# Nonadiabatic transitions in triatomic systems

A. I. Voronin and V. I. Osherov

*Institute of Chemical Physics, USSR Academy of Sciences*
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The model of conical term crossing is considered for a triatomic system in the $E$ state, and the problem of resonant scattering by a conical well is solved. The scattering phase shifts and the level positions and their widths are obtained for linear ($E \gg m^{2/3}$) and circular ($E \approx 3m^{2/3}/2$) trajectories are obtained. Unlike the previously known expressions, the expressions derived here are applicable for all values of the Landau–Zener parameter that characterizes the problem. The obtained widths coincide with those calculated numerically in the common energy region.

## INTRODUCTION

Many physical problems connected with energy transfer in molecular systems call for the investigation of nonadiabatic transitions. Such transitions have been investigated most thoroughly at the present time for two-atom quantum systems[1]. Nonadiabatic transitions in two-atom systems occur with largest probability for those states whose energy terms are close enough to one another. This is usually due to the fact that the zeroth-approximation terms have different symmetry and intersect; in this case the transition is effected under the influence of a relatively weak coupling between the considered states (spin-orbit interaction, interaction of the electron angular momentum with the rotation of the quasimolecule). In this sense, nonadiabatic transitions in polyatomic systems differ in principle. This difference is determined by the fact that in this case terms of identical symmetry can intersect, and this should lead to appreciable transition probabilities.

This was indeed first demonstrated by Teller[2] and later by Nikitin[3] for the semiclassical model of motion in two dimensions (two-dimensional Landau-Zener model). The very possibility of using the concept of a trajectory in a problem in which the potential surfaces have a complicated shape (double cone) remained unclear in this case, however. Therefore the problem of a nonadiabatic transition of this type was reviewed in[4] in the quasiclassical limit, in a range of parameters where the transition probability is exponentially small. A rigorous expression for the transition probability in a wide range of parameters, including the region where it becomes appreciable, had not been derived to this day.

## 1. FORMULATION OF PROBLEM. DERIVATION OF EQUATIONS FOR THE TRANSITION AMPLITUDES

The simplest equation for the investigation of nonadiabatic transitions in three-atom systems is produced when three identical atoms in the $^2S$ state form a configuration that is close to that of an equilateral triangle (doubly-degenerate molecular state E). The motion of the system along the normal coordinates x and y, which violate the symmetry, leads to a lifting of the degeneracy in accordance with the Jahn-Teller effect. Near the symmetrical configuration, the nuclear Hamiltonian of the system can be represented in the form[5]

$$H=\frac{p_x^2+p_y^2}{2M}+F(x\sigma_x+y\sigma_y), \tag{1}$$

where $p_x$ and $p_y$ are momentum-projection operators, and $\sigma_x$ and $\sigma_y$ are Pauli matrices. The adiabatic terms corresponding to this Hamiltonian are solutions of the equation

$$\det(\varepsilon-F[x\sigma_x+y\sigma_y])=0 \tag{2}$$

and form a double circular cone

$$\varepsilon_{1,2}=\pm Fr. \tag{3}$$

In the upper term (conical well) there exist nonstationary states that decay under the influence of the nonadiabatic coupling between the electrons and the motion of the nuclei. The stationary states of the problem

$$H\Psi=E\Psi,\quad \Psi=\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} \tag{4}$$

are standing waves that correspond to elastic resonant scattering by the conical well at $E > 0$, and to scattering by the conical peak at $E < 0$ (the latter are not of great interest, since they are not connected with nonadiabatic transitions in this problem). Thus, the problem (4) should be regarded as the problem of elastic resonant scattering in which it is necessary to find the corresponding phase shifts, meaning also the positions and widths of the levels corresponding to quasistationary states in the conical well.

