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Quantum Dynamics in a Thin Film. II. Stationary States

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Abstract. The spectrum of quantum waveguides simulating thin toroidal tubes and thin spherical surfaces is investigated. Asymptotic formulas are obtained and a geometric classification using the so-called Reeb graphs is carried out.

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1. INTRODUCTION

It is assumed that the quantum dynamics of charged particles in thin films in the one-particle approximation is described by the Pauli–Rashba operator

$$i\hbar\Psi_t = \widehat{\mathcal{H}}\Psi, \qquad \widehat{\mathcal{H}} = \frac{\widehat{\mathbf{P}}^2}{2m} + v_{\text{int}}(\mathbf{r},\mu) + v_{\text{ext}}(\mathbf{r},t) - \frac{e\hbar}{2mc}\langle\boldsymbol{\sigma},\mathbf{H}\rangle + \widehat{\mathcal{H}}_{\text{SO}}. \tag{1}$$

Here $\widehat{\mathbf{P}} = -i\hbar\nabla - \dfrac{e}{c}\mathbf{A}(\mathbf{r},t)$, $\hbar$ stands for the Planck constant, e for the effective charge, m for the effective mass of a quasiparticle, c for the velocity of light, $v_{\text{ext}}(\mathbf{r},t)$ and $\mathbf{A}(\mathbf{r},t)$ for the potentials of the external electric and magnetic fields. $\mathbf{H} = \operatorname{rot}\mathbf{A}(\mathbf{r},t)$ for the magnetic intensity, $\boldsymbol{\sigma} = \{\sigma_1,\sigma_2,\sigma_3\}$ for the standard Pauli matrices, and $\widehat{\mathcal{H}}_{\text{SO}} = \alpha\langle\boldsymbol{\sigma},[\nabla v_{\text{int}},\widehat{\mathbf{P}}]\rangle$ for the interaction of the spin with the intrinsic electric field (this interaction is determined by an effective constant α). The fact that the problem is treated in a thin layer (the domain Ω) is reflected by the existence of the so-called confinement potential $v_{\text{int}}(\mathbf{r},\mu)$ in the operator $\widehat{\mathcal{H}}$; this potential vanishes on some "middle" smooth two-dimensional surface Γ and rapidly increases along the normal to the surface. This very potential keeps the particle in a small neighborhood of the "middle" surface Γ. The fact that the layer is thin means that the typical "longitudinal" size of the layer is much greater than the normal size. It is clear from physical considerations that the dynamics of charged particles must be two-dimensional and is determined by operators defined on the "limit" middle surface. In the first part of the paper (see [1]), it was shown that, under appropriate conditions, the nonstationary equation given by the operator $\widehat{\mathcal{H}}$ is reduced to a nonstationary equation for a scalar function given on the "limit" surface

$$i\mu\frac{\partial\psi}{\partial t} = \Big(-\frac{1}{2}\mu^2\Delta_M + \mathrm{v}_{\text{ext}}(x) + \varepsilon_\perp(x) + \mu^2\mathcal{G}(x)\Big)\psi, \tag{2}$$

where $\mu^2\Delta_M$ stands for the Laplace operator on the surface with regard to the curvature and the presence of a magnetic field (this consideration is expressed in replacing the derivatives by "long" derivatives with the magnetic potential A_i), $x = (x_1,x_2)$ for the pair of coordinates on the surface, $\mathrm{v}_{\text{ext}}(x_1,x_2)$ for the potential of the external electric field, and $\varepsilon_\perp(x_1,x_2)$ for the energy of transversal quantization. Moreover, $\mathcal{G}(x) = -\frac{(\varkappa_1-\varkappa_2)^2}{8}$, the symbols $\varkappa_1$ and $\varkappa_2$ stand for the principal curvatures, and μ for a small dimensionless parameter characterizing the ratio of transversal sizes of the film to the longitudinal ones (see part I [1], references [25, 30]).

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If an exact (or an asymptotic) solution ψ of the last equation is constructed, then the "intertwining" pseudodifferential operator $\hat{\chi}$ defined in [1] enables one to construct (some) asymptotic solutions of the original nonstationary equation

$$\Psi(x,y,t) = \hat{\chi}\psi(x,t), \qquad \hat{\chi} = \chi_0(x,y) + \mu\chi_1(\overset{2}{x},\overset{1}{\hat{p}},y) + \cdots .$$

In this part of the paper we study the asymptotic solutions of stationary equations posed in quantum waveguides of special form. The spectral problem for the operator $\widehat{\mathcal{H}}$ can be reduced according to the scheme used for the nonstationary equation. The answer can be obtained immediately from the nonstationary equation (2) by the formal change $i\mu\frac{\partial}{\partial t} \to E$. Finally, the reduced equation for the spectral problem becomes[1]

$$\begin{gathered}\Big(-\frac{1}{2}\mu^2\Delta_M + \mathrm{v}_{\mathrm{ext}}(x) + \varepsilon_\perp(x) + \mu^2\mathcal{G}(x)\Big)\psi = E\psi,\\ \mu^2\Delta_M = \frac{\mu^2}{\sqrt{g}}\frac{\partial}{\partial x^i}\sqrt{g}g^{ij}\frac{\partial}{\partial x^j} + 2g^{ij}A_i\Big(-i\mu\frac{\partial}{\partial x^j}\Big) - g^{ij}A_iA_j - \frac{i\mu}{\sqrt{g}}\Big(\frac{\partial}{\partial x^i}\sqrt{g}g^{ij}A_j\Big),\end{gathered} \tag{3}$$

where x_i are local coordinates on the surface, g_{ij} is the metric tensor in these coordinates, and $g = \det g_{ij}$, $i = 1, 2$. We also denote by A_n the normal component of the vector potential at the points on the limit surface ($A_n = A_n(x) = \langle \mathbf{A}(x), n(x)\rangle$), by w_c the cyclotron frequency ($w_c = \frac{eB}{mc}$), and by $\Phi_0 = 2\pi\hbar c/e$ the quantum of magnetic flux.

