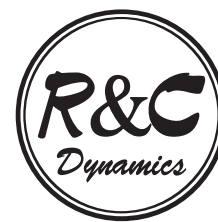


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UNSTABLE CLOSED TRAJECTORIES, LIBRATIONS AND SPLITTING OF THE LOWEST EIGENVALUES IN QUANTUM DOUBLE WELL PROBLEM

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We discuss the structure of asymptotic splitting formula for the lowest eigenvalues of multidimensional quantum double well problem. We show that the change of instanton by closed unstable trajectory of appropriate Hamiltonian system gives more natural and simpler preexponential factor (amplitude) in splitting formula. The projection of this trajectories onto configuration space are well know librations in classical mechanics.

1. Splitting of eigenvalues and closed trajectories in the 1D quantum double well problem

The symmetric potentials $V(x)$, $x \in \mathbb{R}^n$, with two minimum points play an important role in problems of quantum mechanics related to the tunneling effect. Under appropriate conditions, these effects can be well described within the framework of the semiclassical approximation appealing to trajectories of classical mechanics.

First, we recall several simple facts and formulas concerning the one-dimensional case ($n = 1$). We assume that $V(x) = V(-x)$ is a smooth function increasing at infinity with two minimum points x_{\pm} such that $V(x_{\pm}) = 0$. Then the spectrum of the Schrödinger operator $-\frac{\hbar^2}{2} \frac{d^2}{dx^2} + V(x)$ behaves as follows as $\hbar \rightarrow 0$. The eigenvalues of this operator located between $V(x_{\pm}) = 0$ and $V(0)$ turn out to be twice degenerate asymptotically. We denote them by E_n^{\pm} . The difference between the values E_n^+ and E_n^- (the splitting value) is exponentially small in \hbar and we have $E_n^+ - E_n^- = o(\hbar^{\infty})$, $E_n^{\pm} = E_n + o(\hbar^2)$. Here E_n is an asymptotics of E_n^{\pm} in the parameter \hbar . For large $n \gg 1$, $n \sim 1/\hbar$ (excited states in quantum mechanics), the E_n are determined by the Bohr–Sommerfeld quantization rule

$$\frac{1}{2\pi} \oint p dx = \left(n + \frac{1}{2}\right) \hbar, \quad (1.1)$$

and the splitting value is given by the asymptotic formula [24] (see also [16], [28])

$$E_n^+ - E_n^- = \frac{\omega \hbar}{\pi} e^{-\pi J/\hbar} (1 + O(\hbar)). \quad (1.2)$$

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The integral in Bohr–Sommerfeld rule (1.1) can be interpreted as an integral taken along the periodic trajectory of Hamiltonian system $p = -V_x$, $\dot{x} = p$ with the classical energy lying at level E_n : $H \equiv \frac{p^2}{2} + V(x) = E_n$. This system is equivalent to the Newtonian system

$$\ddot{x} = -V_x. \tag{1.3}$$

ω in (1.2) is the frequency of motion along this trajectory. The quantity J has the form $J = \frac{1}{\pi} \int_{b_-}^{b_+} \sqrt{-2(E_n - V(x))} dx$, where $b_+ = -b_-$ are the roots of the equation $V(x) = E_n$ that are the nearest to $x = 0$ (see Fig. 1, (a)).

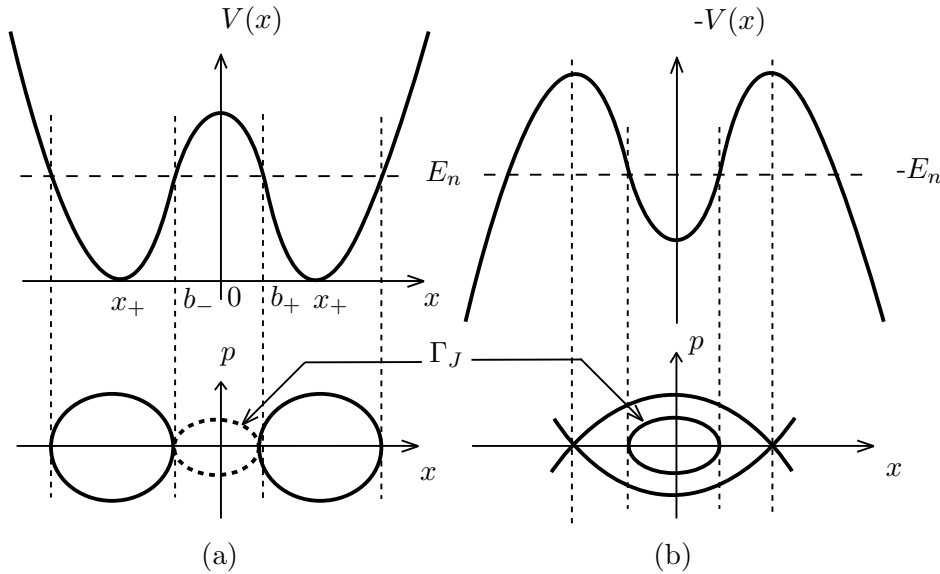


Fig. 1. The phase–plane portraits corresponding to the Hamiltonians H (a) and \mathcal{H} (b).

Both formula (1.1) for the energy and formula (1.2) for the splitting have an explicit geometric interpretation, namely, the integral in the Bohr–Sommerfeld condition is the *action* along the closed curve, which is invariant under the flow of the Hamiltonian system with Hamiltonian $H = \frac{p^2}{2} + V(x)$ lying at level E_n . As was already noted, the frequency ω in formula (1.2) is the frequency of motion along the corresponding trajectory. The exponent J in (1.2) can be interpreted as follows. Consider the analytic continuation of the Hamiltonian $H = \frac{p^2}{2} + V(x)$ to the domain of imaginary momenta, $p \rightarrow ip$, multiplying by -1 , we obtain the Hamiltonian

$$\mathcal{H}(p, x) = -H(ip, x) \equiv \frac{p^2}{2} - V(x). \tag{1.4}$$

In the domain (b_-, b_+) (corresponding to the energies $(-V(0), 0)$), this Hamiltonian also has closed trajectories (see Fig. 1, (b)), which can be parameterized by the action variable J . Precisely this action, which corresponds to the closed trajectory Γ_J (see Fig. 1) lying at the energy level $\mathcal{H} = -E_n$, determines the exponent in the formula for the splitting. The projection of this trajectory on the x -axis connects the turning points b_- and b_+ and is called a libration ([26], [27]). We also call the corresponding trajectory in the phase space by the same name.

