Nonadiabatic transition in triatomic systems

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A two-dimensional model for nonadiabatic transitions in triatomic systems is considered. The phase shifts for resonance scattering by a potential surface having the shape of a slightly elliptic ($\tau \ll 1$) double cone are found in the quasiclassical approximation. The widths of the obtained resonances exhibit a threshold dependence on the magnitude of the orbital quantum number m for $m_c = 2\sqrt{2}\pi^{-1}E^{3/2}\tau$. The existence of such a threshold in partial cross sections is, from the point of view of classical mechanics, connected with oscillations in the angular momentum of the motion in the elliptic conical well.

The chief characteristic of nonadiabatic transitions in triatomic systems is the multidimensional nature of the motion of the atoms. In the simplest case such a motion is two-dimensional. An example is the quantum system consisting of three identical atoms in the ^2S states and having a configuration close to an equilateral triangle, when the role of the two coordinates essential for a transition is played by nonsymmetric normal coordinates that destroy the symmetry of the regular triangle. The adiabatic terms of such a system form a double circular cone, which makes it possible to separate the motion of the system in the variables r and φ, and solve the nonadiabatic-transition problem in the quasiclassical approximation [1].

Under certain limitations, the two-dimensional nature of the motion is sufficient for the investigation of the transitions that occur in collisions of atoms with diatomic molecules and in triatomic nonlinear molecules [2]. As an example, we can cite the electronic transitions induced in atoms by collisions with rigid molecules, when the vibrational quantum number of the molecule does not change as a result of the collision. In accordance with the general rules [3], terms of the same symmetry intersect in this case on the surface of a double cone arbitrarily positioned above the plane of the two configurational coordinates, as which we can choose the distance **R** between the atom and the center of gravity of the molecule and the angle between **R** and the molecular axis. The forces acting on a representative point along the chosen coordinate axes are, in this case, different, and, even if the cone is positioned vertically, the curves of its intersection with the constant-energy planes are ellipses. Exact separation of the variables for the entire adiabatic surface is impossible to attain in this case. The resulting problem cannot be solved with the aid of the known methods of investigating problems with boundary conditions defined on an ellipse [4].

However, the problem of nonadiabatic transitions in systems with elliptic conical terms is fairly easy to solve in the semiclassical approximation if it is assumed that the classical trajectories of the motion are rectilinear [5,6]. To what extent such an assumption is justified is a question that can be answered only after the consistent solution of the pertinent quantum problem.

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

In the basis of the nonadiabatic electronic wave functions in the dimensionless variables characteristic of linear fields, the chosen model reduces to the Schrödinger equation

$$\left(\frac{p_x^2+p_y^2}{2}+f_1\sigma_x x+f_2\sigma_y y\right)\Psi=E\Psi, \tag{1}$$

where p_x and p_y are momentum-component operators, σ_x and σ_y are Pauli matrices, and f_1 and f_2 are the dimensionless components of the force along the important coordinate axes:

$$f_{1,2}=F_{1,2}\left(\frac{2}{F_1+F_2}\right)^{1/2}.$$

The adiabatic terms of the system under consideration form the double elliptical cone

$$E_{1,2}=\pm(f_1^2x^2+f_2^2y^2)^{1/2}.$$

Therefore, as in [1], when $E > 0$, we can consider the problem of the elastic resonance scattering by the conical well of the upper adiabatic state. But the problem of the computation of the corresponding phases in the present case requires the prior determination of the correct asymptotic forms of the wave functions, since there is no cylindrical symmetry in the chosen coordinate system. This is extremely complicated to do in the r-representation, since the simple partial waves $\psi = e^{im\varphi}F(r)$ get strongly mixed up as $r \to \infty$. Also strongly coupled are the elliptic waves $\psi = M(r, \varphi)F(r)$ (where the $M(r, \varphi)$ are suitable angular functions that take the elliptical symmetry of the cone into account).

It is more convenient in this sense to use the momentum representation:

$$\Psi_{1,2}=\iint dk_x\,dk_y\,\Psi_{1,2}(k_x,k_y)\exp(ik_xx+ik_yy). \tag{2}$$

In this case the amplitudes $\Psi_{1,2}(k_x, k_y)$ do not change upon going round the coordinate origin and, in polar coordinates,

$$k_x=f_1p\cos\varphi,\quad k_y=f_2p\sin\varphi$$

satisfy the system of equations

$$\begin{pmatrix} -i\varepsilon, & e^{i\varphi}\left(\dfrac{\partial}{\partial p}+\dfrac{i}{p}\dfrac{\partial}{\partial\varphi}\right) \\ e^{-i\varphi}\left(\dfrac{\partial}{\partial p}-\dfrac{i}{p}\dfrac{\partial}{\partial\varphi}\right), & -i\varepsilon \end{pmatrix}\begin{pmatrix}\Psi_1(p,\varphi)\\ \Psi_2(p,\varphi)\end{pmatrix}=0. \tag{3}$$