If the solutions of (3) with wavelengths $h \gtrsim \mu$ are found, then using them one can construct some (at least formal) asymptotic solutions of the original stationary equation. These solutions are mainly defined as follows:

$$\begin{aligned}\Psi^+(x,y) &= \big(\chi_0(x,y) + \mu\hat{\chi}_1\big)\exp(iyA_n/\Phi_0)\begin{pmatrix}\psi\\0\end{pmatrix}, \qquad \mathcal{E}^+ = +\frac{1}{2}\hbar w_c + \frac{\hbar^2}{md^2}E,\\ \Psi^-(x,y) &= \big(\chi_0(x,y) + \mu\hat{\chi}_1\big)\exp(iyA_n/\Phi_0)\begin{pmatrix}0\\\psi\end{pmatrix}, \qquad \mathcal{E}^- = -\frac{1}{2}\hbar w_c + \frac{\hbar^2}{md^2}E,\end{aligned} \tag{4}$$

here the signs plus and minus correspond to states with positive and negative projection of the spin to the z axis.

Thus, we have the spectral problem (3) for the differential operator on the surface Γ with small parameter μ at all derivatives. This enables one to apply the semiclassical approximation to solve the problem.

2. QUASIMODES

As is well known, in curvilinear coordinates, one can simplify the manipulations by using the function $\psi' = \psi g^{1/4}$ instead of the function ψ. For this reason, we rewrite the original equation in the form of an equation for the function ψ'. Denote by L the symbol of the μ-differential operator thus obtained. We have the expansion

$$L(x,p,\mu) = H(x,p) + \mu L_1(x,p) + \mu^2 L_2(x);$$

here

$$H(x_1,x_2,p_1,p_2) = \frac{1}{2}g^{ij}(x)(p_i - A_i)(p_j - A_j) + \mathrm{v}_{\mathrm{ext}}(x) + \varepsilon_\perp(x)$$

is the leading symbol, $L_1(x,p) = 0$, and the term $\mu^2 L_2(x)$ does not influence the leading term of the semiclassical asymptotics.

[1]Unfortunately, in the similar equation (3.10) in part I [1], we missed the factors μ^{-1} in the second and fourth summands and the factor μ^{-2} in the third summand in the expression for Δ_M.

The semiclassical (stationary) eigenstates ψ (the so-called *quasimodes*) are constructed from objects of classical Hamilton dynamics with Hamiltonian H. These objects are submanifolds of the phase space that are isotropic and invariant with respect to the action of the phase flow g_H^t (generated by the shift along the trajectories of the corresponding Hamiltonian system); for example, stable stationary points, closed trajectories, Liouville tori, and so on [2–5].

Recall that by a *quasimode* (an asymptotic eigenfunction and an eigenvalue) of an operator $\hat{L} = L(\overset{2}{x}, -i\overset{1}{\mu}\nabla, \mu)$ one means formal asymptotic solutions $\mod O(\mu^N)$, $N > 1$ (below we simply call them *asymptotic solutions*), of the spectral problem for the operator $\hat{L}$, i.e., pairs $(E(\mu), \psi(x, \mu))$ satisfying the relations

$$\hat{L}\psi = E\psi + O(\mu^N), \qquad \|\psi\|_{L^2(\Gamma)} = 1,$$

for some $N > 1$, where the estimate for a function in the form $O(\mu^N)$ is treated in the $L^2(\Gamma)$ norm.

The classical dynamics in $T^*\Gamma$ is given by the system of Hamiltonian equations

$$\dot{x}^j = \frac{\partial H}{\partial p_j}, \qquad \dot{p}_j = -\frac{\partial H}{\partial x^j}, \qquad j = 1, 2. \tag{5}$$

Let us recall some formulas for semiclassical states in the following cases.

I) Let system (5) have a stable stationary point $\Lambda_0 = (x_0, p_0)$ (it suffices to have such a point in the linear approximation). In this case, to this point, one can assign a family (a "series") of quasimodes which is well known from the method of oscillatory approximation.

Recall that a stationary point is said to be *stable in the linear approximation* if its linearized system (i.e., the following system in variations)

$$\begin{pmatrix} \dot{Z} \\ \dot{W} \end{pmatrix} = \begin{pmatrix} H_{px} & H_{pp} \\ -H_{xx} & -H_{xp} \end{pmatrix}\Bigg|_{\Lambda_0} \begin{pmatrix} Z \\ W \end{pmatrix} \tag{6}$$

is stable. In this case, by well-known theorems of linear algebra and of the theory of linear differential equations, the above linearization matrix can be reduced to diagonal form, and the eigenvalues form pairs $\pm i\beta, \beta \geqslant 0$. Here the eigenvectors $b_1, b_2, \overline{b}_1, \overline{b}_2$ can be chosen so that

$$\{b_i, b_j\} = 0, \qquad \{b_i, \overline{b}_j\} = 2i\delta_{i,j}, \qquad i, j = 1, 2.$$

In this case, the plane spanned by b_1, b_2 is given by the equation $W = QZ$, where Q is a complex 2×2 matrix; the braces stand here for the skew-inner product (see [2, 3]).

