INELASTIC COLLISIONS OF LIGHT ATOMS IN THE ADIABATIC APPROXIMATION

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Collisions of light atoms are considered in the adiabatic approximation. The integral corresponding to the transition-probability amplitude is computed by the saddle-point method. To determine the transition probability it is sufficient to find the matrix elements of the atom that is produced by combining the nuclei of the colliding atoms. With decreasing relative velocity of the nuclei v, the inelastic scattering cross section first decreases as v^4 and then exponentially. The cross section for charge exchange of protons on helium is computed.

1. Inelastic collisions of slow atoms were investigated by Bates, Massey, and Stewart[1,2]. It was shown that the method of perturbed stationary states can be used in this case, and a connection between this method and the impact-parameter method[3] or other methods was established. However, the results obtained in these investigations are not convenient for practical use. Consequently numerical values for the inelastic transition cross section were obtained[4] only for the cases H(1s) + p → H(2p) + p and H(1s) + H(1s) → H(2p) + H(1s), where the matrix elements were calculated by perturbation theory, the use of which is not valid.

In the present work we study the case when the main contribution to the inelastic scattering cross section is made by small impact parameters. It turns out here that to determine the transition probability it is sufficient to know the matrix element of the atom produced by combining the nuclei of the colliding atoms. The range of applicability of the proposed method to light atoms coincides in order of magnitude with the range of applicability of the adiabatic approximation; this range is sharply decreased with increasing charge of the colliding-atom nuclei.

2. The probability amplitude of electronic transition due to the motion of the nuclei is given in the adiabatic approximation by[5]

$$c_k = \int\limits_{-\infty}^{+\infty} \frac{1}{\omega_{km}} \left(\frac{\partial H}{\partial t}\right)_{km} \exp\left(i \int\limits_0^t \omega_{km}\, dt'\right) dt \qquad (1)$$

(we use a system of atomic units $\hbar = m_{el} = e^2 = 1$). The subscripts k and m stand for the numbers of the stationary states and ω_{km} is the difference between the energies of the corresponding states.

We assume the nuclei to be classical particles. If the exponential function in the integral oscillates strongly, it is convenient to change over to the complex plane of the variable of integration and determine the integral by the saddle-point method.

3. Let us determine the law governing the relative motion of the nuclei. Let the energy of the nuclei in the center of mass system (c.m.s.) be

$$E \gg \tfrac{1}{2} Z Z_{\text{eff}}, \qquad (2)$$

where Z is the nuclear charge of the bombarded atom (the incoming nucleus is assumed singly charged), and Z_{eff} is the effective charge of the system, so that the properties of the system are noticeably modified when the distance between nuclei changes by an amount $1/Z_{\text{eff}}$.

The c.m.s. motion of the particle in the Coulomb field is given in parametric form[6] by

$$t = b(\varepsilon \operatorname{sh} \xi + \xi), \qquad R = a(\varepsilon \operatorname{ch} \xi + 1),$$
$$a = Z/2E, \qquad b = Z/2Ev, \qquad \varepsilon = \sqrt{1 + (\rho/a)^2}, \qquad (3)^*$$

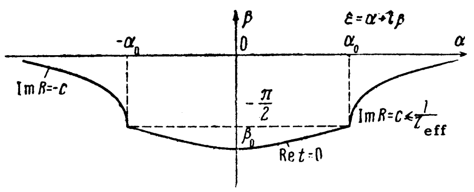
where ρ is the impact parameter.

As $R \to 0$, the interaction between the atoms has a Coulomb-like potential. With increasing R the potential decreases more rapidly than a Coulomb potential, and begins to deviate from the latter noticeably at a distance $R \sim 1/Z_{\text{eff}}$. For a Coulomb interaction potential, it follows from (2) and (3) that $\cosh \xi \gg 1$ at these distances, and since $\epsilon \geq 1$, we have $\epsilon \sinh \xi \gg \xi$, i.e., the particles move as if they were free. Thus, if (2) is satisfied the relative motion of the atoms (ions) is well described by the law (3).

4. Substituting (3) in (1), we evaluate the integral in the complex plane $\xi = \alpha + i\beta$ by the saddle-point method. We introduce $\omega = -\omega_{km}$. The

*sh = sinh; ch = cosh.

matrix elements ω and $R(\partial H/\partial t)_{km}$ are continuous functions of R on the semi axis Im R = 0, Re R $\geq$ 0. In order not to touch the singularities of the intergrand, we confine the contour of integration to the region $|\mathrm{Im}\, R| \lesssim 1/Z_{\mathrm{eff}}$. The integration contour consists of three pieces: Re t = 0, which corresponds to the saddle-point method, and $|\mathrm{Im}\, R| < 1/Z_{\mathrm{eff}}$ (see the figure).