The Hamiltonian \mathcal{H} describes the motions at energy level $-E_n$ in the domain $V(x) > E_n$, where the motion due to “standard” systems (1.3) is impossible. We shall say that the domain $V(x) > E_n$ is

classically prohibited and the domain $V(x) \leq E_n$ is classically allowed. Thus the trajectory Γ_J lies in the classically prohibited domain. We note that the Newtonian system generated by the Hamiltonian \mathcal{H} (describing Γ_J) has the form

$$\ddot{x} = V_x \quad (1.5)$$

and the potential in this system is the “inverted” potential in system (1.3). Such a system with an “inverted” potential (in the classically prohibited domain) can be obtained from the Newtonian system (1.3) in the “classically allowed domain” by replacing the real time t with the imaginary time it . This argument is often used in the physics literature. In our consideration, it is most convenient to pass from Hamiltonian H to (1.4) replacing p with ip (see [15], [40], [29], [34], [20]).

We see that the exponent in the formula for the splitting of eigenvalues for excited states is the action variable of libration lying at the “inverted” energy level of the periodic classical trajectories determining the Bohr–Sommerfeld quantization rule. The splitting amplitude is completely determined by the frequency of motion along the latter trajectories: the splitting formula does not contain any additional Maslov-index-type objects related to the trajectory Γ_J (which contribute $1/2$ to the Bohr–Sommerfeld rule (1.1)). Under appropriate analyticity assumptions, the procedure of calculating the action J can be described as follows. As J is an integral of motion for the Hamiltonian system with Hamiltonian \mathcal{H} , we have $J = J(p, x)$. The analytic continuation $J = J(ip, x)$ gives an integral in the classically allowed domain for the Hamiltonian system with the original Hamiltonian H , which, in turn, must be expressed only in terms of the integral I , i. e., the action variable corresponding to the trajectory in one of the potential wells. This gives the relation $J = J(I)$ equivalent to

$$\mathcal{H}(J) = -H(I), \quad (1.6)$$

and precisely this relation determines the splitting of excited eigenvalues.

We note that the periodic trajectories in the classically allowed domain (in “potential wells”), which generate quantization condition (1.1), are also librations, but the meaning of these trajectories and of Γ_J in the quantum problem is completely different; this difference becomes especially transparent in the multidimensional case.

For lower energy levels ($n = O(1)$ as $\hbar \rightarrow 1$), the Bohr–Sommerfeld formula remains valid, but it is more convenient to use the harmonic oscillator approximation $E_n = \omega_0 \hbar (\frac{1}{2} + n)$, where $\omega_0 = V_{xx}(x_{\pm})$ is the frequency of the “limit periodic motions” in the potential wells. Although the splitting formula (1.2) also permits passing to small n , the direct passage to the limit gives a false result. To obtain the correct formula, we must multiply the right-hand side in (1.2) by $\sqrt{\frac{\pi}{e}}$. This fact was established in [1] by comparing formula (1.2) with the formulas for the lower eigenvalues splitting, which were obtained in [38] and actually related to the limit trajectory (the separatrix) of the system with Hamiltonian \mathcal{H} , lying at zero energy level and connecting the potential maximum points x_{\pm} [17], [18], [19], [23]. This trajectory (the separatrix) in the tunneling problems is called an instanton (see e. g. [36], [7], [8]) and is the path of integration in the splitting formula. In this case, the preexponential factor in the formulas obtained in mentioned papers has a very complicated structure, and precisely passing from the classical zero energy level to the quantum level $E_0 = \hbar \omega_0 / 2$ “removes” the cumbersome expressions in the preexponent and permits reducing the splitting formula to an “elegant geometric form” similar to that obtained in [24]. Of course, passing from the zero level to the lower quantum energy level is equivalent to passing from the (separatrix) instanton to a closed trajectory (libration) lying in a small neighborhood of the separatrix.

The goal of this paper is to derive a formula for the splitting of lower energy levels, which is similar to formula (1.2) (with correction $\sqrt{\frac{\pi}{e}}$) for lower energy levels of the Schrödinger operator with potential of the form of two symmetric potential wells in the multidimensional case.

Before we state the explicit formulas, we note that the formulas for the splitting of excited states in the multidimensional case have been proved accurately only for the case of separating variables,

although several papers present formulas based on completely reasonable considerations [9], [40]. In [10], [11], [12] a two-dimensional analogue of formula (1.2) is constructed (and proved) for several problems with separating variables (treated from a different viewpoint in [25]). In this analogue, the exponent continues to contain a variable of action-variable-type generated by some tunnel cycle (but in the complex phase space in the classically prohibited domain), and the frequency ω is replaced by sum of frequencies $\omega_1 m_1 + \omega_2 m_2$ with integer-valued coefficients, which are the indices of intersection of some cycle with the basis cycles of tori in the potential wells invariant with respect to the Hamiltonian system.

