Dedicated to the memory of V. A. Geyler

Quantum Dynamics in a Thin Film, I. Propagation of Localized Perturbations

J. Brüning*, S. Yu. Dobrokhotov**, R. V. Nekrasov**, and T. Ya. Tudorovskiy**

*Institut für Mathematik, Humboldt-Universität zu Berlin Rudower Chaussee 25, 12489 Berlin, Germany E-mail: bruening@mathematik.hu-berlin.de **Institute for Problems in Mechanics RAS, pr. Vernadskogo 101-1, Moscow, 119526 Russia E-mail: dobr@ipmnet.ru, logno@rambler.ru, timtudor@mail.ru

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Abstract. In the one-particle approximation, the quantum behavior of a (quasi-)particle is studied in a thin waveguide having the form of a thin curvilinear film (in three-dimensional space) placed in external magnetic and electric fields. Objects of this type arise in the actively developing physics of nano-structures and, in particular, in the theory of ballistic transport of electrons. The corresponding quantum-mechanical equation is a Pauli-type equation with nonrelativistic Rashba spin-orbital interaction for a two-dimensional vector function. Asymptotic solutions of the Cauchy problem with special localized initial data and those of the spectral problem are obtained. The construction of asymptotic solutions is carried out in two stages. At the first stage, in the framework of the adiabatic approximation, using the "operator separation of variables" (the "generalized adiabatic principle") for a rather broad class of quantum states, the original three-dimensional equation is reduced to a two-dimensional surface (the limit film), and then diverse solutions of this reduced equation are constructed. The first part of the paper is devoted to the reduction and the solutions of the Cauchy problem. Spectral problems will be treated in the second part.

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1. INTRODUCTION

In the paper, we study the quantum behavior of a (quasi-)particle in a thin waveguide having the form of a thin curvilinear film (in three-dimensional space) placed in external magnetic and electric fields. Objects of this type arise in the actively developing physics of nano-structures and, in particular, in the theory of ballistic transport of electrons [11, 10, 34, 16, 19, 33]. In the oneparticle approximation, the corresponding quantum-mechanical equation is a Pauli-type equation with nonrelativistic Rashba spin-orbital interaction for a two-dimensional vector function Ψ with components Ψ_1, Ψ_2 (see [10, 17]),

$$i\hbar\Psi_t = \widehat{\mathcal{H}}\Psi, \qquad \widehat{\mathcal{H}} = \widehat{\mathbf{P}}^2/(2m) + v_{\text{int}}(\mathbf{r}) + v_{\text{ext}}(\mathbf{r},t) - e\hbar/(2mc)\langle\boldsymbol{\sigma},\mathbf{H}\rangle + \widehat{\mathcal{H}}_{\text{SO}}.$$
 (1.1)

Here $\widehat{\mathbf{P}} = -i\hbar\nabla - (e/c)\mathbf{A}(\mathbf{r},t)$, \hbar is the Planck constant, e is the effective charge, m is the effective mass of the quasiparticle, c is the velocity of light, $v_{\text{ext}}(\mathbf{r},t)$ and $\mathbf{A}(\mathbf{r},t)$ are the potentials of the external electric and magnetic field, $\mathbf{H} = \operatorname{rot} \mathbf{A}(\mathbf{r},t)$ is the intensity of the magnetic field, $\boldsymbol{\sigma} = \{\sigma_1, \sigma_2, \sigma_3\}$ stand for the standard Pauli matrices, and $\hat{\mathcal{H}}_{\text{SO}} = \alpha \langle \boldsymbol{\sigma}, [\nabla v_{\text{int}}, \widehat{\mathbf{P}}] \rangle$ is the interaction of the spin with the intrinsic electric field (this interaction is determined by an effective constant α). We restrict ourselves to the case of a homogeneous magnetic field \mathbf{H} . The fact that the problem is treated in a thin film (the domain Ω) is reflected by the existence of the so-called confinement potential $v_{\text{int}}(\mathbf{r},\mu)$ in the operator $\hat{\mathcal{H}}$; 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 film is thin means that the typical "longitudinal" size of the film is much greater than the normal size. Below we return to the problem to define the domain Ω , the surface Γ , etc.

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For Eq. (1.1), we consider special boundary value problems and spectral problems formulated below. It is clear from physical considerations that the dynamics of an electron in the film must be approximately determined by some effective Hamiltonian on the two-dimensional surface Γ ; the Hamiltonian can depend on the geometry of the film, its local thickness, and so on. Therefore, it is natural to decompose the problem to find wave functions on the film into two parts: 1) the reduction of Eq. (1.1) from three-dimensional space to the two-dimensional surface Γ , 2) the construction of solutions of the reduced equation. The first part of the paper is mainly devoted to the accurate derivation of the reduced equation. This procedure uses a special version of the adiabatic approximation, namely, the so-called "operator separation of variables" [5, 14, 1, 2]. We also consider here problems concerning the propagation of localized perturbations for the reduced equations thus derived; in this consideration, we use the Maslov canonical operator [26, 29] to construct asymptotic solutions of these equations and complete the exposition with several simple examples. The spectral problems are treated in the next part of the paper.

2. OPERATOR \mathcal{H} IN CURVILINEAR COORDINATES

Curvilinear coordinates. When seeking solutions of Eq. (1.1), it is natural to use appropriate curvilinear coordinates. The surface Γ can be, for instance, a cylinder or a sphere, and therefore the coordinates (the longitudinal coordinates $\mathbf{x} = (x^1, x^2)$ and the transversal coordinate y) can be defined in general only locally, in a small neighborhood of an arbitrary (but connected) part of the surface Γ . Let the surface Γ be (locally) equipped with some coordinates x^1, x^2 . Suppose that Γ is defined by a vector function $\mathbf{R}(x^1, x^2)$ by the rule $\Gamma = {\mathbf{r} \in \mathbb{R}^3 | \mathbf{r} = \mathbf{R}(x^1, x^2)}$. Let \mathbf{n} be a unit vector orthogonal to the surface Γ . In this case, the coordinates x^1, x^2, y can be defined by setting $\mathbf{r} = \mathbf{R}(\mathbf{x}) + y\mathbf{n}(\mathbf{x})$.

Note that the coordinates x^1, x^2 need not be orthogonal in general; however, we always have $\langle \mathbf{n}, \mathbf{n} \rangle = 1$ and $\langle \mathbf{n}, \partial_i \mathbf{R} \rangle = 0$, i = 1, 2. Thus, the metric tensor becomes

$$G_{ab} = \left\| \begin{array}{cc} \gamma_{ij} & 0\\ 0 & 1 \end{array} \right\|, \qquad a, b = 1, 2, 3, \tag{2.1}$$

where $\gamma_{ij} = \langle \partial_i \mathbf{r} \partial_j \mathbf{r} \rangle = g_{ij} + y(\langle \partial_i \mathbf{R}, \partial_j \mathbf{n} \rangle + \langle \partial_i \mathbf{n}, \partial_j \mathbf{R} \rangle) + y^2 \langle \partial_i \mathbf{n}, \partial_j \mathbf{n} \rangle$, i, j = 1, 2, and g_{ij} is the metric tensor on Γ . Hereafter, $G = \det G_{ab} = \gamma = \det \gamma_{ij}$, $g = \det g_{ij}$. As is well known, in the curvilinear coordinates, to simplify the manipulations, it is useful to replace the function Φ by the function $\Phi = \Psi G^{1/4}$. Therefore, we immediately represent the original equation in the curvilinear coordinates for the function Φ ,

$$\hbar \Phi_t = \left[G^{1/4} \widehat{\mathcal{H}} G^{-1/4} \right] \Phi.$$
(2.2)

Write out the Hamiltonian in the form $\widehat{\mathcal{H}} = \widehat{\mathcal{H}}_O + \widehat{\mathcal{H}}_S + \widehat{\mathcal{H}}_{SO}$, where

$$\widehat{\mathcal{H}}_{O} = (1/2) \left(-i\hbar\nabla - (e/c)\mathbf{A} \right)^{2} + v_{\text{int}}(x, y) + v_{\text{ext}}(\mathbf{r}, t),
\widehat{\mathcal{H}}_{SO} = \alpha \left\langle \boldsymbol{\sigma}, \left[\nabla v_{\text{int}}, -i\hbar\nabla - (e/c)\mathbf{A} \right] \right\rangle, \qquad \widehat{\mathcal{H}}_{S} = -e\hbar/(2mc) \left\langle \boldsymbol{\sigma}, \mathbf{H} \right\rangle.$$
(2.3)

In the calculation below, it is convenient to use the notation customary for relativity theory, including the *summation with respect to repeated indices*. We also write

$$\partial_j = \partial/\partial x^j, \quad \hat{p}_j = -i\hbar\partial/\partial x^j, \quad \hat{p}_y = \hat{p}_3 = -i\hbar\partial/\partial y$$

Let us use the invariant form of the operator $(-i\hbar\nabla - (e/c)\mathbf{A})^2$ and Coulomb gauge:

$$\left(-i\hbar\nabla - \frac{e}{c}\mathbf{A}\right)^2 = \frac{1}{2}\left(-i\hbar\operatorname{div} - \frac{e}{c}\mathbf{A}\right)G^{ab}\left(-i\hbar\nabla_b - \frac{e}{c}A_b\right), \quad \operatorname{div}\mathbf{v} = \frac{1}{\sqrt{G}}\frac{\partial}{\partial x^a}\sqrt{G}\,v^a, \quad \operatorname{div}\mathbf{A} = 0,$$
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$$G^{1/4}\widehat{\mathcal{H}}_{O}G^{-1/4} = (\gamma^{ij}/2)(\hat{p}_{i}\hat{p}_{j} - 2A_{i}\hat{p}_{j} + A_{i}A_{j}) + v_{\text{ext}}(\mathbf{r}, t) + v_{\text{int}}(x, y) - (i\hbar/2)\partial_{i}(\gamma^{ij})\hat{p}_{j}$$
(2.4)
- $(i\hbar/4)\gamma^{ij}A_{i}\partial_{j}(\ln\gamma) - (\hbar^{2}/2)\gamma^{-1/4}\partial_{i}[\gamma^{1/2}\gamma^{ij}\partial_{j}(\gamma^{-1/4})] - (1/2)\gamma^{-1/4}\partial_{y}[\gamma^{1/2}\partial_{y}(\gamma^{-1/4})],$

where $A_i = (e/c) \langle \partial_i \mathbf{r}, \mathbf{A} \rangle$ and $A_y = (e/c) \langle \mathbf{n}, \mathbf{A} \rangle$. Moreover, it is clear that

$$G^{1/4}\mathcal{H}_S G^{-1/4} = \mathcal{H}_S.$$
(2.5)

Finally, let us represent the operator of spin-orbital interaction in an invariant form,

$$G^{1/4}\mathcal{H}_{SO}G^{-1/4} = \alpha \gamma^{-1/2} \varepsilon^{jkm} \sigma_a(\partial_k v_{\text{int}}) \left(\hat{p}_m - A_m + (i\hbar/4)\partial_m(\ln\gamma) \right), \ \sigma_j = \langle \partial_j \mathbf{r}, \boldsymbol{\sigma} \rangle, \tag{2.6}$$

where j, k, m = 1, 2, 3 and ε^{jkm} stands for the identity completely antisymmetric tensor. Formulas (2.4)–(2.6) define Eq. (2.2) in the curvilinear coordinates.

