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On transfer-excitation in slow ion–helium collisions

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Abstract

Simultaneous transfer and excitation of the two helium electrons in slow collisions of a helium target with multiply charged ions is discussed and calculated for the example of C^{6+} projectiles around 10 keV/u impact energies. The cross section for transfer-excitation is found to be much larger than the cross section for single excitation. There are indications that the cross sections for transfer-excitation scale, with respect to impact energy and projectile charge state, much in the same way as cross sections for transfer ionization.

In slow collisions between multiply charged ions and a helium target, simultaneous transfer and excitation of the two helium electrons is a weak process. Very little is known about this process, even less than about single electron excitation in slow collisions, not in the least because the measurement of electron excitation in slow collisions is difficult. Cederquist [1] analyzed low-energy data on single and double electron removal from the target in Xe^{q+}–He collisions within the classical over-barrier model and found indications for contributions of the transfer-excitation process. An investigation [2] of O^{6+} and N^{6+} collisions with He at 9 keV with the method of energy-gain spectroscopy has also shown a peak which has been attributed to transfer-excitation. Recently it has been found in calculations [3] and in measurements [4] that in the case of slow He^{2+}–He collisions, transfer-excitation cross sections are about as large as cross sections for single electron transfer (which in turn are smaller than the two-electron transfer cross sections in this system). In contrast, at high energies, different transfer-excitation processes have been studied extensively for many systems, notably in view of a resonant transition mechanism, see the contributions in a recent review book [5]. These processes usually involve the excitation of the *projectile* ion and hence differ from the one discussed here.

In this work, we discuss the process of transfer-excitation for the specific case of slow C^{6+}–He collisions. When looking into single electron transfer to $n \geqslant 5$ states of the projectile and into single electron excitation, weak processes that still are important for, respectively, charge exchange and beam emission spectroscopy of fusion plasmas, we realized that the molecular energies in this system are favourable for the process of simultaneous transfer and excitation of the two target electrons. This process may hence, in a close-coupling calculation, influence the magnitude of calculated cross sections for the weaker channels. In this Letter, we will concentrate on the process of transfer-excitation. As it turns out, the results of this and previous [1,3] work allow for an estimate of transfer-excitation cross sections for other systems and other energies.

The transition mechanism in slow C^{6+}–He collisions can be illustrated in a diagram of approximate

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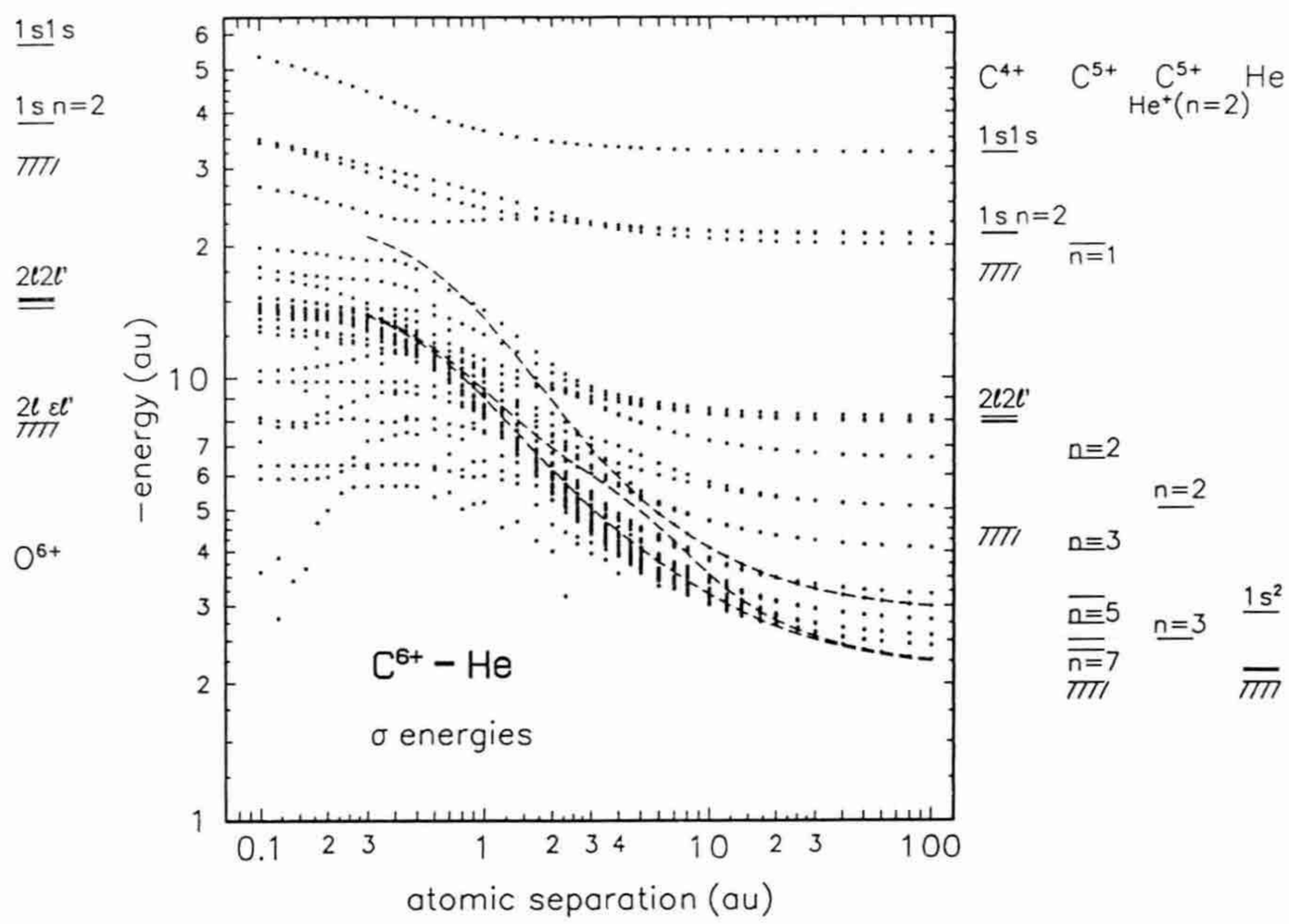

