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Calculations of two-electron transition cross sections between fully stripped ions and helium atoms

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Abstract. One- and two-electron collision processes between fully stripped ions ($Z = 2$-9) and helium atoms have been investigated in the intermediate energy range within the independent electron approximation. The transition probabilities for single excitation, single ionization and electron capture for an effective one-electron helium atom colliding with bare ions calculated in the coupled channel semiclassical impact parameter model employing a travelling atomic orbital expansion were combined to obtain cross sections for two-electron processes, such as transfer ionization, double capture and double ionization. It is found that *all* one-electron processes are well described by an independent electron approximation where the effective potential of the target atom gives the correct single ionization energy, while accurate cross sections for *all* two-electron transitions can be obtained only if one adopts a different effective potential where the single ionization energy of each electron is half the double ionization energy of helium.

1. Introduction

Collisions between fully stripped ions and the helium atom are one of the simplest examples of the interacting two-electron collision systems. The availability of multiply charged ions in a wide range of energies and the ease with which helium can be used as a target has led to a large amount of experimental effort being directed towards the study of these collisions. One- and two-electron transitions have been studied by measuring the charge states of the projectile and/or of target ions, or by detecting the electron spectra emitted in the collisions. For two-electron target atoms, in addition to the one-electron transitions such as single excitation, single ionization and single electron capture, two-electron processes also frequently occur, in particular, for multiply charged projectile ions. These processes can be expressed schematically, right after the collision, as:

(i) double capture (DC)

$$A^{q+} + He \rightarrow A^{(q-2)+} + He^{2+}$$

where the projectile ion $A^{(q-2)+}$ can be in the ground ($1s^2$), singly ($1snl$) or doubly excited state ($nln'l'$);

(ii) double excitation (DE)

$$A^{q+} + He \rightarrow A^{q+} + He^{**}$$

(iii) double ionization (DI)

$$A^{q+} + He \rightarrow A^{q+} + He^{2+} + e^- + e^-$$

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(iv) transfer excitation (TE)

$$A^{q+} + He \rightarrow A^{(q-1)+} + He^{+*}$$

(v) transfer ionization (TI)

$$A^{q+} + He \rightarrow A^{(q-1)+} + He^{2+} + e^{-}$$

(vi) simultaneous excitation–ionization (SEI)

$$A^{q+} + He \rightarrow A^{q+} + He^{+*} + e^{-}.$$

In the above expressions we use a single asterisk to indicate singly excited states and a double asterisk to indicate doubly excited states. Experimentally only the decay products after the collision are measured. Thus, if doubly excited states are formed in the collision, the charge state of the ion depends on whether these states decay radiatively or by autoionization. In this paper, we will focus on experiments where only the charge states of the projectile and of the target are measured, with or without coincidence. Thus transfer ionization cannot be distinguished from double capture to doubly excited states if these states decay by autoionization.

From the theoretical viewpoint, all the one- and two-electron processes can be calculated by solving the time-dependent Schrödinger equation for the two-electron system,

$$\left(H - i\frac{\partial}{\partial t}\right)\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, t) = 0 \tag{1}$$

where

$$H = -\tfrac{1}{2}\nabla_1^2 - \tfrac{1}{2}\nabla_2^2 - \frac{Z}{r_{1p}} - \frac{Z}{r_{2p}} - \frac{2}{r_{1t}} - \frac{2}{r_{2t}} + \frac{1}{r_{12}} \tag{2}$$

using the standard close-coupling impact parameter method, employing travelling molecular orbitals (Kimura *et al* 1983) or travelling atomic orbitals. For the latter, one can use atomic states placed both on the target (t) and the projectile (p) centre as basis functions where each two-electron wavefunction is an eigenstate of the two-electron atomic Hamiltonian in the separated-atom limit. Some calculations of such a nature have been carried out for single excitation and single capture in the energy region where ionization and two-electron processes are not important (Bransden *et al* 1984, Fritsch and Lin 1986, Shingal and Bransden 1989, Shingal *et al* 1989). In others, double capture, transfer excitation and double excitation processes have been studied within the close-coupling scheme for situations where the number of doubly excited states populated is small. For example, $2l2l'$ doubly excited states populated by double capture at lower energies, by double excitations at high energies, and by transfer excitation in $He^+ + H$ have been studied theoretically (Fritsch and Lin 1988, 1990). These limited studies allow us to address, to some extent, the question of the relative importance of the role of the interelectronic interaction in ion–atom collisions.

