathbf{Q}_{\mathrm{t}}),
\tag{7}
$$

and for the 'ionization first' amplitude

$$
f_{\mathrm{ion}} = -\frac{\sqrt{\mu_i \mu_f}}{(2\pi)^4} \int d\mathbf{s}\, \frac{-4\pi Z_{\mathrm{p}}}{|\mathbf{s} - \mathbf{K}|^2} \varphi_{nl}^{\mathrm{F}*}(\mathbf{s}) T(\mathbf{k}_2; \mathbf{s} - \mathbf{K} + \mathbf{Q}, \mathbf{K} - \mathbf{s} - \mathbf{Q}_{\mathrm{t}}),
\tag{8}
$$

where the momenta transfer $\mathbf{Q}$ and $\mathbf{K}$ are defined by

$$
\mathbf{Q} = \frac{M_{\mathrm{t}} + 1}{M_{\mathrm{t}} + 2}\mathbf{K}_i - \mathbf{K}_f, \qquad \mathbf{K} = \mathbf{K}_i - \frac{M_{\mathrm{p}}}{M_{\mathrm{p}} + 1}\mathbf{K}_f,
\tag{9}
$$

$\mathbf{Q}_{\mathrm{t}} \equiv \mathbf{Q}/(M_{\mathrm{t}} + 1)$. T denotes the two-particle transition matrix element

$$
T(\mathbf{k}_2; \mathbf{s}_1, \mathbf{s}_2) = \int d\mathbf{r}_1\, d\mathbf{r}_2\, \psi_{\mathbf{k}_2}^{(-)*}(\mathbf{r}_2)\Phi_i(\mathbf{r}_1, \mathbf{r}_2) \exp(i\mathbf{s}_1\mathbf{r}_1 + i\mathbf{s}_2\mathbf{r}_2).
\tag{10}
$$

The amplitude corresponding to the last term in the interaction potential (5), that is interaction between heavy particles, may be written in a form using the Fourier transform as well, i.e.

$$
f_{\mathrm{pn}} = -\frac{\sqrt{\mu_i \mu_f}}{(2\pi)^4} \int d\mathbf{s}\, \frac{4\pi Z_{\mathrm{p}} Z_{\mathrm{t}}}{|\mathbf{s} - \mathbf{K}|^2} \varphi_{nl}^{\mathrm{F}*}(\mathbf{s}) T(\mathbf{k}_2; \mathbf{s} - \mathbf{K} + \mathbf{Q}, -\mathbf{Q}_{\mathrm{t}}).
\tag{11}
$$

One may see from equation (7) that the transfer and ionization transitions in the 'transfer first' amplitude are separable and can be written as

$$
f_{\mathrm{tr}} = -\frac{\sqrt{\mu_i \mu_f}}{2\pi} \tilde{V}_{nl}^*(\mathbf{K}) T(\mathbf{k}_2; \mathbf{Q}, -\mathbf{Q}_{\mathrm{t}}),
\tag{12}
$$

where $\tilde{V}_{nl}$ is proportional to a matrix element for the capture of a free electron into the bound state of the hydrogen-like atom

$$
\tilde{V}_{nl}(\mathbf{K}) = -\frac{4\pi Z_{\mathrm{p}}}{(2\pi)^3} \int d\mathbf{s}\, \frac{\varphi_{nl}^{\mathrm{F}}(\mathbf{s})}{|\mathbf{K} - \mathbf{s}|^2} = \int d\mathbf{r}\, \varphi_{nl}(\mathbf{r}) \left(-\frac{Z_{\mathrm{p}}}{r}\right) \exp(i\mathbf{K}\mathbf{r}).
\tag{13}
$$

This fact essentially simplifies the calculations of the amplitude f_{tr} which can be performed analytically by means of standard methods.

The evaluation of the amplitudes f_{ion} and f_{pn} requires numerical three-dimensional integration over $\mathbf{s}$.