Fig. 1. Approximate energies of molecular σ states in the $(C–He)^{6+}$ system. The dashed lines denote energies of the Stark states which are formed from the initial ground state and the first excited states of helium by the approaching ion, see text. The energy diagram on the left-hand side gives some of the energies of the united-atom system O^{6+}. The energy diagrams on the right-hand side give, from left to right, energies of the system after two-electron transfer, single-electron transfer, transfer-excitation, and the initial system, respectively.

energies of molecular σ states, see Fig. 1. This has been generated by diagonalizing the two-center two-electron Hamiltonian in a large space of atomic two-electron configurations, see further below. For clarification purposes, the energies of Stark states have also been plotted, which are formed from the initial ground state and the first excited states of helium by the approaching C^{6+} ion. These latter energies are determined by diagonalizing the two-center Hamiltonian in the space of the helium configurations only. They show, at large separations, how the energy of the initial state and the first excited states of helium change with diminishing inter-atomic separations. The internuclear interaction does not lead to electron transitions, it is not included in the Hamiltonian.

From Fig. 1, the initial state is seen to evolve to a molecular orbital which may couple, via radial couplings, to a large number of other orbitals. These are mainly orbitals which correlate to the single-transfer configurations of $C^{5+}(n = 3)$–$He^{+}(1s)$. Among the channels which are populated at smaller impact parameters we count the single-transfer channels to $C^{5+}(n = 2)$ states and the two-electron transfer channels to $C^{4+}(2l2l')$ states. The single-transfer channels to $n \geqslant 4$ states of C^{5+} are populated not through transitions at or around avoided crossings but rather by couplings across energy bands. These states are likely to couple efficiently with the singly excited states as well as the transfer-excitation configurations of $C^{5+}(n = 2–3)$–$He^{+}(n = 2)$.

The partial cross sections for transitions to the various channels are determined within the semiclassical close-coupling description of atomic collisions [6,7]. As basis configurations for the decomposition of the time-dependent two-electron wavefunction we take anti-symmetrized products of travelling hydrogenic orbitals, where plane-wave translation factors describe the rectilinear classical motion of the nuclei. Details of the adaption which we use here have been described earlier [8]. At the helium center we include representations [9] of the ground state and the $^{1}2S$ and $^{1}2P$ states. In the single electron transfer channel we include the $C^{5+}(nl)$–$He^{+}(1s)$ configurations with all orbitals of the $n = 1,\ldots,7$ manifold. At the carbon center, representations of the $C^{4+}(^{1}1S,^{1}2L)$ configurations are included along with doubly ex-

cited ($2l2l'$) configurations. For the techniques of representing two-electron states, including doubly-excited states, by products of scaled hydrogenic orbitals, see Ref. [9]. Out of the transfer-excitation configurations, the $C^{5+}(2p)$–$He^{+}(n = 2)$ and the $C^{5+}(3d)$–$He^{+}(n = 2)$ configurations are included in the basis. Other degenerated transfer-excitation states have not been included for reasons of computational efficiency, on grounds that transitions to states (2p, 3d), which have the same nodal structure as the initial state, should be favoured over other states (2s, 3s, 3p). The energy diagram in Fig. 1 has been determined with the basis which consists of the $m = 0$ subset of all these states.