Modelling the film's boundary: "soft" and "rigid" walls. By problems with "rigid" walls we mean problems with zero confinement potential $v_{int} = 0$ and with the Dirichlet conditions $\Psi|_{\partial\Omega} = 0$. In problems on films with "soft" walls, it is assumed that $v_{int} \neq 0$ and $\Psi(x, y) \in L_2(y)$ for any x. In the latter case, it is further assumed that the potential $v_{int}(x, y)$ is uniquely defined on the entire space \mathbb{R}^3 . The last condition is too strong; however, since the function $\Psi(x, y)$ is usually exponentially small for $y \gg \mu$, any assumptions concerning the function Ψ in this area negligibly influence its behavior. To be definite, assume that $\Psi(x, y)|_{\partial\Omega} = 0$. An "empty" film with "rigid" walls can be regarded as the limit case of soft walls described by a potential with rapid growth near the boundaries. For example, consider the potential $v_{int}(x, y') = (y'/D(x))^{2m}$, $y' = y/\mu$, m > 0. In this case, $v_{int}(x, yd(x)) \to \infty$ as $m \to \infty$. Below we restrict ourselves to the modeling of films using "soft" walls, adding also the hard-wall conditions on the boundary of a certain film neighborhood.

Parameters of the problem. Introduce the typical sizes. Suppose first that the film $\Omega \subset \mathbb{R}^3$ is bounded by two smooth surfaces Γ_1 and Γ_2 without boundaries. The quantum process is described by a wave function $\Psi(\mathbf{r}, t)$ on the domain Ω . Denote by l_0 the typical size of the domain Ω and by d_0 the typical thickness of the film. We assume that $l_0 \gg d_0$, which means that the film is *thin.* This relation leads to the presence of a small parameter $\mu = d_0/l_0$ in the problem under consideration. We refer to μ as the *adiabatic* parameter. Suppose for a while that the film is flat, $\Omega = \{(x_1, x_2, y) \in \mathbb{R}^3 : 0 \leq y \leq d_0\}$, i.e., it is bounded by the planes $\Gamma_1 = \{y = 0\}$ and $\Gamma_2 = \{y = d_0\}$, that there are no electric and magnetic fields, and that the model with rigid walls is treated. In this case, instead of (1.1), we have the Schrödinger equation corresponding to a free particle with Dirichlet conditions on Γ_1 and Γ_2 . In this case, one can construct the wave function $\Psi(x, t)$ in the form of a plane wave $\Psi(\mathbf{r}, t) = \exp(-i\omega t + i\langle k_{\parallel}, x \rangle) \sin(k_{\perp} y)$. This function is characterized by two wavelengths, the longitudinal length $\lambda = 2\pi/|k_{\parallel}|$ and the transversal length $\lambda_{\perp} = 2\pi/|k_{\perp}|$. We consider processes with transversal wavelengths comparable with the thickness of the film $d_0, \lambda_{\perp} \sim d_0$. This means that the wave function Ψ has only a few (for instance, one or two) oscillations in the transverse direction. The number of oscillations of the wave function in the longitudinal direction has nothing in common in general with the oscillations in the transverse direction and can be characterized by another dimensionless parameter $h = \lambda/l_0$, which we call *semiclassical* or dynamical. In contrast to the parameter μ , the parameter h can take different values corresponding to different wave processes.

Equation in dimensionless variables. Let us now rewrite Eqs. (2.2)–(2.6) in dimensionless coordinates, considering the existence of diverse scales. Write $\mathbf{x}' = \mathbf{x}/l_0$ and $y' = y/d_0$. Introduce the dimensionless time, t' = t/T, $T = md_0l_0/\hbar$ (the unit is the time needed for a free particle with longitudinal energy $\varepsilon_0 = \hbar^2/(md_0^2)$ to travel the distance l_0). We also introduce the dimensionless potentials $v'_{\text{int}} = v_{\text{int}}/\varepsilon_0$, $v'_{\text{ext}} = v_{\text{ext}}/\varepsilon_0$, and $\mathbf{A}' = ed_0(\hbar c)^{-1}\mathbf{A}$, and also the dimensionless magnetic field as the number of quanta of the flow of the magnetic field through the rectangle with the sides l_0 and d_0 , $\mathbf{H}' = 2\pi l_0 d_0 \cdot \mathbf{H}/\Phi_0$ and $\Phi_0 = 2\pi \hbar c/e$, and the dimensionless quantity $\alpha' = \hbar \alpha/l_0 d_0$. The evaluation of the constant $\tilde{\alpha}$ for specific materials and actual magnetic fields shows that α' does not exceed one. For this reason, we divide Eq. (1.1) by the typical energy of the transversal motion, ε_0 . In this case, Eq. (2.2) becomes

where

$$i\mu\Phi_t = \widehat{\mathcal{H}}'\Phi, \quad \widehat{\mathcal{H}}' = \widehat{\mathcal{H}}'_O + \widehat{\mathcal{H}}'_S + \widehat{\mathcal{H}}'_{SO},$$
(2.7)

$$\widehat{\mathcal{H}}_{O}^{\prime} = (\gamma^{ij}/2)(\widehat{p'}_{i}\widehat{p'}_{j} - 2A'_{i}\widehat{p'}_{j} + A'_{i}A'_{j}) + (1/2)(-\partial_{y'}^{2} + 2iA'_{y}\partial_{y'} + A'_{y}^{2}) + v'_{\text{ext}}(x',\mu y',t') + v'_{\text{int}}(x',y')
- i\mu 2\gamma^{ij}_{,i}\widehat{p}'_{j} - (i\mu/4)\gamma^{ij}A'_{i}\partial_{j}(\ln\gamma) - (i/4)A'_{y}\partial_{y'}(\ln\gamma) - (\mu^{2}/2)\gamma^{-1/4}\partial_{i}[\gamma^{1/2}\gamma^{ij}\partial_{j}(\gamma^{-1/4})]
- (1/2)\gamma^{-1/4}\partial_{y'}[\gamma^{1/2}\partial_{y'}(\gamma^{-1/4})], \qquad \widehat{\mathcal{H}}_{SO}^{\prime} = (\mu\alpha'/\gamma^{1/2})\varepsilon^{jkm}\sigma_{j}(\partial_{k}v'_{\text{int}})Q_{m}, \qquad (2.8)$$

$$\begin{aligned} \widehat{\mathcal{H}}'_{S} &= \mu/2 \langle \boldsymbol{\sigma}, \mathbf{H}' \rangle, \qquad Q_{1,2} = \left(\hat{p}'_{1,2} - A'_{1,2} + (i\mu/4)\partial_{1,2}(\ln\gamma) \right), \qquad Q_{3} = \left(-i\partial_{y} + (i/4)\partial_{y}(\ln\gamma) \right), \\ \sigma_{j} &= \langle \partial_{j}\mathbf{r}, \boldsymbol{\sigma} \rangle, \quad \widehat{p}'_{1,2} = -i\mu\partial/\partial x'^{1,2}, \quad \gamma^{jk} = \gamma^{jk}(x',\mu y'), \quad \gamma = \gamma(x',\mu y'), \quad j,k,m = 1,2,3. \end{aligned}$$

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Let us stress that, in contrast to v_{int} , the potential v_{ext} includes the parameter μ at y'. This reflects the rapid growth of v_{int} in the normal direction to the film.

Equation (2.3) with the Hamiltonian (2.8) is the object of our subsequent investigation. In what follows, to simplify the notation, we omit the primes at all variables and functions except for the function \mathcal{H}' and the operator $\hat{\mathcal{H}}'$. The assumption that the external fields and the confinement potential change rather slowly in the longitudinal direction means that the coefficients in the operator $\hat{\mathcal{H}}$ are smooth functions.

Symbol of the operator $\hat{\mathcal{H}}'$ and its expansion. Equation (2.3)–(2.8) belongs to the class of equations with operator-valued symbol [26, 2]. The variables x and y enter the equation in a different way with respect to the parameter μ , namely, the derivatives with respect to x contain μ , whereas the derivative with respect to the other variable does not. This very fact makes it possible to apply the adiabatic approximation in the case under consideration. It is convenient to represent

the operator (2.8) in the form $\hat{\mathcal{H}}' = \mathcal{H}'(-i\mu\partial/\partial x, \hat{x}, \partial_y, y, \mu)$, where the digits over the operators mean the order of their action (see [28]) and the operator-valued function $\mathcal{H}'(p, x, \partial_y, y, \mu)$, is obtained from (2.8) by replacing the operators \hat{p}'_j by the variables p_j . In order to find approximate (asymptotic) solutions of Eqs. (2.3)–(2.8), we need only several first terms of the expansion $\mathcal{H}'(p, x, \partial_y, y, \mu) = \mathcal{H}'_0(p, x, \partial_y, y) + \mu \mathcal{H}'_1(p, x, \partial_y, y) + \mu^2 \mathcal{H}'_2(p, x, \partial_y, y) + \cdots$ in the parameter μ . Using the relations $\mathbf{A} = \mathbf{A}_0 + \mu y \mathbf{A}_1$, $\mathbf{A}_0 = 1/2[\mathbf{H}, \mathbf{R}]$, $\mathbf{A}_1 = 1/2[\mathbf{H}, \mathbf{n}]$, $A_i = A_i^0 + \mu y A_i^1 + O(\mu^2)$, $A_i^0 = \langle \partial_i \mathbf{R}, \mathbf{A}_0 \rangle$, $A_i^1 = \langle \partial_i \mathbf{R}, \mathbf{A}_1 \rangle + \langle \partial_i \mathbf{n}, \mathbf{A}_0 \rangle$, $A_y = A_y^0 + \mu y A_y^1 + O(\mu^2)$, $A_y^0 = \langle \mathbf{n}, \mathbf{A}_0 \rangle$, and $A_y^1 = \langle \mathbf{n}, \mathbf{A}_1 \rangle = 0$ and the Taylor expansions of the functions γ^{jk} , γ , etc., in the parameter μ , we obtain

$$\mathcal{H}_{0}^{\prime}\left(x, p, y, -i\partial/\partial y, t\right) = (1/2)g^{kj}\mathcal{P}_{k}\mathcal{P}_{j} + (1/2)\hat{\mathcal{P}}_{y}^{2} + v_{\text{ext}}\left(\mathbf{R}(x), t\right) + v_{\text{int}}(x, y),$$
(2.9)

$$\mathcal{H}_{1}'(x,p,y,-i\partial/\partial y,t) = (1/2)y\gamma_{1}^{kj}\mathcal{P}_{k}\mathcal{P}_{j} - yg^{kj}\mathcal{P}_{k}A_{j}^{1} + \langle \nabla v_{\text{ext}}(\mathbf{R}(x),t),y\mathbf{n} \rangle - i((1/2)(\partial g^{kj}/\partial x^{k})p_{j})$$

$$+(1/4)g^{kj}A_{k}^{0}\partial_{j}(\ln g)+(1/4)A_{y}^{0}[\partial_{y}(\ln \gamma)]_{y=0}+(1/2)\langle\boldsymbol{\sigma},\mathbf{H}\rangle+g^{-1/2}(\partial_{y}v_{\rm int})(\sigma_{2}\mathcal{P}_{1}-\sigma_{1}\mathcal{P}_{2}).$$
 (2.10)