Here we have used the designation

$$\varepsilon={}^1/{}_2p^2(1+\tau\cos2\varphi)-E, \tag{4}$$

and τ is the eccentricity of the ellipses of intersection of the cones $E_{1,2}$ with the constant-energy planes, i.e.,

$$\tau=(f_1^2-f_2^2)/(f_1^2+f_2^2). \tag{5}$$

Going over to the new functions

$$\Sigma=p^{1/2}(\Psi_1e^{-i\varphi/2}+\Psi_2e^{i\varphi/2}),$$

$$\Delta=p^{1/2}(\Psi_1 e^{-i\varphi/2}-\Psi_2 e^{i\varphi/2}), \tag{6}$$

we obtain the following system of equations:

$$\begin{pmatrix} \frac{\partial}{\partial p}-i\varepsilon, & -\frac{i}{p}\frac{\partial}{\partial\varphi} \\ -\frac{i}{p}\frac{\partial}{\partial\varphi}, & \frac{\partial}{\partial p}+i\varepsilon \end{pmatrix}\begin{pmatrix}\Sigma\\ \Delta\end{pmatrix}=0, \tag{7}$$

which can be reduced to the basic (for what follows) system

$$\begin{pmatrix} \nabla^2+\varepsilon^2-i\left(\varepsilon_p'+\frac{\varepsilon}{p}\right), & -\frac{\varepsilon_\varphi'}{p} \\ \frac{\varepsilon_\varphi'}{p}, & \nabla^2+\varepsilon^2+i\left(\varepsilon_p'+\frac{\varepsilon}{p}\right) \end{pmatrix}\begin{pmatrix}\Sigma\\ \Delta\end{pmatrix}=0, \tag{8}$$

this system being, under certain conditions, weakly coupled.

Let us now construct the momentum representation for the adiabatic functions

$$\Phi(x,y)=U\Psi(x,y). \tag{9}$$

where the matrix U diagonalizes the interaction in Eq. (1):

$$U=2^{-1/2}\begin{pmatrix}1, & 1\\ -1, & 1\end{pmatrix}\begin{pmatrix}e^{-i\delta/2}, & 0\\ 0, & e^{i\delta/2}\end{pmatrix}, \quad \delta=\operatorname{arctg}\frac{f_2}{f_1}\frac{y}{x}. \tag{10}$$

We find in terms of the polar coordinates

$$x=r\cos\varphi_0,\quad y=r\sin\varphi_0$$

with allowance for the formula (6) the expressions

$$\begin{pmatrix}\Phi_1\\ \Phi_2\end{pmatrix}=2^{-1/2}f_1f_2\iint p^{1/2}\,dp\,d\varphi\exp[ipr(f_1\cos\varphi\cos\varphi_0+f_2\sin\varphi\sin\varphi_0)] \times\left[\cos\frac{\delta-\varphi}{2}\begin{pmatrix}\Sigma\\ -\Delta\end{pmatrix}+i\sin\frac{\delta-\varphi}{2}\begin{pmatrix}-\Delta\\ \Sigma\end{pmatrix}\right]. \tag{11}$$

The basic system (8) shows that as $p\to\infty$ the dominant terms of the asymptotic forms of Σ and Δ oscillate ($\tau<1$) like $e^{ip^3k_1}$ ($k_1\sim 1$). Therefore, as in [1], the dominant contributions to the asymptotic forms of $\Phi_{1,2}(r\to\infty)$ is made by the saddle point $p=k_2\sqrt{2r}$ ($k_2\sim 1$). This circumstance enables us to compute the dominant terms of the asymptotic forms of $\Phi_{1,2}(r\to\infty)$, using the method of steepest descent ($pr\gg 1$) to evaluate the φ integral in (11). The saddle points $\varphi_{1,2}$ are determined from the equation

$$f_1\sin\varphi_{1,2}\cos\varphi_0-f_2\cos\varphi_{1,2}\sin\varphi_0=0$$

and are separated by a distance π from each other. As a result, the dominant asymptotic forms of $\Phi_{1,2}(r\to\infty)$ are given by the integrals

$$\begin{pmatrix}\Phi_1(r,\varphi_0)\\ -\Phi_2(r,\varphi_0)\end{pmatrix}=\frac{1}{\sqrt{2\pi\rho}}\int_0^\infty dp\left[e^{i(p\rho-\pi/4)}\begin{pmatrix}\Sigma(p,\varphi)\\ \Delta(p,\varphi)\end{pmatrix}+ie^{-i(p\rho-\pi/4)}\begin{pmatrix}\Delta(p,\varphi+\pi)\\ \Sigma(p,\varphi+\pi)\end{pmatrix}\right], \tag{12}$$

where

$$\rho=r(1+\tau\cos 2\varphi_0)^{1/2},\quad \varphi=\operatorname{arctg}\left(\frac{1-\tau}{1+\tau}\right)^{1/2}\operatorname{tg}\varphi_0. \tag{13}$$

Upon going round the coordinate origin ($\varphi_0\to\varphi_0+2\pi$), the adiabatic functions $\Phi_{1,2}(r,\varphi_0)$ change their signs; therefore, the adiabatic functions in the p-representation should also change their signs:

$$\begin{pmatrix}\Delta(p,\varphi)\\ \Sigma(p,\varphi)\end{pmatrix}=-\begin{pmatrix}\Delta(p,\varphi+2\pi)\\ \Sigma(p,\varphi+2\pi)\end{pmatrix} \tag{14}$$

