Chapter 5

Tunneling, Librations and Normal Forms in a Quantum Double Well with a Magnetic Field

5.1. Introduction

The quantum double-well problem is a famous and remarkable problem in theoretical and mathematical physics. It is stated as follows. Let $V(x)$ be a smooth function growing to $+\infty$ as $|x| \to \infty$, symmetric with respect to the origin or to the hyperplane $x_1 = 0$ and having two global minima $x_\pm$, $V(x_\pm) = 0$. Consider the Schrödinger operator

$$\hat{H} = -\frac{h^2}{2}\left(\frac{\partial^2}{\partial x_1^2} + \ldots + \frac{\partial^2}{\partial x_n^2}\right) + V(x)$$

with a small positive parameter h. Then its spectrum has the following structure near the energy $E = 0$. If all eigenvalues ω_j^2 of the matrix $\frac{\partial^2 V}{\partial x^2}(x_\pm)$ are non-zero, then the eigenvalues of the operator $\hat{H}$ form pairs $E_\nu^\pm$, $E_\nu^+ < E_\nu^-$, numbered by a quantum number (multi-index) $\nu = (\nu_1, \ldots, \nu_n)$ with non-negative integer components $\nu_j = 0, 1, \ldots$, and these pairs have the asymptotic behavior corresponding to the harmonic oscillator approximation

$$E_\nu^\pm = h\sum_{j=1}^{n} \omega_j\left(\frac{1}{2} + \nu_j\right) + o(h). \qquad [5.1]$$

Chapter written by Sergey Y. DOBROKHOTOV and Anatoly Y. ANIKIN.

Nonlinear Physical Systems: Spectral Analysis, Stability and Bifurcations
Edited by Oleg N. Kirillov and Dmitry E. Pelinovsky
© 2014 ISTE Ltd. Published 2014 by ISTE Ltd.

For each quantum number ν, the difference (splitting) $E_\nu^- - E_\nu^+$ is exponentially small as $h \to +0$ and has the form

$$\Delta E_\nu \equiv E_\nu^- - E_\nu^+ = \frac{A_0}{h^\kappa} e^{-\frac{S_0}{h}} (1 + o(1)). \qquad [5.2]$$

This formula is in the framework of semi-classical analysis, and both the phase S_0 and the amplitude A_0 can be expressed via objects related to the "tunnel" Hamiltonian $\mathscr{H} = T - V$ with inverted potential $-V(x)$. One of these objects is the well-known instanton, the singular trajectory (doubly asymptotic to the unstable equilibriums $x_\pm$) of the tunnel Hamiltonian system (or the Newtonian system $\ddot{x} = V_x$). The relationship between the splitting and the instanton and the method to calculate the phase in [5.2] have been discussed in numerous papers and monographs. We mention here [COL 77, COM 83, GIL 77, HAR 78, HAR 80, HEL 84, HEL 85, JON 81, MAS 84, PAN 84, POL 77, SIM 84, SLA 69], where one can also find many references. We point out that the rigorous proof of [5.2] with the instanton phase is absolutely non-trivial.

The formula for the amplitude A_0 presented in [DOB 91, DOB 93] is also based on the tunnel Hamiltonian system, more precisely, on its linearization near the instanton. This cumbersome formula includes several determinants, and its calculation consists of a sequence of steps that are not simple even in the two-dimensional (2D) case. Thus, this formula is more of an "algorithm for calculation" than a true formula.

However, it is possible to use another object instead of the instanton, namely an unstable closed trajectory of the same system known as a *libration*. It leads to a more convenient asymptotic formula because the hard-to-compute part of the amplitude in the instanton-based formula is now attached to the phase S_0. As a result, the amplitude becomes much simpler, more natural from the physical point of view, and more fit for practical application, and the definitive splitting formula is easy to understand (in contrast to its complete and accurate derivation). Indeed, the zero-energy instanton is a bizarre object from the viewpoint of quantum mechanics. On the contrary, the libration with small negative energy corresponding to the minus ground state is much more natural.

These formulas and their derivation appeared in [BRÜ 06, ANI 13a, ANI 13b] and we present them in section 5.3. We also provide the explanations and ideas [BRÜ 06, ANI 13a, ANI 13b] coming from geometry and normal form theory leading to these formulas (see section 5.5). The idea of derivation is given in section 5.7.

Let us say that the methods used for the derivation of the splitting formulas [5.2] work only for the "standard" Schrödinger operator, and the inclusion of, say, a magnetic field into this operator essentially destroys the scheme of derivation of

[5.2]. Here (see section 5.6), following [BRÜ 13], we show that in some cases the splitting problem for the magnetic Schödinger operator could be reduced to the standard Schödinger operator, which allows one to write out the splitting formulas and express some ideas about tunneling in the multidimensional (non-integrable) case.

To make our consideration clearer, we recall the well-known Landau–Lifshitz splitting formula in the one-dimensional (1D) case and give its suitable geometrical interpretation.

5.2. 1D Landau–Lifshitz splitting formula and its analog for the ground states

First, recall the 1D Landau–Lifshitz splitting formula ([LAN 77] problem 3, §50, Chapter VII; see also [ALE 82, FED 65]). Let $V(x), x \in \mathbb{R}$, be a non-negative even C^∞ function such that $V(x) \to \infty$ as $x \to \infty$. Suppose also that $V(x)$ vanishes at exactly two points (wells) $x = x_\pm = \pm x_+$. For simplicity, we assume that $V(x)$ has only one local point of maximum $x = 0$. Then, as said earlier, the eigenvalues of the 1D Shrödinger operator $\hat{H} = -h^2 \frac{d^2}{dx^2} + V(x)$ lying lower than $V(0)$ form pairs $E_\nu^\pm$, and the difference $E_\nu^- - E_\nu^+$ has the form [5.2]. Let us present the geometric interpretation of the formulas for $E_\nu^\pm$ and ΔE_ν.

Consider two Hamiltonians associated with the operator $\hat{H}$: the classical Hamiltonian $H = \frac{p^2}{2} + V(x)$ and the tunnel Hamiltonian $\mathscr{H} = \frac{p^2}{2} - V(x)$. Consider the following closed trajectories $\Lambda^\pm$ and Γ of these Hamiltonians, which are contour lines of the functions H and $\mathscr{H}$ on the phase plane $\mathbb{R}^2_{px}$ with coordinates (p,x):

$$\Lambda^\pm = \Lambda^\pm(E) = \{p = P(\varphi,E), x = \pm X(\varphi,E) | H = E\},$$
$$\Gamma = \Gamma(E) = \{p = \mathscr{P}(\phi,E), x = \mathscr{X}(\phi,E) | \mathscr{H} = -E, x_- < \mathscr{X}(\phi,E) < x_+\}.$$

We assume that $0 < E < V(0)$. These curves are smooth and homeomorphic to a circle. We assume that φ and ϕ are angle coordinates on $\Lambda^\pm$ and Γ such that the functions $\big(P(\varphi,E), X(\varphi,E)\big)$, $\big(\mathscr{P}(\phi,E), \mathscr{X}(\phi,E)\big)$ are 2π-periodic in φ and ϕ. Let us construct two expressions

$$I = \frac{1}{2\pi} \oint P(\varphi,E) d X(\varphi,E) = \frac{1}{\pi} \int_a^b \sqrt{2(E - V(y))} d y, \qquad [5.3]$$

$$\mathscr{I} = \frac{1}{2\pi} \oint \mathscr{P}(\phi,E) d \mathscr{X}(\phi,E) = \frac{1}{\pi} \int_{-a}^a \sqrt{2(V(y) - E)} d y; \qquad [5.4]$$

here $V(a) = V(b) = E$, and $0 < a < b$. I and $\mathscr{I}$ are the action variables dual to the angles φ and ϕ, respectively, in the classical and tunnel Hamiltonian systems with Hamiltonians H and $\mathscr{H}$ (see Figure 5.1).

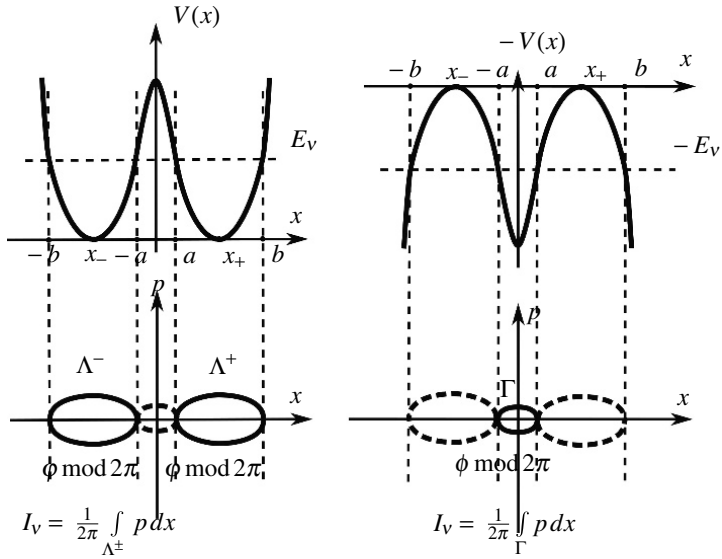

Figure 5.1. *Tunneling between highly excited states*

As $E \to +0$, the curves $\Lambda^{\pm}$ tend to the stable equilibria ($p = 0, x = x_{\pm}$), and Γ tends to the separatrix $\Gamma(0)$, which is the instanton in the 1D quantum double-well problem. One can solve [5.3] and [5.4] for E and express the Hamiltonians via the action variables, $H = H(I)$ and $\mathscr{H} = \mathscr{H}(\mathscr{I})$. Let us assume that the action I takes the discrete values

$$I = I_\nu \equiv h(\frac{1}{2} + \nu);$$

then by the Bohr–Sommerfeld quantization rule, we have the asymptotics

$$E_\nu^{\pm} = H(I_\nu) + O(h^2) \qquad [5.5]$$

for the eigenvalues. It can also be shown that $E_\nu^- - E_\nu^+ = O(h^\infty)$. We take $\mathscr{I}_\nu$ so that $-E = -\mathscr{H}(\mathscr{I}_\nu)$ in [5.4]. Then the Landau–Lifshitz formula reads (for $E_\nu = O(1)$ as $h \to +0$)

$$\Delta E_\nu \equiv E_\nu^- - E_\nu^+ = \frac{\omega^\Lambda h}{\pi} e^{-\frac{\pi \mathscr{I}_\nu}{h}} (1 + O(h)); \qquad [5.6]$$

here ω^Λ is the frequency along the classical trajectory $\Lambda^{\pm} = \Lambda^{\pm}(E)$ of the potential V.