For lower energy levels in multidimensional case, the splitting formulas appealing to instantons were proved accurately [22], [35], [34], [29], [37], [20], [30] without any assumptions on the integrability. Moreover, constructive but very cumbersome formulas for the preexponential factor were obtained in [13], [14]. Again, for the path of integration in calculating the exponent in the formulas given in [33], [29], [37], [20], [3], we choose a trajectory of the system (1.5) (an instanton), which does not corresponds to the lowest energy level in quantum mechanics problem. We show that passing from the instanton to closed trajectories (which are unstable in the multidimensional situation, and proved to be librations) with the correcting factor $\sqrt{\frac{\pi}{\epsilon}}$ introduced for lower energy levels permits writing (accurately proved) formulas for the splitting of lower energy levels in the form [13], [14] which is a generalization of formula (1.2). Apparently, the existence of such a representation proved to be related to the fact that the Hamiltonians H and \mathcal{H} in a neighborhood of the zero energy level can be replaced by their normal forms, which generate already integrable Hamiltonian systems.

To simplify our presentation, we only consider the two-dimensional case, and, sometimes, our reasoning is on a physics level of rigor.

2. Statement of the main result: librations and splitting for lower energy levels of the two-dimensional Schrödinger operator

Restrict ourselves to the case of two degrees of freedom and consider a two-dimensional Schrödinger operator in $L^2(\mathbb{R}^2)$ with the potential $V(x)$ having the properties described above:

$$\widehat{H}\psi = \left[\frac{1}{2} \left(-ih \frac{\partial}{\partial x_1} \right)^2 + \frac{1}{2} \left(-ih \frac{\partial}{\partial x_2} \right)^2 + V(x) \right] \Psi, \quad x = (x_1, x_2)^t \in \mathbb{R}^2 \quad (2.1)$$

We also assume that $V(x)$ is in general position. In particular, the eigenvalues ω_1^2 and ω_2^2 of the matrix of second derivatives $\partial^2 V / \partial x^2$ at the points x_- and x_+ are different. Let $\omega_1 < \omega_2$.

In a neighborhood of the lower energy levels, the structure of the spectrum of this operator is similar to the structure of the spectrum of the one-dimensional operator. In particular, there are two smallest eigenvalues E_0^+ and E_0^- such that

$$E_0^\pm = E_0 + O(h^2), \quad E_0 = \frac{h}{2}(\omega_1 + \omega_2). \quad (2.2)$$

The distance between these eigenvalues is, in fact, exponentially small in the parameter h : $E_0^+ - E_0^- = o(h^\infty)$.

Consider a Hamiltonian system equivalent to Newtonian system (1.5) (with the inverted potential $-V(x)$). It follows from the results of [37], [20], [21], [30], [12], [13], [14] that this system has a trajectory connecting the maximum points x_- and x_+ of the inverted potential $-V(x)$ in infinite time. In general, such a trajectory need not be unique, but we assume that it is unique. In general position, where, in particular, the frequencies of the limit motion ω_1 and ω_2 are different, we can use the theory of the Hamiltonian systems to prove that the instanton is entering singular points and issuing from singular points in the direction of the eigenvector of the matrix $\frac{\partial^2 V}{\partial x^2}$ corresponding to the smaller frequency ω_1 .

Let us consider the problem of trajectories of the Hamiltonian system with Hamiltonian $\mathcal{H} = \frac{p^2}{2} - V(x)$. For the energies $\mathcal{H} = -E < 0$, the domain of possible motions in the configuration space \mathbb{R}^2 is the plane without two nonintersecting symmetric domains Ω_- and Ω_+ diffeomorphic to disks. It follows from [26], [27] that, in the phase space with energy $-E$, there exists at least one closed trajectory whose projection on the configuration space is a curve diffeomorphic to an interval connecting the boundaries $\partial\Omega_-$ and $\partial\Omega_+$ and normal to them (see Fig. 2). Such a trajectory is called a libration. In this domain, we consider the action functional $\int_0^T \sqrt{2V(x(t))} |\dot{x}(t)| dt$, where the

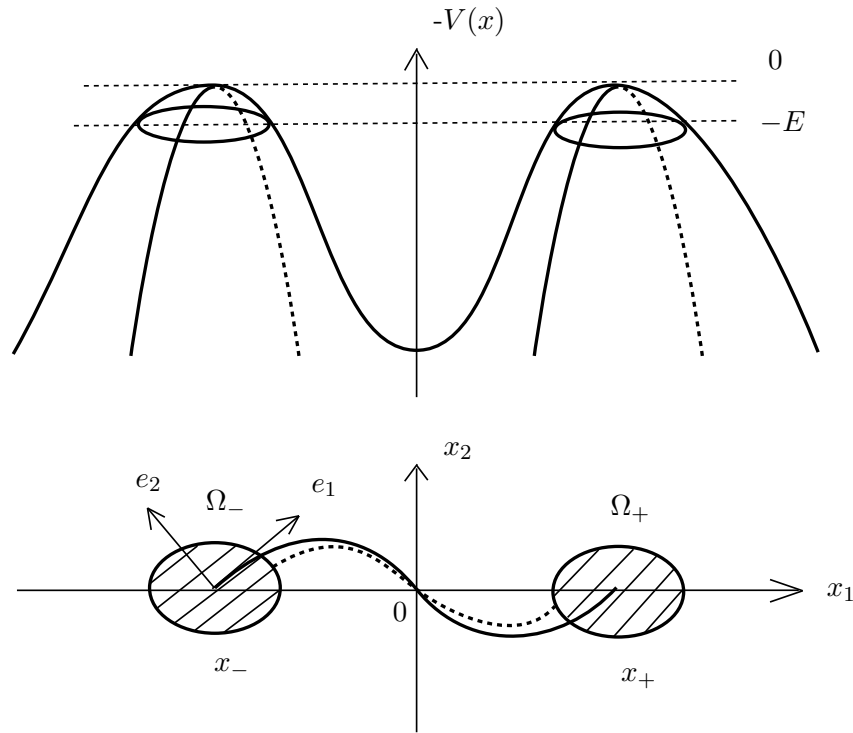


Fig. 2. The potential $-V(x)$ and the domain of possible motions for the energies $\mathcal{H} = -E < 0$. The solid curve is instanton trajectory, the broken curve is libration corresponding to the energy $-E$. e_1 and e_2 are eigenvector

minimum is sought among piecewise smooth curves $x(t)$ connecting the boundaries of the domain of possible motions in different times T . The librations are the trajectories on which this functional attains its minimum. Taking into account well-known results from the theory of periodic trajectories and from variational calculus, it is reasonable to assume that the librations form a one-parameter family of trajectories parameterized by the energy $-E$, and, moreover, the librations converge to an instanton solution as $E \rightarrow 0$. In general, the librations need not be unique for each E . On the other hand, it follows from the theory of the Hamiltonian systems that the librations are unstable trajectories for small E . Therefore, it is natural to assume that the librations form one-parametric continuous family.

