Ion-atom charge exchange at low energies

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The cross section for charge exchange of ions on atoms in slow collisions has been calculated for the case where the concept of a classical trajectory is not applicable to the description of their relative motion. In the limiting case of fast collisions the formula obtained coincides with the Rosen-Zener-Demkov formula. An expression is obtained for the Massey parameter which is suitable for description of inelastic reactions at low collision energies. The results of the present work are compared with the results of a numerical calculation of the cross section for charge exchange of slow protons on hydrogen atoms.

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1. INTRODUCTION

The main features of the charge exchange of ions on atoms

$$A^+ + B \to A + B^+ \tag{1}$$

have been studied in the framework of the two-level approximation (see for example Refs. 1–3), which is applicable if the relative motion of the nuclei is described by the laws of classical mechanics and the difference of the electron binding energies in atoms B and A is small in comparison with the excitation energies of the atoms.

As a rule the interatomic distance R characteristic of the charge-exchange process (1) is large:

$$\gamma R \gg 1, \tag{2}$$

where

$$\gamma = \frac{1}{2}(\gamma_1+\gamma_2), \quad \gamma_1 = (2|\varepsilon_1|)^{1/2}, \quad \gamma_2 = (2|\varepsilon_2|)^{1/2}, \tag{3}$$

and ε_1 and ε_2 are the electron binding energies respectively in atoms B and A (here and below $\hbar = m_e = e = 1$).

Under condition (2), a natural basis for the electron wave functions is the diabatic basis, which in the two-level approximation consists of wave functions $\varphi_2(\mathbf{r},\mathbf{R})$ and $\varphi_2(\mathbf{r},\mathbf{R})$. As $R \to \infty$ the functions φ_1 and φ_2 coincide with the wave functions of the electrons in the isolated atoms B and A, respectively. For finite R the electron wave function is[1–3]

$$\psi = C_1(t)\varphi_1 + C_2(t)\varphi_2,$$

where the probability amplitudes C_1 and C_2 obey the equations

$$i\frac{dC_1}{dt} = \frac{1}{2}\Delta(t)\exp\left(-i\int^t \Delta E(t')\,dt'\right)C_2,$$

$$i\frac{dC_2}{dt} = \frac{1}{2}\Delta(t)\exp\left(i\int^t \Delta E(t')\,dt'\right)C_1. \tag{4}$$

Here $\Delta(R(t))$ is the exchange interaction at a distance R between A^+ and B and $\Delta E(R) = H_{11}(R) - H_{22}(R)$ is the difference of the diagonal matrix elements of the electron Hamiltonian calculated on the basis of the wave functions φ_1 and φ_2. For the initial condition $C_1(-\infty) = 1$, $C_2(-\infty) = 0$ the probability of charge exchange for a given trajectory of the relative motion of the atoms $\mathbf{R}(t)$ is $W = |C_2(+\infty)|^2$.

The two-level-approximation models most characteristic and most amenable to solution are the following:

1) resonance charge exchange (Firsov[4])

$$\Delta E(R) = 0, \quad W = \sin^2\eta, \quad \eta = \frac{1}{2}\int_{-\infty}^{\infty}\Delta(t)\,dt; \tag{5}$$

2) the Rosen-Zener-Demkov model[5,6]

$$\Delta = \Delta_0/\mathrm{ch}\,\alpha t, \quad \Delta E = \text{const}, \quad W = \frac{\sin^2\eta}{\mathrm{ch}^2(\pi\Delta E/\alpha)}; \tag{6}$$

3) the Landau-Zener model[7,8]

$$\Delta = \text{const}, \quad \Delta E = \alpha t, \quad W = 2p(1-p), \quad p = \exp(-\pi\Delta^2/2\alpha). \tag{7}$$

The initial and final states in (1) correspond to two electronic terms with a characteristic energy difference $\sim$3–5 eV, which in play the Born-Oppenheimer approximation the role of the potential energy of the atoms. Therefore in the case of collisions with low energy

$$E \lesssim 3\text{–}5 \text{ eV} \tag{8}$$

the assumption that a classical trajectory $R(t)$ exists becomes invalid.

