LENINGRAD

I.C.P.E.A.C. 1967

V INTERNATIONAL CONFERENCE ON THE PHYSICS OF ELECTRONIC AND ATOMIC COLLISIONS

Leningrad, USSR, july 17—23, 1967

Abstracts of papers

TRANSITIONS BETWEEN DEGENERATED STATES OF THE UNITED ATOMS IN THE CLOSE COLLISIONS

Yu. N. Demkov, G. V. Dubrovsky, A. M. Ermolaev

(Leningrad State University, USSR)

In the close collisions between atoms and ions when the internuclear distance R approaches its minimum value R_0 small in comparison with the electron shell dimensions the united atom approximation can be used.

In such collisions the angular velocity of the internuclear axis can be large enough to make the non-adiabatic transitions possible. The general treatment of such transitions for the non-degenerated states is given in [1].

The case of the degeneracy of several molecular states in the united atom limit is of special interest. In this case the probabilities of corresponding transitions can increase considerably. The simplest example is the proton-hydrogen scattering in the Σ_u state of the quasimolecule H_2^+. This state at $R=0$ turns into $2p$=state of He^+ and the energy of this state coincides with the energies of Π_g and Σ_g states. Thus the excitation of $2p$ hydrogen states becomes possible. Such calculation are given for example in [2].

We consider the problem in a general form simplifying it to the maximum extent enabling us to study the general properties of the process and the transition to limiting cases. We assume the splitting of the energies to be $\Delta E = 2AR^2$ i. e. we consider only the leading term in the expansion of ΔE in powers of R. If the particles move in XY plane, all the states are divided into two groups — symmetric and antisymmetric with respect to reflection in this plane.

No transitions occur between these groups. For the p-state of the united atom the process is described by the system of equations

$$i\hbar\dot{a} = A\,[X^2 - Y^2)\,a + 2XYb],$$
$$i\hbar\dot{b} = A\,[2XYa + (Y^2 - X^2)\,b]$$

where a, b are the probability amplitudes for the states degenerated at $R=0$ (in the fixed coordinate system), $X(t)$, $Y(t)$ are the relative coordinates of the nuclei ($R=\sqrt{X^2+Y^2}$). Assuming the function X, Y to be known we can integrate the system. In the simplest approximation of the rectilinear motion $X=vt$, $Y=R_0$ the process is described by a single parameter $s=\frac{AR_0^3}{\hbar v}$ — the Massey adiabatic parameter. Two limiting cases are possible.

1) $s \ll 1$ — the fast passage. Then the process can be considered as a sudden turning over of the internuclear axis and the probability of transition is small, but the phase of the adiabatic Σ_u-function changes its sign, i. e. it obtains additional phase shift equal to π. The perturbation theory can be used in this case.

2) Adiabatic case $s \gg 1$. Then the system follows the adiabatic states, so that the additional phase and the transition probability are exponentially small.

The approximate formulas are obtained for both cases. For the intermediate values of s the equations are integrated numerically. The maximum probability $\left(\text{equal to } \frac{1}{2}\right)$ occurs at $s=0.5$.

A more realistic approximation, where the motion of nuclei along the Coulomb trajectory is assumed, is also considered. At large scattering angles the transition probability can reach values close to 1 (the sudden turning of the axis through the angle $\pi/2$).

The influence of this effect upon the decrease of the Σ_u state amplitude in $H^+ + H$ and $He^+ + He$ charge transfer is discussed. This results in the smoothing and the shift of the interference maxima of the differential cross section.

REFERENCES

1. B. M. Smirnov. Optics a. Spectroscopy (USSR), 17, 504 (1964).
2. D. R. Bates, D. A. Williams, Proc. Phys. Soc., 83, 425 (1964).