The wave function of the lower energy state is defined by the formula

$$\psi_0 = \mu^{-n/4} e^{\frac{i}{\mu}\left((p_0, x - x_0) + \frac{1}{2}(x - x_0, Q(x - x_0))\right)}.$$

The creation operators which enable one to construct from this function a family ψ_{n_1,n_2}, $n_i = 0, 1, \dots$, of higher excited states of the oscillator approximation are of the form

$$\hat{a}_i = a(\overset{2}{x}, -i\overset{1}{\mu}\nabla), \qquad a_i(x, p) = \frac{1}{\sqrt{\mu}}\{b_i, (x - x_0, p - p_0)\}, \quad i = 1, 2.$$

Proposition 1. *The following values and functions define an asymptotic solution* $\mod O(\mu^{3/2})$ *of equation* (3):

$$E_{n_1,n_2} = H(\Lambda_0) + \mu L_1(\Lambda_0) + \mu\beta^1(n_1 + \tfrac{1}{2}) + \mu\beta^2(n_2 + \tfrac{1}{2}), \quad \psi_{n_1,n_2} = \hat{a}_1^{n_1}\hat{a}_2^{n_2}\psi_0, \quad n_i = O(1). \tag{7}$$

The distance from the values E_{n_1,n_2} to the spectrum of the operator (3) *does not exceed* $O(\mu^{3/2})$.

Remark. If the equilibrium is nondegenerate, then one can construct corrections which give quasimodes of arbitrary order $N > 1$ (see [3]).

II) Let the Hamiltonian system (5) have a family (depending on the parameter $I \in [I_{\min}, I_{\max}]$) of closed orbitally stable trajectories with period $T = T(I)$,

$$\Lambda^1(I) = \{x = \mathcal{X}(t, I), p = \mathcal{P}(t, I)\}.$$

Suppose (without loss of generality) that the parameter I is the action

$$I = \frac{1}{2\pi} \oint_{\Lambda^1(I)} (p, dx)$$

and the coordinate on $\Lambda^1(I)$ is the angle $\phi(t, I) = \frac{2\pi t}{T}$.

For any chosen μ, the Bohr–Sommerfeld quantization conditions

$$I = \mu m, \qquad m \in \mathbb{Z}, \tag{8}$$

define a discrete family of values $I = I^m$ in $[I_{\min}, I_{\max}]$; m is a quantum number (thus, the numbers m are nor absolutely arbitrary, and they are chosen in such a way that $I^m \in [I_{\min}, I_{\max}]$). Thus, a discrete family of curves $\Lambda^1_m = \Lambda^1(I^m)$ is defined, on which one can construct the canonical operator

$$K_{\Lambda^1_m} : C^\infty(\Lambda^1_m) \to C^\infty(\Gamma \times (0, 1])$$

and the creation operator $\hat{a}_{\Lambda^1_m}$ (see [2, 4], and also [13]).

These operators define the basic states $\psi_m = \psi_{0,m}$ and the states $\psi_{n,m}$ excited in the transversal direction,

$$\psi_m = K_{\Lambda_1}[f]; \qquad f = e^{-i\int_0^\phi L_1(I,\tau) - \langle L_1\rangle \mathrm{d}\tau}, \qquad \psi_{n,m} = \hat{a}^n \psi_m.$$

Proposition 2. *If Λ^1 are orbitally stable in the linear approximation, then the following family of values and functions defines an asymptotic solution* $\operatorname{mod} O(\mu^{3/2})$ *of problem* (3):

$$E_{n,m} = H(\Lambda^1_m) + \mu\langle L_1\rangle|_{\Lambda^1_m} + \mu\beta(n + \tfrac{1}{2}), \qquad \psi_{n,m} = \hat{a}^n \psi_m, \qquad n = O(1), \tag{9}$$

where $e^{i\beta T}$, $\beta > 0$, stands for an eigenvalue of the monodromy operator of the periodic system of the form (6) *given on the curve Λ^1_m.*

III) Let the Hamiltonian system (5) have a family of two-dimensional invariant compact Lagrangian manifolds $\Lambda^2(I)$. This case occurs if the Hamiltonian system is completely integrable and $\Lambda^2(I)$ are the Liouville tori (see, e.g., [9]). For any Λ_0 in $\Lambda^2(I)$, there is a neighborhood of Λ_0 in which the phase space is foliated into Liouville tori and in which one can introduce the action-angle coordinates. Two action variables I_1, I_2 parametrize the family of tori $\Lambda^2(I) = \Lambda^2(I_1, I_2)$ and, for a chosen neighborhood in the phase space, belong to some domain $\mathcal{M} \subset \mathbb{R}^2_I$.

For any chosen μ, the Bohr–Sommerfeld–Maslov quantization conditions

$$I_i = \frac{1}{2\pi} \oint_{\gamma_i} (p, dx) = \mu\Big(n_i + \frac{\operatorname{Ind}\gamma_i}{4}\Big), \qquad n_i \in \mathbb{Z}, \tag{10}$$

define a discrete family of values $I^n = (I_1^{n_1}, I_2^{n_2})$ in the domain $\mathcal{M}$ (thus, the numbers n_i are not absolutely arbitrary, and they are chosen in such a way that $I^n \in \mathcal{M}$), where γ_i are the basis cycles on the Liouville torus $\Lambda^2_{n_1,n_2} = \Lambda^2(I_1^{n_1}, I_2^{n_2})$ and $\operatorname{Ind}\gamma_i$ is their Maslov index (independent of I), while the n_i are quantum numbers.

