The shape of the total inelastic cross section curves for atomic collisions

M. Ya. Ovchinnikova
Institute of Chemical Physics, USSR Academy of Sciences
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The possibility of extracting additional information about the terms of diatomic systems from the curves of the total inelastic cross section due to the quasi-crossing of the terms is studied. For this purpose a systematic investigation of the influence of the characteristic parameters (6) on the shape of the energy dependence of the total inelastic cross section when a method more accurate than the Landau-Zener (LZ) model is used to compute the transition probability is carried out. It is shown that the maximum value of the cross section can exceed the value given by the LZ theory by a factor 1.5—2, depending on the magnitude of the interaction (the parameter A), and that the position of the peak with respect to energy varies appreciably as the rate of change of the interaction (the parameter ν) is varied.

A great number of the charge-transfer and excitation processes that occur in atomic collisions is determined by transitions in the quasi-crossing region $R \approx R_0$ of the terms usually characterized by the diabatic terms $U_1(R)$ and $U_2(R)$ and the interaction $V_{12}(R)$ between them[1,2]. The computation of the inelastic cross section, which can be represented as an integral over the impact parameters

$$\sigma = 2\pi \int_0^\infty P(\rho)\,\rho\, d\rho \tag{1}$$

then requires knowledge of the transition probability $P(\rho)$. In the simplest method of describing such processes, when the well-known Landau-Zener (LZ) formula for $P(\rho)$[3,4] is used, the inelastic cross sections are described by a single universal function[5]:

$$\frac{\sigma_{LZ}^{(E)}}{\pi R_0^2} = \frac{y}{y + U_0/E_1} f(y), \tag{2}$$

$$f(y) = \int_0^y dx\, 2\exp(-x^{-1/2})\,(1 - \exp(-x^{-1/2})). \tag{3}$$

Here U_0/E_1 is the potential at the crossing point in units of E_1,

$$y = \frac{E - U_0}{E_1}; \quad x = \frac{E_R}{E_1} = \frac{1}{E_1}\left[E\left(1 - \frac{\rho^2}{R_0^2}\right) - U_0\right] \tag{4}$$

are the dimensionless relative energy of the atoms above the threshold, i.e., the energy measured form the value U_0, and the dimensionless radial energy at the crossing point.

Thus, the cross section (2) is determined in the LZ model by two scale factors:

$$\sigma_0 = \pi R_0^2, \quad E_1 = {}^1/_2 m(2\pi V_0^2/\hbar\Delta F)^2, \tag{5}$$

where $V_0 = V_{12}(R_0)$ and $\Delta F = F_1 - F_2$ is the ρ-independent difference between the slopes of the terms at the crossing point.

Comparison of the experimental cross sections with the theoretical curve shows, however, that the formula (2) leads to a systematic underestimate of the maximum value of the cross section and to a shift in its position along the velocity axis. The reasons for the deviation of the cross sections from σ_{LZ} have been repeatedly analyzed[6,7] and can be reduced to the following:

1) The dependence of the interaction V_{12} on R, which cannot be taken into account in the LZ calculation, usually has the form

$$V_{12}(R) \approx V_0 \exp[-\alpha(R - R_0)].$$

The influence of the parameter $\nu = 2\alpha V_0/\Delta F = 2\alpha\delta R$ on the transition probability has been investigated by Bykhovskiĭ and Nikitin[8]. From their results one can draw qualitative conclusions about the effect on the shape of the cross sections: the displacement of the cross section peak with the growth of ν.

2) The LZ formula for the transition probability does not take into account the considerable interference of the contributions from the transitions which occur during the forward and backward flights, the nonuniformity of the motion in the transition region when this region is close to the distance of closest approach, as well as the presence of tunneling when the point R_0 is classically inaccessible. The effect of these factors on the transition probability has been investigated by Bykhovskiĭ et al.[9]. Owing to the contribution of the peripheral collisions with $\rho \sim R_0$, we can expect that allowance for these effects will lead to a maximum cross section which is larger than the value $\sim 0.45\pi R_0^2$ given by the LZ formula (2).

The computation of the reaction $Be^{++} + H \rightarrow H^+ + Be^+$ carried out by Bates et al.[10] on the basis of a numerical solution of the equations demonstrates these effects.