Here $p = (p_1, p_2)$, $\mathcal{P}_k = p_k - A_k^0$, $\hat{\mathcal{P}}_y = p_y - A_y^0$, $g^{kj} = \gamma^{kj}|_{y=0}$, and $g = \gamma|_{y=0}$. The last summand in \mathcal{H}'_1 corresponds to the spin-orbital interaction and the coefficients g^{ij} define the elements of the metric tensor of the surface Γ . The summands \mathcal{H}'_j with indices j exceeding 2 have a complicated structure; however, they are not needed to construct the leading term of the asymptotic solutions of the original equation, except for the value of \mathcal{H}'_2 for $\mathcal{P}_i = 0$ and $v_{\text{ext}} = 0$. For $\mathcal{H}'_2|_{\mathcal{P}_i=0, v_{\text{ext}}=0}$, we have

 $\mathcal{H}'_2(x,0,y,-i\partial/\partial y,t) \equiv \mathcal{G}(x) - (1/2)g^{-1/4}\partial_i [g^{1/2}g^{ij}\partial_j (g^{-1/4})], \quad \mathcal{G}(x) = -(\varkappa_1 - \varkappa_2)^2/8.$ (2.11) This term does not depend on y and \hat{p}_y and contains geometric characteristics only, namely, characteristics of the embedding of the film Γ in three-dimensional space. We refer to $\mathcal{G}(x)$ as the geometric potential; its role in the theory of waveguides and resonators was first discovered by V.P. Maslov [25, 30].

Remark. With regard to specific numerical values of the intensities of the magnetic and electrical fields, one actually can and must often assume that the potentials $v_{int}(x, y)$, $v_{ext}(\mathbf{R}(x), t)$, and A_j depend on μ regularly, and thus the formulas for \mathcal{H}'_0 and \mathcal{H}'_1 can also include summands of order $O(\mu)$. However, it seems to be hardly reasonable to immediately make the corresponding re-expansions because the formulas become significantly more awkward. For the same reason, we omit this dependence in the arguments of these functions.

3. REDUCTION TO AN EQUATION ON A TWO-DIMENSIONAL SURFACE

Adiabatic approximation and the "operator separation of variables". As we said above, since the problem has different scales in the longitudinal and transversal directions of the film, it is natural to assume that the original problem can be reduced to a family of two-dimensional problems describing the longitudinal motion. Certainly, an exact reduction of this kind can be carried out precisely only for a few models, and the reduction is usually carried out in an approximate or, more exactly, in an asymptotic sense. As a rule, the full asymptotic expansion is rather complicated and has a rather puristic interest. For physical applications, it suffices to construct the

leading term of the expansion (and sometimes several corrections to the leading term). From the "asymptotic point of view," the reduction is related to the presence of the small parameter μ and can be realized in the framework of the adiabatic approximation, which we apply in the form of an "operator separation of variables" (the "generalized adiabatic principle", [14, 5, 2, 1], see also [31, 13]). This approach amalgamates the classical Born–Oppenheimer approximation [6, 7], the theory of equations with operator-valued symbols [26], the operator methods [28], and also the "Peierls substitution" from the physics of solids [32, 22].

As was noted above, in the problems under consideration there is another "semiclassical" parameter h characterizing the longitudinal wavelengths in the film. In every specific problem, it is natural to assume that these parameters are related, and we set $h = \mu^{\alpha}$, where $2 \ge \alpha \ge 0$. This relation between the parameters was discussed in detail in [1, 2, 8, 3], where a classification of the longitudinal waves is carried out (based on a relation of this type) and some remarks are expressed explaining that, in fact, under the corresponding conditions on the potentials, it suffices to restrict ourselves to the relations h = O(1) ("long" waves), $h = O(\sqrt{\mu})$ ("medium" waves), $h = O(\mu)$ ("short" waves), $h = O(\mu^{3/2})$ ("ultrashort" waves), and $h = O(\mu^2)$ and higher (states). The reduction we make includes the case of $\alpha \leq 3/2$, and the two-dimensional reduced equation thus obtained (on the surface Γ) enables one to describe all cases with these values of α . Moreover, this equation describes solutions whose structure varies in time and solutions containing singularities with respect to h related to the presence of focal points. (One of the simplest examples of this kind, namely, a Cauchy problem with localized initial data, is considered in the next subsection.) In the case of "superexcitated" states, the adiabatic approximation is no longer applicable, the reduced equation is not related to the original one, and one must use other approaches. We also note that there are many monographs and publications concerning adiabatic problems, and we mention only the sources [10, 12, 13, 17, 18].

Let us now discuss the operator separation of variables for Eq. (2.7). Since there are different scales in the longitudinal and in the transversal directions of the film, one can separate the modes adiabatically. The standard adiabatic approach enables one to separate the modes as follows: starting from the fundamental papers of Born and Oppenheimer [6, 7], the leading part of the wave function in the adiabatic approximation is sought in the form of a product

$$\Phi(x, y, t, \mu) \approx \chi(y, x, \mu)\psi(x, t, \mu).$$
(3.1)

However, this representation can be used only if the function $\psi(x, t, \mu)$ is rather smooth, and it works badly for sufficiently large energies of longitudinal motion. If the function $\psi(x, t, \mu)$ has rapid oscillations (for instance, if ψ is a WKB-solution $\psi(x, t, \mu) = \exp(iS(x, t, \mu)/h)\varphi(x, t, \mu, h))$, then the representation (3.1) is inconvenient for the decomposition, and it becomes necessary to include the momentum $\partial S/\partial x$ into the factor $\chi(y, x, \mu)$ and use the formula [26]

$$\Phi(x, y, t, \mu) \approx \chi(y, x, \partial S / \partial x, \mu) \psi(x, t, \mu)$$
(3.2)

instead of formula (3.1). Recall that the phase S is a solution of the Hamilton–Jacobi equation $\partial S/\partial t + H^h_{\text{eff}}(\partial S/\partial x, x, t) = 0$ with the so-called effective Hamiltonian $H^h_{\text{eff}}(p, x, t)$. Formula (3.2) is still not satisfactory because, if focal effects exist (like turning points or caustics), the WKB-representation is wrong, and the form of ψ and χ must be changed. We want to "correct" formula (3.2) so that the new formula will be valid for focal points and turning points as well. This correction is based on the observation that, in the case of WKB solution, the right-hand side of Eq. (3.2) is preserved (up to a small correction, see [26]) if we assume that the first factor is a

(pseudodifferential) operator $\chi(\hat{x}, -i\mu\partial/\partial x, y, t, \mu)$ represented as a function (its symbol) of noncommuting operators x and $\hat{p} = -i\mu\partial/\partial x$. Thus, in the adiabatic approach, it is suggested to seek $\Psi(x, y, t)$ in the form

$$\Phi(x, y, t, \mu) = \chi \left(\hat{x}, -i\mu \,\partial /\partial x, y, t, \mu \right) \psi(x, t, \mu), \tag{3.3}$$

where $\hat{\chi}$ is a 2 × 2 matrix whose elements are pseudodifferential operators. The indices over the operators mean the order of their action. From the physical viewpoint, we "freeze" not only the slow variables x (as in the adiabatic approximation) but also the slow momentum which is the differential operator $-i\mu\partial/\partial x$ in quantum mechanics.

We still have not fixed an equation for the function ψ (which describes the longitudinal motion). Following the idea of Peierls substitution in the physics of solids (see [32, 22]), assume that ψ is a

solution of the following equation describing the longitudinal dynamics:

$$i\mu\psi_t = L(\hat{x}, -i\mu\,\partial/\partial x, t, \mu)\psi, \qquad (3.4)$$

where \hat{L} stands for the effective Hamiltonian with the essential part $H_{\text{eff}}(\hat{x}, -i\mu\partial/\partial x, t)$. The objective of the present paper is to evaluate the operators \hat{L} and $\hat{\chi}$ and to construct the semiclassical asymptotics of Eq. (3.4). The evaluation of the operators \hat{L} and $\hat{\chi}$ is reduced to the evaluation of their symbols, i.e., of the functions $L(p, x, t, \mu)$ and $\chi(p, x, t, y, \mu)$. As a rule, this evaluation cannot be carried out exactly, and we restrict ourselves to the evaluation of the coefficients $L_0, L_1, L_2 | p = 0, \chi_0, \text{ and } \chi_1$ in the expansions $L = L_0(p, x, t) + \mu L_1(p, x, t) + \mu^2 L_2(p, x, t) + \cdots$ and $\chi = \chi_0(p, x, t, y) + \mu \chi_1(p, x, t, y) + \mu^2 \chi_2(p, x, t, y) + \cdots$. This turns out to be sufficient to find the leading term of the asymptotic solutions (with respect to the parameters μ or h (see [1, 2, 8])) we are interested in. The description of the operator separation of variables is presented in these papers; for completeness of our exposition, we also present it in the appendix.