For collisions where many doubly excited states are populated and/or where the ionization process is important, the two-electron time-dependent Schrödinger equation (1) cannot be easily solved by the close-coupling method as the number of states to be included in the basis set becomes prohibitively large. To provide a reasonable theoretical model where the two-electron processes (i)–(v) can be evaluated simultaneously, some simplifications are thus desired at the present time. For collisions between multiply charged ions and helium atoms, one may argue that the interelectronic

interaction is weak compared with the electron–projectile interaction, thus the Coulombic repulsion between the electrons can either be dropped or partially taken into account through a central field (for example, McGuire and Richard 1973, McGuire and Weaver 1977, McGuire 1987, Ben-Itzhak and McGuire 1988). Such a theoretical model is discussed briefly in section 2. Within such an independent electron model, we discuss how the various two-electron transitions can be evaluated. The calculated cross sections for the collisions between bare ions ($Z = 2$–9) and helium atoms are compared with experiments in section 3. Finally in section 4 some conclusions are given.

2. Theory and calculation

2.1. The collision model

Within the independent electron approximation it can be assumed that each electron in the ground-state helium atom moves under the influence of a central potential $V_t(r)$. The resulting Hamiltonian can then be written as

$$H = -\tfrac{1}{2}\nabla_1^2 - \tfrac{1}{2}\nabla_2^2 - \frac{Z}{r_{1p}} - \frac{Z}{r_{2p}} + V_t(r_{1t}) + V_t(r_{2t}). \tag{3}$$

For this approximate Hamiltonian, the time-dependent Schrödinger equation (1) is separable and the two-electron wavefunction can be written as a product of two one-electron wavefunctions

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, t) = u(\boldsymbol{r}_1, t)u(\boldsymbol{r}_2, t) \tag{4}$$

where the one-electron wavefunction $u(\boldsymbol{r}, t)$ satisfies the equation

$$\left(-\tfrac{1}{2}\nabla^2 - \frac{Z}{r_p} + V_t(r_t)\right)u(\boldsymbol{r}, t) = \mathrm{i}\frac{\partial}{\partial t}u(\boldsymbol{r}, t). \tag{5}$$

Equation (5) can be solved by expanding the wavefunction u

$$u = \sum_n a_n\phi_n(\boldsymbol{r}_t) + \sum_m b_m\phi_m(\boldsymbol{r}_p) \tag{6}$$

in terms of the travelling atomic orbitals ϕ placed on the target and the projectile centre and assuming that the nuclei follow straight-line trajectories. Here r_t and r_p represent the distances of the active electron from the target and the projectile nucleus, respectively. Substituting (6) into (5) and following the standard procedure a set of coupled first-order differential equations for the expansion coefficients can be derived. The set of equations is then solved with the proper initial condition to extract the excitation (a_n) and electron transfer (b_m) amplitudes at $t \to +\infty$. Pseudostates are included at each centre to account for direct ionization and electron capture to the continuum.

2.2. Evaluation of one- and two-electron transition cross sections

From the scattering amplitudes the total excitation (P_{ex}), total electron capture (P_c) and total ionization (P_i) probabilities at each impact parameter, b, can be calculated. Since

$$1 = P_{el} + P_{ex} + P_c + P_i \tag{7}$$

where P_{el} is the probability for elastic scattering, the expansion

$$1 = (P_{el} + P_{ex} + P_c + P_i)^2 \tag{8}$$

then allows for the identification of both the one- and two-electron transition probabilities. For example, single capture probability to all bound states of the projectile is given by $2P_{el}P_c$ total double capture probability is P_c^2 and total transfer ionization probability is given by $2P_cP_i$.

It is also straightforward to calculate one- and two-electron processes to specific states. For example, single capture to a given nl state is $2P_{el}P_c(nl)$ where $P_c(nl)$ is the calculated single capture probability to the nl states. The question of calculating the probability to populate specific doubly excited states cannot be tackled in the present approach and is addressed elsewhere (Jain *et al* 1989, Chen *et al* 1990). On the other hand the probabilities for capture or excitation to a given (n, n') manifold of doubly excited states can be obtained. For example, total double capture to the (3, 4) manifold can be calculated by $P_c(3)\ P_c(4)$, where $P_c(n)$ is the calculated single capture probability to the state n (=3 or 4).

The cross section σ_i for each one- or two-electron process i can then be calculated from

$$\sigma_i = 2\pi \int_0^\infty b\ \mathrm{db}\ P_i(b) \tag{9}$$

where $P_i(b)$ is the corresponding probability for the ith transition.