Study of the process of ion-atom charge exchange in the energy range (8) presents significant interest from the theoretical and practical points of view. This study is carried out in the present work.

2. BASIC ASSUMPTIONS

The Schrödinger equation for the system of the electron and the cores of the atoms has the form

$$\left[-\frac{\nabla_R^2}{2\mu} + \hat{H}_e(\mathbf{r},\mathbf{R}) + \frac{1}{R} - E\right]\psi(\mathbf{r},\mathbf{R}) = 0, \tag{9}$$

where $\mathbf{r}$ are the electron coordinates, $\mathbf{R}$ is the vector connecting the cores, μ is the reduced mass of the atoms, and $\hat{H}_e$ is the Hamiltonian of the electron for fixed $\mathbf{R}$. We shall show below that the condition (2) is preserved also for quantum-mechanical motion of the atoms, and therefore choose as the basis of the electron wave functions the diabatic basis (see the Introduction). We shall assume also that in atoms B and A the electron is in S states and the ionization potentials of the atoms are nearly the same. Under these conditions the basis consists of two real wave functions: $\varphi_1(\mathbf{r},\mathbf{R})$, $\varphi_2(\mathbf{r},\mathbf{R})$.

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The solution of Eq. (9) can be looked for in the form

$$\psi(\mathbf{r}, \mathbf{R}) = \psi_1(\mathbf{R})\varphi_1(\mathbf{r}, \mathbf{R}) + \psi_2(\mathbf{R})\varphi_2(\mathbf{r}, \mathbf{R}), \tag{10}$$

where the wave functions $\psi_{1,2}(\mathbf{R})$ describe the relative motions of the atoms. Substituting (10) into (9), we obtain the equations[1]

$$\begin{aligned}[E+\nabla_R^2/2\mu - E_1(R)]\psi_1(\mathbf{R}) &= {}^1/_2\Delta(R)\psi_2(\mathbf{R}),\\ [E+\nabla_R^2/2\mu - E_2(R)]\psi_2(\mathbf{R}) &= {}^1/_2\Delta(R)\psi_1(\mathbf{R}),\end{aligned} \tag{11}$$

where $E_1(R) = H_{11}(R) + 1/R$, $E_2(R) = H_{22}(R) + 1/R$.

The equations (11) are valid if the conditions (2) are satisfied and also if

$$KR \gg 1, \quad R|\Delta E|/\gamma \ll 1, \tag{12}$$

where K is the momentum of the relative motion of the atoms.

In what follows we shall discuss reactions induced by singly charged ions, and therefore

$$E_{1,2}(R) = E_{1,2}(\infty) - \alpha_{1,2}/2R^4 \tag{13}$$

where $E_{1,2}(\infty)$ are the energies of the isolated atoms B and A and $\alpha_{1,2}$ are their polarizabilities.

For $R \to \infty$ we have $\Delta(R) \propto \exp(-\gamma R) \to 0$ and the relation between ψ_1 and ψ_2 is "turned off," so that

$$\begin{aligned}\psi_1(\mathbf{R}) &\to e^{i\mathbf{K}_1\mathbf{R}} + \frac{1}{R} f_1(\mathbf{n}) e^{iK_1R},\\ \psi_2(\mathbf{R}) &\to \frac{1}{R} f_2(\mathbf{n}) e^{iK_2R}, \quad \mathbf{n} = \mathbf{R}/R,\end{aligned} \tag{14}$$

where $K_{1,2}$ are defined by the equations

$$K_{1,2}^2(\infty) = 2\mu[E - E_{1,2}(\infty)]. \tag{15}$$

The cross section for charge exchange is expressed in terms of the amplitude f_2:

$$\sigma = \frac{K_2}{K_1}\int d\sigma_{\mathbf{n}} |f_2(\mathbf{n})|^2. \tag{16}$$