2.2. The second-Born amplitude

The amplitude for the transfer ionization in the second-Born approximation may be written in the form similar to a single capture transition, i.e.

$$
f^{\mathrm{B2}} = -(2\pi)^2 \sqrt{\mu_i \mu_f} \langle \Psi_f | V_f \hat{G}_0^+(E) V_i | \Psi_i \rangle,
\tag{14}
$$

where V_i is the interaction potential in the incoming channel (5), V_f is the interaction potential in the outgoing channel,

$$
V_f = -\frac{Z_{\mathrm{t}}}{r_1} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} - \frac{Z_{\mathrm{p}}}{|\mathbf{r}_2 - \mathbf{R}|} + \frac{Z_{\mathrm{p}} Z_{\mathrm{t}}}{R},
\tag{15}
$$

and $\hat{G}_0^+$ is a Green operator. The spectral form of the Green operator can be written as

$$\hat{G}_0^+(E) = \lim_{\varepsilon \to 0} \sum_n \int d\mathbf{K}_\alpha \frac{|\Phi_n\rangle\langle\Phi_n|}{E - E_n - K_\alpha^2/2\mu_i + i\varepsilon} \frac{\exp[i\mathbf{K}_\alpha(\mathbf{R} - \mathbf{R}')]}{(2\pi)^3}. \qquad (16)$$

Here the sum on n is over all discrete and continuum states Φ_n of the target, and E_n is the energy of the state Φ_n.

Exact calculation of the second-order terms is a very challenging computational problem. One of the simplest but efficient methods for performing the sum over n, and the one adopted here, is to use the closure approximation (Massey and Mohr 1934). In this approximation, E_n is set to an average value E_{av} so that the denominator becomes independent of n. Using the completeness of the states

$$\sum_n |\Phi_n\rangle\langle\Phi_n| = 1, \qquad (17)$$

and integrating over $\mathbf{R}'$ one would easily get the second Born amplitude of transfer ionization in the closure approximation

$$f^{B2}(E_{av}) = \frac{Z_p}{(2\pi)^4}\sqrt{\mu_i\mu_f} \lim_{\varepsilon \to 0} \int \frac{d\mathbf{K}_\alpha}{E - E_{av} - K_\alpha^2/2\mu_i + i\varepsilon} \frac{4\pi}{p_\alpha^2}$$
$$\times \int d\mathbf{r}_1 \, d\mathbf{r}_2 \, d\mathbf{R} \, \varphi_{nl}^*(\mathbf{r}_1 - \mathbf{R})\psi_{\mathbf{k}_2}^{(-)*}(\mathbf{r}_2)V_f(\mathbf{R}, \mathbf{r}_1, \mathbf{r}_2)$$
$$\times \exp(i\mathbf{q}_\alpha\mathbf{R} + i(\mathbf{Q} - \mathbf{K})\mathbf{r}_1 - i\mathbf{Q}_t\mathbf{r}_2)$$
$$\times \left[\exp(i\mathbf{p}_\alpha\mathbf{r}_1) + \exp(i\mathbf{p}_\alpha\mathbf{r}_2) - Z_t\right]\Phi_i(\mathbf{r}_1, \mathbf{r}_2), \qquad (18)$$

where the intermediate momenta are defined as

$$\mathbf{p}_\alpha = \mathbf{K}_i - \mathbf{K}_\alpha, \qquad \mathbf{q}_\alpha = \mathbf{K}_\alpha - \frac{M_p}{M_p + 1}\mathbf{K}_f. \qquad (19)$$

This is a six-dimensional integral and generally it is still a cumbersome computational task, particularly for $1/|\mathbf{r}_1 - \mathbf{r}_2|$ electron–electron interaction term in V_f potential. In fact, the first two terms in the potential V_f (15) describe the interaction of the 'transferred' electron with the residual ion of the target. We may consider that as an interaction with a particle with a net charge $(Z_t - 1)$. In this way the potential V_f can be approximated as

$$V_f \approx -\frac{(Z_t - 1)}{r_1} - \frac{Z_p}{|\mathbf{r}_2 - \mathbf{R}|} + \frac{Z_p Z_t}{R}. \qquad (20)$$

