# Asymptotic theory of transmission of fast diatomic ions through thin films

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The general characteristics of the transmission of fast $H_2^+$ and $^4HeH^+$ ions through thin films are formulated on the basis of the theory of multiple scattering. It is demonstrated that two asymptotic regimes exist and the explicit dependence of the number of transmitted phonons on the film thickness is established for each regime. Excellent agreement between theory and experiment is demonstrated.

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**1.** As is well known,[1] for times of flight $\tau > 10^{-15}$ *s* through a film, multiple scattering by atoms of the substance plays a fundamental role, appearing as the mechanism that counteracts the Coulomb repulsion between nuclei in a cluster and allows for the existence of a fraction with low relative velocities and short distances. This fraction can once again form molecular ions in a bound state as it captures electrons on leaving the film. This is what comprises the physics of the so-called *R*-regime of transmission of molecular ions through a material.[1]

Numerical modeling of the process of "reconstruction" of fast $H_2^+$ ions as they exit from carbon films,[1] although leading to satisfactory agreement with experiment, did not permit establishing the general laws governing this phenomenon. This paper is concerned with clarifying these laws for the ions $H_2^+$ and $^4HeH^+$.

**2.** For thick films, when the average internuclear distance in a dicluster exceeds the interatomic distance, the "bare" nuclei in the cluster are scattered independently by the atoms in the film and the kinetic equation for the distribution function $f(\mathbf{r},\mathbf{v},t)$ of nuclei in the cluster over the relative velocities $\mathbf{v}$ and coordinates $\mathbf{r}$ has the following form in the Fokker-Planck approximation:

$$\frac{\partial f}{\partial t} + \mathbf{v}\frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}(\mathbf{r})}{\mu}\frac{\partial f}{\partial \mathbf{v}} = \lambda \Delta_{\mathbf{v}_\perp} f \,. \tag{1}$$

Here $\mu = m_1 m_2/(m_1 + m_2)$ is the reduced mass, and $\mathbf{v}_\perp$ is the component of the relative velocity perpendicular to the velocity $\mathbf{V}_0$ of the ions in the incident beam. The force $\mathbf{F}$ consists of two terms

$$\mathbf{F}(\mathbf{r}) = \frac{Z_1 Z_2 e^2}{r^2}\frac{\mathbf{r}}{r} + \mu Z_1 Z_2 \left[\frac{\mathbf{F}_{12}^{w}(\mathbf{r})}{m_2} - \frac{\mathbf{F}_{21}^{w}(\mathbf{r})}{m_1}\right]. \tag{2}$$

The first term is the Coulomb interaction force and the second term is the so-called wake interaction force[2] between nuclei in the cluster. In the cases of interest to us, the retarding forces acting on the relative motion of nuclei are negligible.

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The constant $\lambda$ is related to the parameters of the film material and of the nuclei in the cluster by the relation

$$\lambda = \lambda_1 + \lambda_2 = \frac{\pi N Z^2 e^4}{V_0}\left(\frac{Z_1^2}{m_1^2}+\frac{Z_2^2}{m_2^2}\right)\ln\left\{NL\frac{7{,}14\pi Z^{4/3}\hbar^2 Z_1^2}{m^2 V_0^2\,\epsilon}\left(\frac{Z_2}{Z_1}\right)^{\gamma}\right\}, \quad (3)$$

where $N$ is the density of atoms in the film, $Z$ is their charge number, $L$ is the thickness of the film in the direction of incidence, $m$ is the mass of an electron, $\varepsilon$ is the base of natural logarithms, and $\gamma = 2/[1 + (Z_1 m_2/Z_2 m_1)^2]$. In deriving (3), we used the well-known expressions for the multiple scattering angle for nonrelativistic particles in a monatomic substance.[3]

**3.** For the process of electron recombination in a cluster resulting in the formation of a bound state of the molecular ion, the region of small $\mathbf{r}$ and $\mathbf{v}$, where the probability $W$ of such a process factorizes

$$W = X(V_0)Y(r) \quad (4)$$

and does not depend on the relative velocity $\mathbf{v}$, is important. Thus the probability of reforming the molecular ion is determined by the expression

$$T = X(V_0)\int Y(r) f(\mathbf{r}, \mathbf{v}, \tau)\, d^3\mathbf{r}\, d^3\mathbf{v}\,, \qquad \mu v^2/2 + U(r) < 0\,. \quad (5)$$

Here $U(r)$ is the effective internuclear interaction potential in a molecular ion, and $\tau = L/V_0$ is the time of flight of the cluster through the film.

**4.** Suppose a molecular ion enters a film at the time $t = 0$ and loses the electrons holding it together. The initial velocity at which the nuclei separate is low and plays no role in the problem being examined.

