Oscillations in the total cross section for the charge-exchange reaction pe + d → de + p

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The two-level approximation of the perturbed-stationary-states method is employed for calculation of the pe + d → de + p charge-exchange reaction cross section. The cross-section curve oscillates, and low-frequency and high-frequency components can be singled out. A partial analysis of the high-frequency component is performed.

1. INTRODUCTION

Study of one-electron molecular systems and the collision processes corresponding to them permits investigation of a large number of interesting physical phenomena which, as a rule, are characteristic also of the more complex scattering problems. At the present time it is possible to calculate for one-electron systems not only the electronic energy as a function of the internuclear distance but also the matrix elements which take into account the coupling between different electronic states. These calculations lead to the equations of the method of perturbed stationary states in the scattering problem (the adiabatic representation).[1,2,3] Solution of the equations obtained in turn permits investigation of the features of the adiabatic representation or any other representation obtained from it by means of an appropriate transformation.[3,4]

In the present article we calculate the cross section for the charge-exchange process

$$(pe)_{1s}+d\rightarrow(de)_{1s}+p \tag{1}$$

(p is a proton, d is a deuteron, and e an electron). In the region of collision energies $E \leq 1$ eV in the center-of-mass system the two-level approximation of the method of perturbed stationary states is sufficient.

Previously we used similar equations in calculation of the reaction[5]

$$(p\mu^-)_{1s}+d\rightarrow(d\mu^-)_{1s}+p, \tag{1a}$$

but technical difficulties associated with the large reduced mass in the case of process (1) did not permit us to use the old algorthm. To overcome these difficulties it was convenient to go over to the adiabatic representation.[3] Then the wave function of the nuclear motion was parametrized in the spirit of the method of phase functions.[6] The equations for the phase functions were integrated numerically, and the successful choice of parameters permitted avoidance of the difficulties characteristic of the algorithm which we used in the previous work.[5]

All of the potentials used are readily available, and the technical details given in our report[7] make it possible to carry out the present calculations.

2. ADIABATIC REPRESENTATION

The two-level approximation of the method of perturbed stationary states in discussion of process (1) leads to a system of radial equations[5]:

$$\left.\begin{aligned}\left(\frac{d^2}{dR^2}+k_1^2-\frac{l(l+1)}{R^2}\right)\chi_1&=K_{11}\chi_1+K_{12}\chi_2+2Q_{12}\frac{d\chi_2}{dR},\\ \left(\frac{d^2}{dR^2}+k_2^2-\frac{l(l+1)}{R^2}\right)\chi_2&=K_{22}\chi_2+K_{21}\chi_1-2Q_{12}\frac{d\chi_1}{dR},\end{aligned}\right\} \tag{2}$$

$$\left.\begin{aligned}K_{11}(R)&=M(W_g+W_u)+(K_{gg}+K_{uu}-K_{gu}-K_{ug})/2,\\ K_{12}(R)&=M(W_g-W_u)+(K_{gg}-K_{ug}+K_{gu}-K_{uu})/2,\\ K_{21}(R)&=M(W_g-W_u)+(K_{gg}-K_{uu}-K_{gu}+K_{ug})/2,\\ K_{22}(R)&=M(W_g+W_u)+(K_{gg}+K_{uu}+K_{gu}+K_{ug})/2,\\ Q_{12}(R)&=-Q_{gu}.\end{aligned}\right\} \tag{3}$$

The matrix elements $K_{gg}, \ldots, K_{ug}, Q_{gu}$ are determined by the equalities $(i, j = g, u)$

$$K_{ij}=\langle i|-\Delta_{\mathbf{R}}|j\rangle,\quad Q_{ij}=\frac{\mathbf{R}}{R}\langle i|-\nabla_{\mathbf{R}}|j\rangle \tag{4}$$

and together with the terms (eigenvalues of the electronic energy operator) $W_g(R)$, $W_u(R)$ are calculated in the solution of the quantum-mechanical problem of two centers. The remaining quantities are found from the equations

$$\begin{gathered}1/M=1/M_p+1/M_d,\quad 1/m=1/m_e+1/(M_p+M_d),\\ k_1^2=2ME,\quad k_2^2=k_1^2+(M_d-M_p)/(M_d+M_p).\end{gathered} \tag{5}$$

Here E is the collision energy in the center of mass, and the system of units is determined by the condition $e = \hbar = m = 1$.