Effective Hamiltonian and corrections to it. To find the effective Hamiltonian L_0 and the function χ_0 in the situation with "soft" walls, one must solve the following auxiliary spectral problem for any chosen x:

$$\left(-(1/2)\partial^2/\partial y^2 + v_{\rm int}(x,y)\right)u(x,y) = \varepsilon_{\perp}(x)u(x,y), \qquad \|u(x,y)\|_y = 1.$$
(3.5)

Denote by $\|\cdot\|$ and $\langle\cdot,\cdot\rangle$ the norm and the inner product in $L_2(\mathbb{R}_y)$, respectively. As is well known, the spectrum of this problem is nondegenerate, all eigenvalues are separated from one another, and the eigenfunctions can be chosen to be real. Therefore, the value of u(x,y) is preserved as the point x bypasses a closed path on Γ , and hence the function u(x,y) (as well as $\varepsilon_{\perp}(x)$) is a one-valued smooth function of x (and y). Let us enumerate the eigenfunctions and the eigenvalues by the index $\nu, \nu = 0, 1, 2...$ We have

$$H_{\text{eff}}^{\nu}(x,p,t) = (1/2)g^{ij}\mathcal{P}_{i}\mathcal{P}_{j} + v_{\text{eff}}, \quad v_{\text{eff}} = v_{\text{ext}} \big(\mathbf{R}(x), t \big) + \varepsilon_{\perp}^{\nu}(x), \quad \chi_{0}^{\nu} = \exp(iy\langle \mathbf{n}, \mathbf{A}_{0} \rangle) u^{\nu} E_{s}, \quad (3.6)$$

where E_s is a unitary 2×2 matrix in the spin space. The index ν is referred to as the index of "subzone of dimensional quantization." We fix this index and, to simplify the notation, omit the dependence on this index in the objects arising below as a rule.

For the model potential $v_{\text{int}}(x,y) = (y/D(x))^{2m}$, m > 0, we obtain $\varepsilon_{\perp}(x) = (d(0)/d(x))^2 \varepsilon_{\perp}(0)$, where $d(x) = D(x)^{\frac{m}{m+1}} d(0)$ is the variance of the state with the energy $\varepsilon_{\perp}(x)$. Assuming that the thickness of the film is proportional to d(x), we see that $D(x)^{\frac{m}{m+1}}$ is the coefficient of the homothety. As $m \to \infty$, this coefficient tends to D(x), which corresponds to a half of the thickness of the film with "rigid" walls.

Let us evaluate the first correction for the effective Hamiltonian of the longitudinal motion, i.e., the matrix L_1 . It is determined by the following formula (see the appendix):

$$L_{1} = \left\langle \chi_{0}^{T}, \mathcal{H}_{1}'\chi_{0} \right\rangle_{y} - i\left\langle \chi_{0}^{T}, \frac{d\chi_{0}}{dt} \right\rangle_{y} - i\left\langle \chi_{0}^{T}, \left[\frac{\partial\mathcal{H}_{0}}{\partial p_{j}} - \frac{\partial H_{\text{eff}}^{\mu}}{\partial p_{j}}\right] \frac{\partial\chi_{0}}{\partial x^{j}} \right\rangle_{y}, \qquad (3.7)$$
$$\frac{d\chi_{0}}{dt} = T\frac{\partial\chi_{0}}{\partial t} - \frac{\partial H_{\text{eff}}^{\mu}}{\partial x^{j}} \frac{\partial\chi_{0}}{\partial p_{j}} + \frac{\partial H_{\text{eff}}^{\mu}}{\partial p_{j}} \frac{\partial\chi_{0}}{\partial x^{j}}.$$

Write $Y = Y^{\nu}(x) = \langle \chi_0, y \chi_0 \rangle_y$. Apply the relations

$$\begin{split} \langle u, \partial_j u \rangle_y &= 0, \quad \left\langle \chi_0, \frac{\partial \chi_0}{\partial t} \right\rangle_y = iY \left\langle \mathbf{n}, \frac{\partial \mathbf{A}_0}{\partial t} \right\rangle, \quad \left\langle \chi_0, \frac{\partial H_{\text{eff}}^{\text{eff}}}{\partial p_j} \frac{\partial \chi_0}{\partial x^j} \right\rangle_y = iY g^{ij} \mathcal{P}_i \partial_j \left\langle \mathbf{n}, \mathbf{A}_0 \right\rangle, \\ Y g^{ij} \mathcal{P}_i \langle \partial_j \mathbf{R}, \mathbf{A}_1 \rangle = -Y g^{ij} \mathcal{P}_i \left\langle \mathbf{n}, \partial_j \mathbf{A}_0 \right\rangle = (1/2) \langle \mathbf{H}, \mathbf{\Lambda} \rangle, \\ g^{ij}_{,i} p_j - \partial_i (g^{ij} A_j^0) = \partial_i (g^{ij} \mathcal{P}_j), \quad \partial_i (g^{ij} A_j^0) + (1/2) g^{ij} A_i^0 \partial_j (\ln g) + A_y^0 [\partial_y (\ln \gamma)]_{y=0} = 0. \end{split}$$

(The last relation is the zero term of the expansion of the gauge rule

$$\partial_i(\gamma^{ij}A_j) + (1/2)\gamma^{ij}A_i\partial_j(\ln\gamma) + \partial_yA_y + (1/2)A_y\partial_y(\ln\gamma) = 0$$

ith respect to the change $y = \mu y'$.) This yields

$$L_{1} = -Y\alpha_{j}^{i}g^{jk}\mathcal{P}_{i}\mathcal{P}_{k} - \left\langle \mathbf{E}(\mathbf{R}(x),t), Y\mathbf{n} \right\rangle - \left\langle \mathbf{H}, \mathbf{\Lambda} \right\rangle + (1/2)\langle \boldsymbol{\sigma}, \mathbf{H} \rangle - (i/2)\partial_{i}(g^{ij}\mathcal{P}_{j}) + g^{-1/2}\langle u, (\partial_{y}v_{\text{int}})u \rangle (\sigma_{2}\mathcal{P}_{1} - \sigma_{1}\mathcal{P}_{2}).$$

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Here $\mathbf{\Lambda} = [Y\mathbf{n}, \mathbf{\mathcal{P}}], \mathbf{\mathcal{P}} = g^{ij}\mathcal{P}_i\partial_j\mathbf{R}$, and $\mathbf{E} = -\nabla v_{\text{ext}} - T(\partial \mathbf{A}_0/\partial t)$. The summand in the last row corresponds to the spin-orbital interaction. Note now that, for any subzone with index ν , one can choose the "middle surface" (by using the change of variable $y \to y - Y^{\nu}(x)$) in such a way that the function $Y = Y^{\nu}(x)$ vanishes. In this case, the first three summands in the formula vanish. Further, we have $\langle u, (\partial_y v_{\text{int}})u \rangle = 0$ (see Appendix A3), and therefore the *spin-orbital interaction makes no contribution to* L_1 . Thus, as the result, we obtain

$$L_1 = (1/2) \langle \boldsymbol{\sigma}, \mathbf{H} \rangle - (i/2) (\partial/\partial x^k) (g^{kj} \mathcal{P}_j), \qquad k, j = 1.$$
(3.8)

Finally, it follows from the formula for L_2 (see Appendix A2) that the contribution into L_2 for $\mathcal{P}_i = 0, v_{\text{ext}} = 0$ is made only by $\mathcal{H}'_2(x, 0, y, -i\partial/\partial y, t) \equiv \mathcal{G}(x) - (1/2)g^{-1/4}\partial_i[g^{1/2}g^{ij}\partial_j(g^{-1/4})]$. Therefore, $L_2|_{\mathcal{P}=0, v_{\text{ext}}=0} = \mathcal{G}(x) - (1/2)g^{-1/4}(\partial/\partial x^k)[g^{1/2}g^{kj}\partial_j(g^{-1/4})]$. Thus, the reduced equation for the longitudinal function ψ becomes (we neglect the correcting summands making no contribution into the leading term of the asymptotic solutions):

$$i\mu\psi_t = \left[H_{\rm eff}(\hat{p}, \hat{x}^2) + \mu L_1(\hat{p}, \hat{x}^2) + \mu^2 \mathcal{G}(x)\right]\psi, \tag{3.9}$$

where H_{eff} is determined by formula (3.6), L_1 by (3.8), and $\mathcal{G}(x)$ by (2.11).

The matrix part of the operator on the right-hand side is the constant matrix $(1/2)\langle \boldsymbol{\sigma}, \mathbf{H} \rangle$, which can be eliminated by the substitution¹ $\psi = \exp(-(i/2)\langle \boldsymbol{\sigma}, \mathbf{H} \rangle t)\varphi$. Furthermore, it is convenient to present φ in the form $\varphi = g^{1/4} \begin{pmatrix} \psi^+ \\ \psi^- \end{pmatrix}$. In what follows, we assume that this substitution is carried out and that ψ^{\pm} are the amplitudes corresponding to the spin that is codirected or counterdirected to the magnetic field. To simplify the notation of the equation derived above, we also note that the summand $-(i\mu/2)\partial_i(g^{ij}\mathcal{P}_j^{\mu})$ in (3.8) should be referred to the operator \hat{L}_0 as an addition needed for \hat{L}_0 to be self-adjoint and occurring due to asymmetric (non-Weyl) quantization of the "kinetic" part of its symbol $(1/2)g^{ij}\mathcal{P}_i\mathcal{P}_j$; the same holds for the second \mathcal{G} -summand in (2.11) which occurs in the Laplace–Beltrami operator due to the modification of the measure of vector functions under the change $\Psi \to \Phi = \Psi G^{1/4}$. Finally, for the functions ψ^{\pm} , we have

$$i\mu \frac{\partial \psi^{\pm}}{\partial t} = \left(-\mu^2 \Delta_M + v_{\text{ext}} \left(\mathbf{R}(x), t\right) + \varepsilon_{\perp}(x) + \mu^2 \mathcal{G}(x)\right) \psi^{\pm}, \qquad (3.10)$$
$$-\Delta_M = -\frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} \sqrt{g} g^{ij} \frac{\partial}{\partial x^j} + 2i g^{ij} A_i \frac{\partial}{\partial x^j} + g^{ij} A_i A_j + \frac{i}{\sqrt{g}} \left(\frac{\partial}{\partial x^i} \sqrt{g} g^{ij} A_j\right),$$

where $\mathcal{G}(x) = -(\varkappa_1 - \varkappa_2)^2/8$, Δ_M stands for the Laplace operator on the surface Γ with regard to the curvature and the presence of magnetic field (which manifests itself in the replacement of the derivatives by "long" derivatives). We especially note that the spin in the preserved summands in the equation thus obtained is totally absent, which means that effects related to the spin are inessential for the leading term of the asymptotics.

The recovering of a solution of the original equation from the functions ψ^{\pm} is carried out by the formula

$$\Psi = g^{1/4} G^{-1/4} \Big(\exp(iy\langle \mathbf{n}, \mathbf{A}_0 \rangle) u^{\nu} + \mu \chi_1 (-i\mu \partial/\partial x, \hat{x}, y, t) \Big) \exp(-(i/2) \langle \boldsymbol{\sigma}, \mathbf{H} \rangle t) \Big(\psi^+_{\psi^-} \Big).$$
(3.11)

Note that, first, the summand $\mu\chi_1(-i\mu\partial/\partial x, \tilde{x}, y, t)$ (in contrast to χ_0) is really an operator rather than a function and, second, this summand gives only a correction to the leading term; however, if we do not take it into account, then the function thus constructed is not an asymptotic solution of the original equation. These problems were discussed in detail in [1, 2, 8].

