Nonadiabatic transitions and spectra induced by atomic collisions in the weak coupling limit: Uniform formula for superbarrier and subbarrier transitions

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A formula is derived for the transition probability or shape of the electron or photon spectrum arising from the motion of atoms in potentials without bound states. The wave functions are asymptotic involving Bessel functions, and the interaction is exponential. The formula is a generalization of the various results for intersecting and parallel terms. The dynamics of the position of the transition region is considered, as well as the dependence of the probability and shape of the spectrum on the impact parameter. The Landau method for calculating integrals of rapidly oscillating functions is discussed.

1. INTRODUCTION.

The treatment of transitions in atoms and molecules with weak coupling between states, e.g., in collisions with large impact parameters, reduces to the calculation of the integral of the overlap between the wave functions $\Psi_{i,f}(r)$, which describe the radial motion in the quasimolecular potentials of the initial and the final states $\Psi_{i,f}(r)$, and the transition matrix element averaged over the electronic interaction $V(r)$ [Ref. 1]

$$J=C\int^{\infty}\Psi_i^{*}V\Psi_f r^2\,dr, \tag{1}$$

where C is a constant which is determined by the normalization of $\Psi_{i,f}$. If $\Psi_{i,f}$ are normalized to a δ-function of energy, then the probability of a nonadiabatic transition is given by $P_{i,f}=|J|^2$ for $C=2\pi$.

The problem of the spectra of electrons and photons formed in pairwise atomic collisions[2,3] also reduces to the evaluation of such integrals. This process can also be represented as a pairwise transition between terms $U_{i,f}$ where the term U_f is shifted by $\hbar\omega$ from the boundary of the continuous spectrum of the term $\tilde{U}_f$ (see Fig. 1). The spectral distribution over the energy of the free electrons or photons is given here by Eq. (1) with the substitution $CV=(2\pi\Gamma)^{1/2}$, where Γ is the auto-ionization or radiative width.

The numerous articles that have appeared that deal with the calculation of J can be separated into two groups depending on whether the terms intersect or not. In the first case it is assumed that the main contribution to the integral comes from the vicinity of the point of intersection of the terms or the Condon point (as it is called in spectral theory) r_c (see e.g., Ref. 3), which is determined by the condition

$$U_i(r_c)-\tilde{U}_f(r_c)=\hbar\omega \quad \text{or} \quad U_i(r_c)=U_f(r_c). \tag{2}$$

The matrix element is assumed to be constant and equal to $V(r_c)$. This case also includes, for example, the calculation of J to first order in the terms in the vicinity of r_c when the turning points for classical motion in the potentials $U_{i,f}$ are far from r_c. Such a calculation leads to a formula for the quasiustatic limit in the theory of line broadening (e.g., Ref. 3) or the well-known Landau formula in the theory of nonadiabatic transitions (Ref. 4, §90). The case which arises when the turning points are close to the point where the lines intersect was considered in Ref. 5 in the context of problems of collision theory, and the oscillatory structure of the spectrum, connected with the emission of particles when the atoms approach and divergence, was considered in Ref. 6, in which the terms were also linearly approximated in the semiclassical approximation, and in which damping was also taken into account. A uniform formula was proposed by Miller[7] for arbitrary repulsive potentials and positions of the Condon point and the turning points, and proven, for example, in Ref. 8.

In the case of parallel terms the calculation of J is linked with an account of the dependence of $V(r)$, which is carried out, as a rule, for model problems which permit the calculations of J in closed form. Of recent works we note Ref. 9, where the quantum motion of the atoms in linear parallel terms with exponential interaction is considered, and also Refs. 10 and 11, which describe the quantal motion of the atoms in the potentials $A_1\exp(-\alpha r)+\Delta\varepsilon$ and $A_2\exp(-\alpha r)$ and the exponential interaction on the basis of a closed expression for the overlap integral from Ref. 12. This preference for model problems is not accidental. The location of the transition region in the case of parallel or close-to-parallel terms is not so obvious. A general principle for estimating integrals involving oscillating wave functions was formulated in Ref. 4, §51; however, the conclusion reached here concerning the location of the transition region (the singular points $U_{i,f}$ and the roots of Eq. (2)) is criticized in Refs. 13 and 14 on the basis of specific examples of atomic and molecular collisions. Deviations from Eq. (2) can also be expected when $V(r)$ varies rapidly in the vicinity of the turning point. Such a situation is frequently encountered in the description of forbidden optical and electronic transitions and collisions at thermal energies.

In these papers the dependence of J on orbital angular momentum was not considered. Between them the question of the asymptotic behavior of the amplitude of the transition at large l always arises in the calculation of the cross sections or the absorption coefficients. It is commonly assumed that this dependence can be found using the modified-wave-function approximation.[15] However, it was long ago established [Ref. 1, §22; Refs. 16 and 17] that this approximation does not permit a valid description of the behavior of the probability of the transition and, consequently, not of the modification of the line shape at large l, either.

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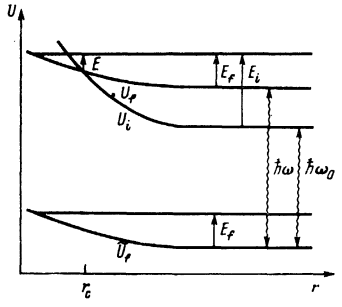

FIG. 1. Transition for motion of atoms in potentials $U_{i,f}$ or emission of an electron or a photon with energy $\hbar\omega$ for motion in the potential U_i. The boundary of the continuous spectrum is determined by the term $\tilde{U}_f$; $E_{i,f}$ are the kinetic energies of the atoms at infinity, E is the kinetic energy at the point $r = r_c$, determined by condition (2). The center of the line corresponds to the energy $\hbar\omega_0 = U_i - \tilde{U}_f$ at large r.

In the present article an expression is obtained for the integral (1) under quite general conditions with regard to $\Psi_{i,f}$ and V and without the usual reduction to the problem on the entire axis. this expression encompasses various formulas for J in the case of intersecting and parallel terms and enables one to find a connection between the Landau–Ziner and Demkov models of nonadiabatic transitions (this question was considered in the semiclassical formulation in Refs. 18 and 19), to refine the formulation of the Landau method for calculating the integrals of rapidly oscillating functions, and to determine how J depends on the orbital angular momentum.

We note that the question of a uniform formula for J was apparently first posed by Child,[20] but the formula which he obtained is in fact valid only in a certain parameter region, which can be qualitatively described as the superbarrier transition for slow variation of $V(r)$ (for a more detailed discussion of this point, see Section 2).

