

Formation and decay of the intermediate quasistationary ion N_2^- during charge exchange between fast H^- ions and nitrogen molecules

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The detachment of the electron from the H^- ion during a collision with the nitrogen molecule at 1–6 keV occurs as a result of charge transfer to an unstable intermediate state of the molecular ion N_2^- and the subsequent decay of the ion. The formation process is described in the impulse approximation, and the motion of nuclei in the ion is treated quasiclassically. Expressions are obtained for the spectrum of emitted electrons and for the energy-loss spectrum of heavy particles. These expressions relate the spectra to the cross sections for the vibrational excitation of N_2 by electron impact. A convenient expression for the amplitude for the formation of the intermediate state is obtained in the “boomerang” model, and it is shown that one of the parameters, considered to be adjustable in traditional theory, can be calculated.

1. INTRODUCTION

The detachment of electrons in collisions between negative ions and molecules has been the subject of a large number of investigations (see Ref. 1). In particular, there has been considerable interest in the strong perturbation^{2–5} of the spectrum of electrons emitted as a result of $H^- + N_2$ collisions, which is related to the formation and decay of an intermediate state of the molecular ion N_2^- . Processes of this type have now been extensively investigated,^{6–9} using different partners ($H^-, D^-, F^-, I^-, Cl^-; N_2, CO, O_2$), different collision energies (ranging from 1 eV to energies of the order of 10 keV), and two different methods of detecting the final states (spectrum of emitted electrons and energy-loss spectrum of the heavy particle). However, these processes have not been adequately investigated from the theoretical point of view. For example, an attempt was made in Ref. 4 to provide a theoretical analysis of the process, but the description of the process of formation and decay of the intermediate ion was too approximate and was based on a representation of the vibrational levels of the intermediate molecular ion N_2^- that was shown in Refs. 10 and 11 to be invalid. An unpublished investigation by Herzenberg and Gayak is mentioned in Ref. 8, but no information is provided therein of the method used for the results obtained.

In this paper, we shall examine the most extensively investigated case, namely, $H^- + N_2$ at collision energies $E \sim 5$ keV. Experiment shows^{2–5} that the charge-transfer process is enhanced in this energy range. Physically, this is due to the “quasiresonant” character of the charge-transfer process at this collision energy for which the translational energy of the electron in the H^- ion is sufficient to compensate the difference between the energy of the intermediate state $E \sim 2$ eV and the binding energy of the electron in the ion ($\epsilon_0 = -0.75$ eV). Experiment thus supports the impulse description of the process, which is an alternative to the usual adiabatic description. Since the shape of the adiabatic energy curves for this system is not known, this mechanism will not be examined in this paper. The important feature of the process is the long (as compared with the transit time) lifetime of the intermediate state of N_2^- , which enables us to

look upon its formation as a step-type perturbation and neglect the decay of N_2^- during this process. In this connection, we must mention the work of Baz'¹² (see also Ref. 13), who investigated the effect of the intermediate quasistationary state on the spectrum of reaction products. We must also mention the deuteron stripping reaction,¹⁴ in which the neutron in the deuteron penetrates the nucleus which subsequently decays. In our case, the intermediate state has an additional vibrational degree of freedom which has been extensively investigated.^{15–17;10,11}

2. FORMAL STATEMENT OF THE PROBLEM

In this section, we turn our attention to the necessity for including accurately the mass of the electron, which is small in comparison with the masses of the nuclei. This mass is important because, when we analyze the energy-loss spectrum of the heavy particle, we must correctly take into account energy transfer between the nuclei and the electron.

In the static approximation to the state of the electron shell of the N_2 molecule, the system is described by the Hamiltonian

$$\hat{H} = \hat{T}_e + \hat{T}_H + \hat{T}_m + \hat{H}_0(q) + V_{em}(\mathbf{R}_m - \mathbf{r}, \mathbf{n}; q) + V_{eH}(\mathbf{r} - \mathbf{R}_H) \quad (1)$$

where \hat{T}_e , \hat{T}_H and \hat{T}_m are the kinetic energies of the electron, hydrogen atom, and molecule, respectively, \mathbf{r} , \mathbf{R}_m and \mathbf{R}_H are the position vector of the electron, the center of mass of molecule, and the center of mass of the hydrogen atom, respectively, V_{eH} and V_{em} are the electron-atom and electron-molecule interactions, \mathbf{n} is the unit vector in the direction of the line joining the nuclei in the molecule (this direction will be assumed to be fixed during the collision), \hat{H}_0 is the Hamiltonian describing the vibrational motion of the nuclei in the molecule, and q is the separation between the nuclei.