Substituting into (11) the expansions

$$\psi_1(\mathbf{R}) = \frac{1}{R}\sum_{l=0}^{\infty} U_l(R) P_l(\cos\theta),$$

$$\psi_2(\mathbf{R}) = \frac{1}{R}\sum_{l=0}^{\infty} V_l(R) P_l(\cos\theta),$$

where θ is the angle between $\mathbf{n}$ and $\mathbf{K}_1$, we obtain equations for the functions U_l and V_l (we shall omit the subscript l):

$$\frac{d^2U}{dR^2} + K_1^2(R)U = \mu\Delta(R)V, \quad \frac{d^2V}{dR^2} + K_2^2(R)V = \mu\Delta(R)U, \tag{17}$$

where

$$K_{1,2}^2(R) = 2\mu[E - E_{1,2}(R) - l(l+1)/2\mu R^2]. \tag{18}$$

For $\mu \to \infty$ the equations (11) reduce to a system of algebraic equations, and from the condition of compatibility of these equations we obtain an expression for the energies of the adiabatic terms

$$E_{u,g} = {}^1/_2(E_1 + E_2) \pm {}^1/_2[(\Delta E)^2 + \Delta^2]^{1/2}.$$

Let us define the effective terms

$$U_{u,g}(R) = E_{u,g}(R) + l(l+1)/2\mu R^2. \tag{19}$$

For the case $E_1(\infty) > E_2(\infty)$ the terms $U_{u,g}$ are plotted in Fig. 1. The dashed line shows the energy level of the system of the electron + the cores of the atoms. R_u is the turning point of the classical motion in the repulsive u term, and R_g is the turning point in the attractive term.

From the stationary equations (11) we obtain after the substitution $E \to i\partial/\partial t$ the nonstationary equations. If the kinetic energy of the atoms is large in comparison with the characteristic difference $E_u - E_g \sim 3$–5 eV, we shall seek the solution of the nonstationary equations in the form

$$\psi_1 = C_1(t)\exp[iS(\mathbf{R}, t)], \quad \psi_2 = C_2(t)\exp[iS(\mathbf{R}, t)].$$

Then for S we obtain the Hamilton-Jacobi equation, and for the coefficients C_1 and C_2 we obtain the system (4). Consequently the equations (11) are a quantum-mechanical generalization of the two-level approximation (4).

Stuckelberg[9] discussed on the basis of the Eqs. (11) the quantum-mechanical analog of the Landau-Zener model.[7] Resonance charge exchange (5) for quantum-mechanical motion of the atoms was investigated by Massey and Smith.[10]

In the present work we shall assume that, generally speaking, $E_1(R) \neq E_2(R)$ and in this case there is no crossing of the diabatic terms $E_1(R)$ and $E_2(R)$.

The condition that the motion of the atoms (12) be quasiclassical is equivalent at low energies to the assumption

$$N \gg 1, \quad K_{1,2}(\infty)(\mu\alpha_{1,2})^{1/2} \gg 1, \tag{20}$$

where N is the number of vibrational levels of the ion $(AB)^+$. The first of the conditions (20) is as a rule satisfied. The second condition arises on taking into account the acceleration of the atoms in the polarization potential (13). According to the criterion (20), the equations (11) are valid down to collision energies $(\mu^2\alpha_{1,2})^{-1} \sim 0.1$ K for light atoms and still lower for heavy atoms.

3. CHARGE-EXCHANGE CROSS SECTION

Near the turning point R_u (see Fig. 1) $\Delta(R)$ varies exponentially:

$$\Delta(R) = \Delta_0 \exp[-\gamma(R - R_u)], \tag{21}$$

and $K_{1,2}(R)$ depend on R according to a power law; therefore at $R \approx R_u$ we shall replace the quantities $K_{1,2}(R)$ by constants $K_{1,2}(R_u)$:

$$\begin{aligned}\frac{d^2U}{dx^2} + q_1^2 U &= \alpha \exp\left(-\frac{1}{2}x\right) V,\\ \frac{d^2V}{dx^2} + q_2^2 V &= \alpha \exp\left(-\frac{1}{2}x\right) U,\end{aligned} \tag{22}$$