2.3. Two models for the description of helium atoms

Model A. In the independent electron model there are many ways to approximate the helium atom. We have chosen the active electron of the helium atom to move in an effective potential V_t, generated by the alpha particle and the passive electron. The parameters of the potential and the powers and the exponents of the Slater-type orbitals were adjusted such that the energies of the ground state and the first few singly excited states are well reproduced. Following Shingal (1988) the effective potential was represented by

$$V_t(r) = -Z_1/r - (a + br)\exp(-\beta r)/r \tag{10}$$

where $Z_1 = a = 1.0$, $b = 0.4143$, and $\beta = 2.499$. This potential gives an ionization energy of 0.9 au.

In the independent electron model, with the potential V_t given above, the double ionization energy is $2 \times 0.9 = 1.8$ au which is much smaller than the experimental value of 2.9 au. In section 3, we will show that calculations based on model A tend to give cross sections for two-electron transitions which overestimate the experimental data.

Model B. To show the effects of the binding energy of helium on the calculated cross sections we also use a different model for helium where each electron is assumed to be in a Coulomb potential $V_t = -Z_{eff}/r$ with an effective charge Z_{eff} such that the binding energy of each electron is half of the double ionization energy. We will show in section 3 that this model provides a better prediction for all the two-electron transitions.

3. Results and discussion

In this section we present results for one- and two-electron transitions in the collision of bare ions of charge $+q$ colliding with helium atoms. We consider experiments (i) where only the charge states of the projectiles are measured, and (ii) where charge states of the projectiles and the target ions are both measured. To compare theoretical calculations with results from such experiments, one needs to know the decays of the populated doubly excited states. For example, double capture to doubly excited states are indistinguishable from transfer ionization if the doubly excited states decay by autoionization since each ends up in a projectile of charge $+(q-1)$ and a He^{2+} recoil ion. We will show that this is indeed the main 'source' of transfer ionization at lower energies for multiply charged ion projectiles. If these doubly excited states decay radiatively, the projectile charge is $+(q-2)$ with a He^{2+} recoil ion. They will be observed as 'true' double capture together with double capture to ground and to singly excited states. In the present article we did not calculate double capture to individual doubly excited states (see, for example, Chen *et al* 1990). Furthermore, we assume that each doubly excited state decays by electron emission. Thus double capture to doubly excited states is counted as transfer ionization, and double excitation of He is treated as single ionization. In experiments where only the charge state of the projectile is measured, single capture would not only consist of 'true' single capture from the one-electron process, but also include transfer ionization and transfer excitation from the two-electron processes. In the following we analyse the predicted cross sections from our calculations for different collision systems and compare them with experiments.

3.1. $He^{2+} + He$

A basis set consisting of a total of 79 atomic states (s, p, d and f) on both the target and the projectile centre was used to study the collision between an alpha particle and a helium atom for impact energies lying between 50.0 and 300 keV amu^{-1}. This basis set contains some bound and positive energy pseudostates in addition to the exact $n=1$-3 states of He^+ and $n=1$-3 singly excited states of He calculated from the potential (10), i.e. model A. The calculated single ionization (SI), single capture (SC), double ionization (DI) and transfer ionization (TI) cross sections are shown in figure 1. They are compared with experimental data (Shah and Gilbody 1985) where the charge states of the projectile and the target were measured. The single electron capture cross section includes two reactions: (i) single electron capture leaving the helium ion in the ground state and (ii) single electron capture leaving the helium ion in the excited states. In the impact energy range under consideration the calculated total cross section is dominated by the first reaction. The cross section for single ionization comprises: (i) direct ionization and charge transfer to continuum, in addition to (ii) the contribution from double excitation to doubly excited states and (iii) simultaneous excitation and ionization of helium. Most of the contribution to the calculated single ionization cross section comes from the reaction (i) followed by the processes (iii) (about 5%) and process (ii) (less than 1%). The transfer ionization process removes two electrons from the helium atom while the charge state of the projectile decreases by one unit. The theoretical cross section has two components: (i) capture of one electron by the projectile leaving the second electron in the continuum, and (ii) capture of the two electrons into the doubly excited states of the projectile which subsequently decay by autoionization (radiative decay being assumed to be