It is most expedient to use for the solution of (4) a momentum representation, putting in the first step

$$\psi_{1,2}=\frac{1}{2\pi}\int_{-\infty}^{\infty}dp_x\int_{-\infty}^{\infty}dp_y\exp\{ip_xx+ip_yy\}\varphi_{1,2}(p_x,p_y) \tag{5}$$

and then introducing a polar coordinate system in the coordinate and momentum spaces:

$$x=r\cos\varphi,\quad y=r\sin\varphi,\quad p_x=p\cos\alpha,\quad p_y=p\sin\alpha.$$

We now expand in partial waves

$$\begin{aligned}\psi_{1,2}(r,\varphi)&=\sum_m\psi_{1,2}^m(r)e^{i(m\pm1/2)\varphi},\\ \varphi_{1,2}(p,\alpha)&=\sum_{m'}\varphi_{1,2}^{m'}(p)e^{i(m'\pm1/2)\alpha}.\end{aligned} \tag{6}$$

Here m takes on only half-integer values; this is a manifestation of the existence of singularities of the terms at the origin and follows from the requirement that the total electron-hole wave function be unique on going around $r = 0$[5]. Using subsequently the length and energy units $(\hbar^2/FM)^{1/3}$ and $(F^2\hbar^2/M)^{1/3}$, we obtain

$$\begin{aligned}\left(\frac{p^2}{2}-E\right)\varphi_1^m+i\left(\frac{d}{dp}-\frac{m-1/2}{p}\right)\varphi_2^m=0,\\ \left(\frac{p^2}{2}-E\right)\varphi_2^m+i\left(\frac{d}{dp}+\frac{m+1/2}{p}\right)\varphi_1^m=0.\end{aligned} \tag{7}$$

More convenient for the study are the functions

$$\begin{aligned}\sigma_m(p)&=\exp\left\{-i\int^p\left(\frac{p^2}{2}-E+\frac{i}{2p}\right)dp\right\}(\varphi_1^m(p)+\varphi_2^m(p)),\\ \delta_m(p)&=\exp\left\{i\int^p\left(\frac{p^2}{2}-E-\frac{i}{2p}\right)dp\right\}(\varphi_1^m(p)-\varphi_2^m(p)),\end{aligned} \tag{8}$$

  

which satisfy the system of equations

$$\frac{d}{dp}\sigma_m(p)=-\frac{m}{p}\exp\left\{-2i\int^p\left(\frac{p^2}{2}-E\right)dp\right\}\delta_m(p),$$
$$\frac{d}{dp}\delta_m(p)=-\frac{m}{p}\exp\left\{2i\int^p\left(\frac{p^2}{2}-E\right)dp\right\}\sigma_m(p). \quad (9)$$

Solutions of this system, which is the basis for all the further investigations, have the following fundamental property:

$$|\sigma_m(p)|^2-|\delta_m(p)|^2=\text{const}, \quad (10)$$

Thus revealing that the system is non-Hermitian, meaning that it is impossible to introduce a single classical trajectory[6]. Knowledge of $\varphi^m_{1,2}(p)$ makes it possible to obtain the wave functions

$$\psi^m_{1,2}(r)=i^{m\pm 1/2}\int_0^\infty p\,dp\,\varphi^m_{1,2}(p)J_{m\pm 1/2}(pr), \quad (11)$$

satisfying the condition that they be finite as $r\to 0$ ($J_{m\pm 1/2}(pr)$ are Bessel functions); this condition must be satisfied in order that the solutions of the scattering problem be physically meaningful.

The behavior of the solutions as $r\to\infty$ is investigated in the following manner: We set up the functions

$$\Psi^m_{1,2}(r)=\psi_1^m(r)\pm\psi_2^m(r), \quad (12)$$

which are solutions of the problem (4) in an adiabatic basis:

$$\left(\frac{1}{2r^2}(rp_r)^2+\frac{m^2+1/4}{2r^2}-r-E\right)\Psi_2^m(r)+\frac{m}{2r^2}\Psi_1^m(r)=0,$$
$$\left(\frac{1}{2r^2}(rp_r)^2+\frac{m^2+1/4}{2r^2}+r-E\right)\Psi_1^m(r)+\frac{m}{2r^2}\Psi_2^m(r)=0, \quad (13)$$