The amplitude corresponding to the first term in the potential above can be written as

$$f_f^{B2}(E_{av}) = -\frac{\sqrt{\mu_i\mu_f}Z_p}{(2\pi)^4} \lim_{\varepsilon \to 0} \int \frac{d\mathbf{K}_\alpha}{E - E_{av} - K_\alpha^2/2\mu_i + i\varepsilon} \frac{4\pi}{p_\alpha^2}\tilde{\phi}_{nl}^{F*}(\mathbf{q}_\alpha)[T'(\mathbf{k}_2; \mathbf{Q}, -\mathbf{Q}_t)$$
$$+ T'(\mathbf{k}_2; \mathbf{Q} - \mathbf{p}_\alpha, \mathbf{p}_\alpha - \mathbf{Q}_t) - Z_t T'(\mathbf{k}_2; \mathbf{Q} - \mathbf{p}_\alpha, -\mathbf{Q}_t)], \qquad (21)$$

where

$$T'(\mathbf{k}_2; \mathbf{s}_1, \mathbf{s}_2) = \int d\mathbf{r}_1 \, d\mathbf{r}_2 \, \psi_{\mathbf{k}_2}^{(-)*}(\mathbf{r}_2)\frac{1}{r_1}\Phi_i(\mathbf{r}_1, \mathbf{r}_2) \exp(i\mathbf{s}_1\mathbf{r}_1 + i\mathbf{s}_2\mathbf{r}_2). \qquad (22)$$

The contribution of the last two terms of the final interaction potential V_f after introduction of the Fourier transform (6) and integration in (18) over coordinate $\mathbf{R}$ may be represented in

the following form:

$$
\begin{aligned}
f_i^{B2}(E_{av}) = {}&-\frac{\sqrt{\mu_i\mu_f}Z_p^2}{(2\pi)^4}\lim_{\varepsilon\to 0}\int\frac{d\mathbf{K}_\alpha}{E-E_{av}-K_\alpha^2/2\mu_i+i\varepsilon}\frac{4\pi}{p_\alpha^2}(2\pi)^{-3}\int d\mathbf{s}\,\tilde\phi_{nl}^{F*}(\mathbf{s})\frac{4\pi}{|\mathbf{q}_\alpha-\mathbf{s}|^2}\\
&\times[T(\mathbf{k}_2;\mathbf{Q}-\mathbf{q}_\alpha+\mathbf{s},\mathbf{q}_\alpha-\mathbf{Q}_t-\mathbf{s})+T(\mathbf{k}_2;\mathbf{Q}-\mathbf{K}+\mathbf{s},\mathbf{K}-\mathbf{Q}_t-\mathbf{s})\\
&-Z_tT(\mathbf{k}_2;\mathbf{Q}-\mathbf{K}+\mathbf{s},\mathbf{q}_\alpha-\mathbf{Q}_t-\mathbf{s})]
\end{aligned}
\tag{23}
$$

$$
\begin{aligned}
f_{pn}^{B2}(E_{av}) = {}&\frac{\sqrt{\mu_i\mu_f}Z_p^2 Z_t}{(2\pi)^4}\lim_{\varepsilon\to 0}\int\frac{d\mathbf{K}_\alpha}{E-E_{av}-K_\alpha^2/2\mu_i+i\varepsilon}\frac{4\pi}{p_\alpha^2}(2\pi)^{-3}\int d\mathbf{s}\,\tilde\phi_{nl}^{F*}(\mathbf{s})\frac{4\pi}{|\mathbf{q}_\alpha-\mathbf{s}|^2}\\
&\times[T(\mathbf{k}_2;\mathbf{Q}-\mathbf{q}_\alpha+\mathbf{s},-\mathbf{Q}_t)+T(\mathbf{k}_2;\mathbf{Q}-\mathbf{K}+\mathbf{s},\mathbf{p}_\alpha-\mathbf{Q}_t)\\
&-Z_tT(\mathbf{k}_2;\mathbf{Q}-\mathbf{K}+\mathbf{s},-\mathbf{Q}_t)].
\end{aligned}
\tag{24}
$$

The two-particle transition matrix element T is defined by (10).

