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Calculation of partial electron-transfer cross sections in 1–84-keV/amu $He^{2+}+H$ collisions

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Results of large-scale close-coupling calculations are reported for the $He^{2+}+H$ collision system at energies of 1–84 keV/amu. The calculated transfer cross sections are seen to agree very well with most of the available experimental data at lower energies. At higher energies they constitute improved predictions of cross sections, which are needed for plasma diagnostics purposes. A previously proposed model which neglects intershell couplings in the final capture states is assessed with respect to the accuracy of its results for this collision system.

In this paper we discuss calculations of electron-transfer cross sections for the process

$$He^{2+}+H \rightarrow He^{+}(n,l)+H^{+} \qquad (1)$$

in the energy region 1–84 keV/amu and present some representative results. The calculations are performed within the semiclassical close-coupling method with atomic-orbital (AO) basis sets which have been augmented, at low energies, by united-atom orbitals[1] and, at high energies, by pseudostates which are designed to represent ionization channels.[2] Originally this investigation was taken up with a view to the needs of the plasma physics community, as the knowledge of the small cross sections for populating high-n states in process (1) at about 40–80 keV/amu is instrumental for visible-light charge exchange spectroscopy of helium nuclei in fusion plasmas. From a fundamental point of view, this investigation addresses also the basic question of reliability of small cross sections from close-coupling studies,[3] since experimental transfer cross sections for a number of channels in process (1) at energies 1–10 keV/amu are already available[4] and even more have become available[5] in the course of this investigation. In addition, previously proposed simplified prescriptions[6] on how to calculate cross sections for capture into high-n orbitals can be well tested for collision system (1), for which consistent close-coupling calculations can be performed for principal quantum numbers n well beyond its value n_0 for the dominant capture channel.

The calculations for electron transfer were done mainly with two different basis sets for different energy regions. Both basis sets contain all 84 He^{+} states with $n=1-7$ at the helium center, and the $n=1-2$ H states as well as the $n=2$ united-atom (Li^{2+}) states at the hydrogen center. In addition to these states, target-centered hydrogenic states 1s and 2p with effective charges $Z=3,1.7,0.6$ have been included at higher energies, $E>40$ keV/amu, in order to represent, to some extent, target ionization. Starting with the electron in the 1s H state, the coupled equations have been set up and solved in the customary way.[1,2] From the final occupation probabilities of atomic states, calculated with these basis sets, the partial cross sections for all $He^{+}(n,l)$ channels with $n=1-6$ were integrated. The results for the highest n shell, $n=7$, were considered unreliable because of a "wall effect," i.e., since electrons may be trapped in this shell merely because orbitals with higher quantum numbers n are not available in the basis. Indeed, in actual calculations, the population of the highest projectile n shell of the basis turned out to be distinctively larger than would be consistent with the trend of the population of lower-n states. As tests of the convergence of results with respect to alterations of the basic set have been done only in a very limited sense (cf. below), the accuracy of results, particularly the small channels, has to be estimated from comparison to experiment.

In this paper we present only some portion of the calculated *nlm* partial transfer cross sections; the complete set of results is available from the author, in tabular form, upon request. In Fig. 1 we compare calculated cross sections for the population of $He^{+}(n,l)$ states in $He^{2+}+H$ collisions to the measured results by Ciric *et al.*[4] Except for the population of the metastable $He^{+}(2s)$ state the results of experiment and theory are seen to agree very closely, and still agree reasonably well for the $He^{+}(2s)$ cross sections which, experimentally, are determined by taking the difference of measured cross sections. A comparison to results of other theoretical descriptions is already given in Ref. 4. As discussed there, the measured results for the sensitive 2s channel and for the smaller $n=3$ channels agree with the respective cross sections from other close-coupling calculations[7–9] within typically 30% (and so do results from this work) except for the atomic-orbital expansion results by Bransden *et al.*[10] which, for the $n=3$ channels, decrease much faster with decreasing energy than all other results do. We do not know the precise reason for the deviation of the results of Ref. 10 from the predictions of all other theories and from experiment. Even with a minimal basis set of $n=1-3$ He^{+} states we get, e.g., at 7.5 keV/amu, a cross section $\sigma_{n=3}$ of 0.71×10^{-16} cm^2 which is close to experiment and to the other theories (cf. Ref. 4), while in Ref. 10 this cross section is 0.30×10^{-16} cm^2. It seems, therefore, unlikely that the different types of pseudostates used in Ref. 10 and in this work are the reason for the differences of results.

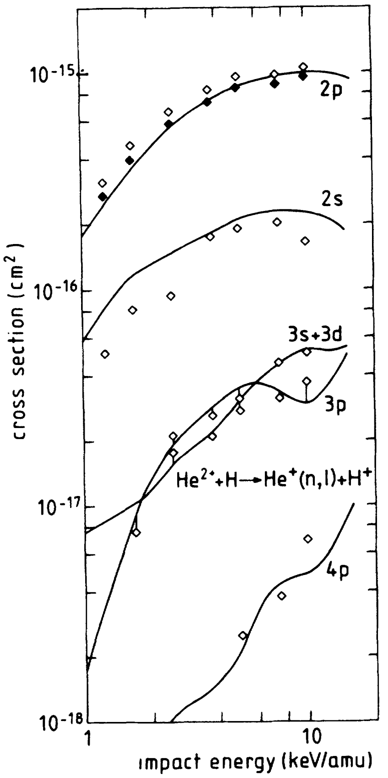

FIG. 1. Comparison of calculated (solid lines, this work) and experimental (Ref. 4, diamonds) partial transfer cross sections in $He^{2+}+H$ collisions. Experimental results are not corrected for the anisotropy of the emitted radiation except for the results given by closed symbols (Ref. 4).