The calculations carried out in Sec. 2 show that this expression corresponds to the condition:

$$\begin{pmatrix}\Delta(p,\varphi+\pi)\\ \Sigma(p,\varphi+\pi)\end{pmatrix}=e^{i(m+1/2)\pi}\begin{pmatrix}\Sigma(p,\varphi)\\ \Sigma(p,\varphi)\end{pmatrix},$$

where m is an integer; therefore

$$\begin{pmatrix}\Phi_1(r,\varphi_0)\\ -\Phi_2(r,\varphi_0)\end{pmatrix}=\frac{1}{\sqrt{2\pi\rho}}\int_0^\infty dp\left[e^{i(p\rho-\pi/4)}\begin{pmatrix}\Sigma(p,\varphi)\\ \Delta(p,\varphi)\end{pmatrix}-(-1)^m e^{-i(p\rho-\pi/4)}\begin{pmatrix}\Delta(p,\varphi)\\ \Sigma(p,\varphi)\end{pmatrix}\right]. \tag{15}$$

For $\tau=0$ this result goes over into the corresponding result of the paper [1]. To investigate the scattering, it is sufficient to consider only the function $\Phi_2(r,\varphi_0)$, which corresponds to standing waves at the conical peak of the lower adiabatic state.

2. THE QUASICLASSICAL APPROXIMATION FOR THE ANGULAR FUNCTIONS AND THE ORBITAL ENERGIES

The determination of the asymptotic forms (15) requires the solution of the complex system of equations (8) with the boundary conditions (14). Significant simplifications of this system are possible if the ellipticity of the terms is sufficiently small. Indeed, the intermixing of the amplitudes of Σ and Δ occurs primarily in the vicinity of the zeros of the adiabatic splitting

$$\left(\varepsilon_p'+\frac{\varepsilon}{p}\right)^2+\frac{(\varepsilon_\varphi')^2}{p^2}=0.$$

For $p\to 0$ and $p\to\infty$, we have $|\epsilon_\varphi'/p|\ll|\epsilon_p'+\epsilon/p|$. Therefore, under the condition that

$$\left(\frac{\varepsilon_\varphi'}{p}\right)^2\ll\left|\frac{d}{dp}\left(\varepsilon_p'+\frac{\varepsilon}{p}\right)\right|,$$

which is equivalent to $p_0\tau\ll 1$, the system (8) splits up into separate equations for Σ and Δ:

$$\left(\nabla^2+\varepsilon^2\mp i\left(\varepsilon_p'+\frac{\varepsilon}{p}\right)\right)\begin{pmatrix}\Sigma\\ \Delta\end{pmatrix}=0. \tag{16}$$

In these equations the term $(\epsilon_p'+\epsilon/p)$ has a significant influence on the behavior of the solutions only for $p\to 0$, when the ellipticity of the terms is negligible, and for $p\sim p_0=\sqrt{2E}$ (see [1]). Consequently, under the condition $p_0\tau\ll 1$, the Eqs. (16) can be further simplified:

$$\left(\nabla^2+\varepsilon^2\mp i\left(\varepsilon_{0p}'+\frac{\varepsilon_0}{p}\right)\right)\begin{pmatrix}\Sigma\\ \Delta\end{pmatrix}=0,\quad \varepsilon_0=\frac{p^2}{2}-E. \tag{17}$$

We shall seek their solutions in the form of an expansion in terms of the complete set of solutions to the equation

$$\left(\frac{d^2}{d\varphi^2}+a_m+p^2(\varepsilon^2-\varepsilon_0^2)\right)M_m(p,\varphi)=0 \tag{18}$$

with a boundary condition corresponding to (14):

$$M_m(p,\varphi)=-M_m(p,\varphi+2\pi), \tag{19}$$

where the a_m are the eigenvalues of the Eq. (18). The functions M_m can clearly be assumed to be orthonormalized. Then for the coefficients Σ_m and Δ_m in the expansions of Σ and Δ in terms of the M_m we obtain the following equations:

$$\left(\frac{d^2}{dp^2}+\varepsilon_0^2-\frac{a_m}{p^2}\mp i\left(\varepsilon_{0p}'+\frac{\varepsilon_0}{p}\right)\right)\begin{pmatrix}\Sigma_m\\ \Delta_m\end{pmatrix}+\sum_{m'}\left(2\left\langle M_m\frac{d}{dp}M_{m'}\right\rangle\frac{d}{dp}+\left\langle M_m\frac{d^2}{dp^2}M_{m'}\right\rangle\right)\begin{pmatrix}\Sigma_{m'}\\ \Delta_{m'}\end{pmatrix}=0. \tag{20}$$

They are the basic equations for the computation of the scattering phase shifts, but they require a preliminary investigation of the orbital equations (18).

