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$H^- + H$ COLLISION INDUCED RADIATIVE TRANSITIONS*

Introduction. The present work is aimed at the theoretical study of radiating transitions produced in slow collisions of negative ions with neutral atoms. The process of radiating is treated as a dipole transition between gerade and ungerade quasimolecular states that is as a transition between two states of the temporary molecule formed during the collisions. The concept of quasi-molecular transitions is widely used to describe various features of the spectral profiles [1].

We used zero range potential (ZRP) approach to study scattering in the $H^- + H$ collision. The ZRP model is widely employed by physicists, mathematicians, and chemists because it usually allows one to obtain exact solutions for a broad variety of model systems. The gist of the method is presented in by Demkov and Ostrovsky [2]. ZRP set impose constraint on the wave function of the boundary conditions of the form:

$$\frac{\big(r(\psi(r))\big)'}{r(\psi(r))} \xrightarrow[r\to 0]{} -\beta,$$

where $\beta = \sqrt{-2\varepsilon}$, ε is the bound energy of the extra electron in a negative ion H^-. However, it turns out that characteristics of process collision can be expressed in terms of the Lambert function which is a solution of the equation

$$z = W[x]\exp(W[x])$$

elaborated in [3].

Calculations and results. The spectral profile produced by radiating transitions can be described in the quasi-static approximation by the formula [1]:

$$I = 4\pi R_c^2 \left(\frac{A(R_c)}{d\Delta E/dR_c}\right) \exp\left(-\frac{U_i(R_c)}{kT}\right),$$

where R_c — the position of the Condon point, i. e. the interatomic distance at which the transition takes place in accordance with the Franck—Condon principle that is the distance at which the frequency of radiation $\omega = \Delta E$, where ΔE — the quasimolecular potential energy curve difference,

$$A(R_c) = \frac{4}{3}\, g\omega^3\alpha^3 |D(R_c)|^2$$

is the probability of radiation or the Einstein coefficient for spontaneous emission; g — statistical factor equal 2 in our case; $\alpha = 1/137$; $U_i(R_c)$ — the adiabatic energy of the initial

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* По материалам международного семинара «Collisional processes in plasmas and gas laser media», 22–24 апреля 2013 г., физический факультет СПбГУ.

Семинар был проведён при софинансировании фондом «Династия».

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ungerade state; D is the electric dipole moment for transitions between the two states involved. Thus, all we need to calculate spectral profiles in the quasi-static approximation is the $\Delta E, U_i, D$ distance dependencies.

We used zero range potential (ZRP) approach to study scattering in the $H^- + H$ collision. Namely

$$\Delta E = \frac{\chi_-^2 - \chi_+^2}{2},$$

where

$$\begin{cases} \chi_- = \beta + W[-\exp(-\beta R_c)]/R_c; \\ \chi_+ = \beta + W[\exp(-\beta R_c)]/R_c, \end{cases}$$

where $R_c = W[\beta/\omega]/\beta$. The adiabatic energy of the initial term is given in the form:

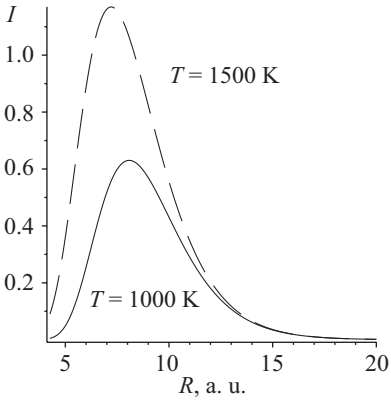
$$U_i(R_c) = -\frac{1}{2}\left(\frac{W^2[-\exp(-\beta R_c)]}{R_c^2} + 2\beta\frac{W[-\exp(-\beta R_c)]}{R_c} + \beta^2\right).$$

In the frame of the LCAO approach the dipole moment is the equal to:

$$D = -\frac{R_c}{2\sqrt{1-S^2}},$$

where S is an overlapping integral between the wave functions of the gerade and ungerade quasimolecular states.

Figure shows the results for the spectral profiles averaged over Maxwell's distributions [3] in relative units as a function of distance in atomic units for two temperatures.



The averaged spectral profile produced in $H^- + H$ collisions

The maximum of intensity at frequencies approximately 0.01 a. u. is formed by transitions in the region of 7–10 a. u.

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Статья поступила в редакцию 22 апреля 2013 г.