2.3. Cross sections

The total cross section of transfer ionization in the perturbative model through the second order is given by

$$
\sigma = 2\frac{K_f}{K_i}\int |f^{B1}+f^{B2}|^2 k_e\,dE_e\,d\Omega_e\,d\Omega_f,
\tag{25}
$$

where k_e and Ω_e are the momentum and the solid angle for the ionized electron, Ω_f is the scattered angle. The cross section is a coherent sum of the transition amplitudes and thus depends on their interference. The factor of 2 in above equation is a result of spatial antisymmetrization over electron coordinates in the initial and the final state wavefunctions.

3. Calculation method

We calculated the transfer ionization cross sections in various approximations to study the effects of first- and second-order terms, and electron correlation. The first-Born calculations (Born 1) include a coherent sum of three first-order amplitudes, namely, $f^{B1}=f_{tr}+f_{ion}+f_{pn}$. For calculating the second-order terms, we use the Sokhotsky theorem (Sokhotsky 1873)

$$
\lim_{\varepsilon\to\pm 0}\int\frac{f(x)}{x-x_0\pm\varepsilon}\,dx = P\int\frac{f(x)}{x-x_0}\,dx\pm i\pi f(x_0),
\tag{26}
$$

where P stands for the Cauchy principal value integral. Thus, a second-order term can be written as $f^{B2}=f^{B2off}+f^{B2on}$. In atomic and nuclear scattering theory, terms corresponding to the Cauchy principal value integral are usually called off-shell terms. Godunov *et al* (2001) demonstrated that the 'off-shell' terms may lead to time correlation between electrons. The second term in equation (26) is usually called as an on-shell term. As opposed to the f_f^{B2} (21) term, calculations for f_i^{B2} (23) and f_{pn}^{B2} (24) terms require additional three-dimensional integration. However, it is the amplitude f_f^{B2} that corresponds more closely to the concept of the $V_f G_0 V_i$ expansion. We used this amplitude for our calculations to reduce computational time. In the following, we denote the second-order calculations in the 'on-shell' approximation as 'Born 2 on', that is $f=f^{B1}+f_f^{B2on}$. 'Born 2' stands for calculations with both 'on-shell' and 'off-shell' terms, i.e. $f=f^{B1}+f_f^{B2on}+f_f^{B2off}\equiv f^{B1}+f_f^{B2}$. The second-order 'on-shell' calculations without electron correlation are labelled as 'Born 2 unc'.
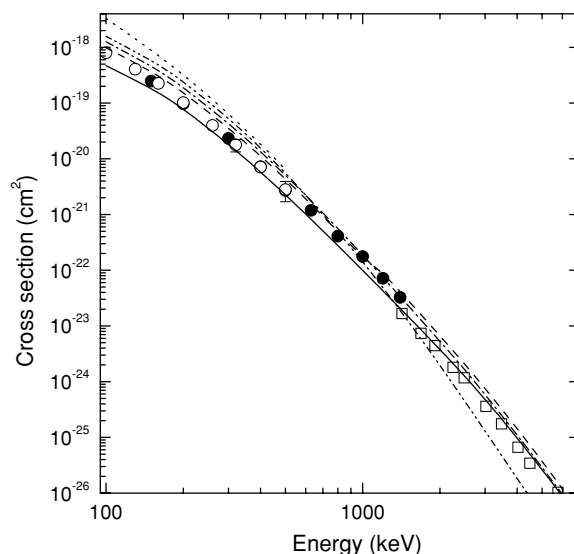
Figure 1. Transfer ionization cross sections for H$^+$ + He collisions. Present theoretical results: - - - -, first Born calculations; — · —, Born 2 on-shell; ——, Born 2 includes both on- and off-shell terms; — · · —, Born 2 on-shell with uncorrelated functions. Experiment: ●, Mergel *et al* (1997); ○, Shah and Gilbody (1985); □, Schmidt *et al* (2005). Other calculations: · · · · · ·, Dunseath and Crothers (1991).

The average energy E_{av} in the closure approximation for the second-order terms can be chosen arbitrarily. In practice, this parameter should correspond to the energy of the most important intermediate states. Since our calculations were quite insensitive to variations of E_{av} within 20 eV–60 eV interval, the calculations presented below were carried out with $E_{av} = 32.5$ eV.