The eigenfunction Ψ of the Hamiltonian (1) that corresponds to the collision between the ion with momentum \mathbf{P}_0 and the resting molecule in vibrational state n_0 characterized by vibrational function $v_{n_0}(q)$ and E_{n_0} is (in atomic units)

$$\Psi = \Psi_0 + \delta\tilde{\Psi}, \quad (2)$$

where

$$\Psi_0 = \exp \left[i \mathbf{P}_0 \frac{M_H \mathbf{R}_H + \mathbf{r}}{M_H + 1} \right] \varphi(\mathbf{r} - \mathbf{R}_H) v_{n_0}(q), \quad (3)$$

$$E = P_0^2/2(M_H + 1) + \varepsilon_0 + E_{n_0}.$$

In these expressions, φ is the wave function of the electron in the ion, ε_0 is the corresponding binding energy, E is the total energy of the system, and M_H is the mass of the hydrogen atom.

The correction $\delta\tilde{\Psi}$ contains contributions corresponding to different physical mechanisms involved in the process and, in particular, takes into account possible multiple scattering of the electron by the potentials V_{eH} and V_{em} . However, since the velocity of the ion is comparable with, or exceeds, the velocity of the electron relative to the ion, and since the lifetime of the intermediate state is long (the width is $\Gamma \sim 0.5$ eV), we may suppose that multiple scattering of the electron has little effect on the charge-transfer process, so that we have the following equation for the corresponding term $\delta\Psi$ in the function $\delta\tilde{\Psi}$:

$$[\hat{T}_H + \hat{T}_e + \hat{T}_m + \hat{H}_0(q) + V_{em}(\mathbf{R}_m - \mathbf{r}, \mathbf{n}; q) - E] \delta\Psi = -V_{em}(\mathbf{R}_m - \mathbf{r}, \mathbf{n}; q) \Psi_0. \quad (4)$$

It is clear from the formulation of the problem that, as $r \rightarrow \infty$, the quantity $\delta\Psi$ should not contain incident-electron waves. The solution of (4) has the form

$$\delta\Psi = \int \frac{d^3k}{(2\pi)^{3/2}} \exp \left\{ i \left[(\mathbf{P}_0 - \mathbf{k}) \mathbf{R}_H + \mathbf{k} \frac{M_m \mathbf{R}_m + \mathbf{r}}{M_m + 1} \right] \right\} f_k(\rho, q), \quad (5)$$

$$\rho = \mathbf{R}_m - \mathbf{r},$$

and f_k satisfies the equation

$$[\hat{T}_\rho + \hat{H}_0(q) + V_{em}(\rho, \mathbf{n}; q) - \tilde{E}] f_k(\rho, q) = -V_{em}(\rho, \mathbf{n}; q) \exp(-i\mathbf{k}\rho M_m/(M_m + 1)) \tilde{\varphi}(\mathbf{k} - \mathbf{v}_0) v_{n_0}(q), \quad (6)$$

$$\tilde{\varphi}(\mathbf{z}) = \int \frac{d^3r}{(2\pi)^{3/2}} \varphi(\mathbf{r}) \exp(-i\mathbf{r}\mathbf{z}),$$

where $\mathbf{v}_0 = \mathbf{P}_0/(M_H + 1)$ is the velocity of the incident H^- ion. The energy $\tilde{E} = E - (\mathbf{P}_0 - \mathbf{k})^2/2M_H - k^2/2(M_m + 1)$ can be interpreted as the energy produced as a result of the capture of the electron by the compound system. Since the Fourier transform of φ has an appreciable magnitude for arguments of the order of the atomic unit, we may suppose that $|\mathbf{k}| \sim 1$ and simplify the expression for \tilde{E} by neglecting the recoil molecule:

$$\tilde{E} = -v_0^2/2 + (\mathbf{v}_0 \mathbf{k}) + \varepsilon_0 + E_{n_0}. \quad (7)$$

We note that this expression has a clear interpretation involving the translational motion of the electron together with the H^- ion.