Formula [5.6] is a masterpiece of theoretical and mathematical physics; it is very clear and includes a minimum of the required objects: *nothing is possible to avoid and nothing is necessary to add*.

The assumption $E_\nu^\pm = O(1)$ means that we consider excited states: the quantum number ν is large, $\nu = O(1/h)$. Note that both formulas [5.5] and [5.6] admit passage to small ν. The corresponding passage for [5.5] is correct, and the well-known simple analysis shows that the Bohr–Sommerfeld rule turns into the harmonic oscillator approximation

$$E_\nu^\pm = \omega_0 h(\frac{1}{2} + \nu) + O(h^2), \qquad [5.7]$$

where $\omega_0 = \sqrt{V''(x_\pm)/2} = \frac{\partial H(I)}{\partial I}|_{I=0}$ is the limit frequency of the classical motion of the Hamiltonian system H in a neighborhood of the minima $(p = 0, x = \pm a)$. This passage is not straightforward for the splitting formula [5.6]: we should include extra factors. For the ground states (i.e. $\nu = 0$), the corresponding factor is $\sqrt{\pi/e}$, and the definitive formula becomes [HAR 78, HAR 80, HEL 84, HEL 85, ALB 04]

$$E_0^- - E_0^+ = \frac{\omega_0 h}{\sqrt{\pi e}} e^{-\frac{\mathscr{I}_0 h}{h}} \big(1 + O(h)\big). \qquad [5.8]$$

In the case of excited lower states (where the quantum number ν is fixed and $h \to +0$), the splitting has a form similar to [5.8], namely,

$$E_\nu^- - E_\nu^+ = b_\nu \frac{\omega_0 h}{\pi} e^{-\frac{\mathscr{I}_\nu h}{h}} \big(1 + O(h)\big). \qquad [5.9]$$

Here, $\mathscr{I}_\nu$ is an action on the periodic trajectory with energy [5.7] and b_ν is a numerical factor (dependent on ν only). It follows from Stirling's formula that b_ν tends to unity as $\nu \to \infty$. On the other hand, $\omega^\Lambda \to \omega_0$ as $E \to 0$. Thus, we see that formulas [5.6] and [5.9] give the same result. This important fact giving a transition between splittings of low lying and highly excited eigenstates was indicated in [HEL 85].

Note that the energy $E = E_0^\pm$, as well as the corresponding curves $\Lambda^\pm(E)$, is small (as $h \to +0$), and the curve $\Gamma(E)$ is close to the separatrix (instanton) $\Gamma(0)$. As said before, one can use the instanton and corresponding "instanton action" in the last formula, but the form of the amplitude becomes much more complicated, especially in the n-dimensional case. We will return to this question later in this chapter.

One of our main results is the claim that the splitting formula for the ground states in the multidimensional case looks like [5.8] *with an appropriate phase* $\mathscr{I}_0$ *and*

frequency ω_0. The question is: what are these phase and frequency? Moreover, it seems to be likely that the splitting formulas in many other tunneling problems are similar to the Landau–Lifshitz formula [5.6] with some dimensionless factors like $\sqrt{\frac{\pi}{e}}$ in [5.8]. *We point out that all objects in formulas* [5.6] *and* [5.8] *are merely integrals and derivatives of the potential* V *and one can avoid discussing their geometrical and dynamical nature. However, this discussion becomes crucial as soon as one passes to the multidimensional case.*

COMMENT 5.1.–

1) Let us discuss the occurrence of the real motion frequency ω_ν in [5.6] and [5.8]. A naive but probably useful explanation is as follows. Both classical trajectories in the left and right wells are characterized by the action variables I^+ and I^-. Because of the symmetry and tunneling, the semi-classical quantization gives $I^+ = I_\nu^+$, $I^- = I_\nu^-$, and $\Delta I_\nu = I_\nu^- - I_\nu^+$. Let us substitute this expression into the formulas relating the classical energy and the action variable, $E = H(I)$. This gives

$$\Delta E_\nu = H(I_\nu^-) - H(I_\nu^+) \approx \frac{\partial H}{\partial I}(I_\nu^+)\,\Delta I_\nu = \omega_\nu \Delta I_\nu.$$

Dividing ΔE_ν, by ω_ν, we obtain a "jump" of the actions appearing due to tunneling and related to the action corresponding to the "tunnel" potential $\mathscr{H}$ alone.

2) We also wish to mention a "recipe" for finding the "tunnel" action $\mathscr{I}_0$. We simply use the relation

$$E_0^\pm = H(I_0) = \frac{\omega_0 h}{2} + O(h^2) = -\mathscr{H}(\mathscr{I}_0) + O(h^2). \qquad [5.10]$$

Thus, $\mathscr{I}^0$ is the action corresponding to the tunnel Hamiltonian at level $-E_0$. This fact will be useful in the multidimensional case.

Let us briefly discuss the asymptotic behavior of the eigenfunctions $\psi_\nu^\pm$. In the case of excited states, their behavior is as follows. Because of the symmetry of the problem, the function ψ_ν^+ is even, and the function ψ_ν^- is odd with respect to x (see Figure 5.2). (That is, the state associated with the even eigenfunction is lower than the state corresponding to the odd one.) The functions $\psi_\nu^\pm$ are the sum and the difference of two WKB-exponential functions $A_\pm(x)\exp\left(\pm\frac{iS(x)}{h}\right)$ (or quasimodes). The phase $S(x)$ is real on the intervals $(-b,-a),(a,b)$, and pure imaginary on the rays $(-\infty,-b)$ and (b,∞) and the interval $(-a,a)$. In a neighborhood of the points $x = \pm a$ and $x = \pm b$, we can use the asymptotics based on the Airy function. By pasting together the different WKB asymptotics and the asymptotics of the Airy functions, we obtain a global description of $\psi_\nu^\pm$ and a method for computing the asymptotics of $E_\nu^\pm$ and $\Delta E_\nu^\pm$.

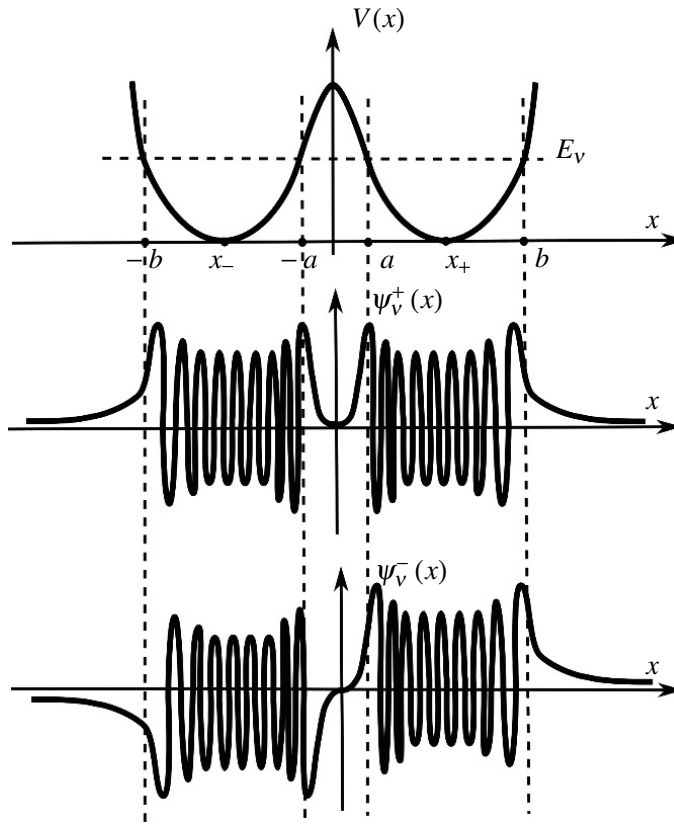

Figure 5.2. *Eigenfunctions: highly excited states*

The construction of asymptotic eigenfunctions $\psi_\nu^\pm$ for small ν, $\nu = O(1)$ as $h \to 0$ (in particular for $\nu = 0$, the ground state), is easier; it is based on the WKB-exponential functions $A\exp\left(-\frac{S(x)}{h}\right)$ on the rays $(-\infty, x_\pm)$ and $(x_\pm, \infty)$ (see Figure 5.3). In fact, these asymptotics lead to a splitting formula based on the instanton, and one can obtain the Landau–Lifshitz-type formula [5.8] after some transformations. We will later discuss some other ideas and procedures leading to the splitting formula [5.8]. Needless to say, an accurate proof of the asymptotic formulas for the functions $\psi_\nu^\pm$ is not trivial even in the 1D case (see [FED 65, SLA 69, ALE 82, POL 77, JON 81, COM 83, COL 77, GIL 77, HAR 78, HAR 80, HEL 84, HEL 85, PAN 84]).