It is significant that of the many characteristic terms in the transition region, only the quantities πR_0^2 and E_1 can be estimated on the basis of the LZ description of the inelastic process. Two questions arise: firstly, how accurate can we take the parameters found in such a treatment to be, and, secondly, can we extract from the deviation of the total inelastic cross section curve from the LZ curve (without the involvement of the differential cross sections) additional information about the terms and the interaction of the system in the transition region? To answer these questions we must ascertain the number of the most important parameters which determine the cross section without the simplifying assumptions of the LZ theory.

In this connection, we analyze in the present paper the total inelastic cross section using a more exact model for the computation of the transition probability; this allows us to distinguish the characteristic parameters and systematically investigate their influence on the shape of the inelastic cross section. As such parameters we can, as we shall see below, choose the

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following dimensionless quantities:

$$A=\frac{2}{\pi}\left(\frac{R_0}{\delta R}\right)^{1/4},\quad \nu=2\alpha\delta R,\quad \Phi=\frac{FR_0}{2E}. \tag{6}$$

Here $\delta R = V_0/\Delta F$; A characterizes the width δR of the transition region compared to the crossing radius, ν characterizes the extent to which the interaction $V_{12}(R) = V_0 \exp[-\alpha(R - R_0)]$ changes in the transition region, and Φ is the average slope $F = (F_1 F_2)^{1/2}$ of the terms in units of $2E_1/R_0$, where the characteristic energy scale E_1 is given by (5) and roughly determines the position of the peak of the cross section.

In subsection (I) below we give the general formulation of the problem. In (II) we reduce the problem to a model problem and separate out the parameters. The final formulas used in the computation are given in (III), and then in (IV) we present the results of the computations and discuss the experimental cross section[11] for the charge-transfer reaction in B^{+3} + He collisions.

I. Since the LZ model is a reasonable approximation, the dimensionless energies (4) with the scales (5) can conveniently be used, as before, for the investigation of the cross sections. Then the cross section (1) can be rewritten in the form

$$\frac{\sigma(E)}{\pi R_0^2}=\frac{y}{y+U_0/E_1}\int_{-\infty}^{y}P(x,y)\,dx. \tag{7}$$

Let us briefly go over the derivation of the equation determining P.

In the basis of two diabatic states χ_1 and χ_2 the wave function of the system has the form

$$\psi=\psi_1(R)\chi_1+\psi_2(R)\chi_2.$$

We shall use the momentum representation for the nuclear functions[12,9]

$$\psi_j(R)=\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\exp\left\{ipR-i\int^{p}R_j(p')\,dp'\right\}\frac{c_j(p)\,dp}{F_j^{1/2}(R_j(p))},\quad j=1,2, \tag{8}$$

where the $R_j(p)$ satisfy the equation

$$\frac{p^2}{2m}+U_j(R_j(p))+E\left[\frac{\rho}{R_j(p)}\right]^2=E,\quad F_j(R)=\frac{dU_j(R)}{dR}. \tag{9}$$

Under quasi-classical conditions the system of second-order quantum equations for $\psi_j(R)$ reduces to semiclassical first-order equations for the amplitudes $c_j(p)$[12]. After the introduction of the dimensionless time variable

$$\tau(p)=\frac{V_0}{\hbar}\int^{p}\frac{dp}{F(p)},\quad F(p)=[F_1(R_1(p))F_2(R_2(p))]^{1/2} \tag{10}$$

these equations have the form

$$i\frac{dc_1}{d\tau}=\frac{V_{12}(R(p))}{V_0}e^{iS(p)}c_2,\quad i\frac{dc_2}{d\tau}=\frac{V_{12}(R(p))}{V_0}e^{-iS(p)}c_1, \tag{11}$$

$$S(p)=\int[R_1(p)-R_2(p)]\,dp,\ R(p)=[R_1(p)R_2(p)]^{1/2};$$

p and τ are connected by formula (10). The transition probability $P_{i\to j}$ is given as usual by $P_{ij} = |c_j(+\infty)|^2$, with the initial conditions $c_j(-\infty) = \delta_{ij}$. It is easy to see that when $\rho^2/R^2 \gg U_j(R)/E$ Eqs. (11) go over into the equations of the impact-parameter method, i.e., into the time-dependent Schrödinger equations with a straight-line trajectory.