Let us integrate along the portion of the contour Re t = 0:

$$c_k = C \int_{-\alpha_0+i\beta_0}^{\alpha_0+i\beta_0} f(R) \exp\left[\frac{b}{a}\int_{i\pi/2}^{\xi} \omega R d\xi'\right] d\xi,$$

where

$$C = \exp\left[-\frac{b}{a}\int_{-\pi/2}^{0} \omega R d\beta\right], \qquad f(R) = -\frac{b}{a\omega} R \left(\frac{\partial H}{\partial t}\right)_{km}.$$

Estimates show that if

$$v/\omega \ll 1/Z_{\mathrm{eff}}, \tag{4}$$

then the exponential function in the integral is strongly attenuated in the region $\alpha \leq \alpha_0$, where R practically remains unchanged ($|\Delta R| < 1/Z_{\mathrm{eff}}$). The integral along the part of the contour $|\mathrm{Im}\, R| \lesssim 1/Z_{\mathrm{eff}}$ is exponentially small [$\sim \exp(-\omega/vZ_{\mathrm{eff}})$] compared with the integral along the portion of the contour Re t = 0. Thus

$$c_k = C \int_{-\infty-i\pi/2}^{\infty-i\pi/2} \exp\left[-\frac{\omega b}{a}\int_{i\pi/2}^{\xi} R d\xi'\right] d\xi$$

$$= 2Cf(0) \exp(\omega b\varepsilon) K_{-i\omega b}(\omega b\varepsilon),$$

where K is the Macdonald function with imaginary index.

We see that the main contribution to the cross section is made by $\rho \ll 1$. In this case

$$C = \exp(-\omega b\varepsilon - \pi\omega b/2),$$

so that

$$c_k = 2\exp(-\pi\omega b/2) f(0) K_{-i\omega b}(\omega b\varepsilon),$$

$$f(0) = -\frac{1}{v\omega}\lim_{R\to 0}\left[R\left(\frac{\partial H}{\partial t}\right)_{km}\right]. \tag{5}$$

The problem is thus reduced to the calculation of matrix elements with $R \to 0$.

5. The Hamiltonian of the electron system under consideration has the form

$$H = -\sum_i \frac{p_i^2}{2} - \sum_i \frac{1}{|\mathbf{r}_i - \mathbf{R}_1|} - \sum_i \frac{Z}{|\mathbf{r}_i - \mathbf{R}_2|} + \sum_{i,k}\frac{1}{r_{ik}},$$

where i and k are the numbers of the electrons, r_{ik} the distance between them, $\mathbf{r}_i$ the coordinate of the i-th electron, while $\mathbf{R}_1$ and $\mathbf{R}_2$ are the coordinates of the nuclei. Hence

$$\frac{\partial H}{\partial t} = \sum_i\left(\frac{v_{1R}^i \cos\theta_1^i}{|\mathbf{r}_i - \mathbf{R}_1|^2} - \frac{Zv_{2R}^i\cos\theta_2^i}{|\mathbf{r}_i - \mathbf{R}_2|^2}\right)$$

$$+ \sum_i\left(\frac{v_{1\tau}^i \sin\theta_1^i \cos\varphi^i}{|\mathbf{r}_i - \mathbf{R}_1|^2} + \frac{v_{2\tau}^i \sin\theta_2^i\cos\varphi^i}{|\mathbf{r}_i - \mathbf{R}_2|^2}\right),$$

where v_{1R}^i, v_{2R}^i, v_{1T}^i, and v_{2T}^i are the relative tangential and normal components of the center of mass velocity of the i-th electron and of the nuclei, $\theta_{1,2}^i$ and φ^i are the polar angles between the vector $\mathbf{r}_i - \mathbf{R}_{1,2}$ and the axis $\mathbf{R} = \mathbf{R}_1 - \mathbf{R}_2$, with φ^i measured from the plane $(\mathbf{v}, \mathbf{R})$.

The choice of the coordinate system, the origin of which coincides with the center of mass of the i-th electron, is in general not trivial and was discussed many times in the literature[1,7]. It depends on which nucleus the electron is bound to before and after the collision. In our case, when the main contribution to the cross section is made by $\rho \sim v/\omega \ll 1$, the transition occurs essentially when $R \lesssim 1$. In this case the center of mass of the electron coincides with the center of the nuclear charge and the initial conditions are immaterial.

We have

$$\mathbf{R}_1 = \frac{Z}{Z+1}\mathbf{R}, \qquad \mathbf{R}_2 = -\frac{1}{Z+1}\mathbf{R}.$$

In the limit as $R \to 0$ we have $\theta_{1,2}^i \to \theta^i$, so that we obtain for the operator $\partial H/\partial t$

$$\frac{\partial H}{\partial t} = \frac{2Z}{Z+1} v_\tau \sum_i \frac{\sin\theta^i\cos\varphi^i}{r_i^2}.$$

Hence ($v_T = \rho v/R$)

$$c_k = \frac{4Z}{Z+1}\frac{\rho}{\omega}\exp\left(-\frac{\pi}{2}\omega b\right)$$

$$\times K_{-i\omega b}(\omega b\varepsilon)\langle k|\sum_i r_i^{-2}\sin\theta^i\cos\varphi^i|m\rangle, \tag{6}$$

where the matrix element is taken over the wave functions of the atom made up of the combined nuclei.