$p_r$ is the radial momentum. For these we get from (8) and (11) the representation

$$\Psi_1^m(r)=\int_0^\infty dp[\alpha_m(p)K_1^m(pr)+\beta_m(p)K_2^m(pr)],$$
$$\Psi_2^m(r)=\int_0^\infty dp[\alpha_m(p)K_2^m(pr)+\beta_m(p)K_1^m(pr)], \quad (14)$$

where

$$\alpha_m(p)=\frac{\sqrt{p}}{2}\exp\left\{i\left(\frac{p^3}{6}-Ep\right)\right\}\sigma_m(p),$$
$$\beta_m(p)=\frac{\sqrt{p}}{2}\exp\left\{-i\left(\frac{p^3}{6}-Ep\right)\right\}\delta_m(p), \quad (15)$$

$$K^m_{1,2}(pr)=i^{m+1/2}(J_{m+1/2}(pr)\mp iJ_{m-1/2}(pr)). \quad (16)$$

The asymptotic representation for $K^m_{1,2}(pr)$ takes, accurate to terms of order $1/(pr)^2$, the form

$$K_1^m(pr)=i^{m+1/2}\sqrt{\frac{2}{\pi pr}}\left[\left(-i+\frac{m^2}{2pr}+\frac{im^2(m^2-1)}{2(2pr)^2}\right)e^{ipr-im\pi/2}+\left(\frac{m}{2pr}-\frac{im(m^2-1)}{(2pr)^2}\right)e^{-ipr+im\pi/2}\right], \quad (17)$$
$$K_2^m(pr)=(-1)^{m+1/2}\bar{K}_1^m(pr).$$

Using only the principal terms of this expansion, we obtain for $\Psi_2^m(r)$ the expression

$$\Psi_2^m(r)\approx\left(\frac{1}{2\pi r}\right)^{1/2}i^{m+1/2}\int_0^\infty dp\left[\exp\left\{i\left(\frac{p^3}{6}-Ep\right)-ipr+i\varphi_0\right\}\sigma_m(p)+\exp\left\{-i\left(\frac{p^3}{6}-Ep\right)+ipr-i\varphi_0\right\}\delta_m(p)\right] \quad (18)$$

in which

$$\varphi_0=\pi(m+1)/2. \quad (19)$$

The main contribution to the integral (18) as $r\to\infty$ is made by the vicinity of the saddle point $p=(2(E+r))^{1/2}$, and as a result we get

$$\Psi_2^m(r)\sim\frac{1}{r^{3/4}}\cos\left(\frac{1}{3}(2(r+E))^{3/2}-\varphi_0-\frac{\pi}{4}-\frac{\chi}{2}\right). \quad (20)$$

We have put here

$$\sigma_m(+\infty)/\delta_m(+\infty)=e^{i\chi}, \quad (21)$$

which corresponds to the choice const = 0 in (10). This choice of the arbitrary constant must be made in order to ensure an elastic character of the scattering.

Expression (20) is the sought asymptotic form of the standing waves for the problem in question. Indeed, from (13) it follows that as $r\to\infty$, when the nonadiabatic coupling vanishes, $\Psi_2^m(r)$ satisfies the equation

$$\left(\frac{1}{2r^2}(rp_r)^2+\frac{m^2+1/4}{2r^2}-r-E\right)\Psi_2^m(r)=0,\quad r\to\infty,$$

which is the two-dimensional analog of the Airy equation describing the scattering states.

The asymptotic form of $\Psi_1^m(r)$ is determined mainly by the nonadiabatic coupling, since the physically meaningful solutions of the equation

$$\left(\frac{1}{2r^2}(rp_r)^2+\frac{m^2+1/4}{2r^2}+r-E\right)\Psi_1^m(r)=0,\quad r\to\infty$$

decrease exponentially as $r\to\infty$. The second equation of (13) shows, together with (20), that the principal term of the asymptotic form of $\Psi_1^m(r)$ should be

$$\Psi_1^m(r)\sim\frac{m}{r^{3/4+3}}\cos\left(\frac{1}{3}(2(r+E))^{3/2}-\varphi_0-\frac{\pi}{4}-\frac{\chi}{2}\right). \quad (22)$$