4. CAUCHY PROBLEM WITH LOCALIZED INITIAL DATA

Let us show by an example of the Cauchy problem with localized initial data how one may find solutions which are related to regimes with diverse wavelengths on one hand, and contain focal points and change their structure in the course of evolution on the other hand.

Representation of initial data in the form of canonical operator. Let us suppose for a while that Γ is a diffeomorphic to the plane \mathbb{R}^2 . Let h be a small positive parameter and let V(z), $z \in \mathbb{R}^2$, be a smooth function decaying at infinity as $1/|z|^k$, $k \ge 1$, where the derivatives $\partial V/\partial z_j$

¹Since the magnetic field is directed along the z axis, the matrix $\langle \boldsymbol{\sigma}, \mathbf{H} \rangle$, and hence the matrix L_1 as well, is diagonal (with the elements $\pm (1/2)|\mathbf{H}| - (i/2)\partial_i(g^{ij}\mathcal{P}_j)$).

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decay as $1/|z|^{k+1}$. Write z = x/h, $x \in \mathbb{R}^2$. The function V(x/h) is localized in a neighborhood of zero. The objective of this section is to construct the asymptotics of the Cauchy problem

$$\psi\big|_{t=0} = V(x/h) \tag{4.1}$$

for the reduced equation (3.10). Here we consider the case in which the parameter h is related to μ by $\mu = h^{\alpha}$, where $\alpha \ge 0$. In particular, we claim that the form of the asymptotic behavior of the Cauchy problem heavily depends on this ratio (i.e., on α). To solve the Cauchy problem, we would like to use the general scheme [26, 29] based on the Maslov canonical operator. To this end, we use the following representation for localized functions. Denote by $\tilde{V}(p)$ Fourier transform of the function V(z),

$$\tilde{V}(p) = \frac{1}{2\pi} \int_{\mathbb{R}^2_y} e^{-i\langle p, z \rangle} V(z) dz.$$

Here the symbol $\langle \cdot, \cdot \rangle$ stands for the real inner product. In this case, we have the formula

$$V(x/h) = \frac{1}{2\pi} \int_{\mathbb{R}^2_p} e^{(i/h)\langle p, x \rangle} \tilde{V}(p) dp.$$

$$(4.2)$$

The function V(x/h) rapidly decreases outside a small neighborhood of the point x = 0. Meaning the study of asymptotic solutions of the Cauchy problem with the initial data of the form (4.2) for partial differential equations, one can represent the expression on the right-hand side in the form of the Maslov canonical operator $K_{\Lambda_0^2}^h$ on the Lagrangian manifold (a plane) given by

$$\Lambda_0^2 = \{ p = \alpha, x = 0 \mid \alpha \in \mathbb{R}^2 \} \text{ acting on the function } \tilde{V}(\alpha) \text{ on } \Lambda_0^2, V(x/h) = (h/i) K_{\Lambda_z^2}^h[\tilde{V}(\alpha)].$$

$$(4.3)$$

The last relation readily follows from the definition of canonical operator with regard to the following facts: (a) we have $\langle p, dx \rangle |_{\Lambda_0^2} = 0$; (b) all points on Λ_0^2 are focal and infinitely degenerate, and thus Λ_0^2 is covered by a single focal map x = 0 with the coordinates (p_1, p_2) ; (c) the Jacobian satisfies the relation det $\partial p / \partial \alpha \equiv 1$. Formula (4.3) defines a δ -shape sequence and, as $h \to +0$, we have

$$h^{-2}V(x/h) \to \delta(x) \int_{\mathbb{R}^2} V(z) dz$$

and, in essence, formulas (4.2),(4.3) give a "spreading" of the Dirac δ -function which is based on the well-known representation

$$\delta(x) = (2\pi)^{-2} \int_{\mathbb{R}^2} e^{i\langle p, x \rangle} dp$$

If Γ is not diffeomorphic to the plane \mathbb{R}^2 , for example, Γ is a sphere or a cylinder, then we assume that V(z) is finite and preserve (4.1), (4.3).

Shortwave asymptotics. First consider the case in which $\mu = h$ in (4.1). Having in mind the representation (4.3) and the general scheme [26, 29], we construct the asymptotics of the solution of the Cauchy problem (3.10), (4.1). By [26, 29], this asymptotics is expressed using the solution of the Hamiltonian system in the phase space with the coordinates $p = (p_1, p_2), x = (x^1, x^2)$,

$$\dot{x}^{i} = \partial H_{\text{eff}}(x, p, t) / \partial p_{i}, \qquad \dot{p}_{i} = -\partial H_{\text{eff}}(x, p, t) / \partial x^{i}.$$
(4.4)

This system generates a canonical transformation $g_{H_{\text{eff}}}^t$ taking a point with coordinates (p^0, x_0) to the point $(p, x) = g_{H_{\text{eff}}}^t(p^0, x_0) = \mathcal{P}(p^0, x_0, t), \mathcal{X}(p^0, x_0, t)$, where $\mathcal{P}(p^0, x_0, t), \mathcal{X}(p^0, x_0, t)$ is the solution of system (4.4) with the initial data

$$P\big|_{t=0} = p^0, \qquad X\big|_{t=0} = x_0.$$
 (4.5)

The transformation $g_{H_{\text{eff}}}^t$ takes the Lagrangian manifold Λ_0^2 to the Lagrangian manifold given by $\Lambda_t^2 = g_{H_{\text{eff}}}^t \Lambda_0^2$ and, for the coordinates on the latter, one can choose the coordinates α induced by the coordinates on the manifold Λ_0^2 . Namely, denote by $(P(\alpha, t), X(\alpha, t))$ the trajectory of (4.4) issued from the point $(\alpha, 0)$. In this case, $\Lambda_t^2 = \{p = P(\alpha, t), x = X(\alpha, t)\}$.

Let us choose a point (x=0,p=0) on the manifold Λ_0^2 and denote by

$$\gamma_0 = \{ p = P^0(t) \equiv P(0, t), x = X^0(t) \equiv X(0, t) \}$$

the trajectory of the Hamiltonian system (4.4) issuing from this point (0,0). For any chosen t, we regard $(P^0(t), X^0(t))$ as a distinguished point on the Lagrangian manifold Λ_t^2 . Let us introduce a function $\tilde{V}(\alpha)$ on the family of Lagrangian manifolds Λ_t^2 , where $\tilde{V}(\alpha)$ is constant on the trajectories $P(\alpha, t), X(\alpha, t)$. On the trajectory γ_0 , we have the action

$$s(t) = \int_0^t \left(\left\langle p, \frac{\partial H_{\text{eff}}}{\partial p} \right\rangle - H_{\text{eff}} \right) \Big|_{\gamma_0} d\eta$$

Recall that a point $(p, x) = (P(\alpha, t), X(\alpha, t))$ (with the coordinates α) on Λ_t^2 is said to be nonsingular if $J(\alpha, t) = \det \partial X / \partial \alpha \neq 0$. This definition works, in particular, for the points $(P^0(t), X^0(t))$ on the trajectory γ_0 (with the coordinates $\alpha = 0$). Let time t be such that the point $P^0(t), X^0(t)$ is nonsingular. In this case, we can define the Morse index m(t) of this point on the trajectory; it is equal to the number of zeros (counted according to their multiplicities) of the Jacobian J(0, t) on the interval (0, t]. Let us construct the Maslov canonical operator $K_{\Lambda_t^2}^{\mu}$ on Λ_t^2 acting on the function

$$V(\alpha)$$
 and write

$$\psi^{\pm}(x,t,\mu) = -i\mu e^{is(t)/\mu - i\pi m(t)/2} K^{\mu}_{\Lambda^{2}_{t}} \tilde{V}(\alpha).$$
(4.6)

One of the main results of this paper is the following assertion.

The function $\psi^{\pm}(x,t,\mu)$ is the leading term of the asymptotic solution of the Cauchy problem (3.10), (4.1) with respect to mod $O(h^2)$ in $L_2(\Gamma)$.

This assertion seems to hold for a wide class of films and external potentials. Under some assumptions, in the second part of this paper, we present a proof using general assertions [26, 29] on solutions of Cauchy problems. Let us now present a realization and simplification of the general formula (4.6) in specific situations.

Example 1. Van-Vleck-type formula for localized initial conditions. A rather general formula can still be obtained under the assumption that the surface Γ (the layer) is diffeomorphic to the plane \mathbb{R}^2 and that the manifold Λ_t^2 is projected onto Γ bijectively. In this case, the Jacobian $J(\alpha, t) = \det \partial X(\alpha, t)/\partial \alpha$ vanishes nowhere, and the equation

$$X(\alpha, t) = x \tag{4.7}$$

can uniquely be solved with respect to α . Therefore, at any point x, we can define (in the coordinates of x) the action $\int_0^{\alpha(x,t)} \langle p, dx \rangle$ and the Jacobian $J(\alpha(x,t),t)$. In this case, formula (4.6) becomes

$$\psi^{\pm}(x,t,\mu) = -i\mu e^{is(t)/\mu - i\pi m(t)/2} e^{(i/\mu) \int_0^{\alpha(x,t)} \langle p, dx \rangle} \tilde{V}(\alpha(x,t)) / \sqrt{|J(\alpha(x,t),t)|}.$$
(4.8)

If the external electric and magnetic fields are absent, the layer is flat, and its thickness is constant, then (3.10) becomes the Schrödinger equation for the free particle, $H_{\text{eff}} = p^2$, $P = \alpha$, $X = 2\alpha t$, and the Jacobian is J = 2t; for t > 0, J does not vanish, the trajectory γ_0 is the point (0,0), m(t) = 0, s(t) = 0, $\int_0^\alpha \langle p, dx \rangle = \alpha^2 t$, and $\alpha(t,x) = x/2t$. Therefore, for t > 0, we obtain a well-known WKB-formula in quantum mechanics,

$$\psi^{\pm}(x,t,\mu) = -i\mu \frac{e^{ix^{-}/(4\mu t)}}{\sqrt{2t}} \tilde{V}\left(\frac{x}{2t}\right).$$
(4.9)

If one replaces the function \tilde{V} by 1 (or, which is the same, the function V by the delta function $\delta(x)$), then formula (4.8) is transformed, up to normalizing factors, to the Van Vleck formula for the semiclassical asymptotics of the Green function for the Cauchy problem for the Schrödinger equation, and this formula is well known in quantum mechanics (see, e.g., [4] and also [9]), whereas formula (4.9) is transformed into an exact formula for the Green function of the Schrödinger equation for a free particle. This example shows that the solution (4.8) can change its structure, but the intertwining operator $\hat{\chi}$ and the reduced equation remain invariant with respect to such transformations, which is the main advantage of the "operator separation of variables."