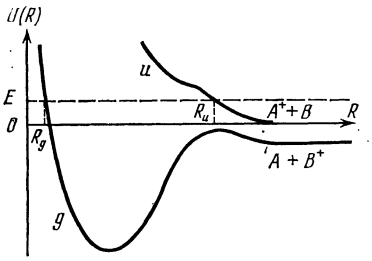

FIG. 1. Diagram of effective adiabatic terms for the case $E_1(\infty) > E_2(\infty)$.

where

$$x=2\gamma(R-R_u), \qquad q_{1,2}=K_{1,2}(R_u)/2\gamma,$$
$$\alpha=\mu\Delta_0/4\gamma^2.$$

For $R<R_u$ the value of $\Delta(R)$ is exponentially large and in the equations (22) we can neglect the terms with $q_{1,2}^2$. Consequently in this region

$$d^2U/dx^2=\alpha\exp(-{}^1/_2x)V,$$
$$d^2V/dx^2=\alpha\exp(-{}^1/_2x)U, \tag{23}$$

or

$$d^2X/dx^2-\alpha\exp(-{}^1/_2x)X=0,$$
$$d^2Y/dx^2+\alpha\exp(-{}^1/_2x)Y=0, \tag{24}$$

where

$$X=U+V, \qquad Y=U-V.$$

For $x\to-\infty$ the function $X(x)$ falls off exponentially, which corresponds to the classically inaccessible region of motion in the u term, and the function $Y(x)$ oscillates. Since in the g term the motion in R also is bounded on the left (see Fig. 1), the solution has the form of a standing wave

$$Y(x)\to e^{x/8}\sin[4\alpha^{1/2}e^{-x/4}+\varphi_l-\pi/4], \tag{25}$$

where $\varphi_l\sim\pi N(l)$ and $N(l)$ is the number of vibrational levels of the ion $(AB)^+$ with orbital angular momentum l. The quasiclassical formula (25) is valid for the condition (20).

Let us apply to the equations (22) the Fourier transformation

$$U(\alpha,p)=\int_{-\infty}^{\infty}dx\,e^{-ipx}U(\alpha,x), \qquad V(\alpha,p)=\int_{-\infty}^{\infty}dx\,e^{-ipx}V(\alpha,x). \tag{26}$$

For these integrals to converge as $x\to+\infty$ we add to p a negative imaginary quantity, $p\to p-i0$. The inverse transformation has the form

$$U(\alpha,x)=\int_{-\infty-i0}^{+\infty-i0}\frac{dp}{2\pi}e^{ipx}U(\alpha,p) \tag{27}$$

and similarly for V. From (22) and (26) we obtain

$$(q_1^2-p^2)U(\alpha,\ p)=\alpha V(\alpha,\ p-i/2),$$
$$(q_2^2-p^2)V(\alpha,\ p)=\alpha U(\alpha,\ p-i/2).$$

The equations (22) are invariant to the transformation $x\to x+a$, $\alpha\to\alpha\exp(1/2a)$. Consequently

$$U(\alpha,\ x)=U(\alpha\exp({}^1/_2a),\quad x+a),$$
$$V(\alpha,\ x)=V(\alpha\exp({}^1/_2a),\quad x+a).$$

Hence

$$U(\alpha,\ p)=\alpha^{-2ip}U(p); \qquad V(\alpha,\ p)=\alpha^{-2ip}V(p),$$

where $U(p)$ and $V(p)$ satisfy the equations

$$(q_1^2-p^2)U(p)=V(p-i/2), \qquad (q_2^2-p^2)V(p)=U(p-i/2). \tag{28}$$

Using the property $\Gamma(x+1)=x\Gamma(x)$ of the Γ function, we obtain from the equations (28)