The wavefunction $\Phi_i(\vec{r}_1, \vec{r}_2)$ for helium, ground state was calculated in the multiconfigurational Hartree–Fock approximation (MCHF) (Froese Fischer 1996). The full set of calculations with both radial and angular correlation include $(n\mathrm{s})^2$, $(p\mathrm{s})^2$ and $(n\mathrm{d})^2$ terms with n through 4. These configurations yield about 97% of the correlation energy. The same correlated wavefunction was used in both the first- and second-order calculations.

Allowance for electron correlation increases computational time by almost a factor of 10. The results presented below were calculated on the 50-processor cluster at Physics Department of Old Dominion University.

4. Results and discussion

In figure 1, we present transfer-ionization cross sections for H$^+$ + He collisions. The first-Born calculations reasonably agree with experimental data for all collision energy. This result is unexpected. Normally, the first-order calculations do not agree with experiments for other two-electron transitions. The second-order terms in the 'on-shell' approximation were calculated with and without electron correlation. For uncorrelated calculations, we used the Hartree–Fock function for the ground state. Calculations allowing for the second-order 'on-shell' terms with correlation show that the cross section is affected slightly. But the ramification of correlation is quite remarkable. As we can see from the figure, at lower energies, the uncorrelated cross
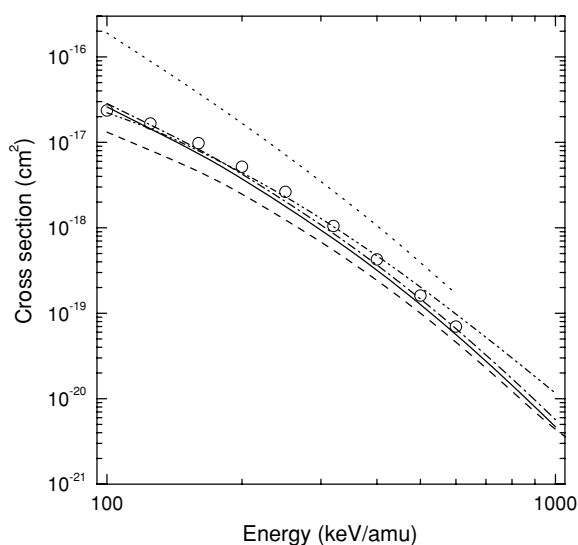
Figure 2. Transfer ionization cross sections for He^{2+} + He collisions. Present theoretical results: - - - -, first-Born calculations; — · —, Born 2 on-shell; ——, Born 2 includes both on- and off-shell terms. Experiment: ○, Shah and Gilbody (1985). Other calculations: · · · · ·, Dunseath and Crothers (1991); — · · —, Belkic *et al* (1997).

section is about 25% larger compared to the correlated calculations, but for higher energies it is about five times smaller. Therefore, we conclude that electron correlation plays an important role in transfer ionization by fast proton impact. Effect of the 'off-shell' is strongest at 100 keV (about a factor 2), but decreases to few per cent at high energies. The second-order calculations of Dunseath and Crothers (1991), which did not include the first-order terms, are much larger than our calculations. Our calculations show that the interference between terms in the cross section (25) affects the coherent sum of the amplitudes.

Cross section for transfer ionization in He^{2+} + He collisions is presented in figure 2. The first-Born calculations strongly disagree with experimental data. Allowing for the second-order terms increases the cross section by a factor 2 at 100 keV amu^{-1}. As the collision energy increases, the difference between the first- and second-order calculations decreases. The effect of off-shell term for He^{2+} impact is rather small (within 15%). Our theoretical results agree closely with the experimental data of Shah and Gilbody (1985) for all energies. Our results are also very close to the theoretical data of Belkic *et al* (1997) in the interval of 100 keV amu^{-1}—400 keV amu^{-1}. However, for higher-collision energies the two methods demonstrate different asymptotic behaviour. There is no experimental data for collision energies above 600 keV amu^{-1}. However, a visual extrapolation of the experimental data of Shah and Gilbody (1985) shows that the expected experimental cross sections would follow the asymptotic behaviour in our calculations.