Example 2. Flat film in a homogeneous magnetic field. In this example, one can again obtain explicit formulas. Let Ω be a flat film of constant thickness ($\varepsilon_1(\mathbf{x}) = \text{const}$), the external electric field being absent, and the magnetic field being everywhere constant and equal to $\mathbf{H} = (H_1, H_2, H_3)$. In this case, the reduced equation (3.10) given on the plane $\Gamma = \mathbb{R}^2$ is simply the equation for a free particle in a constant magnetic field,

$$i\mu\partial\psi/\partial t = (1/2)\left(\left(-i\mu(\partial/\partial x_1) + (\omega/2)x_2\right)^2 + \left(-i\mu(\partial/\partial x_2) - (\omega/2)x_1\right)^2\right)\psi$$

where $\omega = H_3$. The corresponding trajectories of the Hamiltonian system (4.4) are of the form

$$P_{1}(t,\alpha) = \frac{1}{2} \left(\alpha_{1} + \alpha_{1} \cos(\omega t) + \alpha_{2} \sin(\omega t) \right), \quad P_{2}(t,\alpha) = \frac{1}{2} \left(\alpha_{2} + \alpha_{2} \cos(\omega t) - \alpha_{1} \sin(\omega t) \right), \tag{4.10}$$

$$X_{1}(t,\alpha) = \frac{1}{\omega} \left(\alpha_{2} - \alpha_{2} \cos(\omega t) + \alpha_{1} \sin(\omega t) \right), \quad X_{2}(t,\alpha) = \frac{1}{\omega} \left(-\alpha_{1} + \alpha_{1} \cos(\omega t) + \alpha_{2} \sin(\omega t) \right).$$

These very trajectories define the Lagrangian manifolds Λ_t^2 at the time moment t. At the time moments that are multiples of $T = 2\pi/\omega$, the trajectories return to the initial points $(x_1, x_2, p_1, p_2) = (0, 0, \alpha_1, \alpha_2)$, i.e., the Lagrangian manifold comes to the original one, and at the other moments, this manifold is projected to the plane (x_1, x_2) bijectively. The Jacobian J is equal to

$$J = \det \left| \partial x^i / \partial \alpha_j \right| = \omega^{-2} \Big|_{-1 + \cos(\omega t)}^{\sin(\omega t)} \frac{1 - \cos(\omega t)}{\sin(\omega t)} \Big| = 4 \sin^2(\omega t/2) \omega^{-2},$$

J = 0 at the points $t = 2\pi k/\omega$, $k = 0, \pm 1, \pm 2, \ldots$, and the zeros of J are obviously of multiplicity 2. The trajectory of γ_0 is the point (p = 0, x = 0), s(t) = 0 and, when "running along" this trajectory, the Morse index changes by 2 when passing through the points $t = 2\pi k/\omega$. Therefore, after "jumping" over k points of this kind, the index becomes equal to 2k, and one can rewrite the exponential $e^{is(t)/\mu - i\pi m(t)/2}$ in the form $sign(sin(\omega t/2))$. Let us present the asymptotics of the functions ψ^{\pm} at the time instants separated from kT, i.e., for some chosen $\varepsilon > 0$ and any integers $k = 1, 2, \ldots$, the time moments of interest belong to the set $|t - kT| > \varepsilon$. The phase on the Lagrangian manifold (in the variables α , the phase is well defined for any t) is

$$\int_0^\alpha \langle P, dX \rangle = \frac{\alpha^2}{2\omega} \sin(\omega t).$$

To evaluate the phase in the coordinates x, one must express α_1 and α_2 in the last formula in terms of x_1, x_2 by solving Eq. (4.7). Elementary manipulations give

$$\alpha_1 = \frac{\omega}{2} (x_1 \operatorname{ctg}(\omega t/2) - x_2), \qquad \alpha_2 = \frac{\omega}{2} (x_2 \operatorname{ctg}(\omega t/2) + x_1), \qquad \alpha^2 = \frac{\omega^2 (x_1^2 + x_2^2)}{4 \sin^2(\omega t/2)}$$

Therefore, $S(x_1, x_2, t) = (\omega/4)(x_1^2 + x_2^2) \operatorname{ctg}(\omega t/2)$. Thus, formula (4.8) becomes

$$\psi^{\pm} = -\frac{i\mu\omega}{2\sin(\omega t/2)} e^{i\omega x^2 \operatorname{ctg}(\omega t/2)/(4\mu)} \tilde{V}\Big(\frac{\omega}{2} (x_1 \operatorname{ctg}(\omega t/2) - x_2), \frac{\omega}{2} (x_2 \operatorname{ctg}(\omega t/2) + x_1)\Big).$$

As $\tilde{V} \to 1$, we obtain the well-known formula for the Green function for a free particle in a homogeneous magnetic field.

Example 3: Spherical film. Let Ω be a film of constant thickness near the unit sphere and let the external electric and magnetic fields be absent. In this case, the reduced equation is given on the sphere of unit radius $\Gamma = S^2$,

$$i\mu \frac{\partial \psi}{\partial t} = -\frac{\mu^2}{2}\Delta\psi, \qquad \Delta = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2},$$

where $\theta \in [0, \pi], \phi \in [0, 2\pi]$ are the spherical coordinates.

Let us present the asymptotic solution of this equation in the case of initial conditions strongly localized at the "noth pole" ($\theta = 0$), $\psi|_{t=0} = V(x_1/\mu, x_2/\mu)$, where $x_1 = \theta \cos \phi, x_2 = \theta \sin \phi$ are the coordinates in a neighborhood of the pole and V is a smooth compactly supported function. The trajectories of the Hamiltonian system (4.4) that pass through the north pole are the geodesics with

$$\theta(t, \alpha_1, \alpha_2) = \begin{cases} t\sqrt{\alpha_1^2 + \alpha_2^2} \pmod{2\pi} & \text{for } t\sqrt{\alpha_1^2 + \alpha_2^2} \pmod{2\pi} \in [0, \pi], \\ 2\pi - t\sqrt{\alpha_1^2 + \alpha_2^2} \pmod{2\pi} & \text{for } t\sqrt{\alpha_1^2 + \alpha_2^2} \pmod{2\pi} \in [\pi, 2\pi], \\ \phi(t, \alpha_1, \alpha_2) = \arccos\left(\frac{\alpha_1}{\sqrt{\alpha_1^2 + \alpha_2^2}}\right), \qquad p_{\theta}(t, \alpha_1, \alpha_2) = \sqrt{\alpha_1^2 + \alpha_2^2}, \qquad p_{\phi} = 0. \end{cases}$$

Modifying the parameters $(\alpha_1, \alpha_2) \in \mathbb{R}^2$, we obtain a set of points corresponding to the Lagrangian manifold at the time moment t. To any point of the sphere distinct from the poles, at any time moment t > 0, there comes a set of trajectories that are indexed by the number of performed full rotations and by the sign of the direction of motion (from the north pole/to the north pole). This means that, when projecting the Lagrangian manifold from the phase space to the configuration space (the sphere S^2), every point of the sphere distinct from the poles has countably many preimages, $\alpha_1^{(k)} = ((\theta + 2\pi k)/t) \cos \phi$, $\alpha_2^{(k)} = ((\theta + 2\pi k)/t) \sin \phi$, $k = \ldots, -2, -1, 0, 1, 2, \ldots$

Let us find the asymptotic behavior of the function $\psi(\theta, \phi, t)$, t > 0, in the cylindrical band $\theta \in [\varepsilon, \pi - \varepsilon], \varepsilon > 0$. To begin with, let us find the phase on the Lagrangian surface,

$$S(t,\alpha_1,\alpha_2) = \int_0^t \left\{ \mathbf{p}(\tau, P, \phi) \dot{\mathbf{x}}(\tau, P, \phi) - H(x(\tau, P, \phi), p(\tau, P, \phi)) \right\} \mathrm{d}\tau = \frac{(\alpha_1^2 + \alpha_2^2)t}{2}.$$

The Jacobian of the passage from the coordinates α_1, α_2 to the coordinates θ, ϕ of the configuration space is $J = t/\sqrt{\alpha_1^2 + \alpha_2^2}$.

The singular points on Λ_t^2 are the concentric circles $\alpha^2 = \pi n/t$, n = 0, 1, 2, ... (the preimages of the poles of S^2). The Maslov index can change when passing from one map to another. However, since the Jacobian J is everywhere positive, it follows that the modification of the Maslov index is zero, and the index is zero everywhere. Thus, the asymptotic solution in this example is of the form

$$\psi(\theta,\phi,t) = (1/t) \sum_{k=-\infty}^{k=+\infty} \sqrt{|\theta+2\pi k|} e^{i(\theta+2\pi k)^2/(2th)} \widetilde{V}(((\theta+2\pi k)/t)\cos\phi, ((\theta+2\pi k)/t)\sin\phi).$$

Since the function V is compactly supported, the function \tilde{V} vanishes at infinity, and the series can be truncated by replacing the limits $\pm \infty$ by $\pm 1/(\mu)^{\delta}$, where $\delta > 0$ is some small number. This truncation of the series is also useful when justifying the asymptotics.

Example 4: Compact Riemannian manifold. Let Ω be a film of constant thickness near a compact Riemannian manifold Γ and let the electric and magnetic fields be absent ($\mathbf{H} = E = 0$). In this case, the reduced equation is given on Γ and has the form

$$i\mu\frac{\partial\psi}{\partial t} = -\frac{\mu^2}{2}\Delta\psi,$$

where Δ is the Laplace–Beltrami operator on Γ . The initial condition is localized at an arbitrary point $X_0 \in \Gamma$. The Hamiltonian flow given by (4.4) is the geodesic flow. Suppose that all geodesics issuing from X_0 contain no focal points.

Let us present an asymptotic solution of this equation outside a neighborhood of the focal points, i.e., for the points containing no singularities of the projection of Λ_t^2 . To any point of $X \in \Gamma$, at any time moment t > 0, there comes a family of trajectories issuing from X_0 at t = 0. All these trajectories have their own length l(X) and their initial momentum α ; we enumerate them by an index $k \in I(X, t)$. The sets of preimages smoothly depend on $X \in \Gamma, t > 0$, and therefore the entire family of indices is countable and, in what follows, the summation is taken over one and the same set I.