2. SUPERBARRIER TRANSITIONS

We will evaluate the integral (1), setting $V = V_0 \exp(-\alpha r)$, where V_0 is slowly varying in comparison with the exponential function, which, for example, takes into account the incomplete overlap of the continua as a result of the rotation of the internuclear axis.[21,22] The function $\chi_i = r\Psi_i$ satisfies the equation

$$\frac{d^2\chi_i}{dr^2} + k_i^2\chi_i = 0, \quad k_i^2 = \frac{2\mu}{\hbar^2}(E_i - U_i) - \frac{l_i(l_i+1)}{r^2}, \tag{3}$$

with the boundary condition $\chi_i(r=0) = 0$; E_i is the total energy of the colliding atoms with reduced mass μ and angular momentum l_i. In Eq. (3) and below, $E_{i,f}$ and $U_{i,f} \to 0$ as $r \to 0$, and Eq. (2) takes the form

$$U_i(r_c) - U_f(r_c) = E_i - E_f = \hbar(\omega - \omega_0).$$

The potentials $U_{i,f}$ have no bound states, so that the following can serve as a reference equation for Eq. (3)

$$\frac{d^2Y_i}{dx^2} + \tilde{k}_i^2 Y_i = 0, \quad \tilde{k}_i^2 = k_{0i}^2 - \frac{l_i(l_i+1)}{x^2}, \quad k_{0i}^2 = \frac{2\mu}{\hbar^2}E_i, \tag{4}$$

whose solution, normalized to a δ-function in energy, is given by

$$Y_i = \frac{(\mu x)^{1/2}}{\hbar} J_{l_i+1/2}(k_{0i}x), \tag{5}$$

where $J_{l_i+1/2}$ is the Bessel function.[24]

The first term of the asymptotic expansion of χ_i is

$$\chi_i(r) = \left(\frac{dx_i}{dr}\right)^{-1/2} Y_i(x_i), \tag{6}$$

if the function $x_i(r)$ satisfies the condition

$$\int_{\tilde{x}_i}^{x_i} \tilde{k}_i\, dx = \int_{r_i}^{r} k_i\, dr, \quad \tilde{k}_i(\tilde{x}_i) = k_i(r_i) = 0. \tag{7}$$

Using the reference equation (4) with the solution (5) is advantageous with the usual approximation by the Airy function because its solution (5) takes into account not only the variation of the nature of the solution at the turning point r_i, but also the singularity of k_i at $r = 0$. Therefore, Eq. (6) is valid in the asymptotic sense for any value of r or l.

Relations analogous to Eqs. (3)–(7) can also be written out for Ψ_f, so that the integral (1) takes the form

$$J = \frac{\mu C}{\hbar^2}\int_0^\infty \left(x_i x_f \frac{\tilde{k}_i\tilde{k}_f}{k_i k_f}\right)^{1/2} V(r) J_{l_i+1/2}(k_{0i}x_i) J_{l_f+1/2}(k_{0f}x_f)\, dr \tag{8}$$

which, after the use of well-integral transformations for the Bessel function [Ref. 24, p. 543], transforms to

$$J = \frac{\mu C}{(2\pi\hbar)^2}\int_0^\infty dr \int_{L_\theta} d\theta \int_{L_\varphi} d\varphi \left(x_i x_f \frac{\tilde{k}_i\tilde{k}_f}{k_i k_f}\right)^{1/2} V_0 e^{i\psi}, \tag{9}$$

where

$$\psi = i\alpha r - k_{0i}x_i \sin\theta + (l_i + 1/2)\theta - k_{0f}x_f \sin\varphi + (l_f + 1/2)\varphi,$$

and $L_{\theta,\varphi}$ are contours in the θ and φ complex planes.

To evaluate the integral (9), we make use of the technique of the multidimensional method of steepest descent (saddle-point method) [Ref. 25, p. 341]. The coordinates of the saddle points are found by solving the system of equations

$$\begin{aligned} \frac{\partial\psi}{\partial r} &= i\alpha - k_{0i}\sin\theta\frac{dx_i}{dr} - k_{0f}\sin\varphi\frac{dx_f}{dr} = 0, \\ \frac{\partial\psi}{\partial\theta} &= -x_i k_{0i}\cos\theta + (l_i + 1/2) = 0, \\ \frac{\partial\psi}{\partial\varphi} &= -x_f k_{0f}\cos\varphi + (l_f + 1/2) = 0. \end{aligned} \tag{10}$$

The saddle points naturally fall into two groups. We first assume that $z = (l + 1/2)/k_0 x \leqslant 1$. Then the wavenumbers $\tilde{k}$ in reference equation (4) are real. In this case, which we will refer to below as the superbarrier case and denote by the subscript I, the coordinates of the saddle points along the θ and φ axes are real and for one group of roots are equal to

$$\theta_+ = \arccos z_i, \quad \varphi_+ = -\arccos z_f. \tag{11}$$

The coordinates of the saddle points along the r axis for this group of roots are determined by the equation

$$i\alpha = k_i - k_f. \tag{12}$$

For the second group

$$\theta_-=-\arccos z_i,\ \varphi_-=\arccos z_f, \tag{13}$$

and the coordinates along the r axis are determined by the equation

$$-i\alpha=k_i-k_f. \tag{14}$$

We remark that the simple equations (12) and (14) are obtained only by using the well-known Langer substitution $l(l+1)\to(l+1/2)^2$ in Eq. (7), which is assumed below.

In the case of intersecting terms and $z\leqslant 1$ there exists at least one root r_+ of Eq. (12) and one root r_- of Eq. (14), which is complex conjugate to r_+. Assuming that the contribution of the second root is negligibly small, it is possible to evaluate the integral (9) by a formula from Ref. 25 (p. 355), which is symmetric in the locations of the saddle points and which, with the corresponding changes in notation, has the form

$$\int_\gamma f(y)e^{i\Psi}\,dy=\left\{F^+\left[B^{1/4}\Phi(-B)+\frac{i}{B^{1/4}}\Phi'(-B)\right]\right.$$
$$\left.+F^-\left[B^{1/4}\Phi(-B)-\frac{i}{B^{1/4}}\Phi'(-B)\right]\right\}e^{iA}, \tag{15}$$

where $y=(y_1,\ldots,y_n)$, γ is an n-dimension manifold.

$$2A=\psi(y_+)+\psi(y_-),\ {}^4/_3B^{3/2}=\psi(y_+)-\psi(y_-), \tag{16}$$

$$F^+=\frac{(2\pi i)^{n/2}f(y_+)}{[-i\det\psi''(y_+)]^{1/2}},\qquad F^-=\frac{(2\pi i)^{n/2}f(y_-)}{[i\det\psi''(y_-)]^{1/2}}, \tag{17}$$

Φ and Φ' are the Airy–Fock function and its derivative,[4] and $\det\psi''$ is the Hessian.