Since, in this paper, our main interest is in the analysis of the formation and decay of the intermediate resonance, we may suppose that the energy \tilde{E} is close to the corresponding resonance interval. The function f_k in the neighborhood of the molecule will then be dominated by the term proportional to the wave function of the intermediate state. The structure of the intermediate state will be examined in greater detail later. For the moment, it is sufficient to introduce the

wave function ζ^\pm of this state, which satisfies the equation

$$[\hat{T}_\rho + V_{em}(\rho, \mathbf{n}; q)] \zeta^\pm(\rho, \mathbf{n}; q) = \varepsilon(q) \zeta^\pm(\rho, \mathbf{n}; q) \quad (8)$$

(the two signs appear because of the twofold degeneracy of the state, which has the $1\pi_g$ symmetry in the projection of the angular momentum on to the nuclear axis in the case of the N_2 molecule) and contains only the departing wave for $\rho \rightarrow \infty$. The last condition shows that the self-energy of the state, $\varepsilon(q)$, is complex, and the eigenfunctions grow exponentially for large ρ . Nevertheless, we shall use for these functions the norm introduced in Ref. 13, assuming that the contours of all the radial integrals with respect to ρ are deformed so as to ensure convergence. This can be justified by a generalization of the argument put forward in Ref. 13. However, we cannot pause here to examine this question in greater detail.

Thus, for the range of values of the energy \tilde{E} in which we are interested, the solution of (8) has the form

$$f_k(\rho, q) = \xi_{k^+}(q) \zeta^+(\rho, q) + \xi_{k^-}(q) \zeta^-(\rho, q) + \delta f_k, \quad (9)$$

where ξ^\pm can be interpreted as the wave function for the relative motion of the nuclei in the intermediate state, and the correction δf_k can be regarded as small in the neighborhood of the molecule. It was assumed in Ref. 17 that this correction had a different symmetry than the intermediate-state function ζ^\pm , i.e., that scattering through the intermediate resonance provided the predominant contribution to the process only among functions of the same symmetry. To determine the function $\xi_{k^\pm}(q)$, we must solve the equation from (8) on the assumption that $\zeta^\pm(q)$ is a slowly-varying function of the nuclear separation:

$$[\hat{H}_0(q) + \varepsilon(q) - \tilde{E}] \xi_{k^\pm}(q) = -\tilde{\varphi}(\mathbf{k} - \mathbf{v}_0) V^\pm(\mathbf{k}, \mathbf{n}; q) v_{n_0}(q), \quad (10)$$

where

$$V^\pm(\mathbf{k}, \mathbf{n}; q) = \int V_{em}(\rho, \mathbf{n}; q) \zeta^\mp(\rho, q) e^{-i\mathbf{k}\rho} d^3\rho.$$

The probability that the system will undergo a transition to the final state, characterized by momentum \mathbf{P}_j of the hydrogen atom, momentum \mathbf{k}_j of the escaping electron, and final vibrational state n of the molecule, is given by the matrix element

$$T_{\mathbf{P}_j, \mathbf{k}_j, n} = \langle \Phi_{\mathbf{P}_j, \mathbf{k}_j, n} | V_{em}(\rho, \mathbf{n}; q) | \delta\Psi \rangle, \quad (11)$$

$$\Phi_{\mathbf{P}_j, \mathbf{k}_j, n} = \exp \{ i [\mathbf{P}_j \mathbf{R}_H + \mathbf{k}_j \mathbf{r} + (\mathbf{P}_0 - \mathbf{P}_j - \mathbf{k}_j) \mathbf{R}_m] \} v_n(q).$$

Once we know this matrix element, we can find the differential cross section for the complete experiment:

$$d\sigma(\mathbf{P}_0, n_0 \rightarrow \mathbf{P}_j, \mathbf{k}_j, n) = \frac{1}{(2\pi)^2 v_0} |T_{\mathbf{P}_j, \mathbf{k}_j, n}|^2 d^3P_j d^3k_j \delta(E_j - E). \quad (12)$$