Counting the m-multiplicity of the basis configurations, there are altogether 114 two-electron configurations in the basis set. It takes a very large amount of computer time to evaluate the couplings, including the couplings due to the electron–electron interactions, between all these states for the integration of the coupled equations and the extraction of transition probabilities [9]. Typically, the computation of the cross sections at one energy point takes about one week of full access to the CPU of a fast HP Apollo 735 workstation. It is for this reason that we do not include other states, and that we present here only the results at two energy points and defer a full presentation and discussion of results to another paper.

The results of the calculations at 8 keV/u are given in Table 1 for the most important channels. The transfer cross section is seen to be dominated by contributions of single transfer to the $C^{5+}(n = 3)$ shell as expected [8], followed by single transfer to the $n = 4$ shell. Transfer-excitation cross sections to the $n = 2, 3$ shells of C^{5+}, in conjunction with the population of the $He^{+}(n = 2)$ shell, are larger than all other cross sections. Notably direct excitation is a very weak channel. The calculated results at 14 keV/u are qualitatively very similar. We note that about 80% of the transfer-excitation cross sections involve the population of the $He^{+}(2p)$ state rather than the 2s state. A large population of the 2p state would be expected on grounds that the 2s state has one node and hence does not allow conservation of the nodal structure of the initial state in the collisions.

The relative strength of the transfer-excitation channel versus the single-electron excitation channel is not difficult to understand qualitatively since the energy defects of the transfer-excitation channels are favourable. It seems that only a consistent two-electron model can describe this situation. A one-electron model would have to consider electron excitation of either the He atom or the He^{+} ion, depending on whether the transfer process is visualized to occur, respectively, after or before the excitation process. Such a model would always result in excitation probabilities which are too small to explain the transfer-excitation cross sections of Table 1 through products of independent excitation and transfer probabilities. In other words, the transfer-excitation process occurs, at low energies, as a "correlated" transition of the two electrons. On the other hand, at higher energies, one may well employ an independent-electron description of transfer-excitation, in the same way as has been done [10] successfully for other two-electron transitions.

The calculated single-electron transfer cross sections to the $n = 3$ shell compare very well with earlier work [8] in which a much smaller basis set is used, for the $n = 4$ shell the cross sections from this work are about 50% larger. There is no data on the excitation or the transfer-excitation process. The single-electron excitation cross sections can be linked [11], however, with calculated excitation cross sections for other A^{q+}–He systems much in the same way as this has been accomplished for the A^{q+}–H system [12].

Unlikely as this may seem at first, the transfer-excitation cross sections from this work can be linked with the little information on transfer-excitation, that we have for other systems, when using a scheme that has been introduced by Tanis et al. [13] for scaling transfer-ionization cross sections. For this purpose we define the ratio R_E of total transfer cross sections σ_T to transfer-excitation cross sections σ_{TE},

$$R_E = \frac{\sigma_T}{\sigma_{TE}}. \tag{1}$$

We then plot suitably scaled quantities [13], i.e. the scaled ratio $R_E q^3/E$ over scaled energies $\sqrt{E}/q$ where E is the impact energy in keV/u, for A^{q+}–He systems. This plot is shown in Fig. 2. The points for transfer-excitation in He^{2+}–He collisions between 4 and 65 keV/u are taken from a close-coupling calculation [3] similar to the one of this work. The results for Xe^{q+}–He ($q = 11, \ldots, 31$) collisions at an energy of $4q$ keV are from a study [1] within the classical over-barrier

Table 1
Calculated partial cross sections, in 10^{-16} cm^2, for C^{6+}–He collisions at 8 keV/u

Single capture				Excitation	Transfer excitation	
$n = 2$	$n = 3$	$n = 4$	$n = 5$	$n = 2$	C 2p	C 3d
0.14	14	3.0	0.31	0.018	0.78	0.45