We will make use of Eq. (15) to evaluate the integral (9) in the superbarrier case. Taking into account that

$$\det\psi''(y_\pm)=\pm x_ix_f\tilde{k}_i\tilde{k}_f(k_i'-k_f'),$$

we obtain an expression for the integral (9) in region I in the form (15), where

$$F^\pm=F_I^\pm=\frac{\mu C}{\hbar^2(2\pi)^{1/2}}\frac{V_0(r_\pm)}{[k_ik_f(k_i'-k_f')|_{r_\pm}]^{1/2}}. \tag{18}$$

The quantities A and B with the help of Eq. (7) can be expressed in terms of the values of the action

$$S_{i,f}(r_\pm)=\int_{r_{t,f}}^{r_\pm}k_{i,f}\,dr,$$

$$2A_I=i\alpha(r_++r_-)+S_i(r_-)-S_i(r_+)-S_f(r_-)+S_f(r_+), \tag{19}$$

$${}^4/_3B_I^{3/2}=i\alpha(r_+-r_-)+S_f(r_+)+S_f(r_-)-S_i(r_+)-S_i(r_-).$$

On the basis of the assumptions which we have made about $z_{i,f}$ it follows that $|\arg B|<\pi$, so that Eq. (15) describes the interference structure which is associated with the uniform contribution of both saddle points, as should also be the case for the superbarrier transitions.

In reduced form expressions (15), (18), and (19) coincide (to within the assumptions regarding the quantity α) with those obtained by Child[20] by another method. However, the formula obtained by Child is inadequate not only in the fact that its derivation is based on an approximation of the wave functions by Airy functions and therefore does not contain centrifugal terms; these formulas and those obtained above are uniform in the distance between the saddle points only in the region of superbarrier transitions and do not allow one to directly consider subbarrier transitions, which correspond to imaginary wavenumbers for real r. In order to carry out an analytic continuation of expressions (18) and (19) into the region of subbarrier transitions, we consider the dynamics of the saddle points as functions of the parameters. This problem is of independent interest since it allows us to answer the question of the breakdown of the Franck–Condon principle, which is connected with taking the interaction into account.

3. LOCATION OF THE SADDLE POINTS: SUBBARRIER TRANSITIONS

For $z_{i,f}>1$ the wavenumbers in Eq. (4) are imaginary, which, thanks to relation (7), corresponds to imaginary values of $k_{i,f}$ for real r. Below we will call such transitions subbarrier transitions. The saddle points for such transitions, as before, fall into two groups, but the θ and φ coordinates of the points are now imaginary, and the equations which describe the positions of the saddle points along the r axis have the form

$$\pm\alpha=\varkappa_i-\varkappa_f,\ \alpha=\varkappa_i+\varkappa_f,\ \varkappa_{i,f}=|k_{i,f}|. \tag{20}$$

The roots both of Eqs. (20) and of Eqs. (12) and (14) lie among the roots of the equation

$$1+M=4\frac{U_m}{\alpha^2}-\Lambda^2\left(\frac{\Delta U}{2k_m\Delta k}-1\right)^2, \tag{21}$$

in which

$$U_m=(U_i+U_f)/2,\qquad \Delta U=U_i-U_f,$$

$$U_{i,f}=\frac{2\mu}{\hbar^2}U_{i,f}+\frac{(l_{i,f}+{}^1/_2)^2}{r^2}$$

and the dimensionless parameters Λ and M have the values

$$\Lambda=2k_m\Delta k/\alpha^2,\ M=(4/\alpha^2)(k_m^2+\Delta k^2/4),$$

where $k_m=(k_{0i}+k_{0f})/2$ and $\Delta k=k_{0i}-k_{0f}$ are controlled by external conditions.

Let us discuss the nature of the solutions of Eq. (21) qualitatively. For $\Delta U>2k_m\Delta k$ the terms intersect for real $r=r_c>r_m=(r_i+r_f)/2$ and there exists a pair of complex conjugate roots which satisfies Eqs. (12) and (14). Formulas (18) and (19) correspond to this case. In the opposite case $\Delta U\ll 2k_m\Delta k$, i.e., for terms which are close to parallel, we distinguish three limiting situations. For such small collision energies, when $M<1$ and $\Lambda^2<1$, Eq. (21) reduces to $U_m=k_m^2/M$, whose root $r_c\ll r_m$. With increasing collision energy, in the far wings of the lines, when $\Delta k/\alpha>1$, i.e., for $\Lambda^2>M$ and $\Lambda^2>1$ Eq. (21) reduces to $U_m=(k_m\Delta k/\alpha)^2$, wherefore its root $r_0<r_m$. Finally, in the vicinity of the center of the line $\Delta k/\alpha<1$, when $M>1$ and $\Lambda^2>1$, Eq. (21) reduces to $U_m=k_m^2$, so that the root satisfies $r_0\lesssim r_m$. For orientation we point out that for collisions with energy $\sim 10^{-2}$ eV and radiation with $\lambda\sim 5000$ Å, $k/\alpha\sim 10$ and $\Delta k/\alpha\sim 1$ for a wing with $\Delta\lambda\sim 5$ Å.

The foregoing qualitative consideration gives an idea of the locations of the roots in the limiting cases; however, for analytic continuation more detailed information on the be-

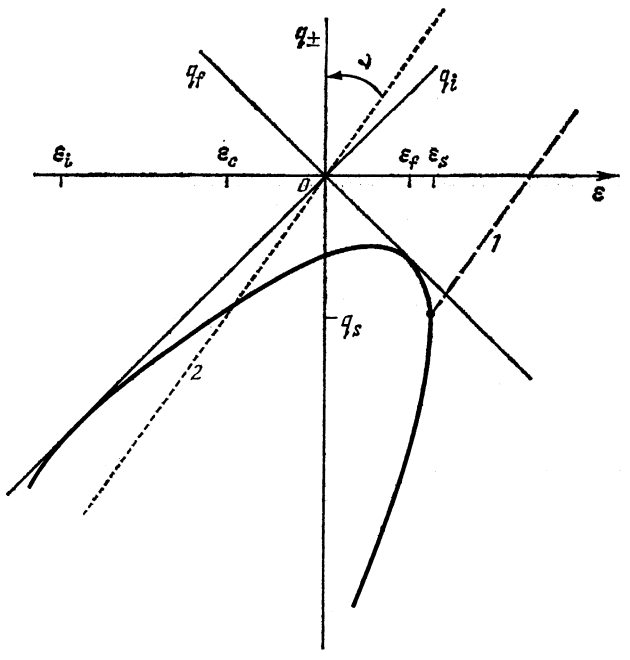

FIG. 2. Qualitative graph of the dependence of the radial coordinates of the saddle points $q_\pm = (r_\pm - r_m)\bar{b}/2\alpha^2$ on the energy ε for linear approximation of the terms. The solid curve is $q_\pm(\varepsilon)$, Eq. (24), the indicated point on which is the point of coalescence of the roots; the dashed line (1) is $\mathrm{Re}\, q_\pm(\varepsilon)$, and dashed line (2) is the locus of points of intersection of the terms $q_c = \varepsilon(1+\delta^2)^{1/2}$; the thin straight lines gives the coordinates of the turning points $q_{i,f} = \pm\delta\varepsilon$, the other notations are defined in the text.