With the exception of the low-momentum region, where

$$a_m=(m+{}^1/_2)^2,\quad M_m=\exp\{\pm i(m+{}^1/_2)\varphi\},$$

Eq. (18) is sufficiently easy to solve only under the assumption that the angular motion is quasiclassical; for in the general case (18) is a Hill-type equation, and even for $p\to\infty$, when it goes over into the Mathieu equation, its solutions (which are then the standard Mathieu functions) do not satisfy the condition (19). The possibility of using the quasiclassical approximation is connected with the fact that in Eq. (18), represented in the form

$$(d^2/d\varphi^2+Z^2(\alpha^2+(\beta+\cos 2\varphi)^2))M_m(\varphi)=0, \tag{21}$$

where

$$\alpha^2=4\frac{a_m-p^2\varepsilon_0^2}{p^6\tau^2},\quad \beta=\frac{2\varepsilon_0}{p^2\tau},$$

the parameter $Z={}^1/_2 p^3\tau$ can, for not too small values of τ, when the solutions to (18) become trivial, be assumed to be large wherever the solution $M_m=e^{i(m+1/2)\varphi}$ is inadmissible. Therefore, with the exception of the regions near the points φ_i, where the quasiclassical approximation breaks down, the principal solutions to (21) can be represented in the form

$$M_m=\frac{A_\pm}{Z^{1/2}(\alpha^2+(\beta+\cos 2\varphi)^2)^{1/4}}\exp\left(\pm iZ\int^{\varphi}(\alpha^2+(\beta+\cos 2\varphi)^2)^{1/2}d\varphi\right). \tag{22}$$

Equation (21) should be solved exactly near the points φ_i. The obtained exact solutions should be matched with the asymptotic forms (22). The computations lead to the following results.

1. The region $|\beta|<1$, $\alpha^2>0$. Near the singular points (see Fig. 1) $\varphi_1={}^1/_2\arccos(-\beta)$, $\varphi_2=\pi-\varphi_1$, φ_3, and φ_4, where above-the-barrier reflection can be important, Eq. (21) can be solved in terms of the parabolic-cylinder functions. This leads to the following transition matrix relating the constants $A_\pm$ to the various sides of the φ_i's:

$$U=\begin{pmatrix}(1+e^{-2\pi\gamma})^{1/2}e^{-i\Delta}, & -ie^{-\pi\gamma}\\ ie^{-\pi\gamma}, & (1+e^{-2\pi\gamma})^{1/2}e^{i\Delta}\end{pmatrix}, \tag{23}$$

where

$$\gamma=\frac{1}{4}Z\frac{\alpha^2}{(1-\beta^2)^{1/2}},\quad \Delta=\arg\Gamma\left(\frac{1}{2}+i\gamma\right)+\gamma-\gamma\ln|\gamma|, \tag{24}$$

and $\Gamma(x)$ is the gamma function. The complete transition matrix connecting $A_\pm(\varphi)$ and $A_\pm(\varphi+2\pi)$ in such a case is determined by the expressions

$$R=L^2,\quad L=\begin{pmatrix}e^{iS_1}, & 0\\ 0, & e^{-iS_1}\end{pmatrix}U\begin{pmatrix}e^{iS_2}, & 0\\ 0, & e^{-iS_2}\end{pmatrix}U, \tag{25}$$

and the quasiclassical actions are computed above the shallow and deep wells (Fig. 1):

$$S_1=Z\int_{-\varphi_1}^{\varphi_1}(\alpha^2+(\beta+\cos 2\varphi)^2)^{1/2}d\varphi,\qquad S_2=Z\int_{\varphi_1}^{\varphi_2}(\alpha^2+(\beta+\cos 2\varphi)^2)^{1/2}d\varphi.$$

Taking into account the fact that the boundary condition

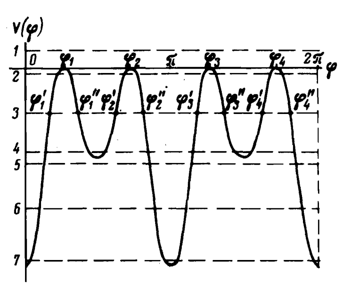

FIG. 1. The potential energy of the orbital motion for $|\beta|<1$. $V(\varphi)=-Z^2(\beta+\cos 2\varphi)^2$.

(19) goes over in the case under consideration into the relation

$$\det(R+1)=0, \tag{26}$$

we find the following equation for the orbital energies a_m:

$$(1+2e^{-2\pi\gamma})\cos\xi\cos\eta=\sin\xi\sin\eta. \tag{27}$$

It contains the total phases above the wells:

$$\xi=S_1-\Delta,\quad \eta=S_2-\Delta$$

with allowance for the shift Δ in the region of maximum reflection. The asymptotic relations in the parameter region under consideration have the forms:

$$\cos(S_1+S_2)=0,\quad \gamma\gg 1,$$
$$\cos(S_1+S_2)=-{}^1/_2\cos(S_1-S_2),\quad \gamma\ll 1.$$