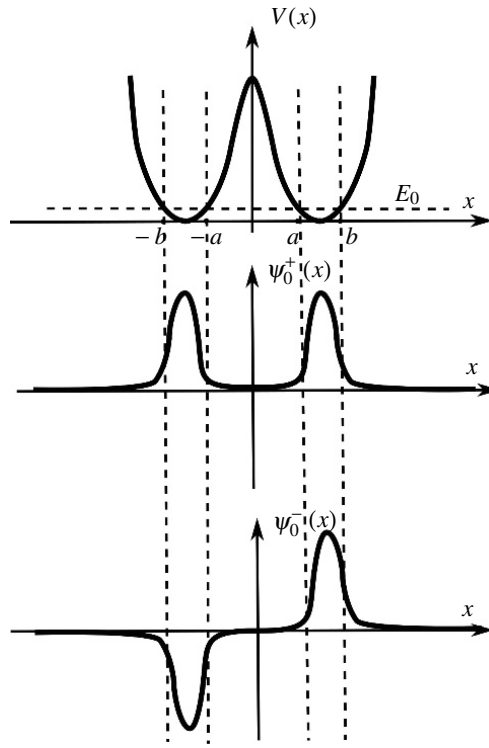

Figure 5.3. *Eigenfunctions: the ground state*

5.3. The splitting formula in multi-dimensional case

Now we present an analog of the splitting formula in the multidimensional case. An attempt to generalize [5.8] to the multidimensional case was made in [BRÜ 06]. This generalization is not straightforward: it is not easy to guess the correct answer. However, some arguments in [BRÜ 06] were not quite rigorous, and the complete proof was given in [ANI 13a], [ANI 13b]. Consider the Shrödinger operator $\hat{H} = -\frac{h^2}{2}\Delta + V(x)$ in $\mathbb{R}^n$ such that we have the following hypotheses:

H1) $V \geq 0$, $V \in C^\infty$,and $V \to \infty$ as $x \to \infty$.

H2) $V(x_1, x_2, \ldots, x_n)$ is symmetric with respect to either the hyperplane $x_1 = 0$ or the origin $x = 0$.

H3) There are exactly two minima $V(x_\pm) = 0$ (symmetric with respect to either the hyperplane $x_1 = 0$ or the origin $x = 0$), and $V''_{xx}(x_\pm)$ has the eigenvalues $\omega_1^2, \ldots, \omega_n^2$, where $2\omega_1 < \min\limits_{j \geq 2} \omega_j$ $(\omega_j > 0)$.

H4) Tunnel Hamiltonian system $\mathscr{H} = K - V$ or the Newtonian one

$$\dot{p} = V_x, \quad \dot{x} = p \qquad \Longleftrightarrow \qquad \ddot{x} = V_x \tag{5.11}$$

with the standard kinetic energy $K = \frac{p^2}{2}$, and the inverted potential $-V$ has a unique trajectory $\Gamma(0)$ (the instanton) doubly asymptotic to the unstable equilibria $x_\pm$. Moreover, the following non-degeneracy conditions hold:

i) $\Gamma(0)$ approaches the equilibria in a non-singular direction (i.e. the direction corresponding to ω_1).

ii) The asymptotic manifolds of the equilibria (in the phase space) intersect transversally along $\Gamma(0)$.

COMMENT 5.2.–

1) The relation between the frequencies in H3 seems to be weird and may probably be omitted. This assumption is essential only when we deal with specific coordinates near the instanton. These coordinates are ill-behaved near the equilibria if H3 does not hold. We might have discarded this assumption if we had used different coordinates. However, what is surely important is that ω_1 is the lowest frequency.

2) To explain H4, we recall that the maxima $x_\pm$ of the potential correspond to the hyperbolic fixed points in the phase space. Each hyperbolic fixed point has its invariant asymptotic stable (respectively unstable) n-dimensional manifold, i.e. the manifold consists of phase trajectories tending to the fixed point as $t \to +\infty$ (respectively $t \to -\infty$). The fixed point is a node singularity for both manifolds, and one of the trajectories approaching it is the instanton. Consider the 2D case for simplicity. It is clear that assumption H4i forbids only two possible directions for the instanton, namely those corresponding to the greater frequency ω_2. Thus, we see that assumption H4i holds for generic systems (takes place in a typical situation). The transversality condition in H4ii is also a generic property.

3) Hypothesis H4ii is very important for several reasons. If the tranversality breaks down, then there can arise pairs of conjugate (or focal) points near the instanton. This makes it more difficult or even impossible to prove the existence of closed trajectories (librations) near the instanton. The problem is that the implicit function theorem cannot be applied because of degeneracy. Focal points lead to another difficulty: the phase $S(x)$ in the WKB method is no longer a smooth function in the vicinity of the instanton. This complicates the calculation of tunnel effects. We will return to this question in section 5.5. The tranversality also ensures that the instanton is unique.

It can be shown that system [5.11] has a one-parameter family of periodic trajectories $\Gamma(\mathscr{E}) = \{p = \mathscr{P}(\phi^t, \mathscr{E}), x = \mathscr{X}(\phi^t, \mathscr{E})\}$ ($\phi^t \bmod 2\pi$). Here the parameter

$\mathscr{E} = -E$, where $E > 0$ is the energy, is sufficiently small). Each $\Gamma(\mathscr{E})$ is a libration (or a brake orbit, or a bounce orbit), i.e. its velocity (or momentum $\mathscr{P}$) vanishes twice per period (see Figure 5.4). The existence of a family of librations is not quite obvious, and this question was studied in a more general situation in [ARN 06], [BOL 78] and [BOL 78b].

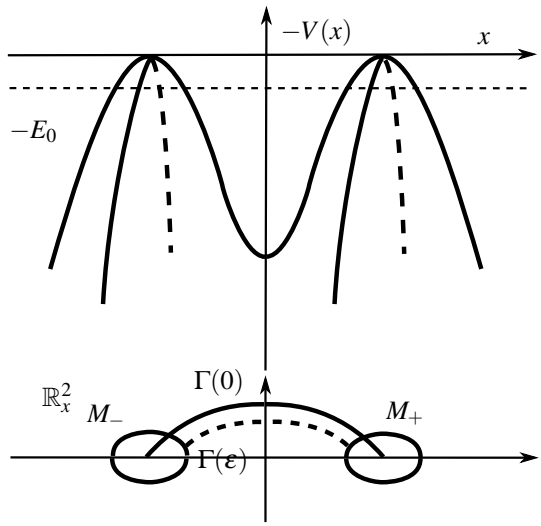

Figure 5.4. *Instanton and libration. Here, $M^{\pm} = \{-V = -\mathscr{E}\}$ is the boundary of the domain of classically allowed motions; $\Gamma(0)$ is the instanton (full curve); $\Gamma(\varepsilon)$ is a libration (broken curve) with energy $\mathscr{E}$*

Now we parameterize the family of librations by the action

$$\mathscr{I} = \frac{1}{2\pi} \oint_{\Gamma(\mathscr{E})} \mathscr{P}\, d\mathscr{X} \qquad [5.12]$$

Also, consider the variational system associated with [5.11] and the libration $\Gamma(\varepsilon)$,

$$\dot{w} = V_{xx}(\mathscr{X}(\phi^t, \mathscr{E}))z, \dot{z} = w \qquad \Longleftrightarrow \qquad \ddot{z} = V_{xx}(\mathscr{X}(\phi^t, \mathscr{E}))z. \qquad [5.13]$$

The libration is a closed unstable trajectory. Because of the structure of the Hamiltonian $\mathscr{H}$, all Floquet exponents are real. Let $-\mathscr{H}_0(\mathscr{I})$ be the energy of a libration with action $\mathscr{I}$, and let $\lambda_j(\mathscr{I})$ be the positive Floquet exponents of the same libration ($2 \leq j \leq n$).

The multidimensional version of [5.8] is our main result and it is stated as follows:

THEOREM 5.1.– [BRÜ 06, ANI 13a, ANI 13b] The difference between the least eigenvalues $E_0^{\pm} = \frac{h}{2}(\omega_1 + \ldots + \omega_n) + O(h^2)$ of the operator $\hat{H}$ satisfying H1–H4 has the asymptotics

$$E_0^- - E_0^+ = \sqrt{\frac{\pi}{e}} \frac{\omega_1 h}{\pi} e^{-\frac{\pi \mathscr{I}_0}{h}} \big(1 + o(1)\big), \qquad h \to 0, \tag{5.14}$$

where $\mathscr{I}_0$ is the solution of the equation:

$$\mathscr{H}_0(\mathscr{I}_0) - \frac{h}{2} \sum_{j=2}^{n} \lambda_j(\mathscr{I}_0) = -(\omega_1 + \ldots + \omega_n)\frac{h}{2}. \tag{5.15}$$

COMMENT 5.3.–

1) In the 1D case, theorem 5.1 gives exactly formula [5.8].

2) Consider the 2D case of separating variables. Suppose that $V = V_1(x_1) + V_2(x_2)$, where V_1 is a 1D double well satisfying assumptions H1–H3 and V_2 is a 1D non-degenerate single well at the origin. It is clear that the splitting is equal to that for the 1D operator with the potential V_1. The asymptotics are then given by [5.8]. On the other hand, $\lambda_2 = \omega_2$ in this case, and hence theorem 5.1 gives the same result.

3) We point out that $\mathscr{I}_0$ in the exponential [5.14] is the action on a libration. However, its energy $\mathscr{H}_0(\mathscr{I}_0)$ is not $-E_0^{\pm}$ as one might naively expect. (This is wrong even in the case of separating variables; see point 2.) Actually, the curve $\Gamma(\mathscr{I}_0)$ is the cycle on a certain complex Lagrangian manifold. We will discuss this question later.