havior of the roots in the vicinity of $r \approx r_m \approx r_c$ is necessary. Toward this end we approximate the potentials by linear functions. Then

$$k_{i,f} = [b_{i,f}(r - r_{i,f})]^{1/2},$$
$$b = \frac{2\mu}{\hbar^2}F = -\frac{2\mu}{\hbar^2}\frac{dU}{dr} + \frac{2(l+1/2)^2}{r^3}\Big|_{r=r_m} \qquad (22)$$

In this case Eq. (22) has two roots $r_\pm$, whose positions depend on the two dimensionless model parameters

$$\delta = \Delta b/2\bar{b},\ \varepsilon = (\mu/\alpha^2\hbar^2)E = \Delta r\Delta b/8\alpha^2\delta^2, \qquad (23)$$

where $\Delta b = b_i - b_f \geqslant 0$, $\bar{b} = (b_i b_f)^{1/2}$, $E = E_{i,f} - U_{i,f}(r_c)$, $\Delta r = r_i - r_f > 0$ for $E > 0$ (see Fig. 1). The dependence of the dimensionless distances $q_\pm = (r_\pm - r_m)\bar{b}/2\alpha^2$ on the parameters δ and ε has the form

$$q_\pm = \varepsilon(1+\delta^2)^{1/2} - (1+\delta^2)^{1/2}/4\delta^2 \pm (1 - 8\varepsilon\delta^2)^{1/2}/4\delta^2. \qquad (24)$$

Here the subscript "$\pm$" has the following meaning: $q_+ > q_-$ or $\mathrm{Im}\, q_+ > 0$.

For fixed δ, i.e., prescribed forces, and real $r_\pm$ Eq. (24) corresponds to a parabola, which reduces to canonical through a rotation of the q and ε axes by an angle ν such that $\mathrm{tg}\ \nu = -(1+\delta^2)^{-1/2}$. The dependence $q(\varepsilon)$ is shown qualitatively in Fig. 2. The position of the intersection point of the terms $q_c = r_c\bar{b}/2\alpha^2 = \varepsilon(1+\delta^2)^{1/2}$ for $\alpha \neq 0$ coincides with q_+ only at the point $\varepsilon_c = -1/8$, i.e., for an r-dependent interaction the Franck–Condon principle is not satisfied. The interaction shifts the transition region from r_c to r_m independent of whether the transition[1)] is superbarrier in the usual sense ($\varepsilon > 0$) or subbarrier ($\varepsilon < 0$). This shift is most important for those terms which are close to parallel, $\delta \ll 1$. In this limit $r_+ - r_m = -\alpha^2/4\bar{b}$ for $\varepsilon = 0$.

If in Fig. 2 we draw the straight lines $q_{i,f} = \pm\varepsilon\delta$, which give the position of the turning point as a function of energy, then we can isolate the three points whose coordinates along the ε axis are ε_s, ε_f, and ε_i. At the point $\varepsilon_s = 1/8\delta^2$, $q_s = -(1+\delta^2)^{1/2}/8\delta^2$, where the tangent to the curve is vertical, there is a double root $r_+ = r_-$, and $\theta = \varphi = 0$. At the point $\varepsilon_f = [(1+\delta^2)^{1/2} - \delta]/4\delta$, the larger of the two roots r_+ equals r_f, and at the point $\varepsilon_i = [(1+\delta^2)^{1/2} + \delta]/4\delta$, r_+ equals r_i.

Figure 3 allows one to trace out the dynamics of the roots $r_\pm$ as functions of the parameter α for fixed values of the distance between the turning points $\Delta r = r_i - r_f$ and the difference of the slopes of the terms Δb. As α varies from zero to $\alpha = (\Delta r\Delta b)^{1/2}$, which corresponds to ε varying over the interval $\varepsilon_s < \varepsilon < \infty$, the roots describe an ellipse in the r plane with axes $\Delta r/\delta$ and $\Delta r(1+\delta^2)^{1/2}/\delta$.

The values $\varepsilon > \varepsilon_s$ correspond to superbarrier transitions, i.e., region I. As should be the case in this region, Eq. (24) determines for such ε two complex conjugate roots, where the one with imaginary part greater than zero (r_+) satisfies Eq. (12), and the one with imaginary part less than zero (r_-) satisfies Eq. (14). For $\varepsilon < \varepsilon_s$ the transitions have a subbarrier character $z_{i,f} > 1$, but are described by different formulas. We will first isolate region II, in which $\varepsilon_f < \varepsilon < \varepsilon_s$, which corresponds in the r plane to motion of the root r_+ from r_s to r_f (see Fig. 3a). In this region both r_+ and r_- satisfy the equation

$$\alpha = \varkappa_i - \varkappa_f, \qquad (25)$$

and

$$\theta_\pm = i\ln\{z_i(r_\pm) + [z_i^2(r_\pm) - 1]^{1/2}\},$$
$$\varphi_\pm = -i\ln\{z_f(r_\pm) + [z_f^2(r_\pm) - 1]^{1/2}\}. \qquad (26)$$

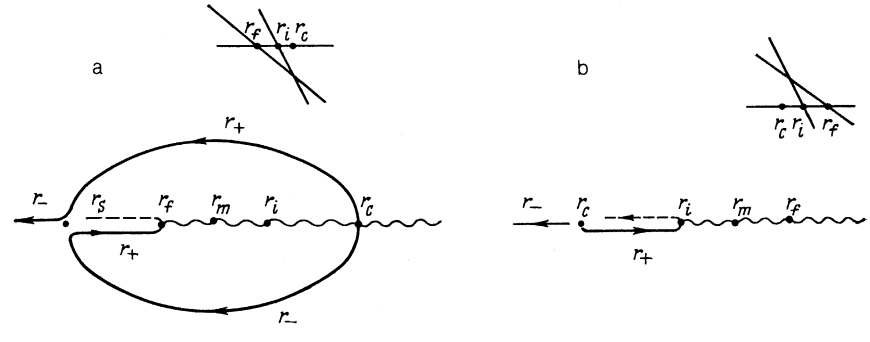

FIG. 3. Location of the saddle points in the r plane as a function of the parameter α for $\varepsilon > 0$ (a) and $\varepsilon < 0$ (b), see text. The solid lines are the location of $r_\pm$, the dashed lines are the location of r_+ on the second sheet, the wavy lines are the branch cuts from the points $r_{i,f}$.