The family of librations can be parameterized by the action variable J . By Γ_J we denote the libration corresponding to J . Then $J = \frac{1}{2\pi} \oint p dx$ and $J \in [0, 2J_{ins}]$, where $J_{ins} = \frac{1}{\pi} \int_{\Gamma} p dx$ is the action on the instanton Γ . As $J \rightarrow J_{ins}$, the parts of the trajectories Γ_J during the motion form the boundary $\partial\Omega_-$ to $\partial\Omega_+$, tend to Γ . Since the librations are closed trajectories in the phase space, they generate a variational system, which is a linear system with periodic coefficients

$$\dot{u} = \hat{J} \frac{\partial^2 H}{\partial y^2} \Big|_{\Gamma_J} \cdot u, \quad \hat{J} = \begin{pmatrix} 0 & -E \\ E & 0 \end{pmatrix}. \tag{2.3}$$

Here $\frac{\partial^2 H}{\partial y^2}$ is the 4x4 matrix of second derivatives of H over the variables $y = (p, x)^t$, E is the 2×2 unit matrix. By $\beta(J)$ we denote the Floquet coefficients corresponding to the motions in direction perpendicular to the motion along the libration. According to the theory of normal forms of Hamiltonian systems in a neighborhood of Γ_J , we can introduce new canonical variables J, ϕ, ξ, η such that the Hamiltonian \mathcal{H} in this neighborhood can be represented in the form

$$\mathcal{H} = \mathcal{H}_0(J) - \beta(J)\xi\eta + O(\xi^2\eta^2).$$

Omitting the terms $O(\xi^2\eta^2)$, we obtain the Hamiltonian (the normal form) of the integrable Hamiltonian system

$$\tilde{\mathcal{H}} = \mathcal{H}_0(J) - \beta(J)\xi\eta,$$

where J and $\tilde{J} = \xi\eta$ are integrals of motion. Thus, in a neighborhood of the libration, our Hamiltonian has the property of being “almost” integrable. These integrals can be expressed in terms of p and x . We assume that, in some complex neighborhood of real p, x , these functions are analytic, one can construct functions of the complex arguments p, x , and, in particular, $J'(p, x) = J(ip, x)$ and $\tilde{J}'(p, x) = \tilde{J}(ip, x)$. These functions are almost integrals of the original Hamiltonian system in the classically allowed domain for the Hamiltonian $H = \frac{p^2}{2} + V(x)$. On the other hand, the original Hamiltonian has “approximate” integrals I_1 and I_2 corresponding to the harmonic oscillator approximation of the Hamiltonian H near the minimum points x_{\pm} at which the Hamiltonian can be represented as $H = \omega_1 I_1 + \omega_2 I_2 + o(I_1, I_2)$. These integrals must be related to the integrals J' and \tilde{J}' . We will show that $\tilde{J}' = I_2 + o(I_2)$. Thus, to find the relation between the integrals J' and I_1 , it is necessary to solve the equation

$$-E \equiv \mathcal{H}_0(J) - \beta(J)I_2 = -\omega_1 I_1 - \omega_2 I_2, \tag{2.4}$$

which determines J as a function of I_1 and I_2 .

The following assertion is the main result of this paper.

Theorem 1. *The formula for the splitting of lower energy levels has the form*

$$E_0^+ - E_0^- \stackrel{\text{def}}{=} \Delta E_0 = \sqrt{\frac{\pi}{e}} \frac{\omega_1 h}{\pi} e^{-\pi J_0(h)/h} (1 + o(1)). \tag{2.5}$$

Here $J_0(h)$ is the solution of (2.4) with $I_1 = I_2 = \frac{h}{2}$.

The goal of the next sections is to derive formula (2.5) from the formulas obtained in [12], [13], [14].

REMARK 1. $J_0(h)$ is the action on the libration, but it is not connected with the energy level $\mathcal{H} = -E_0$. It would be more appropriate to say that this quantity has the following meaning. In the phase space, the equations $J = J_0(h)$ and $\tilde{J} = h$ determine an “almost invariant Lagrangian manifold.” This manifold has a complicated structure, but there is a cycle (a closed path) on it near the libration Γ_{J_0} , and the action integral $\oint p dx$ along this cycle is equal to $2\pi J_0(h)$. This cycle does not coincide with the closed trajectory of the Hamiltonian system lying at the energy level $-E_0$ in the forbidden domain. In the case of separating variables, $V(x) = V_1(x_1) + V_2(x_2)$, where $V_1(x_1)$ is a one-dimensional potential with two wells and $V_1(x_2)$ is a potential increasing at infinity, we have $\beta(J) = \omega_2$ and the motions in a direction perpendicular above-mentioned cycle do not affect the splitting. If the variables cannot be separated, we have $\beta(J) \neq \omega_2$ and the transversal motions deform the action J .

3. 2D Splitting problem for the lowest energy levels and the scattering problem

3.1. Instanton and splitting of the lowest energy levels in two-dimensional case

We first recall the formulas for the splitting of the lowest eigenvalues of the Schrödinger operator (2.1) based on the instanton trajectory.