Equations (11) in the momentum representation do not, in contrast to the coordinate representation, exclude from the analysis the neighborhood of the point of closest approach, and only require for their derivation (besides quasi-classicality) a slow variation of $V_{12}(R)$ as compared to $\tilde{U}_j(R,\rho) = U_j(R) + E\rho^2/R_0^2$:

$$\frac{dV_{12}(R)}{dR}\ll|F_j(R,\rho)|=-F_j(R)+\frac{2E\rho^2}{R_0^3}. \tag{12}$$

Under this condition we can consider the distance R, on which the interaction V_{12} in (11) depends, to be equal to R(p), for example, since we have $R_{1(2)}(p) - R_0 \gg R_1(p) - R_2(p)$ when (12) is fulfilled. At high energies E (the limit of the straight-line trajectories), when

$$2E\rho^2/R^3\gg dV_{12}/dR\sim\alpha V_0,$$

the condition (12) does not impose any restrictions on the ratio of dV_{12}/dR to F_j, i.e., on the parameter $\nu = 2\alpha V_0/\Delta F$.

II. We adopt for the computation of the transition probability a natural model in which we replace the true terms $U_j(R)$ by linear terms. The question, however, arises as to how to carry out such a replacement correctly for different impact parameters. The simplest method is to use the linear expansion of the potentials $U_j(R)$ in the neighborhood of the point R_0.

For above-the-barrier transitions, when $E_R > 0$, or, in terms of the variables (4), when $x > 0$, this simple method is the most judicious, since the point of slowest oscillations of $\exp[iS(p)]$ in the system (11) coincides with the point p_0 for which $R_1(p_0) = R_2(p_0) = R_0$. The departure from linearity of the terms turns out to be substantial only for impact parameters corresponding to high E_R (or x): it leads to inaccuracy in the phase Γ of the oscillations in the transition probability $P(\rho) = 4w(1 - w)\sin^2\Gamma$. But for such ρ the phase Γ is large, and the contribution from these impact parameters to the total cross section (1) will be determined by only the magnitude of the probability w of a single-stage transition, which is accurately reproduced by the model[1)].

Thus, for above-the-barrier transitions, we set

$$V_{12}(R)=V_0\exp[-\alpha(R-R_0)],\ U_j(R)=U_0-E\rho^2/R_0^2+\bar{F}_j(R-R_0),$$
$$\bar{F}_j=-F(R_0)+2E\rho^2/R_0^3=\text{const}.$$

Then

$$R_j(p)=\frac{1}{\bar{F}^j}\left(\frac{p^2}{2m}-E_R\right)$$

and, after the introduction of the new variable $\xi = \frac{1}{2}p(\Delta F/\tilde{F}mV_0)^{1/2}$, the system (11) acquires the form

$$i\frac{dc_1}{d\xi}=\frac{1}{2}b\varphi(\xi)e^{is}c_2,\quad i\frac{dc_2}{d\xi}=\frac{1}{2}b\varphi(\xi)e^{-is}c_1, \tag{13}$$

$$\varphi(\xi)=\exp[-\nu(\xi^2-\varepsilon)],\ S=b\int^{\xi}(\xi^2-\varepsilon)\,d\varepsilon. \tag{14}$$

Here ν is defined in (6), and

$$\varepsilon=\frac{F_R\Delta F}{2V_0\bar{F}},\ b=\frac{4V_0}{\hbar}\left(\frac{mV_0}{\bar{F}\Delta F}\right)^{1/2},\ \bar{F}=(F_1F_2)^{1/2}$$

are the well-known parameters of the model[9] which depend on the impact parameter ρ and the energy E. It is convenient to represent this dependence on E and ρ in terms of the dimensionless variables (5). We then obtain

$$b=A[(\Phi_1+y-x)(\Phi_2+y-x)]^{-1/4},\quad \varepsilon=(\pi b/4)^2x.$$

Here A and Φ_j are given by the formulas (6) with F replaced by F_j. Among actual charge-transfer reactions, those which occur most frequently are the cases when $FR_0 \sim U_0 \sim \Delta E \ll 2E_1$ (the applicability condition for the impact-parameter method) or $\Phi_j \ll 1$. Then, in

the energy range of interest $0.1 < y < 1000$ we can set $\Phi_1 = \Phi_2 = 0$, since $\Phi_j \ll y$[2]. For the other class of processes (excitation reactions with a high energy threshold $U_0 \gg \Delta E$) we can assume that $\Delta F/F \ll 1$, i.e., that $\Phi_1 \approx \Phi_2 \approx \Phi = (\Phi_1\Phi_2)^{1/2}$.