Carrying out the same calculations as in the derivation of formulas (18) and (19), we find that in region II

$$J_{II}=\{F_{II}^{+}[(-B_{II})^{1/4}\Phi(-B_{II})-(-B_{II})^{-1/4}\Phi'(-B_{II})]$$
$$+F_{II}^{-}[(-B_{II})^{1/4}\Phi(-B_{II})+(-B_{II})^{-1/4}\Phi'(-B_{II})]\}e^{iA_{II}}, \tag{27}$$

where

$$F_{II}^{\pm}=\frac{\mu C}{\hbar^2(2\pi)^{1/2}}\frac{V_0(r_\pm)}{[\varkappa_i\varkappa_f(\pm\varkappa_i'\mp\varkappa_f')|_{r_\pm}]^{1/2}},$$
$$-2iA_{II}=\alpha(r_+-r_-)-\sigma_i(r_+)-\sigma_i(r_-)+\sigma_f(r_+)+\sigma_f(r_-), \tag{28}$$
$$^4/_3(-B_{II})^{3/2}=\alpha(r_+-r_-)-\sigma_i(r_+)+\sigma_i(r_-)+\sigma_f(r_+)-\sigma_f(r_-)\geqslant 0,$$
$$\sigma_{i,f}(r_\pm)=\int_{r_{i,f}}^{r_\pm}\varkappa_{i,f}\,dr\leqslant 0.$$

Use of the linear approximation (22) allows us to find a single formula not only for regions I and II, but also for the two other cases considered above. In fact, making a branch cut from the point ε_s into the lower half-plane, we obtain the following rules for passage between regions I and II:

$$r_\pm(\mathrm{I})\leftrightarrow r_\mp(\mathrm{II}), \tag{29}$$

$$k_{i,f}(r_+)\leftrightarrow\exp(i\pi/2)\varkappa_{i,f}(r_-),\ k_{i,f}(r_-)\leftrightarrow\exp(3i\pi/2)\varkappa_{i,f}(r_+),$$
$$S_{i,f}(r_+)\leftrightarrow\exp(i\pi/2)\sigma_{i,f}(r_-),\ S_{i,f}(r_-)\leftrightarrow\exp(3i\pi/2)\sigma_{i,f}(r_+),$$
$$F_I^{\pm}\leftrightarrow F_{II}^{\mp}\exp(-i\pi/4). \tag{30}$$

Rules (30) correspond to $\arg k_{i,f}(r_+)=0$ on the upper lips of the branch cuts along the real r axis and to $\arg k_{i,f}(r_-)=2\pi$ along the lower lips of the cuts (see Fig. 3). After establishing relation (29) and choosing the branches of the function $k_{i,f}(r)$, we can assume that formula (15) or (17) uniquely describes both the superbarrier and the subbarrier transitions.

For further decrease of ε, when $\varepsilon_i<\varepsilon<\varepsilon_f$, the roots $r_\pm$ lie in Region III, in which r_+ satisfies the equation

$$\alpha=\varkappa_i+\varkappa_f,$$
$$\theta_+=i\ln[z_i+(z_i^2-1)^{1/2}],\ \varphi_+=i\ln[z_f+(z_f^2-1)^{1/2}]. \tag{31}$$

In the r plane passage from region II to region III is accomplished by making a detour around the point r_f and passing over to the second sheet (see Fig. 3a), in which $\varkappa_f(r_+)\to\exp(i\pi)\varkappa_f(r_+)$. The coordinates of the second saddle point r_-, θ_-, φ_- are determined from the corresponding equations (25) and (26). The quantity J_{III} is given here by formula (27), in which one should set

$$F_{III}^{+}=\frac{\mu C}{\hbar^2(2\pi)^{1/2}}\frac{V_0(r_+)}{[-\varkappa_i\varkappa_f(\varkappa_i'+\varkappa_f')|_{r_+}]^{1/2}},\quad F_{III}^{-}=F_{II}^{-},$$
$$-2iA_{III}=\alpha(r_+-r_-)-\sigma_i(r_+)-\sigma_i(r_-)-\sigma_f(r_+)+\sigma_f(r_-),$$
$$^4/_3(-B_{III})^{3/2}=\alpha(r_+-r_-)-\sigma_i(r_+)+\sigma_i(r_-)-\sigma_f(r_+)-\sigma_f(r_-). \tag{32}$$

The situation is analogous in region IV, where $\varepsilon<\varepsilon_i$, only here passage to the second sheet is accomplished by making a detour already around the point r_i (see Fig. 3b), in which $\varkappa_i(r_+)\to\exp(i\pi)\varkappa_i(r_+)$. Therefore, in this region the coordinates of one of the saddle points are determined by the equations

$$\alpha=\varkappa_f-\varkappa_i,$$
$$\theta_+=-i\ln[z_i+(z_i^2-1)^{1/2}],\ \varphi_+=i\ln[z_f+(z_f^2-1)^{1/2}], \tag{33}$$

and the coordinates of the second point, as before, are given by Eqs. (25) and (26) with the subscript $\langle\langle\text{“}-\text{”}\rangle\rangle$. The expression for J_{IV} has form (27), in which one should set

$$F_{IV}^{\pm}=\frac{\mu C}{\hbar^2(2\pi)^{1/2}}\frac{V_0(r_+)}{[\varkappa_i\varkappa_f(\varkappa_f'-\varkappa_i')|_{r_+}]^{1/2}},$$
$$-2iA_{IV}=\alpha(r_+-r_-)+\sigma_i(r_+)-\sigma_i(r_-)+\sigma_f(r_+)+\sigma_f(r_-), \tag{34}$$
$$^4/_3(-B_{IV})^{3/2}=\alpha(r_+-r_-)+\sigma_i(r_+)+\sigma_i(r_-)-\sigma_f(r_+)-\sigma_f(r_-).$$

A distinguishing feature of the transitions in regions II and III in comparison with region IV consists in the fact that the transitions here for $r_c>r_m$ have a subbarrier character, even though $\varepsilon>0$. The boundary between the sub- and the superbarrier transitions is located at the point where the roots ε_s coalescence, and for $\delta\sim 0.1$ we have $\varepsilon_s\sim 10$, i.e., E is of the order of the thermal energy.

The above use of the linear approximation has an auxiliary character and allows us to determine the signs in front of $\varkappa_{i,f}$ in the equations for the roots (25), (31), and (33), and also in front of $\sigma_{i,f}$ in the expressions for A and $(-B)^{3/2}$. Therefore, the formulas which have been given for J, even though they were obtained with the help of the linear approximation, are still valid for arbitrary potentials which allow the isolation of a single root in Eqs. (12) and (14), or their analytic continuations.