Consider the Newtonian system (1.5) in the “classically forbidden” region. Here $x \in \mathbb{R}^2$ and $V(x)$ is the 2D double well potential described in Section 2. The system 1.5 has the solution (trajectory) $\gamma = \{x = X(t)\}$ satisfying the boundary conditions $X(-\infty) = x_- \equiv (-a, 0)^t$, $X(\infty) = x_+ \equiv (a, 0)^t$. This trajectory gives the minimum of the action functional

$$S_{12} = \int \sqrt{2V(x(t))} |\dot{x}(t)| dt$$

among the piecewise smooth functions $x(t)$ connecting the points x_- and x_+ (the maxima of $-V$) (see [26], [27]). Lifting γ to the phase space by the formulas $p = \dot{X}(t)$, $x = X(t)$, we obtain a trajectory of the Hamiltonian system with Hamiltonian \mathcal{H} , of (1.4). We denote this trajectory by $\Gamma_0 = \{p = \dot{X}(t), x = X(t)\}$, and we have $\mathcal{H}|_{\Gamma_0} = 0$. This trajectory is called the *instanton*. Suppose for simplicity that the instanton is unique¹ (up to a time shift), and normalize the time by the condition $X(0) = 0$. Then for the difference $E_0^+ - E_0^-$ we have

$$E_0^+ - E_0^- = A(h) \exp\{-S_{12}/h\} (1 + O(\sqrt{h})). \tag{3.1}$$

In order to construct the amplitude $A(h)$ (see [12], [13], [14]), we must consider the variational system

$$\ddot{Z}(t) = \left. \frac{\partial^2 V}{\partial x^2} \right|_{\gamma} Z(t) \tag{3.2}$$

corresponding to the instanton γ and find its matrix solution with the boundary conditions

$$Z(-\infty) = 0, \quad Z(0) = E_2, \tag{3.3}$$

where E_2 is the 2×2 identical matrix. This solution is unique and we have the limit

$$\mathcal{J}_1^{-1} = \lim_{t \rightarrow -\infty} e^{-(\omega_1 + \omega_2)t} \det Z(t).$$

Let λ be the matrix element of $B = O\dot{Z}(0)O^t$ in the second column and the second row, where O is a rotation matrix such that $O\dot{x}_0(0) = (|\dot{x}_0(0)|, 0)^t$. According to [12], [13], [14], the amplitude $A(h)$ in formula (3.1) has the form

$$A(h) = 4\mathcal{J}_1^{-1} \frac{\|\dot{x}_0(0)\|}{\sqrt{\lambda}} \sqrt{\frac{h}{\pi}} \sqrt{\omega_1 \omega_2}. \tag{3.4}$$

We want to show that formula (3.1) with amplitude $A(h)$ can be presented in form (2.5).

3.2. Normal coordinates

The system (1.5) is equivalent to the Hamiltonian system

$$\dot{x} = p, \quad \dot{p} = V_x, \quad x \in \mathbb{R}^2, \quad p \in \mathbb{R}^2 \tag{3.5}$$

with Hamiltonian (1.4). The equation $x = X(t)$ gives a curve on the plane R^2 ; let us parameterize this curve by its natural parameter

$$s = \int_{-\infty}^t |\dot{X}(t)| dt, \quad s \in (0, l),$$

where l is the length of the instanton. Denote by $n(s) = \hat{J}_2 X_s$ the normal vector to the instanton, $\hat{J}_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, and by $k(s)$ the curvature of γ . We have $X_{ss} = k(s)n(s)$.

¹ It seems that this assumption is true in the case of general position.

Introduce normal coordinates (s, q) in a neighborhood of the trajectory γ by the formula $x = X(s) + n(s)q$. This change of variables implies a canonical transformation in the phase space (see e.g. [2]). We denote by P and Q the new momentum variables corresponding to s and q , respectively.

In new coordinates, the Hamiltonian \mathcal{H} takes the form

$$\mathcal{H} = \frac{1}{2J^2}P^2 + \frac{1}{2}Q^2 - V(X(s) + n(s)q), \quad J = 1 + k(s)q.$$

The Taylor expansion of $\frac{1}{J^2}$ and V gives $\frac{1}{J^2} = 1 - 2kq + 6k^2q^2 + O(q^3)$ and $V = V(X(s)) + (\partial V/\partial x, n)q + \frac{1}{2}(n, V_{xx}n)q^2 + O(q^3)$. Here $(\partial V/\partial x, n) = -(\ddot{X}, n) = -2V(X(s))kq$. Thus for the Hamiltonian \mathcal{H} , we have the representation

$$\mathcal{H} = \left(\frac{P^2}{2} - V(X(s)) \right) (1 - 2kq) + \frac{1}{2} (Q^2 - \Omega^2 q^2) + O(q^3), \tag{3.6}$$

where $\Omega^2(P, s) = (V_{xx}|_{x=X(s)}n, n) - 3k^2P^2$.

Let us introduce the 1D Hamiltonian

$$\mathcal{H}_0 = \frac{P^2}{2} - V(X(s)). \tag{3.7}$$

The trajectory Γ_0 of the Hamiltonian system with Hamiltonian (3.6) corresponding to the instanton γ is determined by the formulas $Q = 0, q = 0, P = P_0(t)$, and $s = s_0(t)$, where $P_0(t) = \dot{s}_0(t)$ and $s_0(t)$ is the solution of the Newtonian system

$$\ddot{s} = \partial V(X(s))/\partial s. \tag{3.8}$$

3.3. The variational system in the new coordinates

Now let us rewrite the variational system in the new coordinates. We want to show that the solution of (3.2) and (3.3) can be reduced to the problem

$$\ddot{z} = \omega_0^2(t)z, \quad z(0) = 1, \quad z(-\infty) = 0, \tag{3.9}$$

where $\omega_0^2(t) = \Omega^2(P, s)|_{\Gamma_0}$.