Thus, for the indicated types of processes we should assume $\Phi_1 = \Phi_2 = \Phi$ and write the parameters ϵ and b in the form

$$b = \frac{A}{(\Phi + y - x)^{1/2}}, \quad \varepsilon = \left(\frac{\pi b}{4}\right)^2 x, \quad x > 0. \tag{15}$$

Let us now turn to subbarrier transitions, when $E_R < 0$ or $x < 0$. If, as before, we replace the real terms by the tangents to them at the point R_0, we find that as $\rho \to \infty$ ($x \to -\infty$, $b \to 0$, and $\epsilon \to$ const), the probability of a subbarrier transition tends to a constant value and that when $V_{12} = \text{const}$ ($\nu = 0$) the cross section (7) diverges. The reason for this circumstance, first noted by Devdariani and Bobashev in[15], is clear. In such an approximation the slopes $\tilde{F}_j = F_j = F_j + 2E\rho^2/R_0^2$ of the terms grow so rapidly as $\rho \to \infty$, that despite the decrease of the energy $E_R \to -\infty$, the effective barrier which must be overcome before reaching the crossing point does not increase as $\rho \to \infty$, as obtains in reality.

In order to correctly simulate the actual terms by linear ones, let us turn to the basic system (11). The latest oscillation rate for e^{iS} occurs at $p = 0$:

$$\min (dS/dp) = R_1(0) - R_2(0) = R_1^r - R_2^r.$$

Therefore, it is natural to expand the quantities $S(p)$ and $R_i(p)$ in the vicinity of the point $p = 0$. This is equivalent to replacing the actual terms by the tangents to them at the reversal points $R_j^r = R_i(p = 0)$. This yields

$$S(p) \approx -(R_1^r - R_2^r)p - \frac{\Delta F}{|F^r|}\frac{p^3}{6}, \quad F_r = [F_1(R_1^r)F_2(R_2^r)]^{1/2}. \tag{16}$$

The position of the reversal points is determined by the equation

$$F_i(R_i^r - R_0) + E_i y \frac{\rho^2}{R_0^2}\left(\frac{R_0}{R_i^r}\right)^2 + E_i y = 0. \tag{17}$$

Limiting ourselves, as has been noted, to the most interesting cases $\Delta F \ll F$ ($\Delta\Phi \ll \Phi$), or $\Delta\Phi \ll y$, we obtain from (17) when $R_1^r - R_2^r \ll R_1^r - R_0$,

$$\Delta R^r/R_0 = R_1^r R_2^r/R_0 = 2\Phi(1/k - 1),$$

where $\Delta\Phi = \Delta F/2E_1$ and $k = R_0/R^r$ ($R_1^r \approx R_2^r \approx R^r$) is determined from the equation

$$(y - x)k^2 - y = 2\Phi(1/k - 1). \tag{18}$$

Further, after the change of variable $\xi = \frac{1}{2}(\Delta F/\tilde{F}^r m V_0)^{1/2} p$, the system (11) reduces to the same system as for $x > 0$, namely, the system (13)–(14), since we have $-\alpha(R - R_0) \approx -\alpha(R - R^r) - \alpha(R^r - R_0) = \nu\xi^2 + \alpha R_0(1/k - 1) = \nu\xi - \epsilon$. The parameters ϵ and b then turn out to be equal to

$$b = \frac{A}{[\Phi + (y - x)k^3]^{1/2}}, \quad \varepsilon = -2\left(\frac{\pi A}{4}\right)^2\left(\frac{1}{k} - 1\right), \tag{19}$$

where k is a root of Eq. (18).