From the preceding discussion it seems plausible to conclude that the calculated partial transfer cross sections are reliable at least at energies $E \lesssim 10$ keV/amu and for σ_{nl} with $n \leq 4$. In Fig. 2, scaled calculated partial cross sections $n^3\sigma_n$ are shown for $n=2-6$ and compared to results from the unitarized-distorted-wave-approximation (UDWA) work by Ryufuku.[11] We note that these two sets of results deviate more strongly at lower energies, as expected, since the UDWA method should not be appropriate there. At the highest energies of Fig. 2, the results of this work are typically 20% higher than the results of the UDWA work. We take this observation as an indication that interchannel couplings (not included in the UDWA method) do contribute to electron transfer at these energies, or, in other words, that higher-n shells may be populated by some ladder-climbing mechanism. Also we note that the well-known prediction of the Born approximation, $\sigma_n \sim n^{-3}$, is not yet followed by the results of either calculation in the energy region of Fig. 2. The UDWA cross sections seem to approach an n^{-3} behavior with increasing n. This may be a consequence of the specific approximation in Ref. 11 that interchannel couplings between final capture states are neglected.

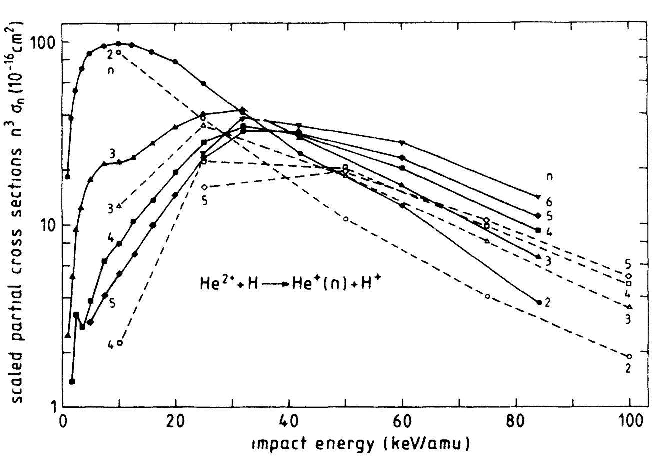

FIG. 2. Scaled partial transfer cross sections in $He^{2+}+H$ collisions from this work (solid lines) and from the UDWA method (Ref. 11, dashed lines).

It is hard to quantitatively assess the accuracy of results presented here since convergence tests with even larger basis sets seem to be impracticable. In Fig. 3, instead, some results of the main calculations are compared to other results derived with *smaller* basis sets. The calculated cross sections from a purely AO expansion scheme appear to be smaller than the results from the main calculations by at most 15% at 25 and at 84 keV/amu. It seems, therefore, that the representation of target excitation and ionization channels in the main calculations is not of critical importance, and little improvement may be gained by further extending the basis with respect to these channels.

In Fig. 3, results are also displayed of calculations which determine the partial cross sections $\sigma_{n'}$ in a two-n-shell AO expansion, i.e., with a basis set consisting of the $n=2$ and n' He^+ orbitals and the 1s H orbital. Such a simplified expansion scheme has been proposed earlier[6] for cases when a full AO expansion scheme cannot be sustained within acceptable computing time limits. Figure 3 shows that the two-n-shell scheme works reason-

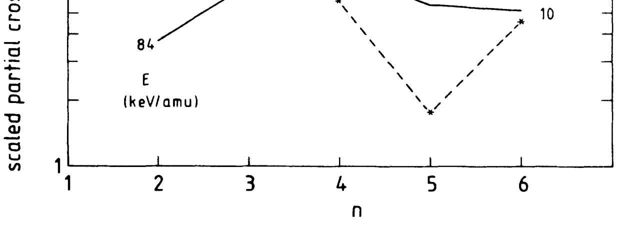

FIG. 3. Scaled partial transfer cross sections derived with various basis sets at three energies (in keV/amu). Solid line, main calculations of this work; triangles linked by dashed lines, pure AO calculation without target excitation states or pseudostates; asterisks linked by dashed lines, two-n-shell AO calculation, see text and Ref. 6.

ably well at the highest energy of 84 keV/amu but becomes increasingly worse for smaller energies and for higher quantum numbers *n*. A related deviation between results of the two-*n*-shell scheme[6] and experimental results[5] has been recently observed for the case of $C^{6+}+H$ collisions at 4–10 keV/amu. This result again emphasizes the importance of interchannel couplings particularly for low energies and high quantum numbers.

While this investigation was being conducted new experimental data on electron transfer in $He^{2+}+H$ collisions has been gathered[5] at energies 1–12 keV/amu. As reported by Ciric *et al.*,[5] the measured line emission cross sections for the $np \rightarrow 1s$ ($n=2$–4) transitions agree very well with corresponding theoretical cross sections determined[5] from the partial cross sections of this work. Surprisingly, other theoretical and experimental line emission cross sections for transitions originating from the same *n* shells, e.g., for the $4 \rightarrow 3$ transitions, are quite different, although sizable lifetime corrections have been applied in the comparison.[5] With respect to this puzzle we note that, in this work, as in any work within the close-coupling method, the various *l*-subshell populations within one *n*-shell are determined all at the same time and certainly not independently from each other. Rather the Stark effect mixes the *l*-subshell orbitals strongly during the collision. It seems, therefore, that the calculated *l*-subshell populations within a given *n* shell should be all equally reliable except for some very small channels within the *l* set.

In summary, the calculated transfer cross sections are seen to agree very well with most of the available experimental data as well as theory at lower energies. At higher energies they should be considered improved predictions of cross sections which are needed for plasma diagnostics purposes. An earlier model which neglects intershell couplings in the final capture states is shown to become increasingly inaccurate for higher-*n* capture channels and for lower energies.

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