Indeed, according to the theory of Hamiltonian systems, the variational system (3.2) in the new coordinates corresponding to (P, Q, s, q) takes the form

$$\dot{\tilde{Z}} = \tilde{W} + K\tilde{Z}, \quad \dot{\tilde{W}} = V_{ss}\tilde{Z}(t) - K^t\tilde{W}, \tag{3.10}$$

$K = \left(\begin{array}{cc} \partial^2 H \partial P \partial s & \partial^2 H \partial P \partial q \\ \partial^2 H \partial Q \partial s & \partial^2 H \partial Q \partial q \end{array} \right) \Big|_{\Gamma} = \begin{pmatrix} 0 & -2k\partial H \partial P|_{\Gamma} \\ 0 & 0 \end{pmatrix}$. Here $\tilde{Z}(t)$ and $\tilde{W}(t)$ are 2×2 matrix functions

related to the matrices $Z(t)$ and $\dot{Z}(t)$ in system (3.2) by the formulas $\tilde{Z} = RZR^t, \tilde{W} = R\dot{Z}(t)R^t$, with $R(t) = \partial(s, q)/\partial x|_{\Gamma}$. It is easy to verify that the functions

$$\tilde{Z}(t) = \begin{pmatrix} \dot{s}_0(t)/\dot{s}_0(0) & C(t)\dot{s}_0(t) \\ 0 & z(t) \end{pmatrix} \quad \tilde{W}(t) = \begin{pmatrix} \dot{P}_0(t)/\dot{s}_0(0) & C(t)\dot{P}_0(t) \\ 0 & w(t) \end{pmatrix}$$

are solutions of the system (3.10), if $z(t)$ is the solution of problem (3.9), $w(t) = \dot{z}(t)$, and $C(t) = -2 \int_0^t k|_{\Gamma} z(t) dt$. The matrix function $Z(t) = R\tilde{Z}(t)R^t, R(0) = O$, implied by this solution is the solution of problem (3.2)–(3.3). Using these formulas, we find that λ and J_1 in (3.4) are given as

$$\lambda = \tilde{W}_{22} = w(0) = \dot{z}(0), \quad \mathcal{J}_1^{-1} = \left(\lim_{t \rightarrow -\infty} e^{-\omega_1 t} \dot{s}_0(t)/\dot{s}_0(0) \right) \left(\lim_{t \rightarrow -\infty} e^{-\omega_2 t} z(t) \right).$$

Note that we can represent problem (3.9) also in the form of a spectral problem on the semiaxis $(-\infty, 0]$, namely

$$\ddot{z} = \omega_0^2(t)z, \quad (\dot{z} - \lambda z)|_{t=0} = 0, \quad \lim_{t \rightarrow -\infty} z(t) = 0, \tag{3.11}$$

together with the normalization condition $z(0) = 1$. If we find the values of λ and $b = \lim_{t \rightarrow -\infty} e^{-\omega_2 t} z(t)$, then we can compute the amplitude (3.4) as

$$A(h) = 4\sqrt{\frac{h}{\pi}} \left[b\sqrt{\frac{\omega_2}{\lambda}} \right] \sqrt{\omega_1} \|\dot{s}_0(0)\| \lim_{t \rightarrow -\infty} e^{-\omega_1 t} \dot{s}_0(t) / \dot{s}_0(0). \tag{3.12}$$

Comparing this formula with the formula given in [39], [1] for the splitting value in the one-dimensional case, we can formulate the following proposition:

Proposition 1. *The amplitude $A(h)$ in (3.1) can be rewritten as*

$$A(h) = \mathcal{T} A_0(h). \tag{3.13}$$

Here $\mathcal{T} = b\sqrt{\frac{\omega_2}{\lambda}}$, and $A_0(h)$ is the amplitude of the splitting between the lowest energy levels of the one-dimensional Schrödinger operator $\hat{\mathcal{H}}_0 = \frac{1}{2} \left(-ih \frac{\partial}{\partial s} \right)^2 + V(X(s))$.

If $\omega_0^2 = \text{const}$ then the coefficient \mathcal{T} is equal to 1 and the splitting problem becomes a one-dimensional problem. In the general case, the splitting value is distinguished from the one-dimensional one by the factor $\mathcal{T} \neq 1$.

3.4. Relationship to the “scattering” problem

Let us now interpret the factor \mathcal{T} . Consider system (3.9) and introduce the function $u(t) = \omega_0^2(t) - \omega_2^2$. It is easy to see that (3.11) can be represented as the spectral problem for the Sturm–Liouville problem $\hat{L} = (-\partial^2 / \partial t^2 + u(t))$,

$$\left(-\frac{\partial^2}{\partial t^2} + u(t) \right) z(t) = -\omega_2^2 z(t). \tag{3.14}$$

We can show that $u(t) = O(e^{-\omega_1 |t|})$, $t \rightarrow \pm\infty$, hence $u(t)$ is a smooth localized potential. It is easy to see that in our case $-\omega_2^2$ does not belong to the spectrum of \hat{L} , thus there exists a solution of problem (3.9) which has the following asymptotic expansion at infinity:

$$\begin{aligned} z(t) &= b e^{\omega_2 t} (1 + O(e^{\alpha t})), & t \rightarrow -\infty, & \alpha > 0, \\ z(t) &= c e^{\omega_2 t} (1 + O(e^{-\alpha t})), & t \rightarrow +\infty. \end{aligned} \tag{3.15}$$

The “scattering amplitude” b/c can be expressed via b and λ . Indeed, the fact that $\Omega^2(t) = \Omega^2(-t)$ implies that $\tilde{z}(-t)$ is also a solution of problem (3.9). The derivative $\dot{z}(t)$ has the following expansion at infinity:

$$\begin{aligned} \dot{z}(t) &= b \omega_2 e^{\omega_2 t} (1 + O(e^{\alpha t})), & t \rightarrow -\infty, & \alpha > 0, \\ z(t) &= c \omega_2 e^{\omega_2 t} (1 + O(e^{-\alpha t})), & t \rightarrow +\infty. \end{aligned} \tag{3.16}$$

At the point $t = 0$, we have $(z(0), \dot{z}(0))^t = (1, \lambda)^t$, $(\tilde{z}(0), \dot{\tilde{z}}(0))^t = (1, -\lambda)^t$. Let us consider the Wronskian $W(t) = z(t)\dot{\tilde{z}}(t) - \dot{z}(t)\tilde{z}(t) = \text{const}$, $W(0) = -2\lambda = \lim_{t \rightarrow -\infty} W(t) = -2bc\omega_2 + O(e^{-\alpha t})$. Hence, the scattering amplitude is equal to

$$b/c = \frac{b^2 \omega_2}{\lambda}.$$

Proposition 2. *The factor \mathcal{T} in (3.13) is equal to the square root of the “scattering amplitude” for the solution of problem (3.14).*

4. Closed trajectories and the amplitude in the 2D splitting formula

Now we want to express the parameters of closed trajectories introduced in Section 2 and the normal form in a neighborhood of these trajectories via the parameters of the instanton and the scattering amplitude \mathcal{T} .