Thus, evaluation of the cross section requires integration of (10), which is similar in form to the basic equation of Herzenberg's theory,¹⁷ followed by integration of the resulting solution with the final-state wave function $v_n(q)$, and integration with respect to the electron momentum k in accordance with (5). Moreover, the electron-capture amplitude on the right-

hand side of (10) differs from the corresponding quantity in Herzenberg's traditional theory, and it is not clear how it can be determined for all nuclear separations. It is probably the combination of these problems that has prevented an acceptable theory from emerging. In this paper, we use the previously developed^{10,11} quasiclassical approach to Herzenberg's theory to show that the basic characteristics of the process can be calculated by performing a single integration, namely, with respect to the electron momentum k , in accordance with (5), and the final result is expressed in terms of the cross section for the vibrational excitation of the hydrogen molecule by electron impact.

3. DESCRIPTION OF THE INTERMEDIATE STATE IN THE HERZENBERG THEORY

It is assumed in the Herzenberg theory that the resonant state is formed as a result of temporary capture of an electron by a vacant orbital of the molecule. In the case of N_2 , the formation of the resonance is examined for the first time (in the approximation of fixed nuclei) in Ref. 18 (see also the review given in Ref. 19) where it is shown that the $N_2 - ({}^2\Pi_g)$ resonance is formed on the basis of the vacant $1\pi_g$ orbital of N_2 . Expansion of the wave function of this symmetry in terms of the partial waves begins with $l = 2$ and contains only even orbital moments. It is this fact which leads to the basic assumption of the theory: it is assumed that the electron becomes bound in the neighborhood of the molecule as a result of a complex nonsingle-particle interaction with the electron shell of the molecule, and the state is prevented from decaying by the centripetal barrier for the lowest orbital angular momentum allowed by the symmetry of the resonance. Hence, the simplest model of the intermediate state is a spherically symmetric well having a depth (and therefore an energy level) that depends on the nuclear separation, and surrounded by the centripetal barrier. In view of the foregoing, we may consider the following simple representation of the wave function ζ^\pm :

$$\zeta^\pm(\rho, \mathbf{n}; q) = Y_{2, \pm 1}(\rho/\rho) \chi(\rho, q), \quad (13)$$

where

$$\chi(\rho, q) = \frac{1}{N} \begin{cases} A\rho^2(\rho-b), & \rho \leq R_0 \\ h_2^+(k\rho), & \rho > R_0 \end{cases} \quad (14)$$

The values of A , b , and N are determined by joining the solutions at $\rho = R_0$ and by the normalization condition, where the quantization axis lies, of course, along the unit vector \mathbf{n} . The momentum k of the state depends on the nuclear separation q and is determined by the eigenenergy $\varepsilon(q)$ (8): $\varepsilon(q) = k^2(q)/2$. The energy $\varepsilon(q)$ of the intermediate state is directly related to the energy curves of the ion and molecule, $W_I(q)$ and $U_0(q)$:

$$W_I(q) = U_0(q) + \varepsilon(q). \quad (15)$$

The quasiclassical analysis of the Herzenberg theory^{10,11} has shown that the main contribution to the formation and decay of the intermediate state is provided by neighborhoods of the nuclei that satisfy the Franck-Condon condition:

$$\tilde{E} - W_I(q_i) = E_i - U_0(q_i), \quad (16)$$

or, in other words,

$$\varepsilon_i = W_I(q_i) - U_0(q_i) = \varepsilon(q_i),$$

where \tilde{E} is, as before, the energy of the compound system, E_i is the energy of the initial or final vibrational states of the molecule, and ε_i is the energy of the captured or emitted electron. The Franck-Condon principle is thus found to determine the Franck-Condon function $q(\varepsilon)$, which is complex for real arguments. It will be useful to consider the function ζ (13) not as a function of the nuclear separation q but as a function of a real argument, namely, the energy of the electron, assuming that the momentum k in (14) is the independent variable. The function defined in this way will not grow exponentially.