Let us find the asymptotics of the function $\psi(\theta, \phi, t)$, t > 0. The phase on the Lagrangian surface is

$$S(t,\alpha) = \int_0^t \left\{ \mathbf{p}(\tau, P, \phi) \dot{\mathbf{x}}(\tau, P, \phi) - H(x(\tau, P, \phi), p(\tau, P, \phi)) \right\} \mathrm{d}\tau = \frac{\alpha^2 t}{2}.$$

Note that, if we know the expression for α_k in terms of X at some moment, then we know this at any time moment, $\alpha_k(X,t) = \alpha_k(X,1)/t$, where α_k^2 can be expressed in terms of the length of the geodesic, $\alpha_k^2(X,t) = l_k^2(X)t^{-2}$. The Jacobian of the passage from the coordinates α to the coordinates of the configuration space is $J_k = J_k(X)t$. The Maslov index vanishes because the focal points are absent by assumption. Thus, in this example, the asymptotic solution is of the form

$$\psi(X,t) = \frac{1}{\sqrt{t}} \sum_{k \in I} \frac{1}{\sqrt{J_k(X)}} e^{il_k^2(X)t/h} \widetilde{V}(\alpha_k(X,t)).$$

Gaussian wave packets and "medium" waves. Let us now consider the situation in which $h = \sqrt{\mu}$ and restrict ourselves to the case in which the initial function has the form of Gaussian exponential $V = \exp(-\langle y, B^0 y \rangle/2)$. Here B^0 stands for a symmetric positive 2×2 matrix. Assume that the initial function is localized in a neighborhood of the point $x = \xi$. In this case,

$$\psi^{\pm}|_{t=0} = A \exp\left(-\langle x - \xi, B^{0}(x - \xi)\rangle/(2\mu)\right),$$
(4.11)

where A is a constant. The application of the above scheme to construct an asymptotic solution without strong additional assumptions is not possible due to a mismatch between the parameters μ and h in the equation and in the initial data. If we take μ for the "basic" parameter, then the corresponding functions V(y) and $\tilde{V}(p)$ should be replaced by $V(y\sqrt{\mu})$ and $\tilde{V}(p/\sqrt{\mu})$, and thus the amplitude in the asymptotics becomes a rapidly varying function, which prevents an application of formula (4.6). In this case, to construct an asymptotic solution, one can use complex germ theory [27, 15]. Let us describe these solutions. They consist of a trajectory $(P(t,\xi), X(t,\xi))$ of the same Hamiltonian system (4.4) issuing from an initial point of the form $(P(0,\xi), X(0,\xi)) = (0,\xi)$; along with this chosen trajectory, one must find matrix solutions $(B(t,\xi), C(t,\xi))$ of the linear system (system in variations which is linearized on the trajectory $(P(t,\xi), X(t,\xi))$ of the system (4.4),

$$\dot{B} = -H_{px}(P(t,\xi), X(t,\xi))B - H_{xx}(P(t,\xi), X(t,\xi))C, \qquad B\big|_{t=0} = B^0, \dot{C} = H_{pp}(P(t,\xi), X(t,\xi))B + H_{px}(P(t,\xi), X(t,\xi))C, \qquad C\big|_{t=0} = E.$$
(4.12)

Note that det $C \neq 0$ for any t [27].

Proposition 4.2. The asymptotics of the solution of the Cauchy problem (3.10), (4.11) is determined by the formula (see [27])

$$\psi^{\pm}(x,t) = (A/\sqrt{\det C(t,\xi)})e^{(i/\mu)\int_{0}^{t} \left(\langle P(\eta,\xi), \dot{X}(\eta,\xi) \rangle - H(X(\eta,\xi), P(\eta,\xi))\right)d\eta} \\ \times e^{(i/\mu)\langle P(t,\xi), x - X(t,\xi) \rangle}e^{(i/2\mu)\langle x - X(t,\xi), BC^{-1}(x - X(t,\xi)) \rangle}.$$
(4.13)

Note now that this formula works for any smooth potentials A_j , v_{eff} , e.g., if $A_j = O(\mu) = \mu A_j^1$ and $v_{\text{eff}} = v_{\text{eff}}^0 + \mu v_{\text{eff}}^1$. In particular, this means that the walls of the film vary rather slowly. However, in this case, the wave packet (its leading part) moves rather slowly and cannot have time to pass the entire wave film at the (dimensionless) time. On the other hand, in this case, we can pass from the functions ψ^{\pm} to the functions

$$\varphi^{\pm} = e^{(i/\mu)v_{\text{eff}}^0}\psi^{\pm} \tag{4.14}$$

(this corresponds to a renormalization of energy) and divide the equation for the functions φ^{\pm} by μ . Further, we can modify the time scale and set $t = t'/\sqrt{\mu}$, assuming that the new time t' varies from 0 to O(1), and thus the "old time" varies up to "larger" values $O(1/\sqrt{\mu})$. However, these are the very times at which the wave packet propagates along the entire film. We can now pass from the parameter μ to the parameter h, and then the equation for the function ϕ becomes

$$ih\partial\varphi^{\pm}/\partial t' = (-h^2\Delta_M + v_{\text{eff}}^1 + h^2\mathcal{G}(x))\varphi^{\pm}.$$
(4.15)

The structure of this equation is the same as that of (3.10); however, this equation now describes "medium" waves with wavelength ~ h. The solution of the Cauchy problem (4.15), (4.1) is determined by formula (4.6) (and its diverse realizations) with the changes $\mu \to h$, $v_{\text{eff}} \to v_{\text{eff}}^1$, and $A_j \to A_j^1$. In essence, we have "renormalized" the momenta p and the Hamiltonian $H_{\text{eff}}(p, x)$ by setting

$$H'_{\text{eff}}(p, x) = (1/\mu)(H'_{\text{eff}}((\mu/h)p, x) - v^0_{\text{eff}}).$$

It is clear that the long-wave geometric potential $\mathcal{G}(x)$ makes here no contribution to the leading term of the asymptotic solution either (with respect to the parameter h). From the point of view of formula (4.6), in this situation, formula (4.13) can be regarded as a realization of the canonical operator at (small) times for which the solution is still localized in a neighborhood of the initial focal point.

Propagation of "widely spread" initial perturbations and the long-wave limit. If oscillations are absent in the initial condition, i.e., in Eq. (4.1) we have h = 1, the function V(X)is compactly supported, and $\partial v_{\text{eff}}/\partial x \neq 0$, then, as a rule, the solutions ψ^{\pm} still oscillate with the frequency $\sim \mu$. These solutions can be constructed by using the same formula (4.6), but with the replacement of the Lagrangian manifold Λ_0^2 by the manifold $\tilde{\Lambda}_0^2 = \{p = 0, x = \alpha\}$ and the function $\tilde{V}(\alpha)$ by $V(\alpha)$. Similarly to the previous subsection, a perturbation of this kind practically does not move along the film at times t O(1) (as $\mu \to 0$) if $A_j = O(\mu^2) = \mu^2 A_j^2$ and $v_{\text{eff}} = v_{\text{eff}}^0 + \mu v_{\text{eff}}^2$. We have weak fields, and the walls of the film vary very slowly. The time at which the initial perturbation propagates along the entire film becomes equal to μ^{-2} , the semiclassical asymptotics do not work, and one should carry out the following procedure: introduce a function by formula (4.14), substitute it into Eq. (3.10), set $t = t''/\mu^2$, and divide the equation for φ^{\pm} by μ^2 . This leads to the equation of long-wave approximation (without a parameter),

$$i\partial\varphi^{\pm}/\partial t'' = (-\Delta_M + v_{\text{eff}}^1 + \mathcal{G}(x))\varphi^{\pm}.$$
(4.16)

This equation must be now solved exactly, and the "geometric potential" $\mathcal{G}(x)$ makes a contribution to the solution. Similarly to the above considerations, we can say that the procedure of derivation is reduced to the "renormalization of momenta" p and of the Hamiltonian $H_{\text{eff}}(p, x)$, namely,

$$H_{\rm eff}''(p,x) = \mu^{-2} \left(H_{\rm eff}'(\mu p,x) - v_{\rm eff}^0 \right)$$

5. APPENDIX

A1. Operator-valued separation of variables. Let $\hat{\mathcal{H}}$ be a μ -pseudodifferential operator of the form

$$\hat{\mathcal{H}} = \mathcal{H}\big(-i\mu\,\partial/\partial x, \hat{x}, y, -i\partial/\partial y, \mu\big) = \|\hat{\mathcal{H}}_{ij}\|_{i,j=1}^s$$

with the operator-valued symbol

$$\mathcal{H}(x,p,y,-i\partial/\partial y,t,h) = \mathcal{H}_0(x,p,y,-i\partial/\partial y,t) + \mu \mathcal{H}_1(x,p,y,-i\partial/\partial y,t) + \cdots$$

We assume that the operator-valued symbol and the coefficients of its expansion are (smoothly dependent on p, x, t) self-adjoint operators acting on an appropriate Hilbert space with respect to the variable y with the inner product $\langle \cdot, \cdot \rangle_y$. Consider an equation (a system of equations) for the vector function $\Psi = (\Psi^1, \ldots, \Psi^s)^T$,

$$i\mu\partial\Psi/\partial t = \mathcal{H}\Psi.$$
 (5.1)

Let us seek solutions of Eq. (5.1) in the form

$$\Psi_{i}(x, y, t, \mu) = \sum_{j=1}^{k} \chi_{ij} \left(-i\mu \partial / \partial x, \hat{x}, y, t, \mu \right) \psi_{j}(x, t, \mu),$$
(5.2)

where $\psi = (\psi_1, \dots, \psi_k)^T$ is the wave function of some chosen *term* (or mode) with multiplicity of degeneration equal to k and $\hat{\chi}$ stands for the "intertwining" matrix pseudodifferential operator

$$\hat{\chi} = \|\hat{\chi}_{ij}\|_{i,j=1}^k, \qquad \chi(p, x, y, t, \mu) = \chi_0(p, x, y, t) + \mu\chi_1(p, x, y, t) + \cdots$$
(5.3)

Concerning the vector function ψ , we assume that it satisfies the "effective" equation

$$i\mu\psi_t = L\big(-i\mu\,\partial^{\dagger}/\partial x, \hat{x}, t, \mu\big)\psi\tag{5.4}$$

given by the matrix operator \hat{L} ,

$$\hat{L} = \|\hat{L}_{ij}\|_{i,j=1}^k, \qquad L(p, x, t, \mu) = L_0(p, x, t) + \mu L_1(p, x, t) + \cdots$$

with a matrix $L_0(x, p, t)$ proportional to the identity $k \times k$ matrix E_k $(L_0(x, p, t) = H_{\text{eff}}^{\mu} E_k)$. The coefficient of proportionality H_{eff}^{μ} is said to be the (classical) effective Hamiltonian. If one defines $\hat{\chi}$ and \hat{L} , then the initial problem (5.1) is reduced to a simpler ("reduced") equation, Eq. (5.4), for the vector function ψ . The original solutions Ψ are recovered via formula (5.2) by using the intertwining operator $\hat{\chi}$. The problem of finding the operators $\hat{\chi}$ and \hat{L} is reduced to finding their symbols (functions) χ and L or the coefficients of their expansion in the parameter μ .