It is convenient to introduce the action-angle variables J, ϕ instead of P and s . To this end, let us consider the one-dimensional potential $-V(X(s))$. It has the structure of the potential well between the points x_- and x_+ . Consider 1D Hamiltonian (3.7). Its trajectories, which are situated below $\mathcal{H}_0 = 0$, are periodic. We can parameterize them by the action variable $J = \frac{1}{2\pi} \oint P ds$ and determine by the equations $P = P(J, \phi + \omega(J)t)$, $s = s(J, \phi + \omega(J)t)$, ϕ is the angle variable conjugated to J , $\omega(J)$ is the frequency of motion along the corresponding closed trajectory, $J \in (0, J_{ins})$, and $J_{ins} = \frac{1}{\pi} \int_0^l \sqrt{2V(X(s))} ds$. We fix the angle ϕ so that $s = s(J, 0) = l/2$.

In the new canonical variables $(J, \phi, q)^t$, Hamiltonian (3.6) takes the form

$$\mathcal{H} = \mathcal{H}_0(J) + \frac{1}{2}(Q^2 - \Omega_1^2 q^2) - 2k\mathcal{H}_0(J)q + O(q^3). \tag{4.1}$$

Here $\Omega_1^2(J, \phi) = \Omega^2(P(J, \phi), s(J, \phi))$ and $k = k(P(J, \phi), s(J, \phi))$.

Our idea is that the librations described in Section 2 are close to trajectories of the Hamiltonian system with “truncated” Hamiltonian

$$\mathcal{H} = \mathcal{H}_0(J) + \frac{1}{2}(Q^2 - \Omega^2 q^2). \tag{4.2}$$

The accurate proof requires some delicate estimates, nevertheless our preliminary estimates allow us to conclude that it is really true. We shall discuss this problem later.

Hamiltonian (4.2) has closed trajectories, which belong to the subspace $Q = q = 0$ and coincide with the closed trajectories of the one-dimensional Hamiltonian system described above.

Denote the period of motion along these trajectories by $T(J)$. These trajectories imply variational systems. In what follows, we need only the parts of these systems corresponding to the perturbations \tilde{w} and \tilde{z} of $Q = 0$ and $q = 0$. These equations take the form

$$\dot{\tilde{w}} = \Omega_1^2(J, \omega(J)t)\tilde{z}, \quad \dot{\tilde{z}} = \tilde{w}. \tag{4.3}$$

According to the theory of linear equations with periodic coefficients, the basis of its solutions can be chosen in the form

$$\begin{aligned} (\tilde{w}, \tilde{z})^t &= v_1(J, \omega(J)t) = V_1(J, \omega(J)t)e^{\beta(J)t}, \\ (\tilde{w}, \tilde{z})^t &= v_2(J, \omega(J)t) = V_2(J, \omega(J)t)e^{-\beta(J)t}, \end{aligned}$$

where $\beta(J) > 0$ is the Floquet index and $V_1(J, \phi)$ and $V_2(J, \phi)$ are smooth functions 2π periodic in the angle ϕ and satisfy the normalization condition $(V_1, \hat{J}_2 V_2) = -1$.

Our aim is to express the Floquet index β via the scattering amplitude \mathcal{T} and the period $T(J) = 2\pi/\omega(J)$ in a neighborhood of the separatrix as J tends to J_{ins} .

Following [31], we assume that, on the interval $t \in [-T(J)/4, T(J)/4]$ up to multiplication by the coefficients $C + O(J - J_{ins})$, $C = const$, the solutions $v_1(J, \omega(J)t)$ and $v_2(J, \omega(J)t)$ coincide with the solutions $(\dot{z}(t), z(t))^t$ and $(\dot{z}(-t), z(-t))^t$ of the variational system from (3.9) (corresponding to the instanton trajectory), where $z(t)$ and $\dot{z}(t)$ have expansions (3.15) and (3.16) at infinity. Then we

estimate $V_1(J, \pm\pi/2)$ and $V_2(J, \pm\pi/2)$ by the formulas

$$\begin{aligned} V_1\left(J, -\frac{\pi}{2}\right) &= Nb \begin{pmatrix} \omega_2 \\ 1 \end{pmatrix} e^{(\beta-\omega_2)T/4} + O(J - J_{ins}), \\ V_1\left(J, \frac{\pi}{2}\right) &= Nc \begin{pmatrix} \omega_2 \\ 1 \end{pmatrix} e^{-(\beta-\omega_2)T/4} + O(J - J_{ins}), \\ V_2\left(J, -\frac{\pi}{2}\right) &= Nc \begin{pmatrix} -\omega_2 \\ 1 \end{pmatrix} e^{-(\beta-\omega_2)T/4} + O(J - J_{ins}), \\ V_2\left(J, \frac{\pi}{2}\right) &= Nb \begin{pmatrix} -\omega_2 \\ 1 \end{pmatrix} e^{(\beta-\omega_2)T/4} + O(J - J_{ins}). \end{aligned}$$

Here the normalizing coefficient N satisfies the equation $-2N^2bc\omega_2 = -1$

It follows from the symmetry properties of system (4.3) that $V_1(J, -\pi/2) = V_1(J, \pi/2)$ and $V_2(J, -\pi/2) = V_2(J, \pi/2)$. From these equalities we can easily derive

$$\beta(J) = \omega_2 + \frac{4 \ln \mathcal{T}}{T(J)} + o(1/T(J)), \tag{4.4}$$

where $\mathcal{T} = \sqrt{\frac{c}{b}}$ is the square root of the ‘‘scattering amplitude’’ introduced above.