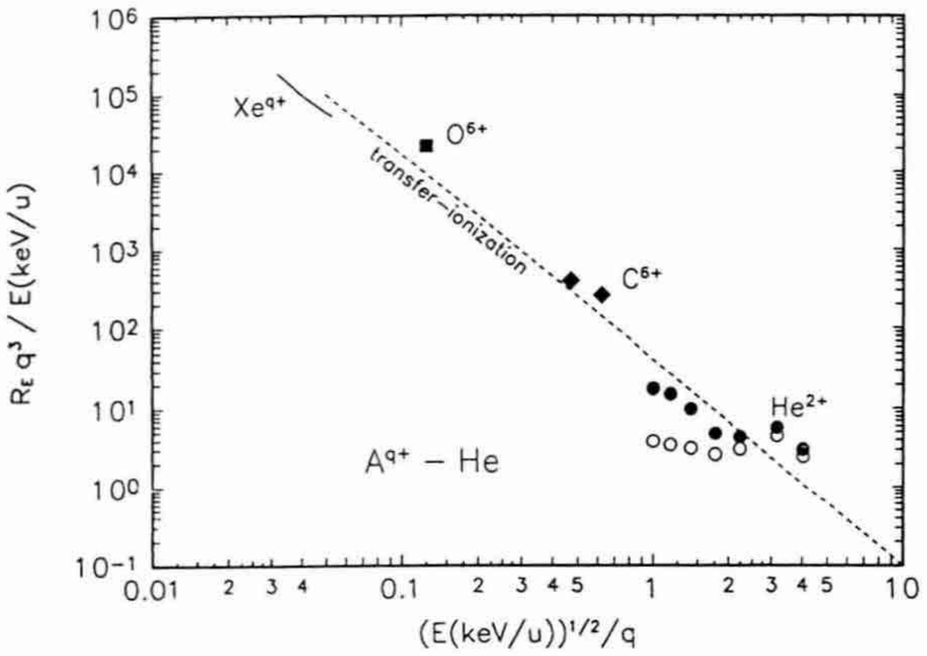

Fig. 2. Scaled ratios R_E of total transfer cross sections to transfer-excitation cross sections, see text, from this work (diamonds), for He^{2+}–He collisions (full circles) [3], for Xe^{q+}–He collisions (solid line) [1], and for O^{6+}–He collisions (square) [2]. The broken line is the line that Tanis et al. [13] used in a similar plot for fitting experimental transfer-*ionization* cross section ratios R'_i. The open circles are for a different ratio R'_E in which only the total *single-electron* transfer cross section for He^{2+}–He collisions is taken in the nominator of Eq. (1).

model, they fit data [14] on one- and two-electron loss from the He target. The data point for O^{6+}–He collisions [2] represents also the result for N^{6+}–He collisions from the same work.

In Fig. 2 we find that all transfer-excitation cross section ratios R_E lie on an approximate universal curve which does not deviate much from the straight line which Tanis et al. used in a study of transfer-*ionization* cross sections [13]. This latter line, which is purely phenomenological, fits ratios of transfer-ionization data over a large range of projectile charge states and energies. It is defined as the ratio R'_i of *single-electron* transfer cross section to the cross section for transfer-ionization. We have preferred here to use the *total* transfer cross section, which includes the two-electron transfer cross sections, in the nominator of R_E, see Eq. (1), since this choice fits better the results for the He^{2+}–He system to the other systems, see Fig. 2. One would expect that low-energy transfer-excitation is caused, at molecular separations between the collision partners, by couplings with a large number of occupied orbitals, not only by couplings to orbitals which are associated with single-electron transfer. In slow He^{2+}–He collisions, this makes a difference because two-electron transfer is by far the strongest channel.

We have refrained from drawing an optimized line through the transfer-excitation results. The line which represents transfer-ionization data appears to serve our purpose sufficiently well. In Fig. 2 one notices deviations from a strictly universal curve which may be drawn through available transfer-excitation cross sections. One may speculate that the calculated transfer-excitation cross sections for the He^{2+}–He system are too small at the higher energies since a larger number of states are populated with increasing energy, states which are not included in the calculation. Also, in general one would expect to see some reflection of the particular level system of a given system in *slow* collision.

The evaluations of transfer-excitation processes for the four systems are hence believed to support each other. The representation of the results in Fig. 2 suggests that transfer-excitation cross sections for other systems and other energies may be readily assessed from the universal curve, with a precision of roughly a factor of two. More work is needed to support this suggestion, notably at higher energies where there are no results available so far. At those higher energies, established independent-electron models [10] may be used to estimate transfer-excitation cross sections. Since the transfer-ionization curve holds at low and at high energies one would expect that also higher-energy transfer-excitation cross section ratios would fall on the universal curve in Fig. 2.

At this point we do not have any physical picture of how the suggested scaling properties of transfer-

excitation cross sections may occur. Such a picture would need to hold in slow collisions where a molecular mechanism supports the transition mechanism of two correlated electrons, and also in faster collisions where the electrons are visualized to move independently from each other. Also in this respect there is more work to be done, much like in the case of transfer-ionization where the phenomenological scaling properties are much better established by data but still there is no explanation in physical terms.

A major portion of the calculations of this work have been performed remotely at a HP Apollo 735 workstation which is operated by the National Institute for Fusion Science at Nagoya, Japan. I am grateful to Hiro Tawara and to the staff at the NIFS Computer Center for granting access to this machine and for technical support.

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