The family $\Lambda^2_{n_1,n_2}$ defines a quantum series of values of energy

$$E_{n_1,n_2} = H(I_1^{n_1}, I_2^{n_2}) + \mu\langle L_1\rangle|_{\Lambda^2_{n_1,n_2}} + O(\mu^2).$$

Here the second summand $\lambda = \langle L_1\rangle|_{\Lambda^2_{n_1,n_2}}$ is the "correcting" term, it occurs due to the presence of L_1. The corresponding correction to the asymptotic eigenfunction is given by the factor $f_{I_1,I_2} \in C^\infty(\Lambda^2(I_1, I_2))$. These factors are defined by the spectral equation

$$\sum_i \frac{\partial H}{\partial I_i}\frac{\partial f}{\partial \phi^i} - L_1 f = \lambda f, \tag{11}$$

which has a unique solution for different L_1 in the case of nonresonant Diophantine torus,

$$\left|\sum_i k_i \frac{\partial H}{\partial I_i}\right| > C|k|^{-\alpha} \qquad \forall k \in \mathbb{Z}^2\backslash\{0\}$$

for some $C, \alpha > 0$.

This family of energies with the corresponding asymptotic eigenfunctions allows us to define a "series" of quasimodes by using the Maslov canonical operator [5].

Proposition 3. *Let the boundary of the neighborhood of $\Lambda^2(\mathcal{M})$ still consist of Liouville tori and let, along with conditions* (10)*, the Diophantine condition additionally hold. In this case, the following set of pairs defines an asymptotic solution* $\operatorname{mod} O(\mu^2)$ *of equation* (3):

$$E_{n_1,n_2} = H(I_1^{n_1}, I_2^{n_2}) + \mu \oint\oint L_1(I_1^{n_1}, I_2^{n_2}, \phi_1, \phi_2)\mathrm{d}\phi_1\mathrm{d}\phi_2, \qquad \psi_{n_1,n_2} = K_{\Lambda^2(I^n)}[f], \tag{12}$$

where $K_{\Lambda^2(I^n)} : C_0^\infty(\Lambda^2(I^n)) \to C^\infty(\Gamma\times(0,1])$ is the Maslov canonical operator for the torus $\Lambda^2(I^n)$ and $I^n \in \mathcal{M}$ satisfies (10).

Remark. As a rule, non-Diophantine tori have zero measure. However, they contain an important class of rational frequencies $\frac{\partial H}{\partial I} \in \mathbb{Q}^2$. In general position, the Diophantine tori are dense in the phase space. It seems, one can assign a quasimode to a non-Diophantine torus with the same accuracy, with the only difference that, instead of the exact solution of equation (11), one can take as exact as desired by a slight perturbation of the torus. If $L_1 = 0$, the Diophantine condition is not required.

Remark. Proposition 3 holds for the phase space of arbitrary dimension. The same holds for the simpler one-dimensional case, see below. In the last case, the Liouville tori are closed curves (trajectories of the Hamiltonian field), there is only one action variable, only one quantum number, and only one angle variable.

The wavelengths of the functions of the series (7)–(12) correspond to either the short-wave approximation $h \sim \mu$ or to the middle-wave approximation $h \sim \sqrt{\mu}$ (see part I [1]), and thus satisfy the desired relation $h \gtrsim \mu$. For the above series, the wave functions and the energy levels of the original three-dimensional Pauli–Rashba operators are defined by formulas (4).

3. INTEGRABLE CASE, EXAMPLES

Spherical nano-film in a magnetic field. Consider a film of constant thickness around the standard unit sphere S^2,

$$r_1 = \cos\theta\cos\phi, \quad r_2 = \cos\theta\sin\phi, \quad r_3 = \sin\theta; \quad \theta \in [-\pi/2, \pi/2], \quad \phi \in [0, 2\pi].$$

Since the principal curvatures coincide, it follows that $\mathcal{G} \equiv 0$. Let the external potential be absent, let $v_{ext} \equiv 0$, and let the confinement potential be homogeneous with respect to the longitudinal coordinates, and thus $\varepsilon_\perp \equiv$ const. In this case, in the spherical coordinates, the reduced equation (3) becomes

$$-\frac{1}{2}\mu^2\Delta_M\psi = \widetilde{E}\psi, \quad \mu^2\Delta_M = \frac{\mu^2}{\cos\theta}\frac{\partial}{\partial\theta}\cos\theta\frac{\partial}{\partial\theta} + \frac{\mu^2}{\cos^2\theta}\frac{\partial^2}{\partial\phi^2} - i\mu w\frac{\partial}{\partial\phi} - \frac{1}{4}w^2\cos^2\theta, \quad \widetilde{E} = E - \varepsilon_\perp.$$

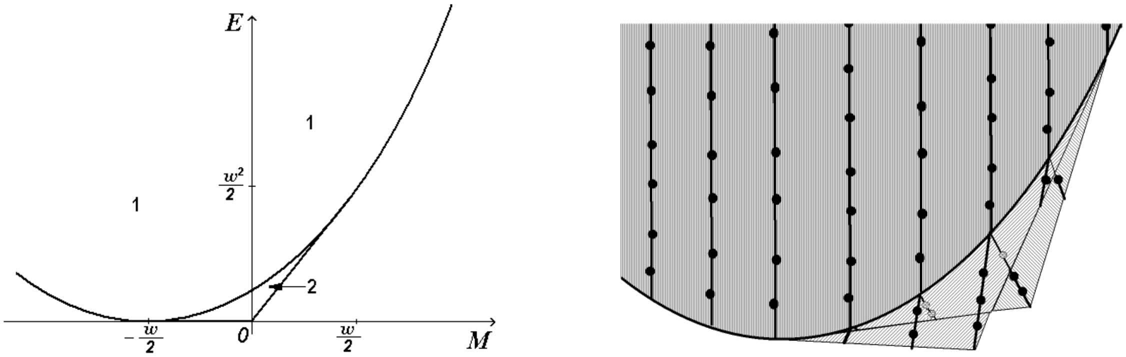

Fig. 1. Bifurcation curves and the set of connected components of the Liouville foliation for the motion on the sphere in a homogeneous magnetic field.