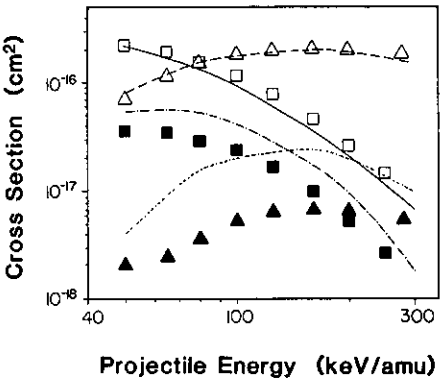

Figure 1. Cross section for various processes in $He^{2+} + He(1s^2)$ collision. Theory (model A, see text): ——, single capture; – – –, single ionization; — · —, transfer ionization; – – · – –, double ionization. Experiment (Shah *et al* 1985): single capture, □; single ionization, △; transfer ionization, ■; double ionization, ▲.

negligible). The process (ii) has also been found to give a very small contribution (less than 1%) to total transfer ionization cross section in the energy range under consideration for the present collision system.

The calculated one-electron removal cross section, charge transfer and single ionization, are in good agreement with the experimental data (figure 1). However, only qualitative agreement is found for the computed transfer ionization and the double ionization cross section. Quantitatively these cross sections are a factor of two to four too large compared with the experiment. This overestimation is not too surprising. In the model under consideration the effective potential for the active electron of the helium atom has been adjusted to give the correct single ionization energy and no account has been taken of the change in binding energy and the relaxation of the second electron when the first electron is removed from helium. To account for the increasing binding for the second electron within the independent electron approximation, model B was used for two-electron processes in which each electron in helium is in a Coulomb potential with the effective charge adjusted to give a binding energy of -1.45 au. We note that the states placed on the projectile remained unchanged in this new basis set.

The calculated double ionization and transfer ionization cross sections from model B are displayed in figure 2, together with the single ionization and single electron capture cross sections calculated using model A. These theoretical results are compared with the experimental data of Shah and Gilbody (1985). A good agreement between the theory and the experiment over the entire energy range under consideration has been achieved within the independent electron model. We emphasize that *two* independent electron models were used: one for *all* one-electron processes, and another for *all* two-electron processes. It is not possible to find a single independent electron model for both the one- and the two-electron processes simultaneously.

The impact parameter weighted total probability as a function of impact parameter, for single capture, single ionization (from model A), and double capture and double ionization (from model B), is shown in figure 3(*a*) and (*b*), for projectile energies of 100 and 300 keV amu^{-1}, respectively. Large impact parameters contribute to single ionization at the two impact energies while single electron transfer moves to small impact parameters as impact energy is increased. In contrast, two-electron removal

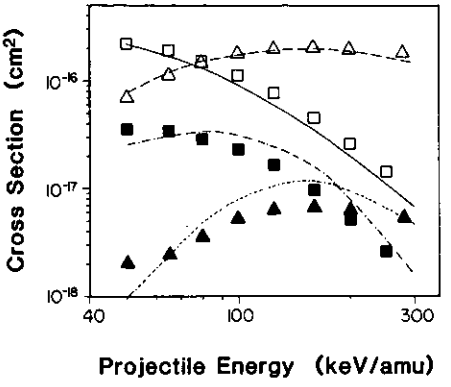

Figure 2. Same as in figure 1 except transfer ionization (—·—) and double ionization (– – –) have been calculated using model B (see text).

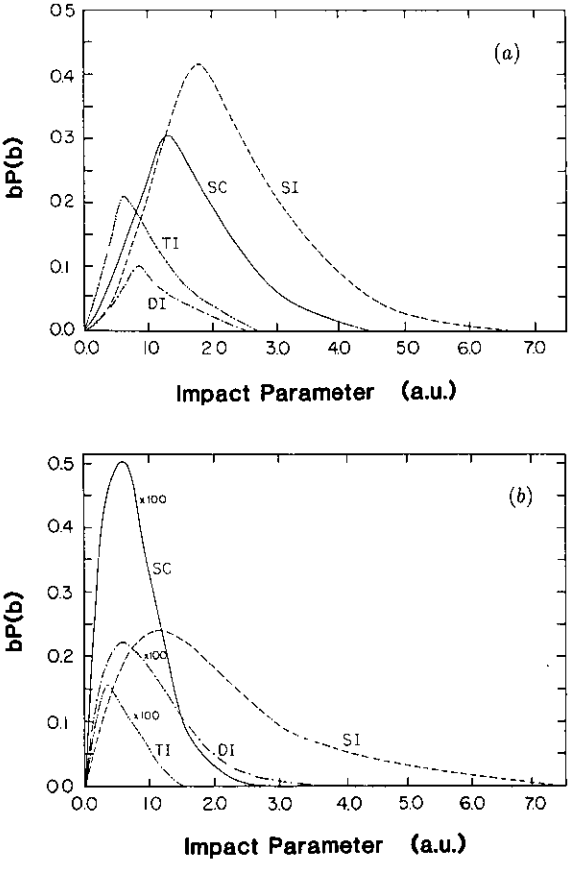

Figure 3. (*a*) Impact parameter weighted probability plotted against impact parameters for various processes in $He^{2+} + He(1s^2)$ collision at an impact energy of 100 keV u^{-1}. Theory (model A): SI, single ionization; SC, single capture. Theory (model B): TI, transfer ionization; DI, double ionization. (*b*) Same as in (*a*) except projectile energy is 300 keV u^{-1}.