We now turn to the analysis of (10). As already noted, this equation is outwardly very similar to the equation in Herzenberg's theory with one minor difference: in Herzenberg's theory, the electron momentum k , the energy \tilde{E} of the compound system, and the energy of the initial vibrational state are related by $\tilde{E} = k^2/2 + E_{n_0}$. This relation indicates that the Herzenberg theory involves only the amplitude $V(k, q)$ for the formation of the intermediate state for which the momentum k coincides with the intermediate state momentum $k(q)$ introduced in the last section. In this connection, we may say that (10) contains on its right-hand side the amplitude for the formation of the compound system "off the mass shell." This quantity was not previously considered in Herzenberg's theory, and its determination is our immediate problem.

Using the definition of the function ζ given by (8), and assuming that $V_{em} = 0$ for $\rho \geq R_0$, we obtain

$$V^\pm(\mathbf{k}, \mathbf{n}; q(\varepsilon)) = (\varepsilon - k^2/2) \int_{\rho \leq R_0} \zeta^\mp e^{-i\mathbf{k}\rho} d^3\rho + \frac{1}{2} \int_{\rho=R_0} d\Omega_\rho \left(e^{-i\mathbf{k}\rho} \frac{\partial}{\partial \rho} \zeta^\mp - \zeta^\mp \frac{\partial}{\partial \rho} e^{-i\mathbf{k}\rho} \right). \quad (17)$$

It is important to note that this result can also be obtained for a nonlocal interaction between the additional electron and the electrons in the molecular shell. Thus, to determine V^\pm , it is sufficient to know the particular representation of the wave function of the external electron in the neighborhood of the molecule. In particular, using representation (14), we can readily evaluate the integrals in (17) in an explicit form (we shall omit the corresponding somewhat unwieldy representation and separate out only the angular dependence of V^\pm):

$$V^\pm(\mathbf{k}, \mathbf{n}; q(\varepsilon)) = \bar{V}(k, \varepsilon) Y_{2, \pm 1}(\mathbf{k}/k). \quad (18)$$

The evaluation of the normalizing integral for the function (14) is not difficult either:

$$N^2 = A^2 (R_0^9/9 - bR_0^8/4 + b^2R_0^7/4) - 1/2 R_0^3 \{ [h_2^+((2\varepsilon)^{1/2}R_0)]^2 + h_3^+((2\varepsilon)^{1/2}R_0) h_1^+((2\varepsilon)^{1/2}R_0) \}.$$

Thus, when (14) is assumed, the amplitude for the formation of the intermediate state is determined by the interaction cutoff radius R_0 . A similar parameter appears in the Herzenberg theory,¹⁷ but the electron-capture amplitude is determined in that theory by the width of the intermediate state,

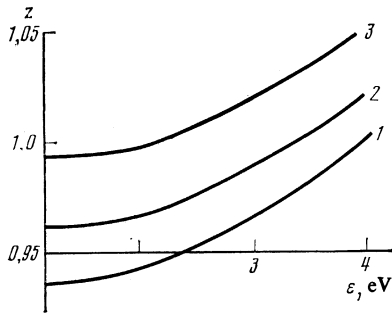


Fig. 1. The ratio z of the absolute amplitude $|\bar{V}(2\varepsilon)^{1/2}, \varepsilon|$, for the formation of the intermediate ion N_2^+ "on the mass shell", calculated in this paper, to the amplitude $V_{DH}(\varepsilon)$ calculated from the formulas in Ref. 17. Different curves correspond to different values of the cutoff radius of the potential V_{em} for the electron-molecule interaction: 1 - $R_0 = 1.41$, 2 - $R_0 = 1.44$; 3 - $R_0 = 1.48$.

which contains an additional parameter $\Gamma(R_0)$. It is therefore very interesting to compare our representation (for $k = (2\varepsilon)^{1/2}$) with calculations based on the formulas given in Ref. 17. Figure 1 shows the ratio of the corresponding quantities. The radius R_0 was assumed in Ref. 17 to be 1.41, whereas here we use 1.44. We note that the difference between these two figures has very little effect on the results given in Ref. 17. We may conclude that the electron-capture amplitude depends on the cutoff radius R_0 but, within the limits of uncertainty of the Herzberg theory (of the order of 5%), the function V (17) is in good agreement with the data in Ref. 17. The difference in the energy dependence of the amplitudes is due to the fact that we take into account the variation of the wave function ξ inside the well with the energy of the intermediate state, whereas this variation was neglected in Ref. 17. We note that allowance for the increase in the amplitude with energy (which is more rapid than is predicted by the Herzberg theory) will correct the cross sections for the resonant vibrational excitation of the molecules at high electron energies in the right direction.

