Charge Transfer in Ionic Systems

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Charge transfer involving multiply charged ions in collision with atomic or molecular targets are determinant processes in controlled thermonuclear fusion research and astrophysical plasmas. In such processes, an electron is generally captured in an excited state of the ion, followed by line emission. The observation of line intensities provides important information on the electron temperature, density and spacial distributions in the emitting region of the plasma.

From a theoretical point of view, different approaches may be used with regard to the collisional energy range of the process. A semi-classical method is currently used at keV energies, but the description of very low-velocity processes requires a complete quantum mechanical treatment of the dynamics of both electrons and nuclei. The first approach extensively used is the resolution of the stationary close-coupling equations, but we have analyzed recently the efficiency of a time-dependent wave packet method [1,2] which provides a clear and physical insight into the dynamics of the processes and may be particularly interesting for polyatomic systems since it allows the possibility of developing a fully quantal mechanical treatment for some degrees of freedom, the other ones being treated classically.

The keV energy range treatment is presented on two examples pointing out the case of complex ion-atom collision systems, as well as the differences between ion-atom and ion-molecule mechanisms. In connection with translation energy spectroscopy experiments of McLaughlin et al [3] in the 4-28 keV impact energy range, we present a complete ab-initio theoretical approach of the $N^{4+}(2s)^2S$ + He system taking into account both single and double
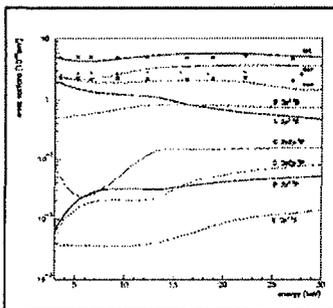
Adiabatic potential energy curves for N^{4+} + He
Full curves, $^2\Sigma^+$ states; broken curves, $^2\Pi$ states.
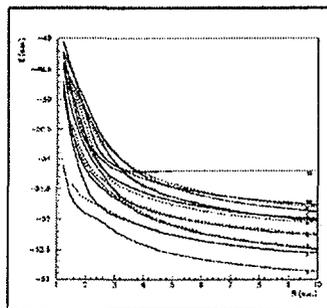
Cross sections for the N^{4+} + He process
Comparison with experimental data [3]

electron capture channels [4]. This is an extremely complex collisional system which involves numerous collision channels with short range interactions and a very intricate interaction region may be observed for interatomic distances around R=3.5 a.u.. In agreement with experimental data, the process is shown to be dominant on the $N^{3+}(2p^2)^1S$ single capture channel, but the double capture process has to be taken into account in the mechanism.

The semi-classical approach may be extended to molecular targets, taking account of the much higher velocity of electronic transitions, with respect to molecular vibration. At the lower level of approximation, the molecular vibration of the molecule can be ignored and the ion-molecule collision may be visualized as an ion bumping an anisotropic atom. This approach has been applied on the $B^{3+}(1s^2) + H_2$ [5] and give reasonable results for energies greater than 100 eV/amu.[6], taking account of the anisotropy effect for the different orientations of the molecule and the dependence on the vibrational coordinate r_{H-H}.

The wave-packet time-dependent treatment has been developed on the Si^{4+} + He collisional system [1,2]. The recombination of silicon ions with atomic hydrogen and helium is a quite important process in astrophysical plasmas which has attracted recently a particular interest as experiments of Fang and Kwong [7] have provided for the first time measurements of rate constants at very low temperatures. The calculation has been performed in both adiabatic and diabatic representations in order to get rid of the ambiguity in defining the unitary transformation, in particular for polyatomic systems and Hanckel-Ricatti functions have been used in order to improve the precision of the calculations. Our results are in good agreement with time independent approaches [8], but a large discrepancy is observed with the ion-trap experiment of Kwong which cannot be explained by the simple electron exchange Si^{4+}/Si^{3+}. Further mechanisms involving impurities or excited states should perhaps be considered.
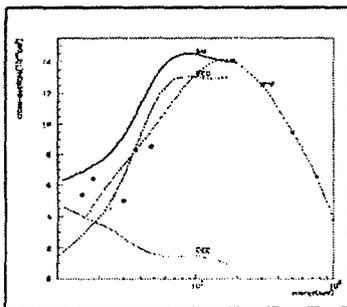
Cross sections for B^{3+} + H_2. Comparison with experimental data [6]
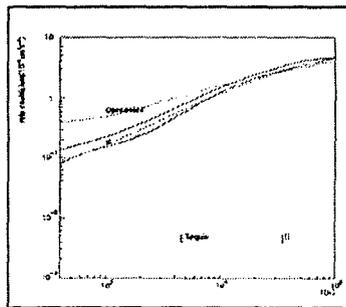
Rate coefficients for Si^{3+}+He (full curve, Hankel- Ricatti functions ; dotted curve, plane waves)

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