from helium is a small impact parameter phenomenon. Furthermore, transfer ionization also shifts to smaller impact parameters, in harmony with single electron capture, with increasing projectile energy.

3.2. $Li^{3+} + He$

To carry out calculations for collisions of helium with bare ions with higher charges ($q > 2$), a modification of the basis set used in the calculation is needed. In contrast to $He^{2+} + He$ collision where the electron is predominantly captured into the $n = 2$ states of the projectile, electron capture shifts to higher principal quantum numbers (n) as the charge on the projectile is increased. Hence the number of projectile centred states has to be increased and the total number of atomic orbitals, though manageable, becomes too large if a basis of 60 states on the target centre, used in the He^{2+}-He system, is retained in the expansion. Henceforth, the f type and some of the s, p and d Slater-type helium orbitals were discarded reducing the total number of travelling atomic orbitals placed on the target to 30. In collisions between fully stripped lithium and helium a basis set consisting of 64 states was used.

In figure 4(a), the calculated total single capture and single ionization cross section is compared with the experimental data (Shah *et al* 1985). The single ionization process is still the dominant contributor to the total calculated single ionization cross section, with the simultaneous excitation ionization and double excitation of the helium atom accounting for about 10% near the maximum of the cross section, a slight increase as compared with the $He^{2+} + He$ collision. The calculated single ionization cross section compares well with the experiment. However, the computed single capture cross section lies slightly below the experimental data, though in qualitative agreement throughout the energy range under consideration.

The predicted and experimental (Shah and Gilbody 1985) cross sections for two-electron processes, are displayed in figure 4(b). The calculated results for TI are in reasonable agreement with the experiment in the energy range considered. Double capture to doubly excited states of lithium becomes an important contributor to transfer ionization for impact energies below 100 keV amu^{-1}. We also show the true double capture in figure 4(b). This corresponds to double capture to the ground and singly excited states. For double ionization, the calculated results are too low at lower energies and too large at higher energies. This is probably a reflection of the smaller number of pseudostates used in the calculation such that ionization channels are inadequately represented.

3.3. $C^{6+} + He$

The collision between a bare carbon ion and a helium atom has been studied using a basis set comprising exact $n = 1$-4 travelling atomic states placed on the projectile centre along with the 30 states centred on the target. In figure 5, the calculated single capture, transfer ionization (which includes double capture to doubly excited states) and the sum are displayed over the 200–1000 keV amu^{-1} impact energy region. Also shown in figure 5 are the recently measured cross section for these individual processes (Shinpaugh 1990, Shinpaugh *et al* 1990). Furthermore, the sum is compared with experimental single electron capture cross sections where the charge state of the target is not measured (Guffey *et al* 1977, Dillingham *et al* 1981). The total single electron capture cross section is in reasonable agreement with the available experimental data. We note that TI is more important than single capture for energies above 250 keV amu^{-1}.