In figure 3, we present transfer-ionization cross sections for Li^{3+} + He collisions. It is clear that the first Born calculations are well lower than experimental data. Allowing for the second order somewhat increases the cross sections, but the calculations are still below the experiment. Inclusion of the off-shell terms dramatically improves the agreement with experimental data. As the collision energy increases, the effect of the second-order terms decreases but remains noticeable.
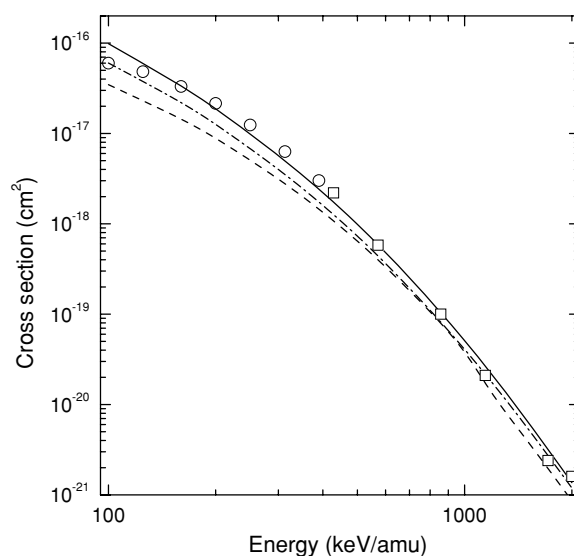
Figure 3. Transfer ionization cross sections for Li^{3+} + He collisions. Present theoretical results: - - - -, first Born calculations; — · —, Born 2 on-shell; ———, Born 2 includes both on- and off-shell terms. Experiment: $\bigcirc$, Shah and Gilbody (1985); $\square$, Woitke *et al* (1998).

Table 1. Coefficients b in the velocity dependence $\sigma \propto v^{-b}$ for cross sections of transfer ionization for H^+ + He collisions.

Experiment		Theory		
Mergel (1997)	Schmidt *et al* (2005)	Born 1	Born 2 on	Born 2
10.02	10.81	11.23	11.31	10.76

Studies of single-electron transfer show that an asymptotic behaviour of cross sections as a function of the collision velocity $\sigma \propto v^{-b}$ may provide information about the most important collision mechanisms. Particularly, the first-order Brinkman and Kramers mechanism would lead to v^{-12} velocity dependence and the second-order Thomas *p–e–n* scattering to v^{-11}. The same v^{-11} trend was expected for the Thomas *p–e–e* mechanism in transfer ionization (Briggs and Taulberg 1979). Mergel (1997) and Schmidt *et al* (2005) studied the contribution and asymptotic dependence for the Thomas *p–e–e* mechanism. Transfer ionization at intermediate collision velocities may proceed via few channels (McGuire 1997). Most of the mechanisms are sensitive to collision velocity. Therefore, we sought to explore the global asymptotic trend for a coherent sum of amplitudes in transfer ionization cross section (25). We fitted our calculation results to the power-law function v^{-b} starting from the collision velocity of 7.75 au. This velocity corresponds to the lower velocities of the Schmidt *et al* (2005) experimental data. Table 1 demonstrates the results of the least-square fit for the total cross sections of transfer ionization of both our theoretical calculations and the experimental data of Mergel (1997) and Schmidt *et al* (2005). The results show that our calculations in the second-order approximation with off-shell terms closely agree with the data of Schmidt *et al* (2005). Furthermore, such a agreement indicates that our perturbative model with electron correlation reasonably describes the physics of transfer ionization at high collision velocities.

5. Conclusions

In summary, we have evaluated the effects of electron correlation and second-order terms on total cross sections of transfer ionization in fast ion–helium collisions. The allowance for electron correlation directly determines how closely theoretical calculations agree with experimental data. Second-order calculations with uncorrelated functions differ considerably from experimental data. The effect of 'off-shell' terms varies for different projectiles. For Li^{3+} impact, it considerably improves the agreement with the experiment. The expansion of the transition amplitude in the Born series through the second order, and allowance for the 'off-shell' terms and electron correlation result in calculations that are in sensible agreement with experimental data, including the v^{-b} dependence.

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