2. The region $|\beta|<1$, $\alpha^2<0$, where the points φ_i', φ_i'' (see Fig. 1) are fairly close to each other. The transition matrices U, L, and R and the condition for the determination of the levels have the same forms as in the case 1. The actions for the wells are computed between the turning points of the classical motion. As a result, we find the equation

$$(1+2e^{-2\pi\gamma})\cos\xi'\cos\eta'=\sin\xi'\sin\eta', \tag{28}$$

in which

$$\xi'=S_1'-\Delta,\quad \eta'=S_2'-\Delta,$$
$$S_1'=Z\int_{-\varphi_1'}^{\varphi_1'}(\alpha^2+(\beta+\cos 2\varphi)^2)^{1/2}d\varphi,$$
$$S_2'=Z\int_{\varphi_1''}^{\varphi_2'}(\alpha^2+(\beta+\cos 2\varphi)^2)^{1/2}d\varphi,$$

and φ_i' and φ_i'' are the turning points:

$$\varphi_1^{\prime,\prime\prime}={}^1/_2\arccos(-\beta\pm\sqrt{-\alpha^2}),\quad \varphi_2'=\pi-\varphi_1'.$$

The first asymptotic relation in this region corresponds to a quasiclassical quantization in isolated wells:

$$\cos S_1'\cos S_2'=0,\quad |\gamma|\gg 1,$$

the second is similar to the corresponding relation in the region 1:

$$\cos(S_1'+S_2')=-{}^1/_2\cos(S_1'-S_2'),\quad |\gamma|\ll 1.$$

3. The region $|\beta|<1$, $\alpha^2<0$, where the turning points φ_i', φ_i'' can be regarded as isolated points. The transition matrix for an individual barrier is constructed, using the exact solutions near φ_i', φ_i'' in the form of linear combinations of the Airy functions $\mathrm{Ai}(\varphi-\varphi_i')$ and $\mathrm{Bi}(\varphi-\varphi_i')$, and has the form

$$U=\begin{pmatrix}e^D+{}^1/_4e^{-D}, & -i(e^D-{}^1/_4e^{-D})\\ i(e^D-{}^1/_4e^{-D}), & e^D+{}^1/_4e^{-D}\end{pmatrix}, \tag{29}$$

where

$$D=Z\int_{\varphi_1'}^{\varphi_1''}(-\alpha^2-(\beta+\cos 2\varphi)^2)^{1/2}d\varphi$$

determines the quasiclassical barrier penetrability. The expressions for L and R and the boundary condition have the same forms as in the region 1. The equation for the determination of the levels can be represented in the form

$$(2e^{2D}+{}^1/_8e^{-2D})\cos S_1'\cos S_2'=\sin S_1'\sin S_2'. \tag{30}$$

On account of the main quasiclassical condition $D\gg 1$, it actually corresponds to quantization in isolated wells and goes over into Eq. (28) when $|\gamma|\gg 1$.

4. The region $|\beta| < 1$, $\alpha^2 < 0$, where the turning points φ_1'' and φ_2' cannot be regarded as isolated points. In this case the solution near φ_1'' and φ_2' can be approximated by the parabolic cylinder functions, and the passage through the isolated points φ_1' and φ_2'' is accomplished with the aid of the Airy functions. As a result, we obtain for L the expression

$$L=\begin{pmatrix} e^{iS_1'}, & 0 \\ 0, & e^{-iS_1'} \end{pmatrix}\begin{pmatrix} e^{-i\pi/4}, & \frac{1}{2}e^{i\pi/4} \\ e^{i\pi/4}, & \frac{1}{2}e^{-i\pi/4} \end{pmatrix}\begin{pmatrix} e^{D}, & 0 \\ 0, & e^{-D} \end{pmatrix} \cdot M\begin{pmatrix} e^{D}, & 0 \\ 0, & e^{-D} \end{pmatrix}\begin{pmatrix} e^{i\pi/4}, & e^{-i\pi/4} \\ \frac{1}{2}e^{-i\pi/4}, & \frac{1}{2}e^{i\pi/4} \end{pmatrix}, \tag{31}$$

in which M corresponds to transitions from the region $\varphi_1' < \varphi < \varphi_1''$ into the region $\varphi_2' < \varphi < \varphi_2''$:

$$M=\begin{pmatrix} -(2/\pi)^{1/2}\Gamma(1+\nu)e^{2\lambda}\sin\lambda\nu, & -\cos\pi\nu \\ \cos\pi\nu, & -\left(\frac{\pi}{2}\right)^{1/2}\frac{e^{-2\lambda}}{\Gamma(1+\nu)}\sin\pi\nu \end{pmatrix}. \tag{32}$$

Here

$$2\lambda=(\nu+\tfrac{1}{2})-(\nu+\tfrac{1}{2})\ln|\nu+\tfrac{1}{2}|,$$
$$\nu+\frac{1}{2}=-\frac{1}{4}Z\frac{\alpha^2-(\beta-1)^2}{(1-\beta)^{1/2}}. \tag{33}$$

Using now the relation (26), we find the following equation for the orbital levels:

$$\left(Be^{2D}+\frac{1}{4B}e^{-2D}\right)\cos S_1'\cos S_2'=\sin S_1'\sin S_2', \tag{34}$$

where

$$B=(2/\pi)^{1/2}\Gamma(1+\nu)e^{2\lambda}, \quad S_2'=\pi(\nu+\tfrac{1}{2}). \tag{35}$$

For the quasiclassical levels in the shallow wells ($\nu \gg 1$), it goes over into Eq. (30). The lowest levels correspond to $B \neq 2$.