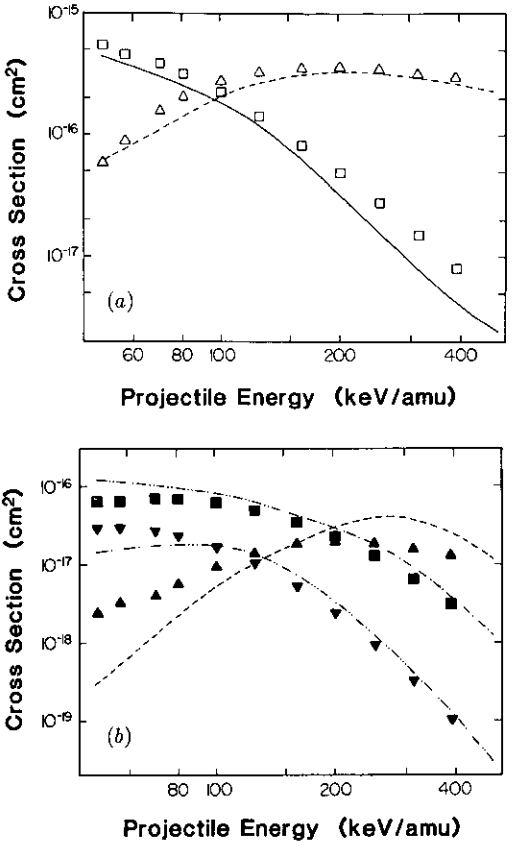

Figure 4. (*a*) Single capture and single ionization cross section in $Li^{3+}+He(1s^2)$ collisions. Theory (model A): -----, single ionization; ——, single capture. Experiment (Shah *et al* 1985): △, single ionization; □, single capture. (*b*) Double capture, double ionization and transfer ionization cross section in $Li^{3+}+He(1s^2)$ collisions. Theory (model B): —···—···, double capture; -···-, transfer ionization; ---, double ionization. Experiment (Shah *et al* 1985): ▼, double capture; ■, transfer ionization; ▲, double ionization.

In other words, it is more difficult to capture an electron without ionizing another electron in collisions between multiply charged ions with helium atoms.

3.4. $O^{8+}+He$

A study, similar to the previous system, for $O^{8+}+He$ is shown in figure 6. Transfer ionization (TI) is always larger than true single capture (SC) over the 250–1000 keV amu^{-1} impact energy region considered. The sum of TI and SC can be compared with the experimental results of Dillingham *et al* (1981) where only the charge state of the projectile was measured. The measured K-shell x-ray cross sections of Guffey *et al* (1977) are also shown in figure 6. Recently Shinpaugh (1990; see also Shinpaugh *et al* 1990) has measured the charge state of the projectile in coincidence with the charge state of the target. These experimental cross sections for TI, SC and the sum at impact energies of 500 and 1000 keV amu^{-1} are also displayed in figure 6. The predicted total single capture cross section (sum) is in reasonable agreement with the corresponding experimental data.

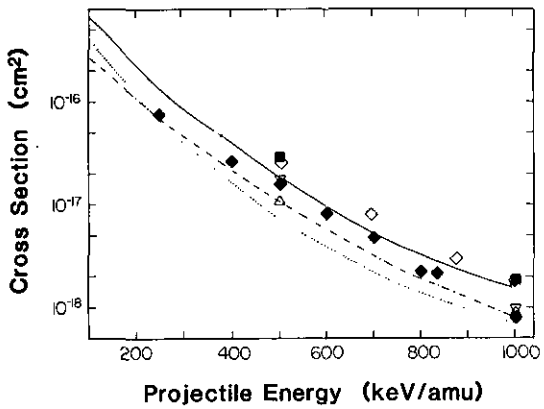

Figure 5. Cross section for various processes in $C^{6+}+He(1s^2)$ collisions. Theory: ·····, single capture (model A); —·—, transfer ionization (model B); ——, total single capture (sum). Experiment (total single capture): ◇, Dillingham *et al* (1979); ◆, Guffey *et al* (1973); ■, Shinpaugh *et al* (1990); △, Shinpaugh *et al* (1990) (single capture); ▽, Shinpaugh *et al* (1990) (transfer ionization).

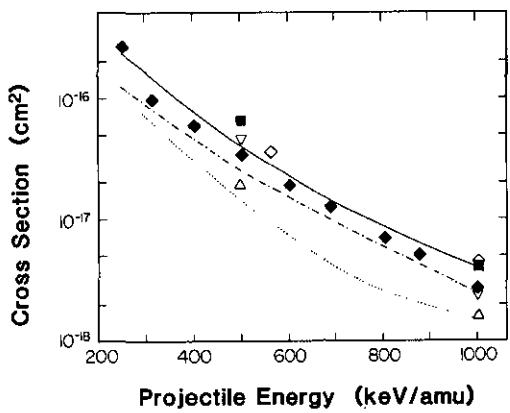

Figure 6. Cross section for various processes in $O^{8+}+He(1s^2)$ collisions. Theory: ·····, single capture (model A); —·—, transfer ionization (model B); ——, total single capture (sum). Experiment (total single capture): ◇, Dillingham *et al* (1979); ◆, Guffey *et al* (1973); ■, Shinpaugh *et al* (1990); △, Shinpaugh *et al* (1990) (single capture); ▽, Shinpaugh *et al* (1990) (transfer ionization).