If the magnetic field is absent, $w = 0$, this is the classical eigenfunction and eigenvalue problem for the Laplace–Beltrami operator on the sphere. The answer is expressed in spherical functions, and the spectrum is $\tilde{E}_n = \mu^2 n(n+1)/2$. However, if the field is present, then the answer cannot be expressed in elementary and/or special functions.

This equation was semiclassically studied in [8] (this work was motivated by studies involving numerical computations [6, 7]). Explicit formulas for the spectrum were successfully obtained only for the asymptotic behavior of the spectrum for high and low values of the magnetic field (shifted Landau levels for high fields and the Zeeman splitting of the eigenvalues that are degenerate on the absence of the magnetic field). To construct a semiclassical approximation, one first studies the classical system of motion of a charged point particle on the surface of the sphere in a homogeneous magnetic field.

The corresponding Hamiltonian in the spherical coordinates (the configuration ones, θ and ϕ, and the conjugate momentum coordinates, p_θ and p_ϕ) on the phase space T^*S is of the form

$$H(\theta, \phi, p_\theta, p_\phi) = \frac{p_\theta^2}{2} + \frac{1}{2}\Big(\frac{p_\phi}{\rho(\theta)} + \frac{w\rho(\theta)}{2}\Big)^2.$$

The Hamiltonian system is integrable, and the second integral is p_ϕ. The phase space is foliated into invariant manifolds, which are the level curves of the first integrals, $H = \text{const} = E$ and $p_\phi = \text{const} = M$. The mapping of the phase space onto the plane of values E, M is referred to as the momentum mapping. The critical values of this mapping form the bifurcation diagram (see [9]). The curves of the bifurcation diagram partition the (E, M) plane into domains in which every point has the union of several Liouville tori as their preimage (the Liouville–Arnold theorem). This preimage continuously depends on the point inside the domain, and the number of its connected components depends on the choice of the domain only. The bifurcation diagram for the motion on the sphere in a homogeneous magnetic field is presented in Fig. 1 on the left.

The points of domain 1 correspond to the same connected component (to a single Liouville torus). The points of domain 2 correspond to two components (one of the tori is entirely placed in the upper hemisphere $\theta > 0$ and the other is symmetrically placed in the lower hemisphere $\theta < 0$). In these domains, one can use the Bohr–Sommerfeld quantization conditions and constructions of the canonical operator to obtain asymptotic solutions.

The parabola $E = \frac{1}{2}(M + \frac{w}{2})^2$ bounds domain 1 and corresponds to motions along the equatorial circle. The points $|M| > w/2$ of this parabola correspond to stable rotations. For these rotations, the asymptotics of the Maslov complex germ method are constructed (see case II),

$$\psi_{nm} = \mathrm{H}_n\left(\theta\sqrt{\Omega/\mu}\right) e^{-\frac{\theta^2\Omega}{2\mu}} e^{im\phi}, \quad E_{nm} = \frac{1}{2}\Big(m\mu + \frac{w}{2}\Big)^2 + \mu\Omega(n + \tfrac{1}{2}); \quad n \sim 1,\ m \sim M/\mu, \tag{13}$$

where H_n stand for the Hermite polynomials and $\Omega = \sqrt{M^2 - w^2/4}$.

Two segments bounding domain 2 from outside also correspond to stable closed invariant curves in the phase space. The first segment is horizontal and corresponds to circles formed of stationary points that are located at the same distance from the vertical axis Z. The other segment is of slope $E = Mw$ and corresponds to the cyclotron rotation along the circles intersecting the sphere orthogonally to the Z axis. The corresponding asymptotics are of the form

$$E_{nm} = \mu w\sqrt{1 - 2m\mu/w}(n + \tfrac{1}{2}); \qquad n \sim 1,\ m \sim -M/\mu, \tag{14}$$

$$E_{nm} = m\mu w + \mu w\sqrt{1 - 2m\mu/w}(n + \tfrac{1}{2}); \quad n \sim 1,\ m \sim M/\mu, \tag{15}$$

respectively.

The point $(0, 0)$ of the plane (E, M) corresponds to two stationary points at the poles of the sphere. Both the points admit an oscillatory approximation, which gives the so-called Landau levels in the first approximation,

$$E_n = \mu w(n + \tfrac{1}{2}); \quad n \sim 1,\ m \sim 1. \tag{16}$$

This series determines the asymptotic behavior of the lower states of the spectrum, and the degeneration with respect to the index m is taken away in the correcting terms (see [10]).

The set of connected components of the foliation of the phase space forms a multisheeted surface (see Fig. 1). The sheets correspond to continuous families of Liouville tori. The boundaries of the sheets correspond to critical invariant submanifolds of the Hamiltonian system, i.e., to singular sets (separatrices) and to degenerations into tori of lesser dimension (circles and points). The section of this surface by $M = \text{const}$ gives the so-called Reeb graph. We discuss this question in the next example (see also [14]).

Preimages of sheets of this surface correspond to maximal domains in the phase space on which one can introduce the action-angle variables. The Bohr–Sommerfeld quantization rules are written out in a unified way on every sheet in the form

$$I_1 = \mu m, \quad I_2 = \mu(l + 1/2), \quad m, l \in \mathbb{Z}. \tag{17}$$

Here the action variables are

$$I_1 = M, \quad I_2 = \oint \sqrt{2E - \left(\frac{M}{\rho(\theta)} + \frac{w\rho(\theta)}{2}\right)^2}\, d\theta.$$

The calculations for the quantization rules (17) in the limit cases, near the boundaries of the sheets, give the spectral series (13)–(16). Nevertheless, the asymptotic *eigenfunctions* (17) do not pass into (13)–(16) and are not asymptotic solutions if they correspond to Liouville tori in a neighborhood of the boundaries of the sheets.