Thus, the computation of the transition probability for any value of the impact parameter reduces to the solution of the system (13)–(14), with the parameters ϵ and b given by (15) when $x > 0$, or by (19) when $x < 0$, and the shape of the inelastic cross section ultimately turns out to be dependent on the three dimensionless parameters (6).

III. Let us briefly discuss the method of integration of the system (13). It is convenient to look for the numerical solution in the adiabatic basis in which Eqs. (13) take the form:

$$i\frac{da_1}{d\xi} = -iHe^{i\Xi}a_2, \quad i\frac{da_2}{d\xi} = iHe^{i\Xi}a_1,$$

$$\Xi = \int^{\xi} L(\xi')d\xi', \quad L(\xi) = -b(t^2 + e^{-2\nu t})^{1/2}, \quad t = \xi^2 - \varepsilon, \tag{20}$$

$$H(\xi) = \xi e^{-\nu t}(1 + \nu t)[1 + e^{-2\nu t}]^{-1}. \tag{21}$$

To find the probability, it is sufficient, on account of the symmetry of the problem, to know the solution only in the interval $(0, \infty)$ of ξ[12].

Let us represent the solution $a_1(\xi)$ and $a_2(\xi)$ with the initial conditions 1 and 0 for $\xi = 0$ in the form

$$a_1(\xi) = (1 - z^2)^{1/2}\exp(i\Gamma_1), \quad a_2(\xi) = z\exp(i\Gamma_2). \tag{22}$$

Then, from (20) and (21) we arrive[12] at the following equations for the real functions z, Γ_1, Γ_2, and Ξ

$$dz/d\xi = -H(\xi)(1 - z^2)^{1/2}\cos(\Xi + \Gamma_2 - \Gamma_1), \quad d\Xi/d\xi = L(\xi),$$

$$d\Gamma_1/d\xi = H(\xi)\frac{z}{(1 - z^2)^{1/2}}\sin(\Xi + \Gamma_2 - \Gamma_1),$$

$$d\Gamma_2/d\xi = H(\xi)\frac{(1 - z^2)^{1/2}}{z}\sin(\Xi + \Gamma_2 - \Gamma_1) \tag{23}$$

with the initial conditions $z(0) = \Gamma_1(0) = \Xi(0) = 0$ and $\Gamma_2(0) = \pi$, and the functions $H(\xi)$ and $L(\xi)$ defined in (21). Using the asymptotic values of z, Γ_1 and Γ_2 for $\xi \to \infty$, we compute the transition probability as follows:

$$P = 4z^2(1 - z^2)\sin^2(\Gamma_1 + \Gamma_2). \tag{24}$$

For $\epsilon > 0$ the system (23) was integrated from the point $\xi = \epsilon^{1/2}$ (the crossing point) to $\xi \to \infty$ and from $\xi = \epsilon^{1/2}$ to $\xi = 0$ (the reversal point), or to the point where $z(\xi)$ first assumes the asymptotic form, with an eye to the possible computation of the average value $\bar{p} = 2z^2(1 - z^2)$ of the probability (24) for the asymptotic region of large phases $\delta = \Gamma_1 + \Gamma_2 \gg 2\pi$. Detailed computational formulas are given in the Appendix. The computation of the cross section (7), in which the probability $P(x, y)$ was found by integrating the system (13), was carried out on the BESM-4 machine.

IV. Let us proceed to discuss the results of the investigation of the influence of the various parameters on the dependence of the dimensionless cross section $\sigma/\pi R_0^2$ on the dimensionless energy $y = (E - U_0)/E_1$. Figure 1 shows the transition cross sections for a constant interaction $V_{12} = \text{const}$, $\nu = 0$, for the computation of which the straightline trajectory approximation was used: $E_1 \gg FR_0$, $\Phi \approx 0$. The varying parameter A (see (6)) characterizes the magnitude of the interaction of the width of the transition region relative to R_0

$$\frac{\delta R}{R_0} = \frac{V_0}{\Delta F R_0} = \left(\frac{2}{\pi A}\right)^2$$