Analysis of Eq. (1) shows that for

$$\tau > t_0 = \frac{Z_1 Z_2 e^2}{12\lambda\mu\bar{r}_0} \quad (6)$$

($\bar{r}_0$ is the average distance between nuclei in the cluster at $t = 0$) its solution in the main region of integration in (4) does not depend on $\mathbf{r}_\perp$ and $\mathbf{v}_\perp$ and is given by the expression

$$f(\mathbf{r}, \mathbf{v}, \tau) = \frac{3}{8\pi^2\lambda^2\tau^4}\int_0^\infty dr_0 f_0(r_0)\int_0^\pi d\theta_0 \sin\theta_0\,\delta(v_\parallel - v_\parallel(r_0, \theta_0))\,\delta(r_\parallel - r_\parallel(r_0, \theta_0, \tau)), \quad (7)$$

where $\mathbf{v}_\parallel(r_0,\theta_0)$ and $r_\parallel(r_0,\theta_0,\tau)$ are the longitudinal components of the relative velocity and the distances, acquired over the time $\tau$ by the pair of separating nuclei as a function of the initial distance $r_0$ and angle $\theta_0$ between $\mathbf{r}_0$ and $\mathbf{V}_0(v_\parallel(r_0,\theta_0) \equiv v_\parallel(r_0,\theta_0,\tau=\infty)$, since for $\tau > t_0$ this component of the velocity as a rule attains its value at $\tau = \infty$, and $f_0(r_0)$ is the initial distribution function over $r_0$.

In calculating $T$, given by Eq. (5), with the help of (7) it is easy to verify that the region of values $\theta_0$, close to $\pi/2$, where

$$v_{\|}(r_0, \theta_0) \cong v(r_0)[\theta_0 - \theta_0^*(r_0)], \; r_{\|}(r_0, \theta_0, \tau) \cong r(r_0, \tau)[\theta_0 - \theta_0^*(r_0)], \tag{8}$$

makes the main contribution to the answer under the conditions (6). Here $\theta^*(r_0)$ is the value of the angle at which $v_{\|}(r_0,\theta_0)$ and $r_{\|}(r_0,\theta_0,\tau)$ vanish. The final result has the form

$$T = \frac{3X(V_0)}{2\lambda^2\tau^4}\left\{\frac{2}{3}\int_0^\infty \frac{dr_0 f_0(r_0)}{v(r_0)} \int dRRY(R)\left|\frac{2}{\mu}U(R)\right|^{3/2}\right.$$
$$\left|\frac{2}{\mu}U(R)\right|^{1/2}/R < v(r_0)/r(r_0,\tau), \; U(R) < 0$$

$$+ \int_0^\infty \frac{dr_0 f_0(r_0)}{r(r_0,\tau)} \int dRR^2 Y(R)\left[\frac{2}{\mu}|U(R)| - \frac{1}{3}\left(R\frac{v(r_0)}{r(r_0,\tau)}\right)^2\right]\Big\}. \tag{9}$$
$$\left|\frac{2}{\mu}U(R)\right|^{1/2}/R > v(r_0)/r(r_0,\tau), \quad U(R) < 0$$

**5.** Expression (9) shows that under the conditions (6), there are two regimes of transmission of ions through the film. We shall denote by $R^*$ the value of $R$ at which the potential $U(R)$ has a minimum. Since for large $\tau$ and $r(r_0,\tau) \approx v(r_0)\tau$, it is clear from (9) that for

$$t_0 < \tau < t_1 = R^*\left|\frac{2}{\mu}U(R^*)\right|^{-1/2} \tag{10}$$

$$T \sim \lambda^{-2}\tau^{-4}. \tag{11}$$

On the other hand, if $\tau \gg t_1$, then

$$T \sim \lambda^{-2}\tau^{-5}. \tag{12}$$

**6.** Precision experiments on the transmission of $^4HeH^+$ ions with energies 0.8–3.63 MeV through carbon films with times of flight $(1.5\text{–}8)\times 10^{-15} s$ have been performed at the Argonne National Laboratory.[4] In this case, $t_0 \approx 3\times 10^{-15}\, s$, $t_1 \approx 8\times 10^{-15}\, s$ therefore, a large part of the experimental data falls into the first asymptotic regime (11).

From (3) and (9) it is easy to obtain an explicit expression for $T$ as a function of the thickness $L$ (in $\mu gm/cm^2$) of the carbon film and of energy $E$ (in MeV) of the incident $^4HeH^+$ ions,

$$T(L, E) = H(E)/\left[\left(\frac{L}{E}\right)^2 \ln(20,8\frac{L}{E})\right]^2. \tag{13}$$

The values of the function $H(E)$ can be determined from the experimental points corresponding to the largest $L$ with fixed $E$.