This asymptotic form can be obtained directly from (14)–(17) by recognizing that, by virtue of the fundamental equations (9), the following representation holds true as $p\to\infty$:

$$\sigma(p)=\sigma(+\infty)-\frac{im}{p^3}\delta(+\infty)\exp\left\{-2i\int^p\left(\frac{p^2}{2}-E\right)dp\right\},$$
$$\delta(p)=\delta(+\infty)+\frac{im}{p^3}\sigma(+\infty)\exp\left\{+2i\int^p\left(\frac{p^2}{2}-E\right)dp\right\}. \quad (23)$$

The use of this representation together with the asymptotic forms of (17) of order not higher than $1/pr$ leads to the vanishing of terms of order $1/r^{3/4+3/2}$ from $\Psi_1^m(r)$. The next term in $\Psi_1^m(r)$ is of order $1/r^{3/4+3}$ and corresponds to the asymptotic representation (22).

The remainder of the problem is to find the phase shift $\chi$. For this it is necessary to solve the system (9).

## 2. SOLUTION OF PRINCIPAL EQUATIONS. QUASICLASSICAL APPROXIMATION

When the conditions

$$E\gg 1,\quad m\gg 1 \quad (24)$$

are satisfied, it is possible to obtain for the functions

$$\Sigma(p)=\exp\left\{i\int^p\left(\frac{p^2}{2}-E\right)dp\right\}\sigma(p),$$
$$\Delta(p)=\exp\left\{-i\int^p\left(\frac{p^2}{2}-E\right)dp\right\}\delta(p) \quad (25)$$

the following quasiclassical representations

$$\Sigma(p)=C_1\cos g\exp\left\{i\varepsilon\int^p\omega(p)dp\right\}+C_2\sin g\exp\left\{-i\varepsilon\int^p\omega(p)dp\right\},$$
$$\Delta(p)=-C_1\sin g\exp\left\{i\varepsilon\int^p\omega(p)dp\right\}+C_2\cos g\exp\left\{-i\varepsilon\int^p\omega(p)dp\right\} \quad (26)$$

in which

$$\omega(p)=\left[\left(\frac{p^2}{2}-E\right)^2-\frac{m^2}{p^2}\right]^{1/2},\quad \varepsilon=\operatorname{sign}\left(\frac{p^2}{2}-E\right),$$
$$g=\frac{1}{2}\operatorname{arctg}\frac{im}{p|{}^1/{}_2p^2-E|} \tag{27}$$

Expression (26) approximates correctly the solution only at a sufficiently large distance from the zeroes of the adiabatic splitting

$$(p^2/2-E)^2-m^2/p^2=0. \tag{28}$$

All the roots of this equation lie on the real p axis. Three of them are positive ($p_0$, $p_1$, $p_2$). By solving the system (9) exactly near $p_0$, $p_1$, and $p_2$ and making these solutions continuous with the quasiclassical asymptotic relations (26) between $p_0$, $p_1$, and $p_2$, we can continue the solutions $\Sigma(p)$ and $\Delta(p)$ along the entire positive p axis. A special role in the solution is played by the point $p = 0$, near which the functions $\Sigma(p)$ and $\Delta(p)$ should be regular, for otherwise $\Psi^m(r)$ acquires unphysical terms $\sim r^m$ as $r\to\infty$. Therefore

$$\Sigma(p)=C_0p^{1/2}(J_{m-1/2}(Ep)-iJ_{m+1/2}(Ep)),$$
$$\Delta(p)=-C_0p^{1/2}(J_{m-1/2}(Ep)+iJ_{m+1/2}(Ep)). \tag{29}$$

Here $J_{m\pm1/2}(Ep)$ are Bessel functions and $C_0$ is an arbitrary constant. The representation (29) plays the role of the boundary condition at any placement of the zeroes $p_0$, $p_1$, and $p_2$.

A concrete continuation of the solutions can be carried out in the following cases.