4) As we have already stated, the splitting formula based on the instanton looks much more complicated and includes, in particular, two $n \times n$ determinants in the amplitude (see [5.22]). Their calculation for large n can be a very difficult problem. This "determinant" problem is replaced by the easier calculation of the Floquet exponents.

5) We point out that *one does not need the instanton* to use in the splitting formula [5.14]; it is replaced by the libration. To find it or calculate it numerically, we can use the following ideas:

i) We can seek a libration as a solution of some variational problem. However, this problem is tricky because librations meet the boundary of the classically allowed domain $\{-V < \mathscr{E}\}$, thus hampering the direct use of the Maupertuis–Jacobi variational principle.

Let us restrict ourselves to the 2D case for simplicity. Let $\Omega^{\pm}$ be sufficiently small fixed closed curves in the configuration space $\mathbb{R}^2$ around $x_{\pm}$. Let $M^{\pm} = M^{\pm}_{\mathscr{E}}$ be two connected components of $\{-V < \mathscr{E}\}$.

Let $\theta_{\pm}$ be the coordinates of the points $x_{\theta_{\pm}}$ on $\Omega^{\pm}$. For any pair $\theta_{\pm} \in \Omega^{\pm}$, we define the trajectory $x = \mathscr{X}_{\theta_-,\theta_+}(t) = \mathscr{X}_{\theta_-,\theta_+}(t,\mathscr{E}), p = \mathscr{P}_{\theta_-,\theta_+}(t) = \mathscr{P}_{\theta_-,\theta_+}(t,\mathscr{E})$ with energy $\mathscr{E}$ to be a solution of the boundary value problem

$$\mathscr{X}_{\theta_-,\theta_+}(t_-) = x_{\theta_-}, \quad \mathscr{X}_{\theta_-,\theta_+}(t_+) = x_{\theta_+}, \tag{5.16}$$

where $t_{\pm}$ are not fixed but can be chosen arbitrarily. By the Maupertuis–Jacobi principle, this solution gives the minimum of the Maupertuis functional $\int_{t_-}^{t_+} p\,dx$ on the set of curves satisfying conditions [5.16].

In a neighborhood of $x_{\pm}$, we use the following property. Let a trajectory $x = x(t), p = p(x)$ start from, say, $x(0) \in M^-$, $p(0) = 0$, and let τ be the first time at which $x(\tau) \in \Omega^-$ (i.e., $x(t) \notin \Omega^-$ for $0 \le t < \tau$). Thus, we have the correspondence between points of M^- and Ω^-. This correspondence is one-to-one if Ω^- is sufficiently small and "not very bad". (The transversality to each trajectory asymptotic to x_- would suffice.) Therefore, to each $\theta_{\pm} \in \Omega^{\pm}$, one can naturally assign a small curve $x = \mathscr{X}_{\theta_{\pm}}(t), p = \mathscr{P}_{\theta_{\pm}}(t)$ starting from $x_{\theta_{\pm}}$, then reaching $M^{\pm}$ with zero velocity and then bouncing back.

By pasting together these trajectories, we arrive at the piecewise smooth curves

$$x = \mathscr{X}_{\theta_-}(t), \quad p = \mathscr{P}_{\theta_-}(t) \quad 0 \le t \le t_-, \qquad \mathscr{X}_{\theta_-}(0) \in M^-, \quad \mathscr{X}_{\theta_-}(t_-) = x_{\theta_-},$$

$$x = \mathscr{X}_{\theta_-,\theta_+}(t), \quad p = \mathscr{P}_{\theta_-,\theta_+}(t) \quad t_- \le t \le t_+, \qquad \mathscr{X}_{\theta_-,\theta_+}(t_{\pm}) = x_{\theta_{\pm}},$$

$$x = \mathscr{X}_{\theta_+}(t), \quad p = \mathscr{P}_{\theta_+}(t) \quad t_+ \le t \le t_0, \qquad \mathscr{X}_{\theta_+}(t_+) = x_{\theta_+}, \quad \mathscr{X}_{\theta_+}(t_0) \in M^+.$$

These curves form a two-parameter family. The libration with energy $\mathscr{E}$ (and also the instanton in the limit case $\mathscr{E} = 0$) is the curve on which the functional

$$\int_0^{t_-} \mathscr{P}_{\theta_-}\, d\mathscr{X}_{\theta_-} + \int_{t_-}^{t_+} \mathscr{P}_{\theta_-,\theta_+}\, d\mathscr{X}_{\theta_-,\theta_+} + \int_{t_+}^{t_0} \mathscr{P}_{\theta_+}\, d\mathscr{X}_{\theta_+}$$

attains its minimum. Generally, minimizing this functional is equivalent to seeking a minimum of a function of two variables.

ii) Let $\mathscr{X}^{\pm} \in M^{\pm}$ be the endpoints of a libration. If $\mathscr{E}$ is sufficiently small, then the libration $\Gamma(\mathscr{E})$ is close to the instanton, and thus the vector $\overline{x_{\pm}\mathscr{X}^{\pm}}$ should be close to the eigenvector $q\mathbf{e}_1^{\pm}$, $|\mathbf{e}_1| = 1$, of the matrix $\frac{\partial^2 V}{\partial x^2}$ (corresponding to its lowest

eigenvalue ω_1^2) with $q = \sqrt{\frac{2\mathscr{E}}{\omega_1}}$.

iii) Assume that a time is chosen so that $\mathscr{X}(0) = \mathscr{X}^-$ and $\mathscr{X}(\frac{T}{2}) = \mathscr{X}^+$, where $T = T(\mathscr{E})$ is the libration period. If the potential V is symmetric with respect to the hyperplane $x_1 = 0$, then the libration crosses this hyperplane normally and we have $\mathscr{P}_1^2(\frac{T}{4}, \mathscr{E}) = 2(\mathscr{E} + V(0, y_2, \ldots, y_n))$, $\mathscr{P}_j(\frac{T}{4}, \mathscr{E}) = 0, j = 2, \ldots, n$, and $\mathscr{X}_1(\frac{T}{4}, \mathscr{E}) = 0, \mathscr{X}_j(\frac{T}{4}, \mathscr{E}) = y_j, j = 2, \ldots, n$. If the potential V is centrally symmetric, then the libration crosses the origin $x = 0$. In this case, $\mathscr{P}^2(\frac{T}{4}, \mathscr{E}) = 2(\mathscr{E} + V(0))$, $\mathscr{P}_j(\frac{T}{4}, \mathscr{E}) = y_j, j = 1, \ldots, n$. Here, y_j are real parameters.

6) One can solve equation [5.15] numerically by using an iteration method. To this end, it is more convenient to parameterize the family of librations by the fictitious energy $\mathscr{E} = \mathscr{H}_0(\mathscr{I})$ and rewrite equation [5.15] in the form

$$\mathscr{E} = (\lambda_2'(\mathscr{E}) + \ldots + \lambda_n'(\mathscr{E}))\frac{h}{2} - (\omega_1 + \ldots + \omega_n)\frac{h}{2}, \qquad \lambda_j'(\mathscr{E}) = \lambda_j(\mathscr{H}_0^{-1}(\mathscr{E})).$$

One can choose the zero approximation by setting, for instance, $\mathscr{E}_0 = -\frac{\omega_1 h}{2}$, and construct the sequence

$$\mathscr{E}_{k+1} = \big(\lambda_2'(\mathscr{E}_k) + \ldots + \lambda_n'(\mathscr{E}_k)\big)\frac{h}{2} - (\omega_1 + \ldots + \omega_n)\frac{h}{2}.$$

To implement this process, one should numerically find the functions $\mathscr{P}(\phi^t, \mathscr{E}_k), \mathscr{X}(\phi^t, \mathscr{E}_k)$ determining the libration $\Gamma(\mathscr{E}_k)$. The main difficulty here is finding these functions (e.g. by using the shooting method for finding the parameters y_j) for the zero approximation because (1) the libration period is unknown *a priori* and (2) the libration is an unstable trajectory. Here one should take into account points 5i–5iii mentioned above. The construction of the next approximation is much easier because $\Gamma(\mathscr{E}_{k+1})$ is close to $\Gamma(\mathscr{E}_k)$ and the iterative process converges very rapidly.

7) Tunneling between low lying excited states was studied by several authors. The upper and lower bounds for a splitting ΔE_ν (where vector ν is fixed) were found in [MAR 87]. They both have a form $Ch^\kappa e^{-\frac{S_0}{h}}$, where powers κ depend on $|\nu|$ quite irregularly. Asymptotic behavior of the splitting was reported in [AVI 75] (though, without necessary subtle estimates on exponential decay). We are planning to prove an analog of theorem 5.1 for excited states when the only non-zero component of vector ν corresponds to the instanton (lowest frequency). It is natural to expect that the final formula will be of the form [5.9].

8) Tunneling between highly excited states is a far more complicated problem. In general, it is hopeless to obtain a multidimensional analog of Landau–Lifshitz formula. It turns out (see [MAR 88, WIL 86, WIL 87a, WIL 87b, CRE 99] for theoretical and numerical analyses) that splitting is very sensitive to the type of

dynamics in wells (e.g. integrable, KAM and chaotic). For instance, an exactly integrable case (see [CRE 94]) differs qualitatively from a nearly integrable case [WIL 86, WIL 87a]. A chaotic case (see, e.g., [WIL 87b, CRE 94]) is the least clear because we do not even have a proper procedure to find eigenfunctions. Our references do not cover all the literature on tunneling between excited states because we focus mainly on the case of the ground state. A more complete list may be found in [CRE 98].