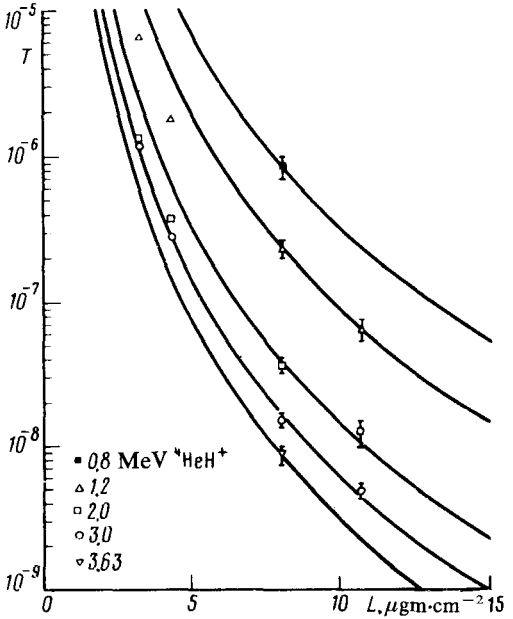


FIG. 1.

The dependences $T(L,E)$ calculated in this maner are compared with the experimental results in Fig. 1.[4] The ratio $T(L,E)/H(E)$, which is a universal function of $L/E$, is shown in Fig. 2. As is evident from Fig. 2, the experimental points from below fall, on a universal curve with increasing $\tau$, which reflects the fact that Coulomb repulsive

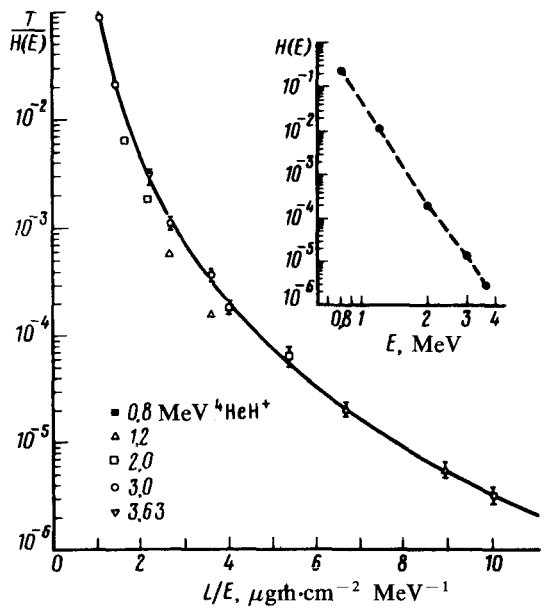


FIG. 2.

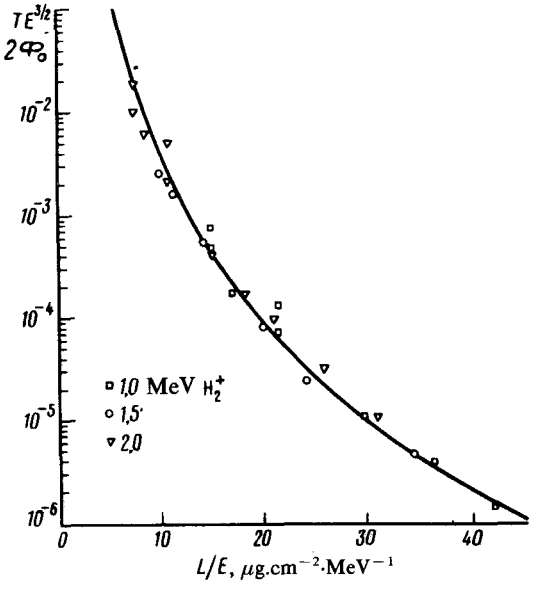


FIG. 3.

forces, which, for small $\tau$, decrease $T$ below its asymptotic value, do have an effect. In the region $t_0 < \tau < t_1$, however, the curves demonstrate excellent agreement between theory and experiment

7. The most acurate experimental data on the transmission of $H_2^+$ ions through a material correspond to the region where the second asymptotic regime (12) is active. These data were obtained by the Lyons group.[5]

Relation (4) in this case has the form[1]

$$W = 2[Z_g(r)]^5 \Phi_0(V_0), \tag{14}$$

where $Z_g(r)$ characterizes the effective charge of a two-proton cluster in the capture of an electron in the $1s\sigma_g$ state, while $\Phi_0(V_0)$ is the probability for capturing an electron by a single proton. Assuming that $v(r_0)$ in (8) and (9) is essentially independent of $V_0$, the theory then shows that the quantity

$$\frac{TE^{3/2}}{2\Phi_0} = \frac{C}{(L/E)^5[\ln(6.32\,L/E)]^2} \tag{15}$$

is a universal function of $L/E$. Here $L$ is the thickness of the carbon film in $\mu gm/cm^2$, and $E$ is the energy of $H_2^+$ ions in MeV.

As is evident from Fig. 3, the experimental points taken from Ref. 5 for $H_2^+$ ions with energies 1–2 MeV, passing through carbon films with a thickness of 15–42 $\mu gm/cm^2$, are described well by the theoretical dependence (15).

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