5. The region $|\beta| < 1$, $\alpha^2 < -(\beta-1)^2$ and sufficiently close to the bottom of the shallow well. In this case $\nu + 1/2 < 0$, and the quantization rules become, for the first time, significantly different from those obtained in the regions 2–4. In particular, in this region, using a method similar to the one used in the region 4, we find

$$\left(Ae^{2D}+\frac{\cos^2 S_2'}{4A}e^{-2D}\right)\cos S_1'=\sin S_1'\sin S_2', \tag{36}$$

where

$$A=\sqrt{2\pi}\frac{e^{2\lambda}}{\Gamma(-\nu)}. \tag{37}$$

The Eq. (36) qualitatively differs from (34), since, in contrast to the first asymptotic relation in the region 2, it yields, when $D \gg 1$, only one condition, $\cos S_1' = 0$, corresponding to quasiclassical quantization in a deep well.

6, 7. The regions $|\beta| < 1$, $\alpha^2 < 0$ and sufficiently large in absolute value. Approximating the solution (21) by Airy functions near the isolated points φ_1' and φ_2'' in the region 6 and by parabolic cylinder functions near the points φ_2'' and φ_3' in the region 7, we find from (26) the following quantization rule: $\cos S_1' = 0$, which is valid for both regions and which is not an asymptotic relation for $D \gg 1$.

8. The region $|\beta| > 1$. In this case there are no shallow wells; therefore, when α^2 is larger than the height of the orbital-potential barrier, the matching reduces to the satisfaction of the condition $\cos S_1 = 0$, and the quantization in the wells follows the equation $\cos S_1' = 0$.

9. The vicinities along the p axis of the points with the parameters $|\beta| = 1$ and $\alpha^2 = 0$ are singular regions of Eq. (21), where the potential figuring in this equation (i.e., in (21)) and having, for $|\beta| < 1$, a very shallow well is replaced by a fourth-order hump when $|\beta| = 1$. The corresponding standard equation has four neighboring singularities, and has not been investigated at all. However, the dimensionless coupling parameter analogous to γ has in this case the form $\gamma' = \alpha^2 Z^{4/3}$, and, in view of the fact that $Z \gg 1$, γ' is almost always large, and a quasiclassical quantization is possible, except in the region of very low orbital energies, through which a small number of terms pass. The latter quantities can be found in these regions by joining the corresponding terms for $|\beta| < 1$ and $|\beta| > 1$, since there are no physical reasons for singular behavior of the terms in this region.

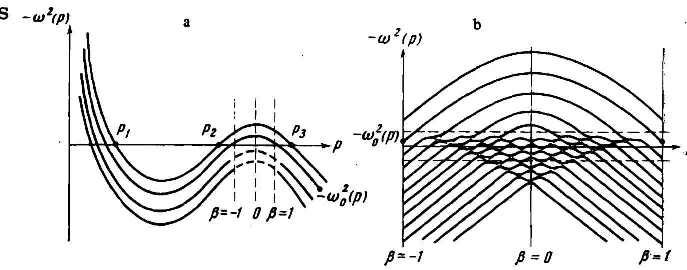

FIG. 2. a) The orbital terms of the problem in the momentum representation; b) the detailed behavior of the orbital terms in the region $|\beta| < 1$.

Thus, with the aid of Eqs. (27), (28), (30), (34), and (36) and the quantization and correspondence rules in the regions 7, 8, and 9, we can find the orbital terms

$$\omega_m^2=\varepsilon_0^2-a_m/p^2 \tag{38}$$

for any momenta. Their qualitative behavior is shown in Fig. 2a and 2b.

With the exception of the strong-interaction region $|\gamma|$, $|\gamma'| < 1$, the orbital terms are quasiclassical and correspond in the region $\gamma < 0$, $|\gamma| \gg 1$ to quantization in two isolated wells or quantization in a single well in the region $\gamma > 0$, $|\gamma| \gg 1$. In particular, in the region of the hump of the potential (Fig. 2b), which determines the resonance-scattering widths, the first asymptotic relation in the region 1 can be reduced to the form

$$((\alpha^2+\beta^2+1)^2-4\beta^2)^{1/4}(E(k)-F(k)+(1+n)\Pi(n,k))=\pi(m+\tfrac{1}{2})/2Z, \tag{39}$$

where E, F, and Π are the complete elliptic integrals of the first, second, and third kind with modulus k and parameter n:

$$k^2=\frac{1}{2}\left[1-\frac{\alpha^2+\beta^2-1}{((\alpha^2+\beta^2+1)^2-4\beta^2)^{1/2}}\right],$$
$$n=\frac{1}{2}\left[\frac{\alpha^2+\beta^2+1}{((\alpha^2+\beta^2+1)^2-4\beta^2)^{1/2}}-1\right]. \tag{40}$$