$$U(\alpha,\ p)=\alpha^{-2ip}\Gamma[i(p-q_1)]\,\Gamma[i(p+q_1)]$$
$$\times\,\Gamma[i(p-q_2)+{}^1/_2]\,\Gamma[i(p+q_2)+{}^1/_2]f(p-i/2),$$
$$V(\alpha,\ p)=\alpha^{-2ip}\Gamma[i(p-q_2)]\,\Gamma[i(p+q_2)]\,\Gamma[i(p-q_1)+{}^1/_2] \tag{29}$$
$$\times\,\Gamma[i(p+q_1)+{}^1/_2]f(p),$$

where $f(p)$ is a still unknown periodic function: $f(p+i)=f(p)$ which we can therefore represent in the form

$$f(p)=\sum_{n=-\infty}^{\infty}C_n\exp(2\pi pn). \tag{30}$$

The Fourier component $V(\alpha,p)$ for complex p located far away in the lower half plane is determined mainly by the asymptotic expression for $V(x)$ as $x\to-\infty$. To find $V(\alpha,p)$ in this region it is necessary to find the Fourier component of the function (25), which reduces to calculation of an integral of the form

$$\int_0^{\infty}dz\,z^{4ip-1/2}e^{iz}.$$

For $z\to+0$ this integral converges since p has a large negative imaginary part. For convergence as $z\to+\infty$ the additional substitution $\exp(iz)\to\exp(iz-\gamma z)$ is required, where $\lambda\to+0$. Omitting unimportant factors which do not depend on p, we obtain

$$V(\alpha,\ p)\propto(16\alpha)^{-2ip}\Gamma(4ip-{}^1/_2)\,\mathrm{ch}(2\pi p-i\varphi_l). \tag{31}$$

From comparison of the formulas (29)–(31) one can conclude that in (30) only the three coefficients $C_{\pm1}$ and C_0 are nonzero, and the term with C_0 is not noticeable against the background of the two other exponentially large terms with $C_{\pm1}$.

To find C_0 we return to the formulas (29). The Γ functions have first-order poles on the real axis and in the upper half plane of complex p. At $x\to+\infty$ the poles from the upper half plane give exponentially decreasing contributions to $U(x)$ and $V(x)$, and the poles on the axis are oscillating terms—traveling waves:

$$U(x)\to Ae^{-iq_1x}+Be^{iq_1x}, \qquad V(x)\to Ce^{-iq_2x}+De^{iq_2x}. \tag{32}$$

The boundary condition (14) for $\psi_2(\mathbf{R})$ contains only the divergent wave, and consequently $C=0$, which is equivalent to the condition

$$f(-q_2)=0. \tag{33}$$

Finally

$$f(p)=\mathrm{ch}(2\pi p-i\varphi_l)-\mathrm{ch}(2\pi q_2+i\varphi_l). \tag{34}$$

The solutions (32) are valid in the region where $K_{1,2}(R)\approx K_{1,2}(R_u)$. Outside this region $(R>R_u)\Delta(R)$ is exponentially small and the relation between $U(R)$ and $V(R)$ is turned off. The conditions (12) and (20) permit use in this region of the WKB approximation, according to which for $R>R_u$ we have

$$U(R)=A\left(\frac{K_1(R_u)}{K_1(R)}\right)^{1/2}\exp\left[-i\int_{R_u}^{R}K_1(R')\,dR'\right]$$
$$+B\left(\frac{K_1(R_u)}{K_1(R)}\right)^{1/2}\exp\left[i\int_{R_u}^{R}K_1(R')\,dR'\right],$$

$$V(R)=D\left(\frac{K_2(R_u)}{K_2(R)}\right)^{1/2}\exp\left[i\int_{R_u}^{R}K_2(R')\,dR'\right]. \tag{35}$$

From Eqs. (14), (16), and (35) we obtain for the cross section for the charge-exchange reaction (1)

$$\sigma=\frac{\pi}{K_1^2(\infty)}\sum_{l=0}^{\infty}(2l+1)\frac{q_2}{q_1}\left|\frac{D_l}{A_l}\right|^2. \tag{36}$$