Case I:

$$\left|\int_{p_i}^{p_k}\omega(p)\,dp\right|\gg1,\qquad p_{i,k}=0,p_0,p_1,p_2. \tag{30}$$

In this case the zeroes of $p_0$, $p_1$, and $p_2$ are far enough from one another and near these zeroes the solution of the system (9) can be approximated by Airy functions. The transition from the region where the solutions increase exponentially or decrease with the coefficients $C^i_{1,2}$ into the region of oscillations with coefficients $C^f_{1,2}$ is effected by the transformation [7]

$$\begin{pmatrix}C_1{}^f\\C_2{}^f\end{pmatrix}=\begin{pmatrix}e^{-i\pi/4}&0\\0&e^{i\pi/4}\end{pmatrix}\begin{pmatrix}{}^1/{}_2i&1\\-{}^1/{}_2i&1\end{pmatrix}\begin{pmatrix}C_1{}^i\\C_2{}^i\end{pmatrix}\equiv S\begin{pmatrix}C_1{}^i\\C_2{}^i\end{pmatrix}. \tag{31}$$

The continuation from $p\ll p_0(C^0_{1,2})$ to $p\gg p_2(C^+_{1,2})$ assumes in this case the form

$$\begin{pmatrix}C_1{}^+\\C_2{}^+\end{pmatrix}=S\begin{pmatrix}0&e^{-D}\\e^D&0\end{pmatrix}S^{-1}\begin{pmatrix}0&e^{-i\Omega}\\e^{i\Omega}&0\end{pmatrix}S\begin{pmatrix}C_1{}^0\\C_2{}^0\end{pmatrix}. \tag{32}$$

Here

$$\Omega=\int_{p_0}^{p_1}\omega(p)\,dp,\qquad D=\left|\int_{p_1}^{p_2}\omega(p)\,dp\right|. \tag{33}$$

We note that the most consistent procedure is that of simultaneously going around the two zeroes $p_1$, and $p_2$ in the complex p plane with a Stokes parameter $\alpha$ $\alpha = i(1+e^{-D})^{1/2}e^{i\varphi}$ ($\varphi$ is an undetermined phase, $\varphi\to0$, $D\to\infty$), as against $\alpha = i$ in the case of (32). However, the approximation (32) is sufficient at the accuracy of interest to us.

Since there is no solution that increases as $p\to0$ in the region $p\ll p_0$, owing to (29) ($C^0_1 = 0$), we obtain the following final coupling formulas:

$$C_1{}^+=e^{-i\pi/4}(2e^D\cos\Omega+{}^1/{}_2ie^{-D}\sin\Omega)C_2{}^0,$$
$$C_2{}^+=e^{i\pi/4}(2e^D\cos\Omega-{}^1/{}_2ie^{-D}\sin\Omega)C_2{}^0, \tag{34}$$

which will be used to determine the phase shift $\chi$.

Case II:

$$E\gg{}^3/{}_2m^{2/3}. \tag{35}$$

The zeroes of the adiabatic splitting are located in this case at the points

$$p_0=m/E,\qquad p_{1,2}=\sqrt{2E}\mp m/2E. \tag{36}$$

The action between the points $p_1$ and $p_2$ no longer satisfies the condition (30) in this case, and the system (9) must be solved exactly in the interval between $p_1$ and $p_2$. This can be done by virtue of the inequality (35), which enables us to regard $p_{1,2}$ as a double root of the adiabatic splitting. The system (9) should then be approximated at $p\approx p_{1,2}$ by a system of the form

$$d\sigma/dz=-i\nu^{1/2}e^{z^2/2}\delta,\qquad d\delta/dz=-i\nu^{1/2}e^{-z^2/2}\sigma, \tag{37}$$

where

$$z=2^{1/2}e^{-i\pi/4}(2E)^{1/4}(p-(2E)^{1/2}), \tag{38}$$
$$\nu=-im^2/2(2E)^{3/2}. \tag{39}$$

The system (37) can be solved in terms of parabolic-cylinder functions $D_\nu(z)$.