We shall now show that the use of the quasiclassical approximation will automatically enable us to integrate with respect to the nuclear separation in (11). In fact, if we introduce the Green function $G(q, q')$ for the differential equation (10), we can show that our integral has the form

$$J_{n_0, \mathbf{k}; n, \mathbf{k}_j} = \langle v_n(q) | V^\pm(\mathbf{k}_j, n; q) G(q, q') V^\mp(\mathbf{k}, n; q) | v_{n_0}(q) \rangle. \quad (19)$$

The quasiclassical analysis given in Refs. 10 and 11 and based on the rapid oscillation of the functions $v_{n_0}(q)$, $v_n(q)$, and $G(q, q')$ as functions of the nuclear separation enables us to take outside the integral sign the values of the amplitudes for the formation of the intermediate state at points satisfying the Franck-Condon principle. Comparison of the resulting integral with the analogous calculations of the amplitude for the resonant vibrational excitation of the molecule by electron impact at $\mathbf{k}_i = \mathbf{k}$, k_i/k , $k_i^2 = 2(\bar{E} - E_{n_0})$, i.e.,

$$A_{n_0, \mathbf{k}; n, \mathbf{k}_j} = \langle v_n(q) | V^\pm(\mathbf{k}_j, n; q) G(q, q') V^\mp(\mathbf{k}_i, n; q) | v_{n_0}(q) \rangle \quad (20)$$

leads to the key conclusion of our work, namely:

$$J_{n_0, \mathbf{k}; n, \mathbf{k}_j} = \frac{\bar{V}(k, \bar{E} - E_{n_0})}{\bar{V}(k_i, \bar{E} - E_{n_0})} A_{n_0, \mathbf{k}_i; n, \mathbf{k}_j}. \quad (21)$$

4. EVALUATION OF CROSS SECTIONS

The complex $P_0, n_0 \rightarrow P_j, k_j, n$ experiment is not possible at present, and measurements are performed of the spectra of emitted electrons or of the energy loss by the heavy particle. The cross section (12) must therefore be integrated with respect to quantities characterizing the part of the complete experiment that cannot be seen in the experiment, and then average over the orientations of the molecule.

Let us examine in greater detail the expression

$$\delta(E_j - E) d^3 P_j d^3 k_j = \delta(\varepsilon_j - v_0 k_{\parallel} + E_n - E_{n_0} + v_0^2/2 - \varepsilon_0) dk_{\parallel} d^2 k_{\perp} d\Omega_{\mathbf{k}_j} (2\varepsilon_j)^{1/2} d\varepsilon_j, \quad (22)$$

where $\varepsilon_j = k_j^2/2$ is the energy of the escaping electron and k_{\parallel} and k_{\perp} are the components of the vector \mathbf{k} respectively along and across the vector \mathbf{v}_0 .

The energy lost by the heavy particle is

$$\delta E = P_j^2/2M_H - P_0^2/2(M_H + 1) = v_0^2/2 - (\mathbf{v}_0 \mathbf{k})$$

($\delta E < \varepsilon_0$ in collisions accompanied by vibrational excitation of the molecule), so that, bearing in mind the fact that we wish to evaluate the spectrum of these losses, we can rewrite (22) in the form

$$\delta(E_j - E) d^3 P_j d^3 k_j = \delta(\delta E - v_0^2/2 + v_0 k_{\parallel}) dk_{\parallel} d^2 k_{\perp} \times d\Omega_{\mathbf{k}_j} (2\varepsilon_j)^{1/2} \delta(\delta E + \varepsilon_j + E_n - E_{n_0} - \varepsilon_0) d\varepsilon_j d(\delta E). \quad (23)$$