9) We point out the works [JON 81], [HEL 84], [HEL 85], and [SIM 85], where the splitting and the eigenfunctions were studied when the symmetric double well was perturbed away from the wells. In this way, one may ask the question: what happens to formula [5.14] in a slightly asymmetric situation? Although this problem is reasonable from the mathematical point of view, we think that it is somewhat unreal in physical applications. It seems that such non-analytical perturbations rarely appear in physics.

5.4. Normal forms and complex Lagrangian manifolds

In this section, we give an interpretation of theorem 5.1 based on the dynamics in the classically forbidden domain (the shadow region). Our argument is rather schematic and sometimes not quite rigorous enough. Generally, throughout the section, we assume the analyticity of the potential rather than the mere smoothness.

5.4.1. *Normal form in the classically allowed and forbidden regions*

Consider the classical Hamiltonian $H = \frac{p^2}{2} + V$. For simplicity, we assume that the frequencies ω_k are non-resonant, i.e. linearly independent over $\mathbb{Z}$. Then in a neighborhood of each stable equilibrium $x_\pm$, there is a Birkhoff normal form (at least formal). This means that for all N there are symplectic coordinates I_k, φ_k such that

$$H = \sum_{m=1}^{N} F_m(I_1, \ldots, I_n) + H_{N+1}(I, \varphi),$$

where F_m is a polynomial of aggregate degree m in I_m. In particular, $F_1 = \omega_1 I_1 + \ldots + \omega_n I_n$. The remainder H_{N+1} contains terms of higher degree in I_k. The truncated Hamiltonian $\check{H} = \sum_{m=1}^{N} F_m$ defines an integrable Hamiltonian system (I_k are the first integrals), which is, at the same time, close to the original system H.

Now let us construct a normal form for the tunnel Hamiltonian $\mathscr{H} = \frac{p^2}{2} - V$ near the family of librations. The normal form of the Hamiltonian system near a periodic

orbit is a standard construction (see [BRU 89]). By generalizing these ideas, we obtain:

$$\mathscr{H} = \mathscr{H}_0(\mathscr{I}_1) - \sum_{k=2}^{n} \lambda_k(\mathscr{I}_1) u_k v_k + \mathscr{H}_3(\mathscr{I}, \varphi, u, v),$$

where $\mathscr{H}_3$ is of total degree ≥ 3 in u, v. Here $\mathscr{I}_1$ is the action variable numbering the librations, and $\varphi \bmod 2\pi$ is its canonically conjugate angle variable. The remaining variables u_k and v_k are canonically conjugate variables in the directions transversal to the libration. The truncated Hamiltonian

$$\check{\mathscr{H}} = \mathscr{H}_0(\mathscr{I}_1) - \sum_{k=2}^{n} \lambda_k(\mathscr{I}_1) \mathscr{I}_k,$$

where $\mathscr{I}_k = u_k v_k$, again defines an integrable system with first integrals $\mathscr{I}_k$.

5.4.2. *Complex continuation of integrals*

Consider the analytical continuation of H and I_k. Obviously, $H(ip,x) = -\mathscr{H}(p,x)$. Therefore, according to the general properties of the Hamiltonian system, $I_k(ip,x)$ should be expressed via $\mathscr{I}_k$. In the case of separated variables, we readily see that $I_k(ip,x) = \mathscr{I}_k$ for $k = 2, \ldots, n$. We believe that this connection also holds in the general case. Then the action $\mathscr{I}_0$ in [5.15] is none other than $I_1(ip,x)$. Thus, we see that the action in the exponent in theorem 5.1 is the action associated with ω_1 continued into the classically forbidden region.

5.4.3. *Almost invariant complex Lagrangian manifolds*

Consider the complex phase space $\mathbb{C}^{2n}_{px}$ with complex coordinates (p,x). The realization of equations $I_j(p,x) = const$, $\mathscr{I}_j(p,x) = const$ in the complex coordinates (p,x) gives $(p = P(\varphi,E), x = X(\varphi,E)) \bigcup (p = i(\mathscr{P}(\phi_1,\mathscr{E}) + w_2(\phi_1,\mathscr{E})\sinh\phi_2 + \ldots + w_n(\phi_1,\mathscr{E})\sinh\phi_n), x = \mathscr{X}(\theta,\mathscr{E}) + z_2(\theta,\mathscr{E})\cosh\phi_2 + \ldots + z_n(\theta,\mathscr{E}))\cosh\phi_n$ (see [5.3] and [5.4]). These equations define two (small) real n-dimensional Liouville tori $\Lambda_0^{\pm}$ connected by a "tunnel" complex band $\tilde{\Lambda}_0$. These objects are the "part of a complex Lagrangian manifold" $\mathscr{L}$ "almost" invariant ($\bmod (I_1^2 + \ldots + I_n^2)^{k/2}$ and $\bmod (\mathscr{I}_2^2 + \ldots + \mathscr{I}_n^2)^{k/2}$) with respect to the Hamiltonian flow g_H^t generated by the Hamiltonian $H = \frac{p^2}{2} + V(x)$ and giving the semi-classical asymptotics of the ground state eigenfunctions. The cycles on $\Lambda_0^{\pm}$, along with the Bohr–Sommerfeld quantization rule (with $\nu_j = 0$), give the asymptotics of the eigenvalues $E_0^{\pm}$ and the cycle on $\tilde{\Lambda}_0$ gives the splitting exponent. Actually, these naive considerations lead to

formula [5.14], although its accurate proof is completely different. We mention here [CRE 94], where similar arguments were applied to calculate the splitting of highly excited states in the integrable non-separable case.

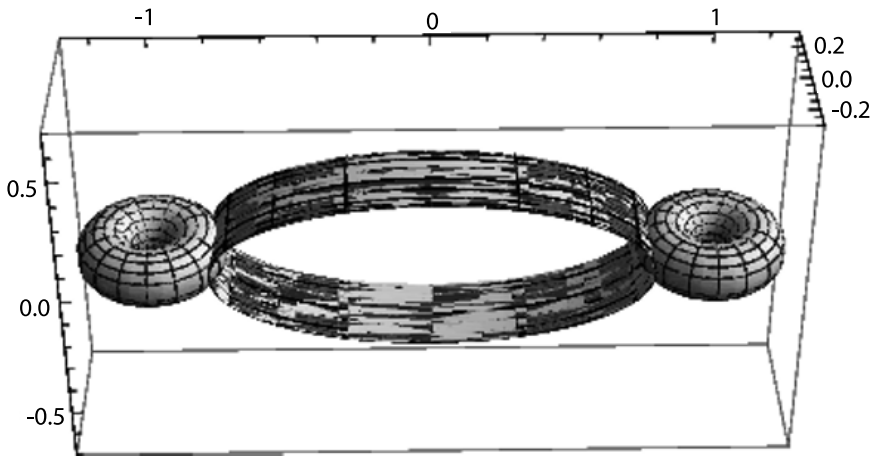

Figure 5.5. *Two Liouville (Lagrangian) tori* $\Lambda_0^{\pm}$ *in the real phase space connected by the "tunnel" Lagrangian band in the complex phase space*

5.5. Constructing the asymptotics for the eigenfunctions in tunnel problems

5.5.1. *Complex WKB-method*

The accurate proof of formulas [5.5] and [5.6], as well as formulas [5.7] and [5.8] in the 1D case could be given using the complex WKB-method (e.g. see [FED 65] and [SLA 69]). This approach is related to the analysis of the original Schrödinger equation on the complex plane and is not possible (at least up to now) in the multidimensional case without some additional conditions like separation of variables in the original Shrödinger-type operator, which implies the complete integrability of the corresponding classical Hamiltonian system. These conditions allow us to reduce the original multidimensional problem to a set of 1D problems and give us the opportunity to apply the 1D complex WKB-method. We point out that the corresponding splitting formulas again have the same Landau–Lifshitz form, although the construction of asymptotics as well as their physical meaning could be very different from the double-well ones and related, for example, to the so-called overbarrier reflection (see [DOB 99]).

5.5.2. *WKB-methods with real and pure imaginary phases*

To construct asymptotic eigenfunctions and calculate the splitting for the ground states, one can use the WKB-method with "pure imaginary phase" (we call it the "tunnel" semi-classical approximation) and seek the solution of the Schrödinger equation $\hat{H}\psi = E\psi$ in the form $\psi = A(x)e^{-S(x)/h}(1 + O(h))$, where the phase satisfies $S(x) \geq 0$ and $A(x)$ is the amplitude. If we substitute this function into the Schrödinger equation and omit the terms $O(h)$, then we obtain the Hamilton–Jacobi equation $\frac{(\nabla S)^2}{2} - V(x) = -E$ or $\mathscr{H}(\nabla S, x) = -E$. Here $\mathscr{H} = \frac{p^2}{2} - V(x)$ is the tunnel Hamiltonian. By matching the coefficients of the higher powers of h, we arrive at the transport equations. Their solutions define formal asymptotic series for the eigenfunctions, which satisfy the Schrödinger equation up to $O(h^\infty)$. The global formal asymptotic series for the eigenfunctions in the quantum double-well problem could be presented in the form of the Maslov tunnel canonical operator [MAS 84, DOB 91]. The main difficulty here is to prove that this series defines the asymptotic behavior of the true eigenfunctions in the sense of the C-norm taking into account the exponential decay of the eigenfunctions outside a neighborhood of the minima $x_\pm$ of the potential $V(x)$.

We recall that one obtains a different (in fact, standard in semi-classical analysis) Hamilton–Jacobi equation $\frac{(\nabla S)^2}{2} + V(x) = -E$ or $H(\nabla S, x) = E$ with the standard Hamiltonian $H = \frac{p^2}{2} + V(x)$ if one seeks the solution of the same Schrödinger equation in the standard WKB form $\psi = A(x)e^{iS(x)/h}(1 + O(h))$ (i.e. with real phase).