This means that, to obtain the semiclassical spectral series, it suffices to use the quantization rules (17). They are satisfied by a discrete set of points on the above surface corresponding to the set of connected invariant submanifolds of the phase space. On any sheet, this gives its own series (see Fig. 1 on the right). The projection of all possible series to the energy axis defines the asymptotic spectrum of the original reduced problem.

The next important classical integrable example is also an axially symmetric surface, namely, the torus.

Toric nano-film in a magnetic field. Consider the three-dimensional figure of rotation about the axis $\mathbf{Z}$ in the form of a thin film around the torus $\Gamma = T^2$,

$$T^2 = \begin{cases} r_1 = (R + \cos\theta)\cos\phi, \\ r_2 = (R + \cos\theta)\sin\phi, \qquad \theta, \phi \in [0, 2\pi], \quad R > 1. \\ r_3 = \sin\theta, \end{cases}$$

For the coordinates on the torus, we choose $x_1 = \theta, x_2 = \phi$, and the metric tensor is of the form

$$g_{ij} = \begin{pmatrix} 1 & 0 \\ 0 & \rho^2(\theta) \end{pmatrix},$$

where $\rho(\theta) = (R + \cos\theta)$ stands for the distance to the axis of rotation.

Assume that the magnetic field is codirectional with the axis of rotation, $\mathbf{B} \upuparrows \mathbf{Z}$, and denote the absolute value of this field by $w = |\mathbf{B}|$. In this case, the components of the vector potential on the surface of the torus are as follows: $A_\theta = 0$, $A_\phi = -\frac{w}{2}$, and $A_n = 0$. The external electric field is absent, $\mathrm{v}_{\mathrm{ext}} = 0$. Assume that $E_1 \equiv \mathrm{const}$ and the shift $\widetilde{E} = E - E_1 \to E$ is also done.

Then the reduced equation (3) is of the form

$$\Big(-\frac{1}{2}\mu^2\Delta_M + \mu^2\mathcal{G}(\theta)\Big)\psi = E\psi. \tag{18}$$

Here

$$\mu^2\Delta_M = \frac{1}{\rho(\theta)}\frac{\partial}{\partial\theta}\rho(\theta)\frac{\partial}{\partial\theta} + \frac{1}{\rho^2(\theta)}\frac{\partial^2}{\partial\phi^2} - iw\frac{\partial}{\partial\phi} - \frac{1}{4}w^2\rho^2(\theta),$$
$$\mathcal{G}(\theta) = -\frac{1}{8} + \frac{\cos\theta}{4(R+\cos\theta)} + \frac{\sin\theta - \cos^2\theta}{8(R+\cos\theta)^2}.$$

One can further immediately pass to the classical system, which is integrable by virtue of the axial symmetry, and then construct a semiclassical approximation similarly to the consideration in the previous example. However, in this case, another order of steps is possible, namely, one can first separate the variables in the quantum equation and then construct the semiclassical approximation for the one-dimensional system.

Substituting

$$\psi(\theta,\phi) = e^{-\frac{iM\phi}{\mu}}\psi(\theta), \qquad M = m\mu, \quad m \in \mathbb{Z},$$

into equation (18), we obtain

$$\Big(-\frac{1}{2}\frac{\mu^2}{\rho(\theta)}\frac{\partial}{\partial\theta}\rho(\theta)\frac{\partial}{\partial\theta} + \frac{1}{2}\frac{M^2}{\rho^2(\theta)} + \frac{1}{2}wM + \frac{1}{8}w^2\rho^2(\theta) + \mu^2\mathcal{G}(\theta)\Big)\psi = E\psi. \tag{19}$$

Let us choose an arbitrary value of M for a while. The semiclassical solutions of problem (19) are defined by using invariant curves of the one-dimensional Hamiltonian system

$$H(\theta,p_\theta) = \frac{p_\theta^2}{2} + W(\theta), \qquad W(\theta) = \frac{1}{2}\left(\frac{M}{\rho(\theta)} + \frac{w\rho(\theta)}{2}\right)^2,$$

in the phase space $(\mathbb{R}_\theta \mod 2\pi) \times \mathbb{R}_{p_\theta}$. The cylinder $(\mathbb{R}_\theta \mod 2\pi) \times \mathbb{R}_{p_\theta}$ and the trajectories on the cylinder can be considered on the plane $\mathbb{R}^2 = \mathbb{R}_\theta \times \mathbb{R}_{p_\theta}$, where the points (θ, p_θ) and $(\theta \pm 2\pi, p_\theta)$ are identified (see Figs. 3 and 4).

The trajectories in the phase space are contained in the level curves $H = \mathrm{const} = E$. The nonsingular curves (where $dH \neq 0$) are closed curves (contractible or wrapping around the cylinder $(\mathbb{R}_\theta \mod 2\pi) \times \mathbb{R}_{p_\theta}$ exactly once), and thus Proposition 3 can be applied to these curves and a series of quasimodes can be constructed. The singular fibers (containing singularities, i.e., points at which $dH = 0$) are separatrices (families of curves with singularities at the endpoints) or stationary points (the quantization of singularities is developed in [11] and, for the quantization of nondegenerate points, the oscillator approximation is usually applied).

The set of connected components of the level curves of the Hamiltonian function H is a graph (see the "Reeb graphs" in [9]). In this case, for the interior points of the edges, we have nonsingular Lagrangian cycles, whereas vertices correspond to components with singularities, namely, for the vertices of strict local minimum, we have stable stationary points, and, for vertices with at least three edges, we obtain separatrices. Accordingly, different semiclassical quantizations can be represented together on different domains of the Reeb graph (see Fig. 5).