Graphs of the matrix elements and terms of the two-center problem are given in a previous article.[5] The effective potentials determined by Eqs. (3) are shown in Figs. 1 and 2. A distinctive feature of the equations in the adiabatic representation is the presence of a term with the first derivative of the wave function, and also the asymmetry, related to this circumstance, of the matrix (3).

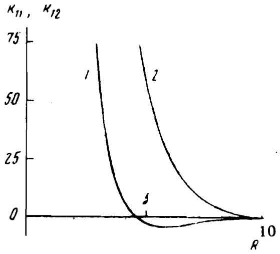

FIG. 1

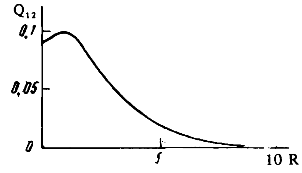

FIG. 2

FIG. 1. Adiabatic matrix elements $K_{11}(R) \approx K_{22}(R)$–curve 1 and $-K_{12}(R) \approx -K_{21}(R)$–curve 2; see Eq. (3).

FIG. 2. Coefficient of the first derivative of the wave function from the equations in the adiabatic representation (2).

3. DIABATIC REPRESENTATION

We will rewrite the system of equations (2) in matrix form

$$L\chi=K\chi+2Qd\chi/dR, \tag{6}$$

where the free motion operator L has the form

$$L=\left(\frac{d^2}{dR^2}-\frac{l(l+1)}{R^2}\right)\begin{pmatrix}1&0\\0&1\end{pmatrix}+\begin{pmatrix}k_1^2&0\\0&k_2^2\end{pmatrix}, \tag{6a}$$

and we will go over to a new basis which is determined by the transformation

$$\chi(R)=W(R)\psi(R). \tag{7}$$

Here W(R) is the unitary matrix:

$$W(R)=\begin{pmatrix}\cos q&\sin q\\-\sin q&\cos q\end{pmatrix}, \tag{8}$$

and the function q(R) is expressed in terms of the matrix element Q_{12}:

$$q(R)=\int\limits_R^\infty Q_{12}(x)\,dx. \tag{9}$$

The transformation performed permits elimination of the terms with the first derivative in Eq. (6), which now takes the form

$$L\psi=\bar{K}\psi. \tag{10}$$

The matrix $\bar{K}(R)$ is given by the equation

$$\bar{K}=W^{-1}\left[K-\frac{dQ}{dR}-Q^2-\begin{pmatrix}k_1^2&0\\0&k_2^2\end{pmatrix}\right]W+\begin{pmatrix}k_1^2&0\\0&k_2^2\end{pmatrix} \tag{11}$$

and turns out to be symmetric.

Equation (10) is the two-level approximation of the scattering problem in the diabatic representation, and the matrix (8) determines the relation between the diabatic and adiabatic bases.[3] The system (10) is completely equivalent to the initial system (6), but for various types of problems one of them may turn out to be preferred. In the present work the diabatic representation was chosen as the result of the diagonality in it of the potential energy matrix (11). The matrix elements $\bar{K}_{ij}(R)$ are shown in Fig. 3.

4. THE VARIABLE PHASE METHOD

We will look for a solution of the matrix equation (10) in the form[6]

$$\psi=(uS_1-vS_2)A \tag{12}$$

with the additional condition

$$\psi_R'=(u'S_1-v'S_2)A. \tag{13}$$

Here

$$u=\begin{pmatrix}u_1&0\\0&u_2\end{pmatrix},\quad v=\begin{pmatrix}v_1&0\\0&v_2\end{pmatrix} \tag{14}$$

are the regular and singular solutions at zero of the free equation

$$L\varphi=0, \tag{15}$$

normalized in such a way that

$$uv'-u'v=1. \tag{16}$$

The matrices $S_1(R)$ and $S_2(R)$ determine the parametrization of the wave function, and the matrix A(R) is arbitrary.

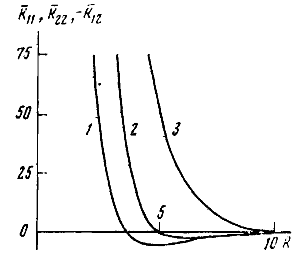

FIG. 3. Diabatic matrix elements defined by Eqs. (8), (9), and (11). Curve 1—for $\bar{K}_{11}$, curve 2—$\bar{K}_{22}$, curve 3—for $-\bar{K}_{12}$.