(for $A = 1.5$, we have $\delta R/R_0 = 0.36$). It can be seen that the variation of A very insignificantly changes the position of the peak of the cross section, but that, owing to the contribution of the peripheral ($\rho \sim R_0$) collisions, the magnitude of the maximum cross section can change considerably. The dependence of σ_{max} on A or δR can be described by the formula

$$\sigma_{max} = 0{,}445\pi(R_0 + 2{,}28\delta R)^2. \tag{25}$$

It is worth noting that for transitions with rotational coupling, which have been investigated by Russek in[16], the cross section can even exceed the value πR_0^2, and

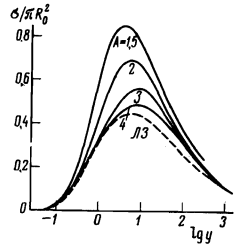

FIG. 1

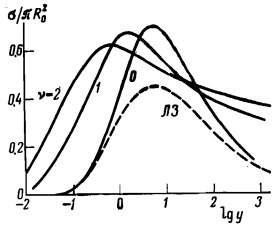

FIG. 2

FIG. 1. The dependence of the cross section on the logarithm of the dimensionless energy $y = (E-U_0)/E_1$ for different values of A at $\nu = \Phi = 0$. The dashed curve is the plot of the Landau-Zener cross section.

FIG. 2. The dependence of the cross section on the logarithm of the dimensionless energy $y = (E-U_0)/E_1$ for different rates of change of the interaction $V_{12}(R)$, which are characterized by the parameter ν. A = 2 and $\Phi = 0$.

does not, on account of the dependence of the interaction $V_{12} \sim E\rho^2/R^2$ on E and ρ, decrease at high energies.

In Figs. 2 and 3 we demonstrate the effect on the shape of the cross section of the exponential dependence of the interaction V_{12} on distance for two values of the parameter A (A = 2 and A = 4) characterizing the interaction strength. As was to be expected from the investigation of the transition probability carried out by Bykhovskiĭ and Nikitin[8], for $\nu \neq 0$ the cross section increases at considerably lower energies than the LZ cross section. Thus, for $\nu = 2$ the peak of the cross section occurs at energies y which are an order of magnitude smaller than the energy $y \sim 5.6$ of the LZ cross section peak. At high energies the cross section does not decrease in a fairly large region, due to the fact that for $\nu \neq 0$ the probability of a single-stage transition does not tend to unity with increasing energy, as obtains in the LZ model with $\nu = 0$, the influence of the second transition region is felt[8]. For $\nu = 0.5$ the energies of the predominant contributions of the two transition mechanisms are separated by a minimum at $y \sim 100$. The difference between the cross sections with A = 2 (Fig. 2) and A = 4 (Fig. 3) consists in the large contribution of the peripheral collisions with $\rho \gtrsim R_0$ to the magnitude of the cross section in the range $0.1 < y < 10$.

In the adiabatic region, the cross section function $\sigma(A, \nu, y)$ for $\nu \neq 0$ can be described with the aid of the cross sections $\sigma(A, \nu = 0, y)$ corresponding to a constant interaction by simply changing the energy scale:

$$\sigma(A, \nu, y) = \sigma(A, \nu = 0, y/y_0(\nu)); \quad y_0(\nu) = e^{-1.54\nu}. \tag{26}$$

In particular, for A > 4 we have in the adiabatic region ($y/y_0 < 2$):

$$\sigma(y) = \frac{y}{y + U_0/E_1} f\left(\frac{y}{y_0(\nu)}\right), \tag{27}$$

where f(y) is a tabulated function (see, for example[5]) defined by the formula (3), while the function $y_0(\nu)$ is given by (26).

The nonvanishing of the parameter $\Phi = FR_0/2E_1$ is characteristic of reactions with a substantial reaction threshold $U_0 \sim FR_0$; the shape of the cross section near the threshold then depends on the threshold energy U_0 (see the factor $y + U_0/E$ in (7)) and on the parameters (6). At high energies $y \gg \Phi$ the cross section curves with the given parameters ν, A, and Φ coincide with the corresponding curves with ν, A, $\Phi' = 0$, which have

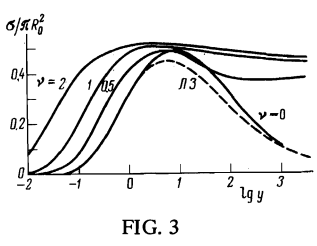

FIG. 3

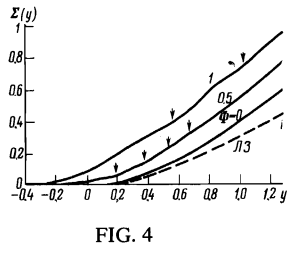

FIG. 4

FIG. 3. The dependence of the cross section on the logarithm of the dimensionless energy $y = (E-U_0)/E_1$ for different rates of change of the interaction $V_{12}(R)$, characterized by the parameter ν. A = 4 and $\Phi = 0$.