The amplitude for splitting between the least eigenstates in the multidimensional case was written out (and proved rigorously) in [DOB 91] using the tunnel semi-classical approximation. Most earlier works treating the 1D case also used this method (see, for instance, [PAN 84, HEL 84, HEL 85] for rigorous proofs). However, we mention [HAR 78] where the WKB-method with real phase was applied. This led to some technical difficulties due to the closeness of the transition points. Moreover, proving that WKB-approximation is accurate relied on very delicate comparison theorems.

Let us recall the key differences between the standard and tunnel semi-classical asymptotic expansions.

1) As a rule, the solution of the Hamilton–Jacobi equation is multivalued and has branching points; the set of the latter consists of focal points and caustics (Lagrangian singularities). In standard semi-classical analysis, this means that the WKB-approximation is typically presented as the sum

$$\sum_j (A_j(x) + O(h))e^{iS_j(x)/h} \qquad [5.17]$$

where each term corresponds to a branch of the solution of the Hamilton–Jacobi equation and affects the asymptotic expansion. The "tunnel" semi-classical approximations are different: one should preserve only one term with the minimum phase $S = \min\{S_j(x)\}$; the other terms are exponentially small with respect to the correction $O(h)e^{-S(x)/h}$, and instead of the sum [5.17] we simply have one term

$$A(x)e^{-S(x)/h}(1+O(h)).$$

That is why it is better to refer to the Hamilton–Jacobi equation arising in tunnel problems as the "Hamilton–Jacobi–Bellman" equation. Its solution is a single-valued continuous but not smooth function. It arises in control theory, in large deviation problems in probability theory, etc. It is an interesting fact that the Hamilton–Jacobi–Bellman equation is linear from the viewpoint of the so-called "tropical mathematics" (in an appropriate semiring); see [MAS 84, KOL 97, LIT 07].

2) One should use the (partial) Fourier transform to construct the asymptotic eigenfunction in a neighborhood of caustics and focal points in the standard semi-classical framework (in the case of "standard" Maslov canonical operator [MAS 81]). This idea seems to be hopeless in the tunnel case, because after the Fourier transform the phase becomes a complex-valued function.

5.5.3. *Variational methods*

Let us restrict ourselves to the case where $V(x_1,x_2,\ldots,x_n) = V(-x_1,x_2,\ldots,x_n)$, i.e. V is symmetric with respect to the hyperplane $x_1 = 0$. This hyperplane divides the configuration space into two symmetric half-spaces, say, $\mathbb{R}^{n\pm}_x$, including the minima $x_\pm$, respectively. The Maslov tunnel canonical operator gives an asymptotic expansion for the eigenfunctions as a sum $\psi = C^+\Psi^+_{as}(x) + C^-\Psi^-_{as}(x)$, where the supports of $\Psi^\pm_{as}(x)$ belong to some small neighborhood of the half-spaces $\mathbb{R}^{n\pm}_x$, $\Psi^-_{as}(x_1,x_2,\ldots,x_n) = \Psi^+_{as}(-x_1,x_2,\ldots,x_n)$ and $C^\pm$ are real constants. The substitution of this sum into the variational principle $\int_{\mathbb{R}_x} \psi\hat{H}\psi dx \longrightarrow \min, ||\psi|| = 1$ readily gives $C^+ = C^-$ for the eigenfunction corresponding to the least eigenvalue and $C^+ = -C^-$ for the next state.This gives

$$\psi^\pm \approx C(\Psi^-_{as} \pm \Psi^+_{as}).$$

As said before, it is reasonable to replace the instanton by an appropriate libration, which is a cycle on a complex Lagrangian manifold. This passage, based on the ideas presented in the previous section, was made at the physical level of rigor in [BRÜ 06], and a rigorous proof is presented in [ANI 13a, ANI 13b]. We discuss it in more detail in section 7.

5.6. Splitting of the eigenvalues in the presence of magnetic field

We start by an important remark about the Schrödinger equation. The WKB solution $A(x)e^{-\frac{S(x)}{h}}$ with pure imaginary phase substituted into this equation gives the Hamilton–Jacobi equation with *real* Hamiltonian, although it is different from the Hamilton–Jacobi equation that we obtain by using the standard WKB solutions $A(x)e^{i\frac{S(x)}{h}}$ with real phase. This property is based on a simple equation $(ip) = -p^2$. If one considers the Schrödinger equation with magnetic field $\frac{(\hat{p}-A(x))^2}{2} + V(x)\psi = E\psi$, where $A(x)$ is the vector potential of the magnetic field $B = \nabla \times A$, then the corresponding "tunnel" Hamiltonian is the complex-valued function $\frac{(ip-A(x))^2}{2} + V(x)$ and all the above considerations become meaningless. Nevertheless, sometimes a certain trick allows us to reduce the quantum double well in a magnetic field to a "standard" quantum double well without the magnetic field and again obtain the Landau–Lifshitz-type splitting formula.

Such an example is given by the 2D Shrödinger operator with the double-well potential $V(y,z) = v_1(y) + \frac{\omega_2^2 z^2}{2}$ in the presence of a homogeneous magnetic field. Here, $v_1(y)$ is a 1D double well having two non-degenerate minima at $y = \pm a$ (e.g. $v_1 = \omega_1^2(y^2 - a^2)^2/(8a^2)$). In the Landau gauge, the Shrödinger operator has the form

$$\hat{H} = -\frac{h^2}{2}\frac{\partial^2}{\partial y^2} + \frac{1}{2}(-ih\frac{\partial}{\partial z} - by)^2 + V(y,z). \qquad [5.18]$$

In the presence of the magnetic field, the lower part of the spectrum of the operator $\hat{H}$ is still regular. As before, the spectrum has power degeneracy, and to find it one can again use the harmonic oscillator approximation. The splitting between the eigenvalues is also exponentially small, but, as explained earlier, the methods in [DOB 91, DOB 93, BRÜ 06, ANI 13a, ANI 13b] do not work in this case.

However, in this special case, the spectral problem for the operator $\hat{H}$ can be reduced to that for the Shrödinger operator with a double-well potential without the magnetic field. Namely, define the Fourier transform with respect to z,

$$\widetilde{\psi}(y,p_z) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \psi(y,z)e^{\frac{i\omega_2 p_z z}{h}}\,dz.$$

Let $x_1 = y$ and $x_2 = p_z$ be the new "mixed" coordinates. Then, in this representation, the operator $\hat{H}$ (see [BRÜ 13]) has the form

$$\hat{H}' = \frac{\hat{p}_1^2}{2} + \frac{\hat{p}_2^2}{2} + v_1(x_1) + \frac{(\omega_2 x_2 - bx_1)^2}{2}, \qquad [5.19]$$

where operators $\hat{p}_1 = -ih\frac{\partial}{\partial x_1}$ and $\hat{p}_2 = -ih\frac{\partial}{\partial x_2}$ correspond to $-ih\frac{\partial}{\partial y}$ and $-\omega_2 z$, respectively. The last two summands in $\hat{H}'$ are a function of $x = (x_1, x_2)$.

We see that the magnetic field appears in $\hat{H}'$ only as a parameter of the potential $\widetilde{V}$. The potential is invariant with respect to the inversion $x_{1,2} \to -x_{1,2}$, and its minima are the points $(x_1, x_2) = (a, \frac{b}{\omega_2}a)$ and $(x_1, x_2) = -(a, \frac{b}{\omega_2}a)$, where $a > 0$ denotes the minimum of v_1. Hence, in this special case, the spectral problem for the operator $\hat{H}$ is reduced to that without the magnetic field, and we can use the methods discussed above as well as the splitting formulas [5.14]–[5.15] (in the case of $n = 2$). Let us return to the original coordinates (y, z) and conjugate momenta (p_y, p_z). The Hamiltonian H corresponding to operator [5.18] is $H = \frac{1}{2}p_y^2 + \frac{1}{2}(p_z^2 - by)^2 + V(y, z)$, and the libration in mixed complex coordinates (we use the objects and notation introduced in section 5.4.3) implies the "complex Lagrangian band "

$$\tilde{\Lambda}_0 = \{p_y = i\big(P_1(\phi_1, \varepsilon) + w_1(\phi_1, \varepsilon)\sinh\phi\big), p_z = X_2(\phi_1, \varepsilon) + z_2(\phi_1, \varepsilon)\sinh\phi,$$

$$y = X_1(\theta, \varepsilon) + z_1(\theta, \varepsilon)\cosh\phi, z = -\frac{i}{\omega_2}\big(X_2(\theta, \varepsilon) + z_2(\theta, \varepsilon)\cosh\phi\big)\}.$$

By fixing the variable ϕ, we obtain the "tunnel" cycle defining the splitting of the lowest eigenvalues. We see again that the splitting has the form of the Landau–Lifshitz formula based on an appropriate cycle on the corresponding complex Lagrangian manifold.

Finally, we mention that all examples related to tunneling in a deterministic situation show that (1) the existence of constructive splitting formulas is related to the integrability or almost integrability of the corresponding Hamiltonian systems; (2) the main object in the splitting formulas is a certain "tunnel" cycle on the complex Lagrangian manifold; and (3) the splitting looks like a Landau–Lifshitz formula with a coefficient universal for each class of tunnel problems.

5.7. Proof of main theorem (a sketch)

We restrict ourselves to the case of a potential symmetric with respect to the hyperplane $\{x_1 = 0\}$. The way of proving theorem 5.1 is somewhat roundabout. We start by writing out the asymptotic splitting formula with the instanton action in the exponential. This step was performed in [DOB 91] using the tunnel canonical operator. The following simple formula plays a key role in the derivation of the formula.