In the remainder of the derivation of the coupling formulas it must be recognized that if the condition (35) is satisfied then the representation (29) is valid also at $p>p_0$ ($p\ll p_{1,2}$). This makes it possible to match together the expressions (29) and the quasiclassical asymptotic relations

$$\Sigma(p)=C_1{}^0\exp\left\{-i\int_{p_0}^{p}\omega(p)\,dp\right\},$$
$$\Delta(p)=C_2{}^0\exp\left\{i\int_{p_0}^{p}\omega(p)\,dp\right\}, \tag{40}$$

by using in (29) the Debye expansions. The transition from $p_0$ to $p_1(C^-_{1,2})$ is given by a diagonal matrix with phase shifts $\pm\Omega$, and for the continuation from $p<p_1$ to $p>p_2$ it is necessary to use the rotation formulas in the solutions

$$\begin{pmatrix}\Sigma\\\Delta\end{pmatrix}=\begin{pmatrix}D_\nu(z_\mp)&D_{-\nu-1}(-iz_\mp)\\i\nu^{1/2}D_{\nu-1}(z_\mp),&-\nu^{-1/2}D_{-\nu}(-iz_\mp)\end{pmatrix}\begin{pmatrix}C_1\\C_2\end{pmatrix},$$
$$\arg z_-=\frac{3}{4}\pi,\qquad \arg z_+=-\frac{\pi}{4} \tag{41}$$

and to match (41) to the quasiclassical asymptotic forms

$$\Sigma(p)=C_1{}^\mp\exp\left\{\mp i\int_{p_{1,2}}^{p}\omega(p)\,dp\right\},$$
$$\Delta(p)=C_2{}^\mp\exp\left\{\pm i\int_{p_{1,2}}^{p}\omega(p)\,dp\right\}. \tag{42}$$

The final coupling formulas are

$$C_1{}^+=\alpha_0[e^{-i\Omega}+(1-e^{-2\pi\mu})^{1/2}e^{i(\Omega+\varphi)}]C_0,$$
$$C_2{}^+=\alpha_0[e^{i\Omega}+(1-e^{-2\pi\mu})^{1/2}e^{-i(\Omega+\varphi)}]C_0, \tag{43}$$

where

$$\mu=\frac{m^2}{2(2E)^{3/2}},\qquad \alpha_0=\sqrt{\frac{2}{\pi E}}e^{\pi\mu}, \tag{44}$$

$$\varphi=-\frac{\pi}{4}-\arg\Gamma(1-i\mu)+\mu-\mu\ln\mu. \tag{45}$$

Case III. At energies close to the resonant-scattering threshold, $E_0 = (3/2)m^{2/3}$, if the inequality

$$(E-E_0)/E_0\ll1 \tag{46}$$

is satisfied, the adiabatic-splitting zeroes that approach each other become $p_0$ and $p_1$:

$$p_{0,1}=m^{1/3}\mp({}^2/{}_3(E-E_0))^{1/2},\qquad p_2=2m^{1/3}+\frac{4}{9}\frac{E-E_0}{m^{1/3}}, \tag{47}$$

so that the standard relation between them can be the equation for the parabolic-cylinder functions[6]. The result for $\Sigma(p)$ is

$$\Sigma(p)=C_1D_\nu(z)+C_2D_\nu(-z), \tag{48}$$

where

$$z=2^{1/2}3^{1/4}m^{1/6}(p-m^{1/3}),\quad \nu=-\frac{1}{2}+\frac{3^{1/2}}{2}m\frac{E-E_0}{E_0}. \tag{49}$$

This solution can be joined together with the quasiclassical solution at $p < p_0$ and, by virtue of the condition (29), we should have $C_1 = 0$. The continuation from $p_1$ to $p_2$ is effected by a diagonal matrix with elements $e^{\pm D}$, the solution (48) is made continuous with the quasiclassical solution near $p = p_1$. The passage through the last zero $p_2$ is given by the matrix (31). We note that both in case I and in case III small imaginary terms are disregarded in the second-order equations for $\Sigma(p)$ and $\Delta(p)$. It is assumed that they exert no strong influence on the Stokes parameter on passing through simple turning points. The final coupling formulas can be expressed in the form

$$C_1^+=\beta e^{-i\pi/4}\left[\frac{\sqrt{2\pi}\,e^\lambda}{\Gamma(-\nu)}e^D+\frac{i}{2}\cos\pi\nu e^{-D}\right]C_2,$$
$$C_2^+=\beta e^{i\pi/4}\left[\frac{\sqrt{2\pi}\,e^\lambda}{\Gamma(-\nu)}e^D-\frac{i}{2}\cos\pi\nu e^{-D}\right]C_2. \tag{50}$$

