§21. Shake-off Mechanism of Two-Electron Transitions in Slow Ion-atom Collisions

I.Yu.Tolstikhina, O.I.Tolstikhin* and H.Tawara

While the physics of the one-electron transfer processes in ion-atom collisions is considered to be well understood both theoretically and experimentally, two-electron transitions (double capture, transfer excitation, transfer ionization) present a much less studied field. Such transitions occur most efficiently in collisions of atom with slow highly charged ions. The interaction between two active electrons here is known to play an important role , because probabilities of *one-step* and *two-step* two-electron transitions for a number of studied cases have comparable values[1].

For qualitative understanding of the inter-electron interaction effects we consider the following simple model. Our collision system consists of two electrons and two bare nuclei of the charges Z_1 (target) and Z_2 (projectile). Both electrons are initially bound on the target. We assume that they are not equivalent, i.e. one of them can be treated as inner and another as outer. For a given internuclear distance R, we approximate wave functions of the inner and outer electrons by solution of the two center Coulomb problem for the pairs of nuclear charges (Z_1, Z_2) and (Z_1-1, Z_2) , respectively. We consider a situation where in the course of the collision an inner electron undergoes a charge transfer transition, i. e. the region of localization of its wave function jumps from Z_1 to Z_2 . This happens while passing some narrow range of R around a point of avoided crossing of the one-electron adiabatic potential curves in the field of the nuclei charges (Z_1, Z_2) . This transition is seen by the outer electron as an abrupt change of the nuclear charges defining its own wave function from (Z_1-1, Z_2) to $(Z_1,$ Z_2 -1), which may result in a change of its state. This shake-off mechanism is of the first order in nonadiabatic coupling at the point of avoided crossing and of the first order in interelectron interaction. It reproduces effect of the inner electron transition on the final state of the outer electron. To our knowledge, this simple mechanism has not been discussed so far (see e.g. Ref.[2]).

As a simple example here we consider ionization of the outer electron (initial state n=2) for $(Z_1, Z_2)=(2,5)$. Fig.1 shows several adiabatic potential curves which interact strongly with the entrance channel. Fig.2 shows corresponding shake-off ionization probabilities.

We also consider double capture and transfer excitation processes.



Fig.1. One-electron adiabatic potentials for nuclear charges $(Z_1-1, Z_2)=(1,5)$. Curves are labeled by elliptic quantum numbers.



Fig.2. Shake-off ionization probability of the outer electron as a function of the internuclear distance at which inner electron transfer occurs.

References

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* Permanent address: P.N.Lebedev Physical Institute, Russian Academy of Sciences, Moscow, Russia.

Present address: Institute for Molecular Science, Myodaiji, Okazaki 444, Japan.