4. LIMITING CASES: EXTREMUM IN THE DIFFERENCE OF TERMS

If we assume, as is customary, for example, in the usual version of the Landau–Ziner model [Ref. 4, §90], that the interaction is constant, but that the terms intersect at $r=r_c$, then regions II and III draw together at the point $\varepsilon=0$, which is now the boundary between the sub- and superbarrier transitions. The radial coordinate of the saddle points is determined either by the equation $k_i-k_f=0$ or the equation $\varkappa_f-\varkappa_i=0$, which $r_\pm=r_c$ satisfies, wherefore we obtain from Eq. (19) or Eq. (34) that

$$J=\frac{\mu C}{\hbar^2(2\pi)^{1/2}}\frac{(-B)^{1/4}}{[\varkappa_i\varkappa_f(\varkappa_f'-\varkappa_i')|_{r_c}]^{1/2}}\Phi(-B), \tag{35}$$

where

$$\frac{2}{3}(-B)^{3/2}=\int_{r_c}^{r_f}\varkappa_f\,dr-\int_{r_c}^{r_i}\varkappa_i\,dr,$$

which coincides with Miller's formula.[7]

A simple formula which does not contain terms with derivatives of the Airy function was also obtained in the problem with linear terms and exponential interaction.[26] but with $V_0=\text{const}$. In this case the overlap integral

$$J=\frac{\beta^{4/3}C}{2\pi^{1/2}}\Phi[-(\varepsilon\beta^{2/3}-a)]\exp\left[\frac{2}{3}(1+\delta^2)^{1/2}a^{3/2}\right] \quad (36)$$

is expressed in terms of the dimensionless parameters

$$\beta^{2/3}=4\mu V(r_c)/\hbar^2(\delta\Delta b)^{1/2},\ \varepsilon=E\delta/V(r_c),$$

which were introduced in Ref. 5 in the treatment of the problem with linear terms and constant interaction, and the parameter a is equal to $(\alpha^3/2\delta\Delta b)^{2/3}$, which is connected with the rate of variation of the interaction.

In this same approximation of linear terms it is also possible to write out the amplitude of the transition in terms of the semiclassical approximation[6]

$$J_{sc}=\frac{1}{i\hbar}\int_{-\infty}^{\infty}V(t)\exp\left(-\frac{i}{\hbar}\int^{t}(U_i-U_f)\,dt'\right)dt. \quad (37)$$

The result which obtains upon prescribing the trajectories in the form

$$r=F_m t^2/2\mu+r_m,\ F_m=(F_i+F_f)/2,$$

coincides with expression (36) for $\delta\ll 1$, i.e., the semiclassical approximation which takes account of the exponential interaction has been validated for terms which almost coincide in the vicinities of the turning points.

Comparison with the semiclassical formula shows that the two saddle points of which we were speaking in Secs. 2 and 3 correspond to the approach and divergence of the particles. This observation enables us to take account of the influence of the rotation of the internuclear axis on the spectrum even in the case of arbitrary terms. Such a problem arises in the investigation of x-ray spectra formed in the collision of ions with atoms. For example, in Ref. 27 it was found that the oscillatory structure of the spectrum in the region around 10 keV in Cl^{16+}–Ar collisions with energies in the range 2–5 meV is connected with the transitions in the vicinity of the turning point and therefore to lowest order is described by a formula of type (35). However, photons of identical energy but emitted at different orientations of the molecular axis with respect to the laboratory frame interfere incompletely. This circumstance is connected with the degeneracy of the states of the continuum and can be described in general form with the help of the overlap integral.[21] If we examine the spectrum averaged over the direction of emission of the photons by the method of coincidences with a ring detector to record scattered particles, which in theory corresponds to averaging over the angle of rotation of the collision plane about the axis of the incident beam, then the comparatively weak dependence of rotation of the axis on r can be included in V_0, after which

$$F^{\pm}=\frac{\mu}{\hbar^2}\left(\frac{4\omega^3}{3c^2k_ik_f(k_i'-k_f')|_{r_\pm}}\right)^{1/2}d\mathbf{n}^{\pm}, \quad (38)$$

where the dipole matrix element is $d=\langle i|e\mathbf{R}\mathbf{n}|f\rangle$, $\mathbf{n}$ is unit vector aligned with the internuclear axis, and c is the velocity of light. Since for dipole transitions the magnitude of the angular momentum depends weakly on r, in Eqs. (12)–(19) one can take $\alpha=0$, so $r_+=r_-=r_c$. Finally, the probability of emission of a photon for fixed impact parameter has the form

$$\frac{dP}{d\omega}=\frac{16\omega^3}{3c^3}\frac{d^2}{v(F_i-F_f)}\times\left[B^{1/2}\Phi^2(-B)\cos^2\tau+\frac{1}{B^{1/2}}\Phi'^2(-B)\sin^2\tau\right], \quad (39)$$

where all quantities, including the radial velocity v and the rotation angle of the internuclear axis measured from the direction of closest approach τ, are given for $r=r_c$. After we go over to the semiclassical approximation for the phases B, Eq. (39) coincides with that obtained in Ref. 28. According to Eq. (39), the complex angle τ formally coincides with the subbarrier transitions $r_c<r_m$. The exponential growth of the overlap integral of the continua in the subbarrier region was noted in Ref. 22 for the electronic spectra.

Equation (15) is also useful in describing the case of an extremum in the difference function $\Delta U=U_i-U_f$. Such a problem arises in nonlinear optics[29] and in the spectroscopy of line wings.[3] In the calculation of spectrum (1) based of the multidimensional approach, the case of an extremum has associated with it the necessity of allowing for four saddle points. Two of them have identical coordinates θ_+, φ_+, and the coordinates $r_{I,II}$ along the r axis are determined by Eq. (12) ($\mathrm{Re}\,r_I>\mathrm{Re}\,r_{II}$), while the other pair r_{III}, r_{IV} are determined by Eq. (14), and θ_- and φ_- are determined by Eq. (13) ($r_{I,II}=r_{III,IV}$). If the coordinates θ_+, φ_+ and θ_-, φ_- are not too close, then by connecting pairs of points with identical θ and φ it is possible to represent the integral (9) as a sum of contributions of each pair $J=J_1+J_2$. Each of the terms $J_{1,2}$ is given by Eq. (15), where for J_1 we have

$$F^{\pm}=\frac{\mu C}{\hbar^2(2\pi)^{1/2}}\frac{V_0(r_{I,II})}{[\pm k_ik_f(k_f'-k_i')|_{r_{I,II}}]^{1/2}},$$

$$2A_1=i\alpha(r_I+r_{II})+S_i(r_I)+S_i(r_{II})-S_f(r_I)-S_f(r_{II}), \quad (40)$$

$$^4/_3B_1^{3/2}=i\alpha(r_I-r_{II})+S_i(r_I)-S_i(r_{II})-S_f(r_I)+S_f(r_{II}).$$

For J_2 the expressions for $F^{\pm}$, A_2, and $B_2^{3/2}$ follow from Eqs. (40) by making the substitutions I → III and II → IV and replacing i by $-i$ in the expression for $B_1^{3/2}$.