An investigation of Eq. (40) shows that near $p = p_0$ its solution for $m \gg 1$ has the form

$$a_m=m^2-m_c^2, \quad m_c=\zeta E^{3/2}\tau, \tag{41}$$

where ζ varies slowly in the interval

$$1\geqslant\zeta\geqslant2\sqrt{2}/\pi$$

as m^2 varies from $m^2 \gg E^3\tau^2$ to values of m^2 satisfying the inequality $(m - 2\sqrt{2}\pi^{-1}E^{3/2}\tau) \ll E^{3/2}\tau$. In this case, in the region of sufficiently low momenta, the interaction

$e^{-2\pi\gamma}$ between the terms becomes appreciable, and the use of the adiabatic terms loses meaning.

3. INVESTIGATION OF THE RADIAL EQUATIONS DETERMINATION OF THE LEVEL WIDTHS

The radial equations (20) describe the motion in a system of coupled orbital terms $-\omega_m^2$. The highest degree of intermixing of the states is then attained in the region $e^{-2\pi\gamma} \sim 1$. In the region $\gamma < 0$, $|\gamma| \gg 1$ the motion occurs along nonadiabatic (intersecting) terms, the probability of transition between which is determined by the exponentially small matrix elements

$$M_1 = \left\langle M_m \frac{d}{dp} M_{m'} \right\rangle, \quad M_2 = \left\langle M_m \frac{d^2}{dp^2} M_{m'} \right\rangle,$$

responsible for transitions between the almost isolated wells shown in Fig. 1. In the region $\gamma > 0$, $\gamma \gg 1$ the system moves along adiabatic terms. In this case the matrix elements of the orbital functions are of order $M_1 \sim 1/p_0$, $M_2 \sim 1/p_0^2$, but the term spacing, even when $m \sim m_c$ and $(a_m - a_{m'})/p^2 \sim p_0\tau$, is considerably larger than M_1 and M_2. Thus, the motion from $p = 0$ along any term lying below the term $-\omega_{m_0}^2$ ($-\omega_0^2$ in Fig. 2a) and reaching into the region of maximum intermixing leads to the appearance, as $p \to \infty$, of the system in all the terms $-\omega_m^2 < -\omega_{m_0}^2$: the states with $-\omega_m^2 > -\omega_{m_0}^2$ intermix slightly. Therefore, in the following computations we shall limit ourselves only to the investigation of scattering with orbital numbers $m > m_0 = 2^{1/2}E^{3/2}\tau$ (which corresponds to $-\omega_m^2 > -\omega_{m_0}^2$), when the Eqs. (20) become uncoupled:

$$\left(\frac{d^2}{dp^2} + \omega_m^2 \mp i\left(\varepsilon_{0p}' + \frac{\varepsilon_0}{p}\right)\right)\begin{pmatrix}\Sigma_m \\ \Delta_m\end{pmatrix} = 0. \tag{42}$$

Then, on account of the condition $p_0\tau \ll 1$ (it implies a small width of the intermixing region), the maximum value of a_m in the region of the hump can be computed with the aid of the formulas (41), assuming that for not too large values of m the hump has a parabolic shape. The latter corresponds to "rectilinear" trajectories in a conical well, when the radial quantum number $n \gg m$ (see [1]). It is precisely this case that is investigated below.

The system (42) with allowance for (7) for the adiabatic terms $-\omega_m^2 > -\omega_{m_0}^2$ has at points far from the turning points (i.e., the zeros of ω_m^2) the following quasiclassical solutions:

$$\begin{aligned}\Sigma_m &= c_1 \cos g \exp\left\{i\int^p \omega_m\, dp\right\} + c_2 \sin g \exp\left\{-i\int^p \omega_m\, dp\right\},\\ \Delta_m &= -c_1 \sin g \exp\left\{i\int^p \omega_m\, dp\right\} + c_2 \cos g \exp\left\{-i\int^p \omega_m\, dp\right\},\end{aligned} \tag{43}$$

where c_1 and c_2 are constants and

$$g = \frac{1}{2}\operatorname{arctg} i \frac{a_m^{1/2}}{p|p^2/2 - E|}.$$

For $p \to 0$, $a_m \to (m + 1/2)^2$ we find, retaining only the regular terms (see [1]), that

$$\Sigma_m = c_0 p^{1/2}(J_{m-1/2}(Ep) - iJ_{m+1/2}(Ep)),$$
$$\Delta_m = -c_0 p^{1/2}(J_{m-1/2}(Ep) + iJ_{m+1/2}(Ep)).$$

In the region of the hump of the potential (Fig. 2a), the Eqs. (42) must be solved exactly. Such solutions are, under conditions when $n \gg m$, expressible in terms of the parabolic cylinder functions, and lead to the following formulas for the continuation of the solutions (43) from the region $p \to 0$ into the region $p \to \infty$:

$$\begin{aligned}c_1^+ &= \alpha(e^{-i\Omega} + (1 - e^{-2\pi\mu})^{1/2} e^{-i(\sigma-\Omega)}),\\ c_2^+ &= \alpha(e^{i\Omega} + (1 - e^{-2\pi\mu})^{1/2}(e^{i(\sigma-\Omega)}).\end{aligned} \tag{44}$$