Here

$$\lambda=(\nu+{}^1/_2)-(\nu+{}^1/_2)\ln(\nu+{}^1/_2), \tag{51}$$

$$\beta=m^{1/6}/2^{1/4}3^{1/8}. \tag{52}$$

The obtained expressions make it possible to connect $\sigma(+\infty)$ with $\sigma(-\infty)$ and to determine the scattering phase shifts $\chi/2$.

## 3. DETERMINATION OF THE SCATTERING PHASE SHIFTS AND THE LEVEL POSITIONS AND WIDTHS

The connection between $\sigma(+\infty)$ and $\sigma(-\infty)$ follows from formulas (25) and (34), (43), (50) and takes the form

$$\sigma(+\infty)/\delta(+\infty)=e^{2i\xi}C_1^+/C_2^+, \tag{53}$$

where

$$\xi=\lim_{p\to\infty}\left(\int_{p_2}^{p}\omega(p)\,dp-\left(\frac{p^3}{6}-Ep\right)\right)+\frac{\pi}{2}. \tag{54}$$

As a result we obtain for $\chi/2$ the expression

$$\frac{\chi}{2}=\xi+\frac{1}{2}\arg\frac{C_1^+}{C_2^+}. \tag{55}$$

Thus, when the inequalities (30) are satisfied we have

$$\frac{\chi}{2}=\xi-\frac{\pi}{4}+\operatorname{arctg}\left(\frac{1}{4}e^{-2D}\operatorname{tg}\Omega\right), \tag{56}$$

in the Landau-Zener region (35) we have

$$\frac{\chi}{2}=\xi+\frac{1}{2}\varphi+\operatorname{arctg}\left[\frac{R-1}{R+1}\operatorname{tg}\left(\Omega+\frac{1}{2}\varphi\right)\right],\quad R=(1-e^{-2\pi\mu})^{1/2} \tag{57}$$

while in the deep tunnel transition region (46) we have

$$\frac{\chi}{2}=\xi-\frac{\pi}{4}+\operatorname{arctg}\left[\frac{\Gamma(-\nu)}{2\sqrt{2\pi}}e^{-\lambda-2D}\cos\pi\nu\right]. \tag{58}$$

Near the resonances $E_n$, the resonant part of the phase shift $\chi/2$ can be represented in the form

$$\frac{\chi_r}{2}=\operatorname{arctg}\frac{\Gamma}{2(E-E_n)}. \tag{59}$$

As seen from (56)–(58), the resonant levels are in this case roots of the equations

$$\Omega=(n+{}^1/_2)\pi, \tag{60a}$$

$$\Omega+{}^1/_2\varphi=(n+{}^1/_2)\pi, \tag{60b}$$

$$\nu=n,\quad n\geqslant 0. \tag{60c}$$

For the widths we obtain respectively

$$\Gamma=\frac{1}{2(d\Omega/dE)_{E_n}}e^{-2D}, \tag{61a}$$

$$\Gamma=\frac{2}{(d\Omega/dE)_{E_n}}\frac{1}{(R+1)^2}e^{-2\pi\mu}, \tag{61b}$$

$$\Gamma=\frac{1}{\sqrt{2\pi}(d\nu/dE)_{E_n}}\frac{\exp\{-(n+{}^1/_2)+(n+{}^1/_2)\ln(n+{}^1/_2)\}}{n!}e^{-2D} \tag{61c}$$