According to the theory of normal forms [2], [5], [6], [32], in a neighborhood of closed trajectories, there exists a change of variables $J, \phi, Q, q \rightarrow J', \phi', \xi, \eta$ such that Hamiltonian (4.2) in the new coordinates takes the form

$$\mathcal{H} = \mathcal{H}_0(J') - \beta(J')\xi\eta + f_1(J', \xi, \phi', \eta). \tag{4.5}$$

This change of variables can be given by the formulas (see e. g. [5], [6], [32], [4])

$$J = J' + f_2(J', \xi, \phi', \eta), \quad \begin{pmatrix} Q \\ q \end{pmatrix} = V_1(J', \phi')\xi + V_2(J', \phi')\eta + g(J', \xi, \phi', \eta), \tag{4.6}$$

To explain the estimates for the scalar corrections f_1, f_2 and the vector correction g , we recall that all our considerations are available in a neighborhood of the instanton, which means that $J - J_{ins}, \eta$ and ξ are small enough: these variables should be connected with a small parameter h in the quantum problem. Namely, an analysis of the splitting formulas shows that

$$J - J_{ins} = O(h \ln h), \quad \eta = O(\sqrt{h}), \quad \xi = O(\sqrt{h}).$$

Taking into account this fact and using formulas [5], [6], [32], [4], we can estimate f_1, f_2 and g in the following way:

$$f_1 = O(h^2), \quad f_2 = O(h^{3/2}), \quad g = O(h).$$

Rough considerations show that these estimates are sufficient to derive formula (2.5) from (3.1)–(3.4).

Now we want to relate the integrals of motion in the classically allowed and classically forbidden regions.

Let us consider a neighborhood of the point x_- . First, let us move and rotate the coordinate system so that the point x_- be the origin O of coordinates and the instanton enter this point in the direction of the Ox_1 -axis (the coordinate system associated with the unite vectors e_1 and e_2 at the point x_- (see the Fig. 2)). Then in the classically allowed region we have two approximate integrals of motion:

$$I_1 = \frac{p_1^2 + \omega_1^2(x_1)^2}{2\omega_1}, \quad I_2 = \frac{p_2^2 + \omega_1^2 x_2^2}{2\omega_2}.$$

The 2D Hamiltonian H can be expressed in the form $H = \omega_1 I_1 + \omega_2 I_2 + O(I_1^{3/2} + I_2^{3/2})$ in a neighborhood of x_- .

Let us take the following point on the torus determined by the integrals I_1 and I_2 :

$$p_1 = p_2 = 0, \quad x_1 = \sqrt{\frac{2I_1}{\omega_1}}, \quad x_2 = \sqrt{\frac{2I_2}{\omega_2}}.$$

Since the point lies in a neighborhood of the instanton trajectory, we can express it in coordinates J, Q, ψ, q . For the coordinates Q and q , we have $Q = 0, q = x_2 = \sqrt{\frac{2I_2}{\omega_2}}$. Using the second formula in (4.6) we get

$$\begin{pmatrix} 0 \\ \sqrt{\frac{2I_2}{\omega_2}} \end{pmatrix} = \frac{1}{\sqrt{2\omega_2}} \begin{pmatrix} \omega_2 \\ 1 \end{pmatrix} \xi + \frac{1}{\sqrt{2\omega_2}} \begin{pmatrix} -\omega_2 \\ 1 \end{pmatrix} \eta$$

and it follows that

$$\xi \eta = I_2.$$

To express J' or J in terms of I_1 and I_2 , we can use relation (2.4). Now we show that the root $J_0(h)$ of this equality gives the splitting value by formula (2.5).

At the lowest quantum energy level, we have $I_1 = I_2 = \frac{h}{2}$. Solving equation (2.4) and using the fact that $\beta(J_0)$ is closed to ω_2 in the first approximation, we obtain $J_0 = J = J_1$, where J_1 is the root of the equation $\mathcal{H}_0(J_1) = h\omega_1/2$. According to [1], this gives an approximation of the splitting value ΔE_{1D} for the lowest energy levels of the one-dimensional Schrödinger operator $\widehat{\mathcal{H}}_0 = \frac{1}{2} \left(-i\hbar \frac{\partial}{\partial s} \right)^2 + V(X(s))$ by the formula $\Delta E_{1D} = \sqrt{\pi} e^{\frac{\omega_1 h}{\pi}} \exp(-J_1 \pi / h)$. Next, we use the expansions $\mathcal{H}_0(J_0) = \mathcal{H}_0(J_1) + \frac{2\pi}{T(J_1)}(J_1)(J_0 - J_1) + \dots$ and $\beta(J_0) = \omega_2 + \frac{4 \ln \mathcal{T}}{T(J_1)} + \dots$. Substituting these formulas into (2.5), we get the next approximation for J_0 :

$$J_0 = J_1 + \frac{h \ln \mathcal{T}}{\pi}$$

Substituting this into formula (2.5), we get the desired asymptotic formula $\Delta E = \mathcal{T} \Delta E_{1D}$.

5. Conclusion

As was mentioned above, the proof of our result rest on several assumptions. In future work, it should be proved that the exact trajectories of the Hamiltonian system with Hamiltonian \mathcal{H} describing librations are approximated by the trajectories determined by the “truncated” Hamiltonian, and also that the normal form is approximated in a neighborhood of librations by the normal form (4.5). The passage from integrals in the “classically prohibited domain” to approximate integrals in the “classically allowed domain” also need a more rigorous derivation.

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