Furthermore, the calculated ratio of TI with respect to SC cross section is in general agreement with the experimental data (Shinpaugh *et al* 1990) except at the lower energies. This is probably a reflection of the insufficient basis set used in the calculation. We will address this question in more detail in the $F^{9+}+He$ collision system.

3.5. $F^{9+}+He$

This system has recently been experimentally studied for a number of projectile energies by Shinpaugh *et al* (1990) and Shinpaugh (1990). In figure 7, the calculated single electron capture, transfer ionization and total one-electron charge transfer cross section (sum), for impact energies lying between 250 and 1500 keV amu^{-1}, is compared with the recent experimental data. The predicted cross section for pure one-electron capture

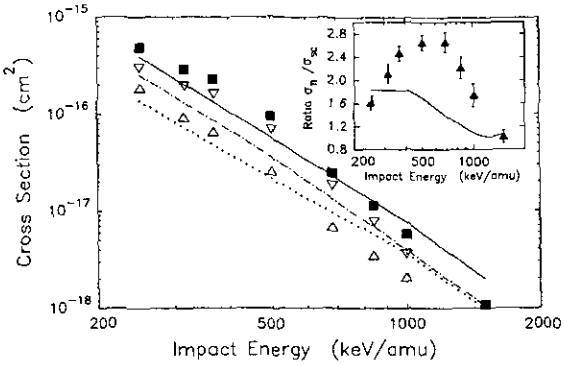

Figure 7. Cross section for various processes in $F^{9+}+He(1s^2)$ collisions. *Theory:* ····, single capture (model A); —·—, transfer ionization (model B); ——, total single capture (sum). Experiment: △, Shinpaugh *et al* (1990) *(single capture)*; ▽, *Shinpaugh et al (1990)* (transfer ionization); ■, Shinpaugh *et al* (1990) (total single capture). Inset: ratio of the transfer ionization to single capture cross section in $F^{9+}+He(1s^2)$ collisions. Theory: ——. *Experiment:* ▲, *Shinpaugh et al (1990).*

comprises of two processes: (i) pure one-electron capture leaving the residual He^+ ion in the 1s state, and (ii) one-electron capture with the ionic He^+ left in the excited states. The later process is only important at the lowest energy where it contributes 25% to the total one-electron capture cross section. We note that the calculated cross section underestimates the experimental data at energies below 500 keV amu^{-1} and overestimates the measurements above these impact energies. Similar trends can be seen also for the transfer ionization cross sections. At lower energies double capture to doubly excited states contributes to TI significantly (more than transfer ionization below 300 keV amu^{-1}). The underestimation of the SC and TI cross sections is also reflected in the ratio of TI/SC, as shown in the inset. The inadequacy of the theory to explain the experimentally determined cross section for total capture and the ratio of transfer ionization to single capture can partly be ascribed to the limited number of projectile centred states ($n = 1$–5 exact and few pseudostates) that are included in the calculation.

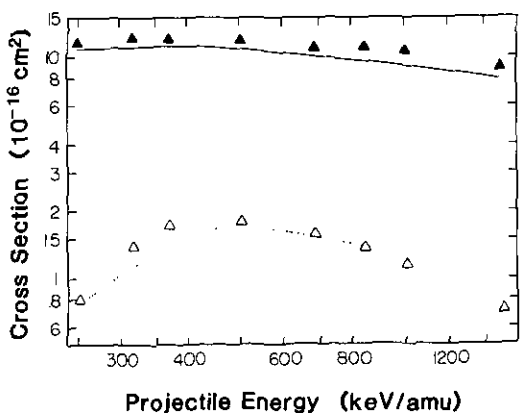

Figure 8. Single and double ionization cross sections in $F^{9+}+He(1s^2)$ collisions. Theory: ——, single ionization (model A); ····, double ionization (model B). Experiment (Shinpaugh *et al* 199): ▲, single ionization; △, double ionization.

Experimental single and double ionization cross sections for F^{9+} + He collisions are also available. The results from our calculations are compared with experimental data (Shinpaugh *1990*, Shinpaugh *et al 1990*) in figure 8. It appears that the calculated results also tend to underestimate for both processes, except that the errors here are smaller. The total single ionization cross section is still dominated by one-electron removal from helium leaving the residual ion in the ground state. However, the process in which the one-electron loss accompanied by an excited residual ion contributes about 20% to the total ionization cross section at the lowest impact energy, reducing to about 10% at the highest energy under consideration. In contrast, the contribution of double excitations to total single ionization (after Auger decay) is less than 5%.