FIG. 4. Threshold behavior of the cross section $\Sigma(y) = E\sigma(E)/E_1\pi R_0^2$ for A = 2, $\nu = 0$, and different values of the parameter Φ.

previously been investigated (but not with the LZ curve, as was supposed in[15]). The extent of the difference between the actual threshold of the process and the classical value $E = U_0$ ($y = 0$) for A = 2 can be seen in Fig. 4. Plotted along the ordinate is the dependence on the dimensionless energy $y = (E - U_0)/E_1$ of the quantity $\Sigma(y) = E\sigma/E_1\pi R_0^2$, which does not depend on the additional parameter U_0/E_1. The value of the cross section at $E = U_0$ sharply decreases like

$$\sigma(E = U_0) \sim 4\frac{E_1}{U_0}\pi R_0^2 \Phi^{3/2} A^{-3} \exp\left(-\frac{1.24A}{\Phi^{1/2}}\right),$$

as A increases and Φ decreases. The experimental detection of the displacement of the actual threshold of the process relative to the classical threshold $E = U_0$ is quite problematic: for this purpose it is necessary to find the other transition parameters with sufficient accuracy from the entire high-energy cross section curve. In view of the large number of parameters such a procedure is not unambiguous, even if, in accordance with the model of the description, the process being measured is due to transitions in only one quasi-crossing region.

The cross sections shown in Fig. 4 also exhibit Stückelberg oscillations connected with the fact that the largest phase $\varphi(\rho)$ for $\rho = 0$ of the oscillations in the transition probability $P(\rho)$ is a small quantity near the threshold. The arrows in Fig. 4 indicate the values of the energy at which $\varphi(E_n, \rho = 0) = \pi n$. The indicated oscillations differ from the Olson-Smith oscillations[17,18] connected with the extremum of the phase $\varphi(\rho)$. They are oscillations in the energy derivative of the cross section and not in the cross section itself, and their amplitude vanishes with growth of the energy, as well as with increasing A and decreasing Φ.

Thus, the results enable us to make an estimate of the degree of accuracy of the parameters E_1 and R_0 found by analyzing the experimental cross sections with the aid of the LZ curve, and in the case, when some of the quasi-crossing parameters (e.g., R_0 and ΔF) are known, they allow a more accurate determination of the other parameters of the model. On the other hand, the proposed computational method is suitable for predicting the cross section when the parameters of the problem are known, since the computation of the probability for any impact parameter reduces to the solution of the same type of system of equations.

Let us briefly touch upon the charge-transfer process $B^{3+} + He \rightarrow B^{2+} + He^+$ for which Zwally and Cable[11] have recently measured the cross section and have discovered that its maximum value differs from that of the LZ cross section by almost a factor of two.

In[11] the parameters R_S, ΔF_S and R_p, ΔF_p characterizing the terms in the two quasi-crossing regions which are responsible for the charge transfer to the $B^{2+}(2s)$ and $B^{2+}(2p)$ states are computed with allowance for Coulomb and polarization potentials, while the interactions inducing the transitions are estimated to be equal to $V_S = 1.14$ eV, and $V_p = 0.043$ eV. If we use these estimates as characteristics of the terms and assume a weak dependence of V_S on distance, then the parameters (6) that determine the cross section in our model will be equal to $A = 2.25$, $\Phi = 0$, and $\nu = 0$. The position of the peak of the cross section will then practically coincide with the position predicted by the LZ theory and given by experiment, while the magnitude of the maximum cross section σ_{max} changes from the value $7.4A^2$ given by the LZ theory to the value $10.2A^2$, which is closer to the experimental value $\sigma_{max} = 14.3A^2$. The remaining difference is possibly due to the fact that the strong exchange interaction which obtains at $R \sim R_S$ and which moves the adiabatic $B^{3+}He$ and $B^{2+}(2p)He^+$ terms apart and leads to an increase in the crossing distance R_S is not taken into account in determining the crossing point R_S.