Here α is an unimportant constant and Ω is the quasiclassical phase in the well of $-\omega_m^2$ (Fig. 2a):

$$\Omega = \int_{p_1}^{p_2} \omega_m(p)\, dp.$$

The principal Landau-Zener parameter μ has, in view of (41), the form

$$\mu = (m^2 - m_c^2)/2(2E)^{3/2}, \tag{45}$$

and σ, the additional phase advance in the transition region, the form

$$\sigma = \pi/4 + \mu \ln \mu - \mu + \arg\Gamma(1 - i\mu).$$

These results and the assumption that the motion (for $m > m_0$) is adiabatic in character enable us to find the scattering phase shifts, using the method of steepest descent to evaluate the p integral in the expression (15). For the asymptotic form of the partial amplitude at the conic peak in this case we obtain

$$\Phi_2(r, \varphi_0) \sim \frac{1}{\rho^{1/2}} M_m(p_0, \varphi) \cos\left(L(\rho) + \frac{\chi}{2}\right), \tag{46}$$

where $L(\rho)$ is the potential-scattering phase shift in the conical well without allowance for the nonadiabatic coupling:

$$L(\rho) = p_0\rho - \int_{p_2}^{p_0} \omega_m dp + \frac{m+1}{2}\pi,$$

and p_0 is the saddle point determined by the equation

$$\omega_m(p_0) = \rho.$$

The resonance phase shift $\chi/2$ has, in view of (44), the form

$$\frac{\chi}{2} = \frac{\sigma}{2} - \operatorname{arctg}\left[\frac{(1 - e^{-2\pi\mu})^{1/2} - 1}{(1 - e^{-2\pi\mu})^{1/2} + 1}\operatorname{tg}\left(\Omega - \frac{\sigma}{2}\right)\right]. \tag{47}$$

For the widths of the resonances E_n in this case, we obtain the expression

$$\frac{\Gamma}{2} = \left(\frac{d\Omega}{dE}\right)_{E_n}^{-1} [1 + (1 - e^{-2\pi\mu})^{1/2}]^{-2} e^{-2\pi\mu}. \tag{48}$$

The dominant exponential behavior is determined here by the formulas (45) and (41).

The main result, as can be seen, consists in the significant increase in the level widths in the elliptical conical well in comparison with the widths in a circular conical well. The width turns out to be comparable to the level spacing for all momenta $m < m_c$. This is a consequence of the fact that for $m < m_c$ there is no decay barrier (Fig. 2b). The exponential decrease of Γ begins only when $m > m_c$.

4. DISCUSSION OF THE RESULTS

The existence of a threshold momentum m_c for the resonance scattering has a classical origin and is connected with the fact that in the case of classical motion in an elliptical conical well the angular momentum is not an integral of the motion. The behavior of the angular momentum

$$M(t) = x\dot{y} - y\dot{x}$$

in time is described by the expression

$$M(t) = M(0) + (f_1^2 - f_2^2)\int_0^t \frac{xy}{(f_1^2x^2 + f_2^2y^2)^{1/2}} dt,$$

which simply follows from the equations of classical motion.

Taking the formula (5) for the case when $\tau < 1$ into account, we can write the last expression in the form

$$M(t)=M(0)+\tau\int_0^t r\sin 2\varphi_0 dt,$$

where the trajectory r(t) is computed for the circular cone. The amplitude of the oscillations in the angular-momentum value

$$\Delta M=\tau\int^t r dt$$

is easy to compute for trajectories that are almost rectilinear between the turning points (i.e., for $n \gg m$), when we can set $dt = dr/\sqrt{2(E-r)}$ and take as the limits of the integration over r the values 0 and E. In consequence, we have

$$\Delta M=\frac{2^{3/2}}{3}E^{3/2}\tau.$$

In the general case the trajectory of the classical motion in a circular cone is not closed; therefore, for $\Delta M > M(0)$ the system will at some moment of time certainly pass through the coordinate origin, where the vertices of the adiabatic terms adjoin. This will lead to a total transition from the well to the conic peak, which corresponds to level widths comparable to the level spacing. The classical value of ζ that follows from the formula for ΔM, $\zeta = 2^{3/2}/3$, falls in the interval $(1, 2\sqrt{2}\pi^{-1})$.

Thus, the primary effect of the scattering—the existence of the threshold angular momentum m_c—is due to the oscillations in time of the momentum, and cannot be obtained under the assumption that the trajectory is linear at any t. The existence of a threshold momentum depending on the collision energy leads to a sharp difference between the partial cross sections with small $m < m_c$ and large $m > m_c$ momenta, when the scattering becomes resonance scattering. The variation of the energy of the colliding particles then enables us, in principle, to find the ellipticity parameter τ of the terms.

An analysis of the corresponding trajectories shows that a threshold angular momentum exists also in scattering in a tilted conical well, and depends on the magnitude of its inclination to the vertical.

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57