For a slowly varying interaction α equals 0, whence the plane in which the four saddle points lie is perpendicular to the $\theta\varphi$ plane. If we further assume $(r_I-r_{II})/r_I\ll 1$, then Eq. (40) simplifies, and we find that

$$J=\frac{2\mu C}{\hbar^2(2\pi)^{1/2}}\left\{\frac{V_0(r_I)}{[k_ik_f(k_f'-k_i')|_{r_I}]^{1/2}}+\frac{V_0(r_{II})}{[k_ik_f(k_i'-k_f')|_{r_{II}}]^{1/2}}\right\}\cos A_1\Phi(-B_1), \quad (41)$$

where it is assumed that $\Delta U<0$ for $r_{II}<r<r_I$. Equation (41) clearly shows that the resulting spectrum in the approximation under consideration is a consequence of two interfering effects. One is connected with the presence of an extremum in the difference function and is described by the factor $\Phi(-B_1)$, and the other arises as a result of the approach and divergence of the particles. The presence of two vibrational modes has been established by experiment in the case of the electronic structure of the quasimolecule

$He(2^3S)$–$He(2^3S)$ at a collision energy of 1.6 meV.[30] Preliminary estimates show that one mode and the main maximum at 14.4 eV are connected with the extremum in the difference of terms $^2\Sigma_g^+ - 1^3\Sigma_u^+$ [the factor $\Phi(-B_1)$ in Eq. (41)], whereas the factor $\cos A_1$ leads to additional minima with a period of 0.13 eV in the vicinity of the main maximum.

In the approximation of the difference of terms by a parabola. Eq. (41) leads to the corresponding equation from Refs. 29 and 31. If the difference in the trajectories is insubstantial ($|\Delta U|/E \ll 1$) and the region of the extremum is far from the turning points, then expression (41) for J, taking into account the noted simplifications, reduces to the uniform equation for the spectrum (5.14) from Ref. 3.

5. THE LANDAU METHOD

The results of Sec. 3 show that a uniform formula whose applicability does not depend on the distance between the saddle points is needed in point of fact only where these points coalesce, i.e., on the boundary between regions I and II. In other regions the saddle points are disposed either by their θ and φ coordinates (as in region I for $\varepsilon \gg \varepsilon_s$) or by their coordinates along the r axis as in regions III and IV. Therefore the situation is typical in which the magnitude of the argument of the Airy function satisfies $|B| > 1$ and it is possible to use the corresponding asymptotic expressions, which in regions I, III, and IV leads to the following expressions:

$$J_{\mathrm{I}} = \frac{\mu C}{\hbar^2 (2\pi)^{1/2}} \left\{ \frac{V(r_-)}{[k_i k_f (k_i' - k_f')]^{1/2}} \exp\left[i\left(S_i - S_f + \frac{\pi}{4}\right)\Big|_{r_-} \right] + \frac{V(r_+)}{[k_i k_f (k_i' - k_f')]^{1/2}} \exp\left[i\left(S_f - S_i - \frac{\pi}{4}\right)\Big|_{r_+} \right] \right\}, \tag{42}$$

$$J_{\mathrm{III}} = \frac{\mu C}{\hbar^2 (2\pi)^{1/2}} \frac{V(r_+)}{[-\varkappa_i \varkappa_f (\varkappa_i' + \varkappa_f')]^{1/2}} \exp(\sigma_i + \sigma_f)|_{r_+}, \tag{43}$$

$$J_{\mathrm{IV}} = \frac{\mu C}{\hbar^2 (2\pi)^{1/2}} \frac{V(r_+)}{[\varkappa_i \varkappa_f (\varkappa_f' - \varkappa_i')]^{1/2}} \exp(\sigma_f - \sigma_i)|_{r_+}. \tag{44}$$

Equations (42)–(44) coincide with the result of evaluating the one-dimensional integral (1) by the method of steepest descent (the saddle-point method) with semiclassical wave functions, so that it is advantageous to consider these formulas from the point of view of the Landau method for calculating integrals of rapidly oscillating functions [Ref. 4, §51].

Comparison with Eqs. (42)–(44) together with the results of Sec. 3 shows that the treatments in Ref. 4 and in Refs. 13 and 14 correspond to two limiting situations. For a slowly varying interaction, the positions of the saddle points, as in Ref. 4, are determined from the equation $k_i = k_f$. In the case of terms which are close to parallel, i.e., for $\delta \gg 1$, the saddle point is located to the left of r_m, which agrees with the analysis of concrete examples for parallel terms with an exponential interaction given in Refs. 13 and 14. In the general case of a variable interaction and arbitrarily disposed terms in the superbarrier region, it is necessary to take into account the contribution of both of the two complex conjugate saddle points which are closest to the real axis and satisfy the equation $\pm i\alpha = k_i - k_f$, while in the subbarrier region, with which are associated transitions between terms which are close to parallel, and where $8\varepsilon\delta^2 < 1$, it is necessary to take into account the contribution only of r_+, which is determined, as before, by Eqs. (12) and (14), but continued into the subbarrier region, i.e., $\alpha = \varkappa_i + \varkappa_f$ for Eq. (43), or $\alpha = \varkappa_f - \varkappa_i$ for Eq. (44). The contribution of the second point $r_- \ll r_m$ can be neglected. We note further that in the subbarrier case the argument of the exponential in the expression for J cannot be the difference of the actions, as is usual, but their sum.