5.7.1. *Lifshitz–Herring formula*

Let χ_1, λ_1 and χ_2, λ_2 be the eigenfunctions and eigenvalues of some certain operator $\hat{L}$ in $\mathbb{R}^n_x$, and let Ω be a domain in $\mathbb{R}^n_x$. Then, we can readily prove that

$$\lambda_1 - \lambda_2 = \frac{\int_\Omega \left(\chi_2 \hat{L}\chi_1 - \psi_1 \hat{L}\chi_2\right) dx^n}{\int_\Omega \chi_2 \chi_1 dx^n}. \qquad [5.20]$$

This type of formula in the 1D case was suggested by Lifshitz and in the n-dimensional case by Herring. Let us apply this formula to the operator $\hat{H}$. By choosing $\Omega = \mathbb{R}^{n-}_x = \{x_1 < 0\}$, $\lambda_1 = \varepsilon^-, \chi_1 = \psi^-, \lambda_2 = \varepsilon^+, \chi_2 = \psi^+$, by assuming that the functions $\psi^\pm$ decay sufficiently rapidly at infinity, and by using the Green's formula, we obtain

$$\varepsilon^- - \varepsilon^+ = \frac{-h^2 \int_{\mathbb{R}^{n-1}} \left(\psi^+ \frac{\partial \psi^-}{\partial x_1} - \psi^- \frac{\partial \psi^-}{\partial x_1}\right)|_{x_1=0} dx^{n-1}}{\int_{\mathbb{R}^{n-}_x} \psi^+ \psi^- dx^n}. \qquad [5.21]$$

5.7.2. *Instanton splitting formula*

Now we replace the functions $\psi^\pm$ with their tunnel WKB approximation and calculate the integrals in [5.21] by the Laplace method. It is easily seen that one can use the oscillator approximation for ψ_+, ψ_- to calculate the integral in the denominator. The stationary point $x = x^0 = (0, x_2^0, , x_2^0 \ldots, 0)$ in the numerator is where the instanton crosses the hyperplane $x_1 = 0$. It is also necessary to find out the determinant of the Hessian $||\frac{\partial S}{\partial x_j \partial x_k}(x^0)||, j,k = 2, \ldots, n$. This gives the formula

$$\Delta E_0 = A_0(h) e^{-\frac{S_0}{h}} (1 + o(1)), \quad A_0(h) = 2\sqrt{\frac{h\omega_1 \ldots \omega_n}{\pi}}\, \mathscr{J}^{-\frac{1}{2}} Q\big|_{x_1=0} |\mathscr{P}_0|. \qquad [5.22]$$

Here, $S(0) = \frac{1}{2} \int\limits_{\Gamma(0)} \mathscr{P}(\phi^t, 0)\, d\mathscr{X}(\phi^t, 0)$ is the instanton action, $\mathscr{P}_0$ is the momentum (or the velocity) of the instanton at the point where it crosses the hyperplane $x_1 = 0$, and $\mathscr{J}$ and Q are the determinants of some matrices.

The next step is to express $\mathscr{J}$ and Q in terms of appropriate matrix solutions of the variational system associated with the instanton. This was done in [DOB 93]; the formula for splitting amplitude becomes more constructive and pragmatic, but nevertheless the problem of finding these determinants does not disappear. It becomes very complicated in the case of large n (for example, in condensed matter physics [KAT 96]).

The remaining part of the proof uses only classical mechanics, not appealing to the semi-classical arguments. The main component here is the following delicate asymptotic formula for the action on librations with small negative energy.

5.7.3. *Asymptotic behavior of the libration action*

Define $\mathscr{I}(\mathscr{E}) = \frac{1}{2\pi} \oint\limits_{\Gamma(\mathscr{E})} p\,dx$. Then (see [ANI 13a])

$$\mathscr{I}(0) - \mathscr{I}(\mathscr{E}) = -\frac{\mathscr{E}}{\pi\omega_1} - \mathscr{E}\frac{2\ln 2}{\pi\omega_1} - \frac{\mathscr{E}T_{\mathscr{E}}}{\pi} + o(\mathscr{E}), \quad \mathscr{E} \to -0. \qquad [5.23]$$

Here, $T_{\mathscr{E}}$ is the time required to cover the distance between the points of the instanton where $-V = \mathscr{E}$.

Let us explain the structure of this formula. Let $\hat{T}_{\mathscr{E}}$ be half of the libration period $\Gamma(\mathscr{E})$. It turns out (see [ANI 13a]) that $\hat{T}_{\mathscr{E}} = T_{\mathscr{E}} + \frac{2\ln 2}{\omega_1} + o(1)$. Hence, the right-hand side of [5.23] acquires the form $-\frac{\mathscr{E}}{\pi\omega_1} - \frac{\mathscr{E}\hat{T}_{\mathscr{E}}}{\pi} + o(\mathscr{E})$. Recall that $-\frac{\mathscr{E}\hat{T}_{\mathscr{E}}}{\pi}$ is none other than the difference between the Maupertuis and Hamilton's actions on the libration. (The Hamilton action is $\frac{1}{2\pi}\oint\limits_{\gamma_{\mathscr{E}}}(p\,dx - H\,dt)$.) Therefore, [5.23] merely states that $-\frac{\mathscr{E}}{\omega_1}$ is the principal term of the difference between the Hamilton actions on the instanton and the libration.

5.7.4. *Reduction to the 1D splitting problem*

Suppose that $x = r(s)$ $(-l \le s \le l)$, $(r(\pm l) = x_{\pm})$ is a natural parameterization of $\Gamma(0)$ with respect to the Euclidean metric and $e_j(s)$, $j = 1, \ldots, n$ is the Frenet–Serret frame. Let $x \to s, q_2, \ldots, q_n$ be the following change of coordinates: $x = r(s) + \sum\limits_{j=2}^{n} q_j e_j(s)$.

Let $\hat{H}^I = -\frac{h^2}{2}\frac{d^2}{ds^2} + V_0$ be the 1D Shrödinger operator, where $V_0(s)$ is the value of the potential V at the point of the instanton with coordinate s.

By using the splitting formula in [DOB 93] for the operators $\hat{H}$ and $\hat{H}^I$, we obtain the relation $E_0^+ - E_0^- = \mathscr{T}(\mu_0^+ - \mu_0^-)(1 + o(1))$, where $\mu_0^{\pm}$ are the least eigenvalues of the operator $\hat{H}^I$. The factor $\mathscr{T}$ (independent of h, because $A_0 \sim \sqrt{h}$ in any dimension) is expressed in terms of some boundary value problem for the variational system near $\Gamma(0)$. It then follows from (5.8) that

$$E_1 - E_0 = \mathscr{T}\sqrt{\frac{\pi}{e}}\frac{\omega_1 h}{\pi} e^{-\frac{\pi\mathscr{I}}{h}}(1 + o(1)), \qquad [5.24]$$

where $\mathscr{H}_0(\mathscr{I}) = -\frac{h\omega_1}{2}$.

5.7.5. *Asymptotic behavior of the Floquet exponents*

The next step is finding the asymptotics for the sum of the positive Floquet exponents λ_j^T of a libration with large period $4T$ (occurring in [5.15]). It is shown in [ANI 13b] that

$$\sum_{j=2}^{n} \lambda_j^T = \sum_{j=2}^{n} \omega_j - \frac{\ln \mathscr{T}}{T} + o\left(\frac{1}{T}\right), \qquad T \to +\infty \qquad [5.25]$$

5.7.6. *Finishing the proof*

By combining [5.15] and [5.25], we obtain

$$\mathscr{H}_0(\mathscr{I}_0) - \frac{h}{2}\left(\sum_{j=2}^{n} \omega_j - 4\frac{\ln \mathscr{T}}{T(\mathscr{I}_0)}\right) = -\frac{h}{2}\sum_{j=1}^{n} \omega_j + O(h^{1+\varepsilon}).$$

By the Taylor formula, $\mathscr{H}_0(\mathscr{I}_0) = \mathscr{H}_0(\mathscr{I}) + \frac{2\pi}{T(\mathscr{I})}(\mathscr{I}_0 - \mathscr{I}) + O(h^{1+\varepsilon})$, and so

$$\frac{2\pi}{T(\mathscr{I})}(\mathscr{I}_0 - \mathscr{I}) + \frac{2h\ln \mathscr{T}}{T(\mathscr{I})} = O(h^{1+\varepsilon}),$$

or $\mathscr{I} = \mathscr{I}_0 + \frac{h\ln \mathscr{T}}{\pi} + O(h^{1+\varepsilon})$. The substitution of the latter formula into [5.24] finishes the proof.

5.8. Conclusion

In this chapter, we discussed the splitting of the least eigenvalues of the multidimensional Shrödinger operator with the double-well potential V. As a rule, the splitting formula is based on the instanton which is a singular trajectory of the Newtonian system with the (inverted) potential $-V$. We showed that this formula takes a more natural "Landau–Lifshitz" form if one changes the instanton by an appropriate libration which is an unstable periodic trajectory of the same system. We explained the main ideas and principal steps of the derivation of the splitting formula, its relationship with the normal form theory, "almost integrability" of a corresponding Hamiltonian system, cycles on a complex Lagrangian manifold, etc. We also considered the splitting of the lowest eigenvalues in the example of 2D Shrödinger operator with the double-well potential placed in homogeneous magnetic field and showed that in this case the splitting formula has again the "Landau–Lifshitz" form.