Experiments²⁻⁵ show that there are no observable anomalies in the distribution of the emitted electrons (this is not surprising because any averaging will smooth out the angular dependence of the cross section). We shall not consider the angular distribution of the electrons, having integrated with respect to σ and Ω_{k_j} . Integrating twice with respect to k_{\perp} , we can readily show that the spectrum of the emitted electrons is given by

$$d\sigma = \sum_{n=0}^{\infty} Q(\varepsilon_i^{(n)}, v_0) \sigma_{n_0 \rightarrow n}(\varepsilon_i^{(n)}) d\varepsilon_j, \quad (24)$$

where

$$\varepsilon_i^{(n)} = \varepsilon_j + E_n - E_{n_0}, \quad (25)$$

$$Q(\varepsilon, v_0) = \frac{(2\varepsilon)^{1/2}}{|\bar{V}((2\varepsilon)^{1/2}, \varepsilon)|^2} \frac{2\pi}{v_0^2} \int_0^{\infty} k_{\perp} dk_{\perp} |\bar{V}(k, \varepsilon)|^2 \times |\bar{\phi}(\mathbf{k} - \mathbf{v}_0)|^2 \Big|_{k_{\parallel} = (\varepsilon + v_0^2/2 - \varepsilon_0)/v_0}$$

The quantity $\sigma_{n_0 \rightarrow n}$ is the total cross section for the $n_0 \rightarrow n$ vibrational transition. Similarly, the energy-loss spectrum of the heavy particle can be shown to have the following form:

$$d\sigma = Q(\varepsilon_0 - \delta E, v_0) \sum_{n=0}^N \sigma_{n_0 \rightarrow n}(\varepsilon_0 - \delta E) d(\delta E). \quad (26)$$

The sum is evaluated only over the channels that are open for the given energy loss, i.e., for $n < N$ we have $\varepsilon_j = E_{n_0}$

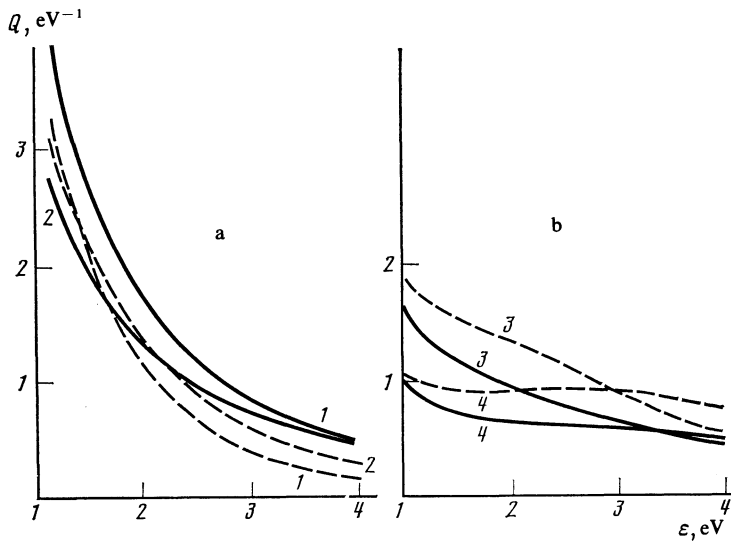


Fig. 2. The function $Q(\varepsilon, v_0)$ plotted against ε . Solid curves correspond to calculations with φ_1 (27). The dashed curve shows calculations with the function given by (28). Different pairs of curves correspond to different collision energies: 1—1 keV, 2—2 keV, 3—4 keV, 4—6 keV.

$+\varepsilon_0 - E_n - \delta E > 0$. We recall that $\delta E < \varepsilon_0$ always.