6. TERMS CLOSE TO PARALLEL: DEPENDENCE OF THE TRANSITION PROBABILITY AND THE SHAPE OF THE SPECTRUM ON THE IMPACT PARAMETER

For terms which are close to parallel, it is possible to use the linear approximation in the vicinity of r_m. Transitions between such terms with $\delta \ll 1$ take place in regions II–IV ($\varepsilon < \varepsilon_s$). In these cases for $b_i \approx b_f \approx b$ we have

$$r_+ = r_m - b\Delta r^2/4\alpha^2 - \alpha^2/4b, \tag{45}$$

Furthermore, for example, from formula (43) for $|\Delta r| < \alpha^2/b$ we obtain

$$J = \frac{\mu C}{\hbar^2} \frac{V(r_m)}{(\pi\alpha b)^{1/2}} \exp\left(-\frac{b\Delta r^2}{4\alpha} + \frac{\alpha^3}{12b} \right), \tag{46}$$

A similar result is also obtained for $|\Delta r| > \alpha^2/b$ in regions II and IV. Formula (46) coincides with the result of an exact calculation for linear, parallel terms and an exponential interaction.[9]

For fixed distance between the turning points, increasing the distance between r_m and r_c leads (independently of the sign of $r_c - r_m$) to a displacement of the region that is most important for the transitions from r_c to r_m. Here the description of the transition differs from the various variants (including the subbarrier ones) of the Landau–Ziner formula (Sec. 4) for intersecting terms up to formula (46), i.e., in essence, the Demkov model with sloping parallel terms. A criterion of the description of the transition within the framework of the model of either intersecting or parallel terms can be estimated from the condition for Eqs. (36) and (46) to coincide, which obtains for

$$\delta < \alpha^{3/2}/4b^{1/2}, \ 8\varepsilon\delta^2 < 1. \tag{47}$$

Such a variation of the nature of the transition also results from variation of the impact parameter $\rho = (l + 1/2)/k$. Even if for small ρ the transition is determined by the intersection of the terms, nevertheless an increase of ρ, as can be seen from Eqs. (22) and (23) by expanding them in the vicinity of r_c, leads to a decrease of δ and the convergence (drawing nearer) of $r_\pm$ and r_m. Thus it is possible to refine the technique proposed in Ref. 17 for reducing the problem of transitions between arbitrary ρ-dependent terms to a problem of linear terms. If the parameters are such that the transitions take place in region I, then it is possible to use the linear approximation for the terms in the vicinity of r_c. For regions II–IV the expansion should be made in the vicinity of r_m.

Let us find the asymptotic form of J in the limiting case which obtains when it is possible to neglect the effect of the potential in comparison with the centrifugal term. In the region of small reaction defects, where $\alpha^2 > |k_{0i}^2 - k_{0f}^2|$ (or

in the vicinity of the center of the line, where $\hbar^2\alpha^2/2\mu > \hbar\omega$) the root r_+ is determined by the equation $\alpha = \varkappa_i + \varkappa_f$ and is equal to

$$r_+ = \frac{(2l+1)\alpha}{\{[\alpha^2+(k_{0i}-k_{0f})^2][\alpha^2+(k_{0i}+k_{0f})^2]\}^{1/2}} < \rho. \quad (48)$$

The matrix element is correspondingly calculated using expression (43)

$$J = \frac{\mu C}{\hbar^2}\frac{\alpha V_0}{\bar{k}^{3/2}(\alpha^2+\Delta k^2)^{3/4}}\left(\frac{l}{2\pi}\right)^{1/2}\exp\left[-\frac{l}{\bar{k}}(\alpha^2+\Delta k^2)^{1/2}\right], \quad \bar{k}=(k_{0i}k_{0f})^{1/2}. \quad (49)$$

Equation (49) gives the desired asymptotic limit at large l. We remark that in the recharging problem the asymptotic limit in ρ for arbitrary velocities is also constructed by the use of a multidimensional variant of the saddle-point method.[32,33]

Since for terms which are close to parallel the transitions are concentrated in the vicinity of the turning point, the centrifugal terms can be approximated in the calculation of J by straight lines, i.e., Eq. (46) should be made to agree with Eq. (49). Indeed, if in Eq. (46) we set $\hbar\Delta\omega = F\Delta r$, the difference in the terms in the vicinity of r_m, and in place of F we substitute the centrifugal force at the turning point, then Eq. (46) takes the form

$$J = \frac{C}{\hbar v}\left(\frac{\rho}{2\pi}\right)^{1/2} V(\rho)\exp\left(-\frac{\Delta\omega^2}{2\alpha v^2}\rho\right), \quad (50)$$

which coincides with Eq. (49), allowing for $\alpha^2 > \Delta k^2$, and leads to a broadening which is proportional to the velocity v.

Above we have compared a general formula in various limiting cases with the exact results available in the literature. For the final case of free motion with arbitrary l and an exponential interaction, a closed formula for the overlap integral with $\Delta k \pm 0$ has apparently not been given. The corresponding formula, which was obtained with the help of Ref. 34, has the form

$$J = -\frac{\mu C V_0 \alpha}{\hbar^2\pi\bar{k}^3}\frac{1}{(z^2-1)^{1/2}}Q_l^1(z), \quad (51)$$

where $z = 1 + (\alpha^2 + \Delta k^2)/2\bar{k}^2$ and Q_l^1 is the associated Legendre function of the second kind. For $l \to \infty$ it is found that[35]

$$J = \frac{\mu C V_0 \alpha}{\hbar^2\pi\bar{k}^3}\frac{l}{(z^2-1)^{1/2}}K_1(l\ln[z+(z^2-1)^{1/2}]), \quad (52)$$

where K_1 is the modified Bessel function. For $z \to 1$, but $l(z^2-1)^{1/2} \gg 1$, Eq. (52) exactly gives Eq. (49), which in the final summation allows us to once more judge the possibilities of the uniform formula (15). In connection with these last arguments it is interesting to note that a solution of the problem of transitions in the limit of weak coupling between the horizontal and the Coulomb terms was obtained in Ref. 36 in closed form, which also included an exponential interaction.

7. CONCLUSION

A multidimensional treatment has been used to obtain a quantum formula for the overlap integral (1) for arbitrary orbital angular momentum in the case of superbarrier transitions in the form (15) with functions $F^{\pm}$, A, and B given by Eqs. (18) and (19). Analytic continuation into the subbarrier region was achieved with the help of rules (29) and (30), where the relation has the form (27) with $F^{\pm}$, A, and B given by Eqs. (28), (32), and (34). As limiting cases it contains various expressions from the theory of nonadiabatic transitions and spectra which are well known in the literature, and which are connected with an exact account of one or two saddle points or an approximate account of four.

The result obtained is applicable under conditions of weak coupling between the states, i.e., the region of strong coupling of the terms is not reached.

$$r_m > (1/\alpha)\ln(V_0/|E_i-E_f|).$$

Another condition is connected with the possibility of neglecting the contribution of other saddle points, besides $r_{\pm}$.

The dynamics of the position of the transition region as a function of the parameters of the problem has been considered. The approach of the terms to parallel shifts the transition region away from where the terms intersect in the region of the turning points, where it is already necessary to explicitly take into account the dependence of $V(r)$. The transitions can have a subbarrier character even for $r_c > r_m$. Taking account of the dependence of $V(r)$ has made it possible to trace out the transition from the case of intersecting terms to the case of parallel terms and the dependence of the transition probability (the shape of the corresponding spectral region) on the orbital angular momentum, and to refine the Landau method for calculating integrals of rapidly oscillating functions.

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[1)] In the case of complex roots $q_{\pm}$ it becomes a question of the value of Re $q_{\pm}$.

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