The coefficients D and A are proportional to the residues of the functions $V(\alpha, p)$ and $U(\alpha, p)$ [see the formulas (29)] respectively at the poles $p=q_2$ and $p=-q_1$. Calculating these residues, we obtain

$$\sigma=\frac{\pi}{K_1^2(\infty)}\sum_l(2l+1)\frac{\operatorname{sh}(2\pi q_1)}{\operatorname{sh}(2\pi q_2)}\left|\frac{f(q_2)}{f(-q_1-i/2)}\right|^2$$

$$=\frac{\pi}{K_1^2(\infty)}\sum_l(2l+1)\frac{\operatorname{sh}(2\pi q_1)\operatorname{sh}(2\pi q_2)\sin^2\varphi_l}{\operatorname{ch}^2[\pi(q_1-q_2)][\operatorname{ch}^2\pi(q_1+q_2)-\sin^2\varphi_l]}. \tag{37}$$

In the theory with classical trajectories[5,6]

$$\varphi_l=\Phi_u-\Phi_g,\quad \Phi_{u,g}=\int_{R_{u,g}}^{\infty}dR[K_{u,g}(R)-K_{u,g}(\infty)],$$

$$K_{u,g}^2=2\mu[E-U_{u,g}(R)]. \tag{38}$$

It is sufficient to extend the summation over l in (37) only to angular-momentum values $l<l_0$, where l_0 is given by the equations[2,3]

$$\varphi_{l_0}=0.28. \tag{39}$$

It is necessary to keep in mind that Eq. (38) is valid only for $l\approx l_0$. In the case $l<l_0$ the phase φ_l is known only in order of magnitude: $\varphi_l\sim\pi N(l)$. As a consequence of this circumstance Eq. (37) contains an uncertainty, which disappears, however, after averaging (37) over the rapid oscillations of $\sin^2\varphi_l$. The final expression for the charge-exchange cross section has the form

$$\sigma=\frac{\pi}{K_1^2(\infty)}\sum_{l=0}^{l_0}(2l+1)W(l), \tag{40}$$

$$W(l)=\frac{\operatorname{sh}(2\pi q_1)\operatorname{sh}(2\pi q_2)\exp[-\pi(q_1+q_2)]}{\operatorname{ch}^2[\pi(q_1-q_2)]\operatorname{sh}[\pi(q_1+q_2)]}. \tag{41}$$

The uncertainty in the phase φ_l does not permit calculation of the cross section for elastic scattering $A^+ + B\to A^+ + B$ by the method described.

4. DISCUSSION OF RESULTS

The expression for $W(l)$ can be understood as the probability of charge exchange if we assign to angular momentum l formally the impact parameter $\rho=l/K_1(\infty)$. In the limiting case of high-energy collisions when the nuclei move along straight trajectories we have

$$q_1-q_2=\frac{1}{2\gamma}[K_1(R_u)-K_2(R_u)]\approx\Delta E(\infty)/2\gamma v_R, \tag{42}$$

where $v_R=(v^2-l^2/\mu^2R_u^2)^{1/2}$. From Eqs. (41) and (42) we obtain the Rosen-Zener-Demkov formula (6) in which averaging over the phase η has been carried out. Thus, Eq. (41) is the quantum-mechanical analog of (6). An important conclusion follows from this. The Massey parameter for classical trajectories

$$\xi=\pi|\Delta E(\infty)|/\gamma v_R$$

in quantum mechanics has the form

$$\xi=\pi\gamma^{-1}|K_1(R_u)-K_2(R_u)|. \tag{43}$$

The agreement in the high-energy limit of Eqs. (41) and (6) permits us to state that Eqs. (40) and (41) are valid if the condition (20) is satisfied and also $v\ll 1$ atomic units.

For the probability of resonance charge exchange we obtain from (41)

$$W=\tfrac{1}{2}[1-\exp(-4\pi q)],\quad q=K(R_u)/2\gamma,$$

$$K(R_u)=\left[K^2(\infty)+\frac{\mu\alpha}{R_u^4}-\frac{l(l+1)}{R_u^2}\right]^{1/2}.$$

However, even for light atoms at zero kinetic energy

$$4\pi q=2\pi(\mu\alpha)^{1/2}/\gamma R_u^2\sim 5,$$

and therefore with high accuracy $W\approx 1/2$, i.e., the theory of resonance charge exchange with classical trajectories of the nuclei is valid in essentially the entire range of energies (20).