The possible Reeb graphs for our model with different parameters M, w are presented in Fig. 7. In this figure, the upper edges correspond to closed cycles wrapping around the cylinder, which corresponds to the overbarrier case $E > E_{s2}$; the other edges correspond to contractible cycles

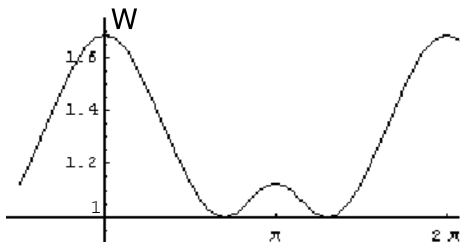

Fig. 2. Potential W for $w = M = 1$ and $R = 2$.

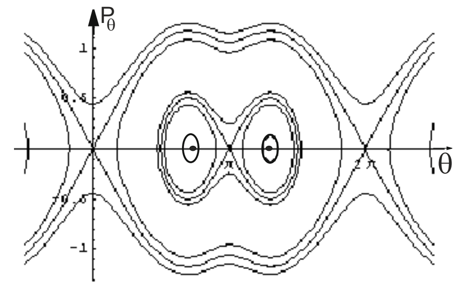

Fig. 3. Level curves of H.

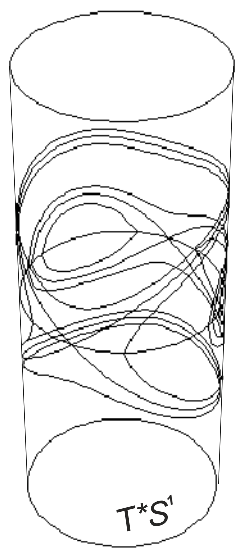

Fig. 4. Phase space and trajectories.

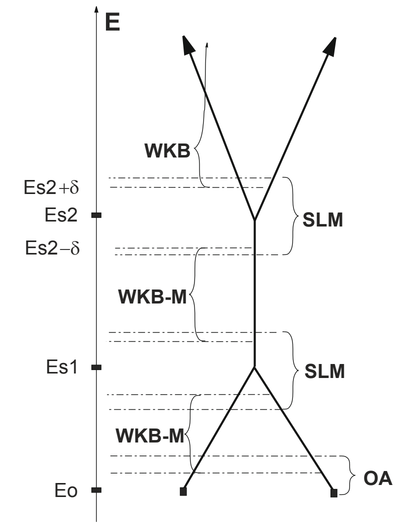

Fig. 5. Reeb graph.

(with "underbarrier reflection" on the circle $S^1 = (\mathbb{R}_\theta \mod 2\pi)$). The lower vertices of the Reeb graph correspond to stable equilibrium points.

For the "over-barrier" case, the classically accessible domain of motion coincides with the entire circle S^1, which enables us to apply the WKB approximation. In this case, every asymptotic spectral value is degenerate of multiplicity two, and the two WKB functions constructed from the same classical motions in opposite directions can be transformed to the real-valued eigenfunctions

$$\psi_1(\theta) = \frac{1}{\sqrt{p_\theta(\theta)}} \cos\Big(\frac{1}{\mu}\int_0^\theta p_\theta(\tau)d\tau\Big), \quad \psi_2(\theta) = \frac{1}{\sqrt{p_\theta(\theta)}} \sin\Big(\frac{1}{\mu}\int_0^\theta p_\theta(\tau)d\tau\Big),$$
$$\frac{1}{\mu}\oint p_\theta(\theta)\,d\theta = 2\pi|l|, \qquad l \in \mathbb{Z}, \tag{20}$$

where the last relation, which is an equation for the asymptotic spectrum, can be regarded as a smoothness condition for the functions $\psi_{1,2}$ at the point $\theta = 0$; the absolute value of the classical momentum is

$$p_\theta(\theta) = \sqrt{2E - \Big(\frac{M}{\rho(\theta)} + \frac{w_c\rho(\theta)}{2}\Big)^2}.$$

Substituting these solutions into the spectral problem (19), we obtain the discrepancy

$$\varepsilon_{1,2}(\theta) = \frac{1}{2}\frac{\mu^2}{\rho(\theta)}\Big(\frac{\partial}{\partial\theta}\rho(\theta)\frac{\partial}{\partial\theta}\frac{1}{\sqrt{p_\theta(\theta)}}\Big)\psi_{1,2}(\theta)\sqrt{p_\theta(\theta)} + \mu^2\mathcal{G}(\theta)\psi_{1,2}(\theta),$$

which can be estimated as

$$|\varepsilon_{1,2}(\theta)| < \mu^2\Big(\frac{(R+1)^2}{(R-1)^2} + \frac{\alpha}{\delta} + \frac{\beta}{(R-1)\delta^{5/4}} + \frac{\beta^2}{\delta^2} + \frac{3\beta}{\delta^{5/2}}\Big).$$

For the "under-barrier" case, in which the corresponding trajectory γ has two turning points $(\theta, p_\theta) = (\theta_{\min,\max}, 0)$, a more general ansatz of the semiclassical approach is to be used, which is based on the construction of the Maslov canonical operator $\psi(\theta) = K_\gamma[1]$, where

$$K_\gamma : C_0^\infty(\gamma) \to C^\infty(S^1 \times (0,1])$$

stands for the Maslov canonical operator on the Lagrangian curve γ. The wave functions $\psi(\theta)$ thus obtained are also "rapidly" oscillating inside the classically accessible domain and damp deep into the inaccessible domain. The following asymptotic expression can be used (where ψ stands for the leading term of the asymptotic for $K_\gamma[1]$):