4. Summary and discussion

In this paper we investigated the one- and two-electron removal processes in collisions of multiply charged ions with helium atoms using the *independent electron picture.* Within this picture, the time-dependent Schrödinger equation for the many-electron wavefunction can be simplified to the time-dependent Schrödinger equation for *each* electron. In this work, the later equation is solved in the semiclassical multichannel impact parameter formulation by expanding the time-dependent wavefunction in terms of atomic orbitals on the two collision centres to give probabilities for excitation, charge transfer and ionization (pseudostates are used to represent continuum states) for each electron. These one-electron probabilities were combined to calculate cross sections for various one- and two-electron processes.

Unlike the atomic or molecular structure calculations, the effective one-electron potential for atomic collisions is *not* chosen variationally in general. (A variational approach would result in a set of time-dependent Hartree–Fock (TDHF) equations which is already quite complicated to solve.) Without such a variational approach, it is important to specify the exact nature of the independent electron approximation adopted in a given theoretical approach. In this paper, we showed that it is *impossible* to adopt a single independent electron model to describe both the one- and two-electron processes *simultaneously.* Instead, two different types of effective potentials are needed to describe one- and two-electron processes separately. To describe *all* one-electron processes, an effective potential which reproduces the energies of the ground and low-lying singly excited states of helium was adopted. To describe *all* two-electron processes, an effective potential which gives the correct double-ionization energy of helium was adopted. The latter potential in effect accounts for the change of the screening between the two electrons from a value when both electrons are in the ground state to a new value when both electrons are excited, captured or ionized. When this change of screening (or relaxation) was included, we showed that the independent electron approximation is capable of predicting total cross sections for all two-electron processes in collisions of multiply charged ions with helium atoms in the cases considered. The discrepancy between the calculated and the experimental cross sections for collisions with ions of higher Z is most likely due to the small size of the basis functions included in the close-coupling calculation, instead of the limitation of the independent electron approximation itself.

We did not investigate the effect of screening of the projectile states since it is known that the probabilities for single excitation, capture and ionization are not very sensitive to the small change of the effective charge of the projectile for collision at

intermediate and higher energies. However, at low energies this effect is expected to be significant.

The conclusion drawn in the previous paragraph is not surprising since the primary interaction responsible for all the inelastic processes is the projectile–target electron interaction which is much larger than the electron–electron interaction. In the independent electron approximation, the electron–electron interaction is *partially* accounted for through the inclusion of screening and our results show that different effective screenings should be used for one- and two-electron processes, respectively. We do not ascribe this change of screening an electron correlation effect. The latter, in our viewpoint, is to be reserved for processes or mechanisms involving electron–electron interaction which cannot be approximated by the screening. In this respect, our viewpoint differs from others given in the literature. For example, in a recent article, Datz *et al* (1990) measured the principal quantum numbers n populated in single capture and in transfer ionization processes in collisions between I^{q+} and U^{q+} (q = 5–44) and He. It was observed that the principal quantum numbers, n, populated in TI processes are smaller than those populated by the single electron capture processes. They attributed this difference to electron correlation effect. However, a smaller n for TI is expected according to present independent electron model because of the larger effective binding energy (-1.45 au) of each electron in helium for the TI process than the single ionization energy of -0.9 au for the single capture process. Furthermore the double capture process becomes an important contributor to TI at lower energies. Autoionization of these doubly excited states also populates smaller n in comparison with the direct single capture process.

The results from the present calculation by no means imply that the independent electron approximation is adequate in describing two-electron processes in general. There is evidence that such models are inadequate for describing collisions at higher velocities for processes such as double excitations (Giese *et al* 1990, Pedersen and Hvelplund 1989), simultaneous excitation and ionization (Pederson and Folkmann 1990), and double ionization (Anderson *et al* 1987). There is also experimental evidence that at higher collision energies the electron–electron interaction cannot be approximated by a screening in transfer excitation (Bhalla 1990, Zouros *et al* 1989, DePaola *et al* 1990), in single excitation and in single ionization processes (Tipping *et al* 1988, Hulskotter *et al* 1989). In these processes, which are often treated in the impulse approximation, interactions between electrons from the two different centres have been shown to account for a major portion of the cross sections. At high collision velocities, the process included in the present model is considered as a two-step process involving double collisions between the electron and the projectile (or target) nucleus. Such two-step processes become small at higher velocities (McGuire 1987) in general. One may expect that there are energy regimes where both the two-step process and the electron–electron interaction make important contributions to the excitation cross sections. In such cases the independent electron approximation would fail and a theoretical formulation including all the electrons in the collision system is necessary.

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