The most substantial deviations from the classical theory occur in nonresonance charge exchange. We shall consider two possible cases.

1) The exothermic charge-exchange reaction $[E_1(\infty)>E_2(\infty)]$. The kinetic energy of collision of the atoms is

$$E_{\text{kin}}=\frac{1}{2\mu}K_1^2(\infty)=E-E_1(\infty).$$

If $E_{\text{kin}}\ll 1/2\alpha_1 R_u^{-4}\sim 10^3$ K, then the quantities q_1 and q_2 do not depend on E_{kin}. According to Eq. (40) in this case $\sigma\propto(E_{\text{kin}})^{-1}$. The dependence is preserved down to $E_{\text{kin}}\sim(\mu^2\alpha 1)^{-1}\lesssim 0.1$ K. At lower energies Eqs. (40) and (41) are not valid, but from the theory of scattering of slow particles it follows that the cross section varies with energy according to the Bethe law $\sigma\propto(E_{\text{kin}})^{-1/2}$.

If the energy transfer is large:

$$\pi\gamma^{-1}(\mu|\delta E|)^{1/2}\gg 1, \tag{44}$$

where

$$\delta E=E_1(\infty)-E_2(\infty)+(\alpha_2-\alpha_1)/2R_u^4,$$

then the main contribution to the cross section is from small angular momenta. Replacing the summation by integration over l in Eq. (40), we obtain

$$\sigma=\frac{4R_u^2\gamma^2}{K_1^2(\infty)}\frac{q_1q_2}{(q_2-q_1)}\exp[-2\pi(q_2-q_1)], \tag{45}$$

where the quantities q_1 and q_2 are calculated for $l=0$.

2) The endothermic charge-exchange reaction $[E_1(\infty)<E_2(\infty)]$. Here

$$E_{\text{kin}}=\frac{1}{2\mu}K_1^2(\infty)=\Delta E(\infty)+\varepsilon,$$

$$\varepsilon=\frac{1}{2\mu}K_2^2(\infty).$$

For $\varepsilon\ll\alpha_2/2R_u^4$ we obtain from (40) and (41) $\sigma=$ const. As in the first case for $\varepsilon\ll(\mu^2\alpha_2)^{-1}$ we have $\sigma\propto\varepsilon^{1/2}$. For a large energy transfer (44), the charge-exchange cross section is determined by Eq. (45), in which for $q_2<q_1$ it is necessary to make the substitution $q_1\rightleftarrows q_2$.

The literature contains a calculation[15] of the cross section for resonance charge exchange $p+\text{H}(1S)\to\text{H}(1S)1p$ at low collision energies based on numerical solution of the three-body problem by the technique described in Refs. 11–

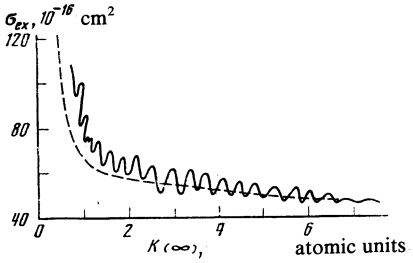

FIG. 2. Cross section for the resonant charge-exchange reaction $p + H \to H + p$ as a function of the relative momentum $K(\infty)$. The solid line shows the result of Ref. 15, and the dashed line is the result of the present work.

15. Comparison of the results of Ref. 15 with the cross-section value calculated with (40) and (41) is carried out in Fig. 2, from which we can obtain an idea of the accuracy of our calculation.

To avoid errors, we emphasize that Eqs. (40) and (41) are applicable only to ion-atom collisions and not to charge exchange of molecular ions. It is well known that in the latter case ion-molecule reactions turn out to be important, for example,

$$H_2^+ + H_2 \to H_4^+ \to H_3^+ + H.$$

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