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APPENDIX

At large ϵ the phase $\delta = \Gamma_1 + \Gamma_2$ of the oscillations in the transition probability (24) is large, so that the contribution of the corresponding range of impact parameters ρ to the cross section will be determined by the average value of the probability $\bar{P} = 2z^2(1 - z^2)$. The quantity z is then determined largely by the solution to the system (23) in the region $\xi \sim \epsilon^{1/2}$. Therefore, it is natural to integrate the system (23) from the point $\xi_0 = \epsilon^{1/2}$. Let $\tilde{z}$, $\tilde{\Gamma}_1$, $\tilde{\Gamma}_2$, $\tilde{\Xi}$ and $\hat{z}$, $\hat{\Gamma}_1$, $\hat{\Gamma}_2$, $\hat{\Xi}$ be the solutions of the system in the intervals $\xi_0 < \xi < \infty$ and $\xi_0 > \xi > 0$ respectively with the initial conditions:

$$\tilde{z}, \tilde{\Gamma}_1, \tilde{\Gamma}_2, \tilde{\Xi}|_{\xi=\xi_0} = \hat{z}, \hat{\Gamma}_1, \hat{\Gamma}_2, \hat{\Xi}|_{\xi=\xi_0} = (0, 0, \pi, 0).$$

Let us denote the values of these solutions at the end points of the integration $\xi = \xi_k (\xi_k \to \infty)$ and $\xi = 0$ by

$$\tilde{z}, \tilde{\Gamma}_1, \tilde{\Gamma}_2, \tilde{\Xi}|_{\xi=\xi_k} = \nu, \delta_1, \delta_2, \Xi_k,$$

$$\hat{z}, \hat{\Gamma}_1, \hat{\Gamma}_2, \hat{\Xi}|_{\xi=0} = u, \gamma_1, \gamma_2, \Xi_0, \quad \Xi_0 = \int_{\xi_0}^{0} L(\xi)\, d\xi.$$

Then the probability (24) can be expressed in terms of these quantities as follows:

$$P = P(\Xi_0) = 4|(1-u^2)v(1-v^2)^{1/2}\sin(\delta_1+\delta_2-2\gamma_1+\Xi_0) - u(1-u^2)^{1/2}(1-2v^2)\sin(\gamma_2-\gamma_1+\Xi_0) - u^2v(1-v^2)^{1/2}\sin(-\delta_1-\delta_2+2\gamma_1+\Xi_0)|^2. \quad (28)$$

This result is easily obtained from the properties of $G(\xi, \xi')$, the matrix of the solutions of the system (20)[11].

Further, the average probability is equal to

$$\bar{P} = 2z^2(1-z^2) = {}^1/_2[P(\Xi_0 = 0) + P(\Xi_0 = \pi/2)],$$

where $P(\Xi_0)$ is determined by the expression (28). Then, to find $\bar{P}$, it is not necessary to find the solution $\hat{z}$, $\hat{\Gamma}_1$, $\hat{\Gamma}_2$, $\hat{\Xi}$ of the system (23) in the entire interval of ξ from ξ_0 to zero if the functions $\hat{z}$, $\hat{\Gamma}_1$, and $\hat{\Gamma}_2$ assume their asymptotic values at some values of ξ greater than zero. This is important for the determination of the contribution to the cross section (7) of the region of small impact parameters, where the probability P oscillates strongly.

[1)] If necessary (e.g., for the differential cross section), the correct phase of the transition probability oscillations can also be computed [13,14].

[2)] Notice that when $\Phi = 0$ and $x \to y$ ($\rho \to 0$), the parameters ϵ and b tend to ∞. However, in this case the average probability $\bar{P} = 2w(1-w)$ is determined by only one parameter $2\pi\delta = \frac{1}{4}\pi b\epsilon^{-1/2} = x^{-1/2}$[9], which does not depend on how good the choice of Φ is if $\Phi \ll 1$.

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