Thus, to determine the loss spectrum and the spectrum of emitted electrons, we must find the function $Q(\varepsilon, v_0)$, and this requires a knowledge of both the amplitude $\bar{V}(k, \varepsilon)$ and the Fourier transform of the wave function of the electron in the ion, $\tilde{\varphi}(\mathbf{k})$. We shall now use two possible parametrizations of this function in configuration space:²⁰

$$\varphi_1(\mathbf{r}) = \left(\frac{\alpha}{2\pi}\right)^{1/2} \frac{e^{-\alpha r}}{r}, \quad \tilde{\varphi}_1(\mathbf{k}) = \frac{\alpha^{1/2}}{\pi} \frac{1}{\alpha^2 + k^2}; \quad (27)$$

$$\varphi_2(\mathbf{r}) = \left[\frac{\beta(\beta + \alpha)\alpha}{2\pi(\beta - \alpha)^2} \right]^{1/2} \frac{e^{-\alpha r} - e^{-\beta r}}{r},$$

$$\tilde{\varphi}_2(\mathbf{k}) = \frac{[\alpha\beta(\alpha + \beta)^3]^{1/2}}{\pi} \frac{1}{(\alpha^2 + k^2)(\beta^2 + k^2)}. \quad (28)$$

Following Ref. 20, we shall suppose that $\alpha = 0.236$ and $\beta = 0.821$ atomic units. It is important to note that the Fourier transforms of the functions φ_1 and φ_2 are close to one another only for $0.25 < k^2 < 0.45$; $\tilde{\varphi}_2$ decreases rapidly with increasing k^2 , and $\tilde{\varphi}_2 > \tilde{\varphi}_1$ for $k^2 < 0.25$.

We now turn to the calculated values of the function Q (Fig. 2). It is clear from these results that, at low collision energies, the result obtained by using φ_1 is much greater than that obtained for φ_2 , whereas the reverse situation obtains for collision energies in excess of 2 keV. The point is that, at low collision velocities, the main contribution to (25) is provided by large arguments of the function φ and, in this region, $\varphi_2 < \varphi_1$. As the collision energy increases, the longitudinal momentum $k_{\parallel} = (\varepsilon - \varepsilon_0)/v_0 + v_0/2$ is found to decrease and, consequently, electrons with low momentum (in the frame in which hydrogen is at rest) begin actively to participate in the process. In this region, φ_2 is much greater than φ_1 , and this is reflected in Fig. 2. The curves corresponding to collision energies of 4 and 6 keV exhibit an appreciable distortion, which is particularly clear at energy ε for which $k_{\parallel} = v_0$, and the region of integration in (25) contains the point at which the argument of the function $\tilde{\varphi}$ vanishes. This distortion is, of course, more appreciable when the calculations are performed with $\tilde{\varphi}_2$.

Unfortunately, our results are difficult to compare with experimental data because, in addition to the resonant de-

tachment of the electron considered here, there are also other mechanisms that lead to the same final state. These mechanisms can be isolated only in a qualitative manner, and the data reported in Ref. 8 can be used as a basis for concluding that the calculations with the function φ_2 yield very reasonable results, whereas those with φ_1 lead to cross sections that are too high at low collision energies.

5. CONCLUSION

The analysis given above is not, of course, very accurate. It is therefore interesting to consider the reasons for, and the character of, the resulting errors.

First of all, one can criticize the impulse mechanism used in this paper as being responsible for the formation of the intermediate states. We have already pointed out that the adiabatic approach is an alternative method of description. On the other hand, the impulse approximation is not very different from the methods developed in Refs. 21 and 22 for the description of the collision between a negative ion and a neutral particle, which have turned out to be quite successful at our collision energies.¹

Next, we have used the quasiclassical approach to the Herzenberg theory, and the error that this introduces in the most unfavorable case of resonant elastic scattering is up to 10%.

Moreover, the assumed behavior of the function ζ^{\pm} in the neighborhood of the molecule, which is used in (14), can be improved.

Finally, the wave function φ of the electron in the ion can also be improved. Here, we must remember that, at low collision energies, the cross section includes an important contribution due to the short-wave part of this function, which is involved in the description of the motion of the additional electron in the immediate neighborhood of the nucleus. This means that the possible effect of electron correlations on this process must be taken into account for slow collisions. At the same time, there is less justification in the case of slow collisions for using the momentum approach to the formation of the intermediate states.

We note that the approach employed above may also be valid for the description of the detachment of an electron from a highly excited atom. In this case, there are no essential difficulties with the determination of the wave function of the electron in the incident particle, and the cross sections for such processes may be very considerable.

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