Let us examine some consequences of the results. First, inasmuch as in the deep tunnel region (49) we have

$$E_n=\frac{3}{2}m^{2/3}+\frac{\sqrt{3}}{m^{1/3}}(n+{}^1/_2),\quad \pi\nu=\Omega-\frac{\pi}{2}, \tag{62}$$

both formula (60b) at $\mu \gg 1$ and formula (60c) reduce to (60a). Second, at $n \gg 1$ formula (61c) yields

$$\Gamma=\frac{1}{2\pi(d\nu/dE)_{E_n}}e^{-2D}. \tag{63}$$

In view of (62), this reduces to (61a). At the same time, when the condition $E \gg {}^3/_2m^{2/3}$ is satisfied we have

$$D=\pi\mu \tag{64}$$

and consequently at $\mu \gg 1$ formula (61b) coincides with (61a). Thus, the expressions

$$\Omega=(n+{}^1/_2)\pi,$$
$$\Gamma=\frac{C}{2(d\Omega/dE)_{E_n}}e^{-2D},\quad C\sim 1 \tag{65}$$

that describe well the resonant scattering by the conical potential in a wide range of parameters. The action varies in this case from

$$\Omega=\pi m^{1/3}(E-E_0)/\sqrt{3},\ n\ll m \tag{66}$$

in the deep tunnel region to

$$\Omega={}^1/_3(2E)^{3/2}-m,\quad E\gg{}^3/_2m^{2/3} \tag{67}$$

near the top of the barrier. For D we have accordingly

$$D=m(\sqrt{3}-\ln(\sqrt{3}+2))-{}^1/_2(n+{}^1/_2)\ln\frac{2m3^{3/2}}{(n+{}^1/_2)}\qquad n\ll m,$$
$$D=\pi\frac{m^2}{2(2E)^{1/2}},\qquad E\gg{}^3/_2m^{2/3}. \tag{68}$$

In the intermediate region, $\Omega$ and D can be expressed in terms of the elliptic integrals

$$\Omega=\frac{1}{4}\int_{x_0}^{x_1}\frac{[(x-x_0)(x_1-x)(x_2-x)]^{1/2}}{x}dx,$$
$$D=\frac{1}{4}\int_{x_1}^{x_2}\frac{[(x-x_0)(x-x_1)(x_2-x)]^{1/2}}{x}dx. \tag{69}$$

Here $x_0$, $x_1$, and $x_2$ are the squares of the zeroes of the adiabatic splitting in increasing order.

The two limiting cases (61b) and (61c), which differ in the form of the energy dependence of the resonance width, differ also with respect to the character of the classical motion. To this end, let us consider an arbitrary linear trajectory in the (x, y) plane. We pass through this trajectory a plane perpendicular to the (xy) plane, and examine the intersection between this plane and the conic surfaces $\pm z$. The hyperbolas $z = \pm(x^2 + b^2)^{1/2}$ produced in this intersection make it possible to reduce the problem to a one-dimensional problem with unit forces and with slopes of opposite sign. It corresponds to a Landau-Zener parameter $\mu = b^2/2v$, where b is the impact distance and v is the velocity of the representative point. We see that

$\mu = m^2/2(2E)^{3/2}$. Such a representation of $\mu$ is obviously possible only at $E \gg 1$ and $E \gg b$, i.e., for classical trajectories that penetrate in the interior of the upper cone. At $E \sim b (E \sim m^{2/3})$ the motion occurs near the surface of the conical well and becomes circular. The decay problem reduces in this case to an investigation of transitions between parallel terms with an action radius determined by the tunnel decay with respect to r.

## CONCLUSION

The results can be used to calculate the cross sections for the scattering of atoms by two-atom molecules and to estimate the lifetimes of three-atom complexes. In the latter case they can be compared with the numerical calculations carried out in[9] for low energies (the initial sequence of values of the principal quantum number) and for a number of angular momenta m. The results of this comparison are perfectly satisfactory in the common region of parameters.

In our case, terms of like symmetry of three-atom systems intersect along a line in three-dimensional space in the absence of spin-orbit interaction, or at the point if this interaction is present. This leads to new possibilities for nonadiabatic transitions.

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