If we assume fulfillment of the condition

$$S_1^{\mathrm{tr}}S_2-S_2^{\mathrm{tr}}S_1=0, \tag{17}$$

then, substituting the solution in the form of (12) into Eq. (10) and taking into account conditions (13), (16), and (17), we obtain the equation

$$S_1^{\mathrm{tr}}\frac{dS_2}{dR}-S_2^{\mathrm{tr}}\frac{dS_1}{dR}=(S_1^{\mathrm{tr}}u-S_2^{\mathrm{tr}}v)\bar{K}(uS_1-vS_2). \tag{18}$$

Discussion of the orginal scattering problem (10) by means of Eq. (18) is known in the physics literature as the variable phase method (method of phase functions).[8] Giving a specific form of the matrices S_1 and S_2 is equivalent to choice of different sets of phase functions, which in turn leads to a definite parametrization of the scattering matrix S or the reaction matrix T. For the latter we have from the definition (12)

$$T=S_2(\infty)S_1^{-1}(\infty). \tag{19}$$

5. WORKING PARAMETERS

For problem (1) it was convenient to use the parameters $\delta_1(R)$, $\delta_2(R)$, and $\epsilon(R)$ given by the matrices

$$S_1=\begin{pmatrix}\cos\varepsilon\cos\delta_1&-\sin\varepsilon\sin\delta_2\\-\sin\varepsilon\sin\delta_1&\cos\varepsilon\cos\delta_2\end{pmatrix}$$
$$S_2=-\begin{pmatrix}\cos\varepsilon\sin\delta_1&\sin\varepsilon\cos\delta_2\\\sin\varepsilon\cos\delta_1&\cos\varepsilon\sin\delta_2\end{pmatrix} \tag{20}$$

It is easy to see that the left-hand side of Eq. (18) in this case takes the form

$$S_1^{\mathrm{tr}}S_2'-S_2^{\mathrm{tr}}S_1'=\begin{pmatrix}\delta_1'&\varepsilon'\cos(\delta_1-\delta_2)\\\varepsilon'\cos(\delta_1-\delta_2)&\delta_2'\end{pmatrix} \tag{21}$$

and identity (17) is satisfied.

The suitability of the parameters (20) is determined by the fact that for reaction (1) over the entire integration region $0 < R < \infty$ the quantity $\cos(\delta_1-\delta_2)$ does not go to zero and, consequently, the system of equations (18) can be solved for the derivatives. This fact is to a substantial degree a fortunate accident, although we counted on its existence, on the basis of the quasisymmetry of the reaction being studied.

6. DISCUSSION OF RESULTS

Figure 4 shows the cross section for the charge-exchange reaction (1) σ_{ex} as a function of the relative velocity v of the nuclei. The general behavior of the curve is characteristic of processes of this type: a sharp drop in the region $v < 0.2$, a broad maximum at $v \sim 0.4$, and a smooth decrease of the cross section with increasing velocity (v is in units of 10^6 cm/sec, $v = 1.695\times10^6\sqrt{E[\mathrm{eV}]}$ cm/sec). At low velocities a transition is observed to the resonance scattering region. The cross-section values at certain points are given below:

$v\cdot10^{-6}$, cm/sec:	0.51	0.54	0.565	0.59	0.62	0.64	0.675	0.695	0.73	1.5	1.7
$\sigma_{cx}\cdot10^{16}$, cm^2:	50	61	48	61	51	60	52	60	51	48	46

Substantially greater interest is presented by the oscillations in the total cross section. They are located beginning with $v \sim 0.3$, and their amplitude first rises, reaching a maximum at velocities $v \sim 0.5$, and then begins to drop. The period of these oscillations increases with increasing velocity from $\Delta v \sim 0.09$ to $\Delta v \sim 0.11$ for the velocity interval $0.3 < v < 1.2$. Considerably less apparent is the presence of a low-frequency component of oscillations with a period $\Delta v \sim 0.38$, although without this it is difficult to explain the sharp minimum in the cross section at $v = 0.565$ and the not so apparent maximum at $v = 0.76$.