5.9. Acknowledgments

Sergey Yu. Dobrokhotov was supported by the grant RFBR 11-01-12058 and project DFG-RAS (DFG 436 RUS 113/572). Anatoly Yu. Anikin was partially supported by RFBR, research project No. 12-01-00441, and by the Program for Supporting Leading scientific schools (under grant no. NSh-2519.2012.1). We express our gratitude to S. Bolotin, V. Nazaikinskii and D. Treschev for useful discussions.

5.10. Bibliography

[ALB 04] ALBEVERIO S., DOBROKHOTOV S.Y., SEMENOV E.S., "Splitting formulas for the higher and lower energy levels of the one-dimensional Schrödinger operator", *Theoretical and Mathematical Physics*, vol. 138, no. 1, pp. 98–106, 2004.

[ALE 82] ALENITSYN A.G., "Spectrum splitting caused by a potential barrier in problems with symmetrical potential", *Differentsial'nye Uravneniya*, vol. 18, no. 11, pp. 1971–1975, 1982.

[ANI 13a] ANIKIN A.Y., "Asymptotic behaviour of the Maupertuis action on a libration and a tunneling in a double well", *Russian Journal of Mathematical Physics*, vol. 20, no. 1, pp. 1–10, 2013.

[ANI 13b] ANIKIN A.Y. "Libration and splitting of the ground state in multidimensional double well problem", *Theoretical and Mathematical Physics*, vol. 175, no. 2, pp. 609–319, 2013.

[ARN 06] ARNOL'D V.I., KOZLOV V.V., NEJSHTADT A.I., *Mathematical Aspects of Classical and Celestial Mechanics. Dynamical Systems III*, Series: Encyclopaedia of Mathematical Sciences, vol. 3, Springer, 2006.

[AVI 75] AVILOV V.V., IORDANSKII S.V., "Calculation of exchange corrections for a crystal", *Journal of Experimental and Theoretical Physics*, vol. 42, pp. 638–689, 1975.

[BOL 78] BOLOTIN S.V., "Libration motions of natural dynamical systems", *Vestnik Moskovskogo Universiteta, Seria. I Matematika. Mekhanika*, vol. 6, pp. 72–77, 1978. [In Russian].

[BOL 78b] BOLOTIN S. V., KOZLOV V. V., "Libration in systems with many degrees of freedom", *Journal of Applied Mathematics and Mechanics*, vol. 42, no. 2, pp. 256–261, 1978.

[BRÜ 06] BRÜNING J., DOBROKHOTOV S.Y., SEMENOV E.S., "Unstable closed trajectories, librations and splitting of the lowest eigenvalues in quantum double well problem", *Regular Chaotic Dynamics*, vol. 11, no. 2, pp. 167–180, 2006.

[BRÜ 13] BRÜNING J., DOBROKHOTOV S.Y., NEKRASOV R.V., "Splitting of the lowest energy levels in quantum double well in magnetic field and tunneling of wave packets in nanowires", *Theoretical and Mathematical Physics*, vol. 175, no. 2, pp. 620–636, 2013.

[BRU 89] BRUNO A.D., "Normalization of a Hamiltonian system near an invariant cycle or torus", *Russian Mathematical Surveys*, vol. 44, no. 2, pp. 53–89, 1989.

[COL 77] COLEMAN S., "The uses of instantons", *Proceedings of the International School of Physics*, Erice, 1977.

[COM 83] COMBES J.M., DUCLOS P., SEILER R., "Krein's formula and one-dimensional multiple-well", *Journal of Functional Analysis*, vol. 52, pp. 257–301, 1983.

[CRE 94] CREAGH S.C., "Tunnelling in multidimensional systems", *Journal of Physics A: Mathematical and General*, vol. 27, pp. 4969–4993, 1994.

[CRE 98] CREAGH S.C., "Tunnelling in two dimensions", *Tunnelling in Complex Systems*, World Scientific Publishing Co. Pte Ltd, Singapore, 1998.

[CRE 99] CREAGH S.C., WHELAN N.D., "A matrix element for chaotic tunnelling rates and scarring intensities", *Annals of Physics*, vol. 272, no. 2, pp. 196–242, 1999.

[DOB 91] DOBROKHOTOV S.Y., KOLOKOL'TSOV V.N., MASLOV V.P., "Splitting of the lowest energy levels of the Schrödinger equation and asymptotic behavior of the fundamental solution of the equation $hu_t = h^2\Delta u/2 - V(x)u$", *Theoretical and Mathematical Physics*, vol. 87, no. 3, pp. 561–599, 1991.

[DOB 93] DOBROKHOTOV S.Y., KOLOKOL'TSOV V.N., "Splitting amplitudes of the lowest energy levels of the Schrödinger operator with double-well potential", *Theoretical and Mathematical Physics*, vol. 94, no. 3, pp. 300–305, 1993.

[DOB 99] DOBROKHOTOV S.Y., SHAFAREVICH A.I., "'Momentum' tunneling between tori and the splitting of eigenvalues of the Beltami-Laplace operator on Liouville surfaces", *Mathematical Physics, Analysis and Geometry*, vol. 2, no. 2, pp. 141–177, 1999.

[FED 65] FEDORYUK M.V., "Asymptotics of the discrete spectrum of the operator $w''(x) - \lambda^2 p(x)w(x)$", *Matematicheskiy Sbornik (N.S.)*, vol. 68(110), no. 1, pp. 81–110, 1965.

[GIL 77] GILDENER E., PATRASCIOIU A., "Pseudoparticle contributions to the energy spectrum of a one-dimensional system", *Physical Review D.*, vol. 16, pp. 425–443, 1977.

[HAR 78] HARRELL E., "On the rate of asymptotic eigenvalue degeneracy", *Communications in Mathematical Physics*, vol. 60, pp. 73–95, 1978.

[HAR 80] HARRELL E., "Double wells", *Communication in Mathematical Physics*, vol. 75, pp. 239–261, 1980.

[HEL 84] HELFFER B., SJÖSTRAND J., "Multiple wells in the semi-classical limit. I", *Communications in Partial Differential Equations*, vol. 9, no. 4, pp. 337–408, 1984.

[HEL 85] HELFFER B., SJÖSTRAND J., "Puits multiples en limite semi-classique. II. Interaction moléculaire. Symétries. Perturbation", *Annales de l'institut Henri Poincaré (A) Physique théorique*, vol. 42, no. 2, pp. 127–212, 1985.

[JON 81] JONA-LASINIO G., MARTINELLI F., SCOPPOLA E., "New approach to the semiclassical limit of quantum mechanics. I. Multiple tunnelings in one dimension", *Communication in Mathematical Physics*, vol. 80, pp. 223–254, 1981.

[KAT 96] KATSNELSON M.I., VAN SCHILFGAARDE M., ANTROPOV V.P., *et al.*, "*Ab initio* instanton molecular dynamics for the description of tunneling phenomena", *Physical Review A*, vol. 54, pp. 4802–4809, 1996.

[KOL 97] KOLOKOL'TSOV V.N., MASLOV V.P., *Idempotent Analysis and its Applications*, Kluwer Publishing House, 1997.

[LIT 07] LITVINOV G.L., "The Maslov dequantization, idempotent and tropical mathematics: a brief introduction", *Journal of Mathematical Sciences*, vol. 140, no. 3, pp. 426–444, 2007.

[LAN 77] LANDAU L.D., LIFSHITZ E.M., *Quantum Mechanics: Non-Relativistic Theory*, Pergamon Press, 1977.

[MAR 87] MARTINEZ A., "Estimations de l'effet tunnel pour le double puits I", *Journal de Mathématiques Pures et Appliquées*, vol. 66, pp. 195–215, 1987.

[MAR 88] MARTINEZ A., "Estimations de l'effet tunnel pour le double puits II - Etats hautement excités", *Bulletin de la Société Mathématique de France*, vol. 116, pp. 199–229, 1988.

[MAS 84] MASLOV V.P., "Global exponential asymptotic behavior of solutions of the tunnel equations and the problem of large deviations", *Proceedings of the Steklov Institute of Mathematics*, vol. 163, pp. 150–180, 1984.

[MAS 81] MASLOV V., FEDORYUK M., *Semiclassical Approximation in Quantum Mechanics*, Reidel, Dordrecht, 1981.

[PAN 84] PANKRATOVA T.F., "Quasimodes and splitting of eigenvalues", *Doklady Akademii Nauk SSSR*, vol. 276, no. 4, pp. 795–798. [In Russian].

[POL 77] POLYAKOV A.M., "Quark confinement and topology of gauge theories", *Nuclear Physics B.*, vol. 120, pp. 429–458, 1977.

[SIM 84] SIMON B., "Semiclassical analysis of low lying eigenvalues II", *Annals of Mathematics*, vol. 120, pp. 89–118, 1984.

[SIM 85] SIMON B., "Semiclassical analysis of low lying eigenvalues IV. The flea on the elephant", *Journal of Functional Analysis*, vol. 63, pp. 123–136, 1985.

[SLA 69] SLAVYANOV S.Y., "The asymptotic behavior of singular Sturm-Liouville problems with respect to a large parameter in the case of nearby transition points", *Differentsial'nye Uravneniya*, vol. 5, no. 2, pp. 313–325, 1969. [In Russian].

[WIL 86] WILKINSON M., "Tunnelling between tori in phase space", *Physica D: Nonlinear Phenomena*, vol. 21, pp. 341–354, 1986.

[WIL 87a] WILKINSON M., "Narrowly avoided crossings", *Journal of Physics A*, vol. 20, pp. 635–645, 1987.

[WIL 87b] WILKINSON M., HANNAY H., "Multidimensional tunnelling between excited states", *Physica D: Nonlinear Phenomena*, pp. vol. 27, 201–212, 1987.