6. We write the inelastic scattering cross section

$$\sigma_{km} = \int_0^\infty 2\pi\rho d\rho\, |c_k|^2$$

in the form

$$\sigma_{km} = \frac{64\pi v^4}{\omega^6}\left(\frac{Z}{Z+1}\right)^2 \exp(-\pi b\omega) \left|\langle k\right|\sum_i r_i^{-2}\sin\theta^i\cos\varphi^i\left|m\rangle\right|^2$$
$$\times \{I_1(\omega b) - \omega^2 b^2 I_2(\omega b)\};$$
$$I_1(y) = \int_y^\infty |K_{-iy}(x)|^2 x^3 dx,$$
$$I_2(y) = \int_y^\infty |K_{-iy}(x)|^2 x dx = \frac{y^2}{2}|K'_{-iy}(y)|^2. \qquad (7)$$

We see that as $v \to 0$ the cross section attenuates exponentially. If $y \gg 1$, then

$$I_1(y) - y^2 I_2(y) = \pi y e^{-3y}[1 + O(1/y)],$$

so that when $\omega b \gg 1$

$$\sigma_{km} = \frac{64\pi^2 v^4}{\omega^6}\omega b\left(\frac{Z}{Z+1}\right)^2 \exp[-(\pi+3)\omega b]$$
$$\times \left|\langle k\right|\sum_i r_i^{-2}\sin\theta^i\cos\varphi^i\left|m\rangle\right|^2. \qquad (8a)$$

Since $I_1(0) = 1/3$ and $I_2(0) = 1/2$, we have for $\omega b \ll 1$

$$\sigma_{km} = \frac{64\pi v^4}{3\omega^6}\left(\frac{Z}{Z+1}\right)^2 \left|\langle k\right|\sum_i r_i^{-2}\sin\theta^i\cos\varphi^i\left|m\rangle\right|^2. \qquad (8b)$$

(Summation is carried out here over the index m.)

7. Let us discuss the limits of applicability of the method. The upper limit (4) is connected with the applicability of the adiabatic approximation, while the lower limit (2) enables us to replace the interaction potential of the atoms by a Coulomb potential. For example, in the case of the Thomas-Fermi atomic model the region of applicability of the method has the form ($Z_{eff} = Z^{1/3}$)

$$Z^{4/3}/2 \ll E \ll \mu\omega^2/Z^{2/3};$$

here E is the c.m.s. energy of the atoms and μ is the reduced mass.

8. Let us use the obtained results to calculate the cross section for the charge exchange of a proton on a helium atom. To find the matrix elements we must establish the correspondence between the stationary states of our system as $R \to 0$ and as $R \to \infty$. We use the Neumann-Wigner theory, according to which there is no crossing of energy levels of electron terms of like symmetry. We list below the established correspondence:

$R \to 0$ Li^+ nlm	$R \to \infty$
100	$He + H^+$
200	$He^+ + H$ 100
210	$He^+ + H$ 2^1_00
211	$He^+ - H$ 211

We take the value[9] $\langle 100|\omega|211\rangle = 2.28$. Furthermore, $\langle 10|r^{-2}|n1\rangle \underset{n\to\infty}{\sim} 1/n^{3/2}$, so that the main contribution of the cross section is made by transitions with small n (in the language of the Li^+ states). This result is common to problems of this class, for in such cases the electronic Ψ functions have the same form as the Ψ functions of the hydrogen atom.

The cross section for the charge exchange of a proton on a helium atom with transition to the 211 state will be $\sigma = 1.13 \times 10^{-8} E_p^2$, where E_p is the proton energy in the laboratory system, with $20 \ll E_p \ll 1000$.

The results of this investigation were used to study the behavior of a μ^+ meson in hydrogen.

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Translated by J. G. Adashko
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ERRATA

Volume 16 (Russ. v. 43)

No. 1, p. 81 (Russ. p. 112), article by B. M. Smirnov.

The article contains an error. In the calculation of the matrix element $(\partial H/\partial t)_{km}$ contained in the formula of the adiabatic perturbation theory, an error was made in the sign of one of the terms, leading to a non-zero result, and the order of the expansion in the small parameter is lower than actual. A corrected paper will be published in "Optika i spekroskopiya."

Volume 17 (Russ. v. 44)

No. 2, p. 518 (Russ. p. 766), article by E. P. Shabalin

Right hand side of Eq. (3) should read

$$\frac{f_1 f_2 G^2 \sin(\varphi_0 - \varphi_1)}{2^8 \pi^4 7!! M} (Q^2 - 4m^2)(M - Q)^5 \left(1 + \frac{5Q}{M} + \frac{Q^2}{M^2}\right)$$

No. 5 p. 999 (Russ. p. 1485), article by D. K. Kopylova et al.

Caption to Fig. 7 should read:

Distribution of two-prong stars by "target mass": Continuous histogram - cases with $M_X^2 > 0$, dashed - with $M_X^2 < 0$.

Volume 18 (Russ. v. 45)

No. 4, p. 1100 (Russ. p. 1598), article by S. I. Syrovat-skiĭ et al.

Values of the fragmentation coefficient: in place of $a_{321} = -4.3618$ read $a_{321} = -3.3618$.