The results of the calculations permit a partial analysis of the oscillations in the charge-exchange cross section to be performed without difficulty. In Fig. 5 we are shown the partial cross sections for $v = 0.565$ (the minimum in the cross section) and $v = 0.59$ (the neighboring maximum). It is easy to see that in the case of the minimum the group of waves with $l = 30$, 31, and 32 does not contribute to the total cross section, while the sum of the cross sections for $0 \leq l \lesssim 30$ provides a smooth component of σ_{ex} for a velocity interval of the order of the period of oscillation. As seen in Fig. 6, with increasing v there appears in the cross-section plot a stable tail whose relative contribution to the total cross section increases. Now the oscillations are provided by a group of waves with l appreciably smaller than l_{max}. As a result the amplitude of the oscillations decreases.

With increasing collision energy the accurate solution of Eq. (18) becomes impractical as the result of the large number of partial waves contributing to the cross section. Approximate, more rapid methods of calculation[4] are appropriate here. The maximum value of E for which calculations were carried out was 1 eV, $l_{max} \sim 100$, $v = 1.7$.

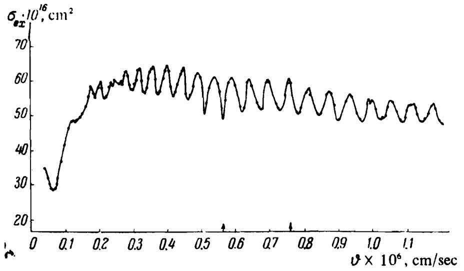

FIG. 4. Total cross section for the charge-exchange reaction (1) as a function of the relative velocity of nuclear motion v. The arrows show the minimum and maximum in the cross section, which can be explained by the existence of low-frequency oscillations of the total cross section. The extreme right-hand point in the graph corresponds to E = 0.5 eV.

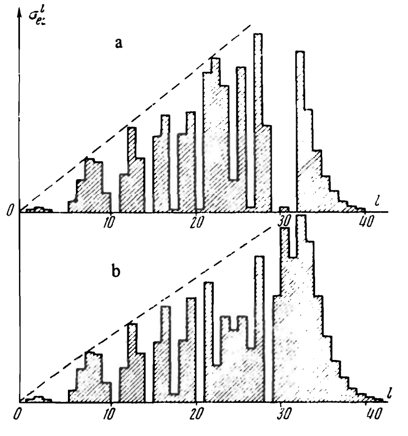

FIG. 5. Partial cross sections for charge exchanges for the minimum of the cross section (a—v = 0.565) and the neighboring maximum (b—v = 0.590). In the case of the minimum the group of waves hardly takes part in the charge-exchange process.

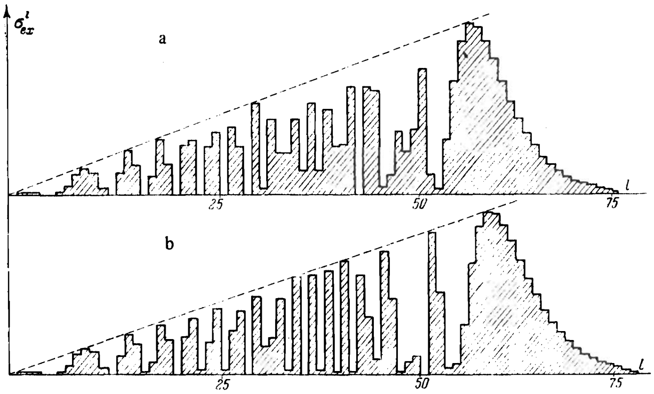

FIG. 6. Partial cross sections for charge exchange for the case where more than 70 waves contribute to the cross section: a—v = 1.15, b—v = 1.20. A stable tail is formed which leads to a decrease in the oscillation amplitude with increasing collision energy.

7. CONCLUSION

A considerable number of accurate experiments[9] have been carried out recently in which oscillations of the total cross section for charge exchange have been observed, in particular, for alkali atoms. It is quite interesting that in the case of the simple reaction (1) the charge-exchange cross section behaves in a similar way. In our opinion there is no satisfactory interpretation of this phenomenon at the present time. In this connection it is particularly valuable that one-electron systems provide the possibility of calculation with high accuracy of a number of physically interesting problems, and simultaneously the investigation of various types of coupling in the equations of the scattering problem. We hope that this program of research, together with the experimental study of the same processes, will turn out to be interesting and productive.

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