$$\begin{gathered}\psi(x \in D_{in}(\mu)) = \frac{1}{\sqrt{p_\theta(\theta)}} \cos\Big(\frac{1}{\mu}\int_{\theta_{\min}}^{\theta} p_\theta(\tau)d\tau - \frac{\pi}{4}\Big),\\ \psi(x \in D_\pm(\mu)) = \mu^{-1/6} Ai(\mu^{-2/3}\beta_\pm^{1/3}(\theta - \theta_{\max/\min})),\\ \frac{1}{\pi\mu}\int_{\theta_{\min}}^{\theta_{\max}} p_\theta(\theta)\, d\theta = l - \frac{1}{2}, \qquad l \in \mathbb{N}, \quad l \sim \frac{1}{\mu},\end{gathered} \tag{21}$$

where $D_{in}(\mu) = [\theta_{\min} + \sqrt{\nu}, \theta_{\max} - \sqrt{\nu}\,]$ is the accessible domain placed at a distance $\sim \sqrt{\nu}$ from the boundaries, $D_-(\mu) = [0, \theta_{\min} + \sqrt{\mu}]$ and $D_+(\mu) = [\theta_{\max} - \sqrt{\mu}, \pi)$ are the complements of $D_{in}(\mu)$, and $\beta_\pm = \pm\big|2W'(\theta_{\max\,/\,\min})\big|$. The discrepancy of these solutions has a much more complicated form; however, it is mainly determined by the same expression $\mu^2\big(\frac{1}{\sqrt{p_\theta(\theta)}}\big)''$ inside the classically accessible domain and is exponentially small outside.

The oscillator approximation gives the quasimodes corresponding to the stationary points θ^* in a stable nondegenerate equilibrium; it is obtained by replacing the potential W by its quadratic part at the minimum point near which one studies small oscillations,

$$\psi_n = \sqrt[4]{\Omega/\mu}\, \mathrm{H}_n\big((\theta - \theta^*)\sqrt{\Omega/\mu}\,\big) e^{-\frac{(\theta-\theta^*)^2\Omega}{2\mu}}, \qquad E_n = W(\theta^*) + \Omega\mu(n + \tfrac{1}{2}), \qquad n = O(1); \tag{22}$$

here $\Omega = \sqrt{W''(\theta^*)}, \mathrm{H}_n$ stand for the Hermite polynomials. The following cases are possible:

$$\begin{aligned} &\theta^* = \pi, && \Omega = \sqrt{\frac{w^2(R-1)}{4} - \frac{M^2}{(R-1)^3}}, && |M| < \frac{w(R-1)^2}{2},\\ &\rho^2(\theta^*) = \frac{2|M|}{w}, && \Omega = w|\rho'(\theta^*)|, && \frac{w(R-1)^2}{2} < |M| < \frac{w(R+1)^2}{2},\\ &\theta^* = 0, && \Omega = \sqrt{\frac{M^2}{(R+1)^3} - \frac{w^2(R+1)}{4}}, && \frac{w(R+1)^2}{2} < |M|. \end{aligned}$$

As the energy of a trajectory is reduced up to the minimum, conditions (21) pass to conditions (13)[2].

Proposition 4. *The set of points E that satisfies the quantization conditions in* (20) *and* (21) *and is located at a distance from the values of energy on a separatrix approaches the exact spectrum,*

$$\mathrm{dist}(E, \mathrm{spec}(\hat{H})) < C\mu^2.$$

Moreover, beginning from some μ, different points of this set approximate different exact eigenvalues of problem (19).

Thus, the set of all possible semiclassical solutions corresponds to a discrete set of points of the Reeb graph of the function H in a one-to-one way. The projection of this set to the axis E gives the

[2]However, when approaching a separatrix, one must use the Bohr–Sommerfeld singular rules [11].

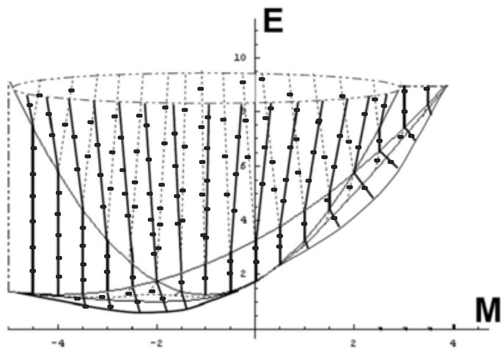

Fig. 6. Reeb graphs as a function of M.

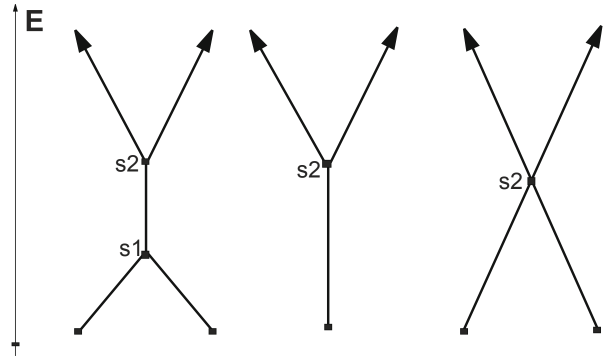

Fig. 7. Possible Reeb graphs.

asymptotic spectrum (19) of states with a certain projection of the momentum $M = m\mu$. Taking the union of the Reeb graphs for diverse M, we obtain a multisheeted surface (see Fig. 6). To any point of the surface that satisfies the quantization conditions (20) and (21), one can assign a pair $(E, \psi(\theta, \phi))$ approximately satisfying the spectral problem (3).

This assertion holds in the arbitrary integrable case. For example, the semiclassical solutions of an abstract problem on a compact surface of constant negative curve for which the form of the magnetic field is proportional to the area form were obtained in a similar way [12]. Nonintegrable case, proof of some assertions of part I, and some physical applications of the constructed spectral series will be published in part III.

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