THEORY OF CHARGE EXCHANGE AND IONIZATION IN ION-ATOM (ION) COLLISIONS

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INTRODUCTION

The present review will deal with the theoretical methods for study of single electron transfer and ionization processes in ion-atom and ion-ion collisions,

\[ A + B^{q+} \rightarrow A^+ + B^{(q-1)+}, \quad q \geq 1 \] (1.1a)

\[ \rightarrow A^+ + B^{q+} + e \] (1.1b)

\[ A^{q_1+} + B^{q_2+} \rightarrow A^{(q_1+1)+} + B^{(q_2-1)+}, \quad q_1, q_2 \geq 1 \] (1.2a)

\[ \rightarrow A^{(q_1+1)+} + B^{q_2+} + e \] (1.2b)

We shall also briefly discuss some conceptual aspects of the transfer ionization process

\[ A + B^{q+} \rightarrow A^{2+} + B^{(q-1)+} + e \] (1.3)

which is the simplest example of correlated multi-electron transition processes.

From the point of view of basic electron transition mechanisms, there is no substantial difference between the processes (1.1) and (1.2). The Coulomb repulsion in the initial channel of ion-ion reactions becomes important at low collision energies only, and for charge transfer reactions governed by a localized nonadiabatic transition mechanism it introduces a threshold. Thus, for energies below its maximum, the charge exchange cross section in ion-ion collision systems decreases more rapidly than for ion-atom systems (where the fall-off is exponential). In the case of ion-ion ionization, the Coulomb repulsion introduces an additional factor in the transition probability which exponentially decreases with decreasing collision velocity. Further, the density of interacting states in ion-atom systems is higher than in ion-ion systems, which enhances the possibility for getting an energy quasi-resonance for electron capture in ion-atom systems. With these remarks in mind, we shall not make any further distinction between the ion-atom and ion-ion charge-exchange and ionization processes, and present the theoretical methods for their description in a form identical for both types of collisions.
When presenting the theoretical methods for the inelastic processes in heavy particle collisions, it is convenient to introduce three dynamical regions defined by the ratio of the relative collision velocity $v$ and the characteristic velocity $v_0$ of active bound electrons. For $v \ll v_0$, the collisional regime is adiabatic. A quasi-molecular description of collisional system is appropriate, and inelastic transitions in the system generally occur due to well localized nonadiabatic couplings between a restricted number of electronic states. For $v \gg v_0$, the collisional regime is such that transition amplitudes of inelastic processes can be expanded in terms of the small parameter $V_{\text{int}}/E$ where $V_{\text{int}}$ is the interaction inducing electron transitions and $E$ is the collision energy. Finally, for $v \sim v_0$ no small dynamical parameter exists in the problem, and the collisional dynamics has to be solved in its whole complexity. Physically speaking, in this region there is a strong coupling between many (both discrete and continuum) electronic states of the colliding system, and the role of virtual transitions (through intermediate states) may become very pronounced. While in the high velocity region ($v \gg v_0$) a perturbational approach (such as the Born series) may be considered as an appropriate one for description of inelastic ion-atom collision processes (with proper account of continuum states in the case of electron transfer), in the intermediate and adiabatic velocity regions, the methods based on an expansion of total electronic wave function over a set of suitably chosen functions have proved to provide a good description of collisional dynamics. Apart from the perturbation and expansion methods, direct solution of the Schrödinger or classical equations of motion can be used in the intermediate velocity region to treat the charge exchange and ionization ion-atom collisions.

In the present lectures we shall confine ourselves to the methods based on the wavefunction expansion (or the coupled channel) formalism within the framework of semiclassical approximation. In the intermediate and low-energy regions this approach allows to treat the electron capture and ionization processes on the same footing and, under certain circumstances, to obtain approximate analytical solutions for the multistate close-coupling problem. Standard formulations of coupled-channel formalism for charge exchange can be found in the monographs\textsuperscript{1, 2} and review articles\textsuperscript{3-6}. Coupled equations for ionization have been derived by using continuum pseudostates\textsuperscript{2, 7}. Here we shall develop a formulation of the close coupling method which provides a unified description of charge exchange, ionization and transfer - ionization processes (Sect. 2). A more complete account on the expansion methods for charge exchange at low and intermediate collision velocities will be given in Sects 3 and 4, respectively, while for ionization in Sect. 5.

Throughout these lectures we shall use atomic units ($e = \hbar = m_e = 1$), unless otherwise is explicitly stated.

GENERAL FORMULATION OF EXPANSION METHOD

Within the semiclassical approximation, the electronic motion in a colliding diatomic system is described by the time-dependent Schrödinger equation

$$i \frac{\partial \Psi}{\partial t} = H(\vec{r}; \vec{R}) \Psi(\vec{r}; \vec{R})$$  \hspace{1cm} (2.1)

where $H$ is the electronic Hamiltonian, $\vec{r}$ is the set of electron position vectors and $\vec{R} = \vec{R}(t)$ is the internuclear position vector, on which $H$ and $\Psi$ depend parametrically. The expansion method starts, with defining a complete basis set $\{ \chi \}$ over which the total electronic wavefunction is expanded. If Eq. (2.1) is to describe processes both in the discrete and continuous spectrum of the system $\{ \chi \}$ should contain both discrete