Substituting the function Ψ from (5.2) into Eq. (5.1), we obtain $i\mu\hat{\chi}\psi_t + i\mu\hat{\chi}_t\psi = \hat{\mathcal{H}}\hat{\chi}\psi$. Using condition (5.4), we represent this equation in the form $(\hat{\chi}\hat{L} + i\mu\hat{\chi}_t - \hat{\mathcal{H}}\hat{\chi})\psi = 0$. A sufficient condition for the validity of the last formula is the relation $\hat{\chi}\hat{L} + i\mu\hat{\chi}_t - \hat{\mathcal{H}}\hat{\chi} = 0$. Let us pass in this relation from the operators to their symbols [26] by using the following formula: the symbol of the product of two operators, $A(x^2, -i\mu \partial^1/\partial x, \mu)B(x^2, -i\mu \partial^1/\partial x, \mu)$, is expressed using their symbols by

the rule $A(x, p - i\mu \partial/\partial x, \mu)B(x, p, \mu)$ (for a correct derivation of this formula for pseudodifferential operators and the description of the conditions on their symbols, see [28]). This leads to the equation 1

$$\begin{split} \chi \big(p - i\mu \,\partial /\partial x, \hat{x}, y, t, \mu \big) L(p, x, t, \mu) &+ i\mu \chi_t(p, x, t, y, \mu) \\ &= \mathcal{H} \big(\hat{x}, p - i\mu \,\partial /\partial x, y, -i \,\partial /\partial y, t, \mu \big) \chi(x, p, y, t, \mu). \end{split}$$

To solve this equation, we use regular perturbation theory in powers of the parameter μ . Collecting terms of zero order with respect to μ , we obtain a family of spectral problems (depending on x, p, t) for the self-adjoint operator $\mathcal{H}_0(x, p, y, -i\partial/\partial y, t)$,

$$\mathcal{H}_0(x, p, y, -i\partial/\partial y, t)\chi_0(x, p, y, t) = \chi_0(x, p, y, t)L_0(x, p, t).$$
(5.5)

Suppose that the asymptotics of the desired function (5.2) is completely determined by an eigenvalue (effective Hamiltonian or term) $H^{\mu}_{\text{eff}}(x, p, t)$ whose multiplicity is equal to k and does not depend on x, p, t. In this case,

$$L_0(x, p, t) = H^{\mu}_{\text{eff}}(x, p, t)E, \qquad (5.6)$$

where E is a unitary $k \times k$ matrix and the matrix $\chi_0(x, p, y, t)$ formed by orthonormal column vectors (eigenfunctions of the operator \mathcal{H}_0 which correspond to the eigenvalue $H^{\mu}_{\text{eff}}(x, p, t)$) is the projection to the eigensubspace generated by the eigenvalue. It is natural to assume that $\chi_0(x, p, y, t)$ depends smoothly on all its arguments.

Collecting the terms at μ^{j} , we obtain nonhomogeneous equations for χ_{j} and L_{j} ,

$$(\mathcal{H}_0 - H^{\mu}_{\text{eff}} E)\chi_j = F_j - \mathcal{H}_j \chi_0 + \chi_0 L_j,$$

where the summands F_j depend on $\chi_0, \ldots, \chi_{j-1}$ and L_0, \ldots, L_{j-1} ; in particular, $F_1 = \hat{\mathcal{D}}\chi_0$ with

$$\begin{split} \hat{\mathcal{D}} &= i \frac{\partial \chi_0}{\partial t} + i \Big[\frac{\partial \mathcal{H}_0}{\partial p_j} \frac{\partial \chi_0}{\partial x^j} - \frac{\partial H_{\text{eff}}^{\mu}}{\partial x^j} \frac{\partial \chi_0}{\partial p_j} \Big] = i \frac{d \chi_0}{dt} + i \Big[\frac{\partial \mathcal{H}_0}{\partial p_j} - \frac{\partial H_{\text{eff}}^{\mu}}{\partial p_j} \Big] \frac{\partial \chi_0}{\partial x^j},\\ &\frac{d \chi_0}{dt} = \frac{\partial \chi_0}{\partial t} - \frac{\partial H_{\text{eff}}^{\mu}}{\partial x^j} \frac{\partial \chi_0}{\partial p_j} + \frac{\partial H_{\text{eff}}^{\mu}}{\partial p_j} \frac{\partial \chi_0}{\partial x^j}. \end{split}$$

Since the operator $(\mathcal{H}_0 - H^{\mu}_{\text{eff}}E)$ is self-adjoint, it follows from the Fredholm alternative that the solvability condition for this equation is equivalent to the condition that the right-hand side is orthogonal to the column vectors of the matrix χ_0 . This yields $L_j = \langle \chi_0^T, \mathcal{H}_j \chi_0 \rangle - \langle \chi_0^T, F_j \rangle$ (see [26]), in particular,

$$L_1 = \left\langle \chi_0^T, \mathcal{H}_1 \chi_0 \right\rangle_y - i \left\langle \chi_0^T, \frac{d\chi_0}{dt} \right\rangle_y - i \left\langle \chi_0^T, \left[\frac{\partial \mathcal{H}_0}{\partial p_j} - \frac{\partial \mathcal{H}_{\text{eff}}^{\mu}}{\partial p_j} \right] \frac{\partial \chi_0}{\partial x^j} \right\rangle_y.$$
(5.7)

Assuming that L_1 is of the form (5.7), one can find a correction, i.e., the matrix

$$\chi_1 = (\mathcal{H}_0 - H_{\text{eff}}^{\mu} E)^{-1} (F_1 - \mathcal{H}_1 \chi_0 + \chi_0 L_1),$$

choosing it (to be definite) by the condition of orthogonality to the column vectors of the matrices χ_0 and χ_1 . The repetition of this procedure leads to the evaluation of L_m and χ_m . Formulas (5.6), (5.7), etc., give the coefficients of the expansion for the symbol of the reduced equation (5.4).

A2. In order to evaluate the symbol L_2 , one needs an expression for F_2 . Let us write it out,

$$F_{2} = \hat{\mathcal{D}}\chi_{1}^{\nu} - \mathcal{H}_{1}\chi_{1}^{\nu} + \chi_{1}^{\nu}L_{1} + i\left[\frac{\partial\mathcal{H}_{1}}{\partial p_{j}}\frac{\partial\chi_{0}^{\nu}}{\partial x^{j}} - \frac{\partial\chi_{0}^{\nu}}{\partial p_{j}}\frac{\partial L_{1}}{\partial x^{j}}\right] + \frac{1}{2}\left[\frac{\partial^{2}\mathcal{H}_{0}}{\partial p_{i}\partial p_{j}}\frac{\partial^{2}\chi_{0}^{\nu}}{\partial x^{i}\partial x^{j}} - \frac{\partial^{2}H_{\text{eff}}^{\mu}}{\partial x^{i}\partial x^{j}}\frac{\partial^{2}\chi_{0}^{\nu}}{\partial p_{i}\partial p_{j}}\right].$$
(5.8)
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By setting A = 0, $\mathcal{P}_i = 0$, $v_{\text{ext}} = 0$ here and using Eqs. (2.9), (2.10), and (2.11), we obtain

$$L_2 = \mathcal{G}(x) - \frac{1}{2g^{1/4}} \frac{\partial}{\partial x^k} \Big[g^{1/2} g^{kj} \partial_j \Big(\frac{1}{g^{1/4}} \Big) \Big], \qquad \mathcal{G}(x) = \frac{1}{\gamma^{1/4}} \frac{\partial}{\partial y} \Big[\gamma^{1/2} \frac{\partial}{\partial y} \Big(\frac{1}{\gamma^{1/4}} \Big) \Big].$$

Denote by α_i^j the coefficients of the first fundamental form on Γ . In this case, $\partial_i \mathbf{n} = \alpha_i^j \partial_j \mathbf{R}$, and $\partial_j \mathbf{r} = \partial_j \mathbf{R} + y \partial_j \mathbf{n} = (\delta_j^k + y \alpha_j^k) \partial_k \mathbf{R}$. For the matrix γ_{ij} , we have

$$\gamma_{ij} = \langle \partial_i \mathbf{r}, \partial_j \mathbf{r} \rangle = (\delta_i^k + y \alpha_i^k) g_{kl} (\delta_j^l + y \alpha_j^l),$$

and thus $\gamma = (E + y\alpha)^T g(E + y\alpha)$,

$$\gamma^{-1} = (E + y\alpha)^{-1}g^{-1}(E + y\alpha)^{-1T} = g^{-1} - y(\alpha g^{-1} + g^{-1}\alpha^{T}) + O(y^{2}).$$

Hence, $\gamma_1^{-1} = -(\alpha g^{-1} + g^{-1} \alpha^T)$ and $\gamma_1^{ij} p_i p_j = -2\alpha_j^i g^{jk} p_i p_k$. The eigenvalues λ_j of the matrix α are equal to $(-\varkappa_j)$, and thus

$$J = \det(1 + y\alpha) = (1 - \varkappa_1 y)(1 - \varkappa_2 y),$$

so that

$$\frac{1}{\gamma^{1/4}}\frac{\partial}{\partial y}\left[\gamma^{1/2}\frac{\partial}{\partial y}\left(\frac{1}{\gamma^{1/4}}\right)\right] = \frac{(\varkappa_1 - \varkappa_2)^2}{4(1 - \varkappa_1 y)^2(1 - \varkappa_2 y)^2}.$$
(5.9)

A3. Let us choose an arbitrary point x on the surface (but omit it in the notation as an argument in quantities depending on it); then we have

$$\langle u, (\partial_y v_{\text{int}})u \rangle = \int_{-\infty}^{\infty} u^*(y)v'_{\text{int}}(y)u(y)\mathrm{d}y = -\int_{-\infty}^{\infty} v_{\text{int}}(y)\big(u^*(y)u'(y) + {u^*}'(y)u(y)\big)\mathrm{d}y,$$

expressing the products $v_{int}(y)u(y)$ and $v_{int}(y)u^*(y)$ in Eq. (3.5) (and its complex conjugate), we continue,

$$\begin{split} -\int_{-\infty}^{\infty} u'(y) \Big(\varepsilon_{\perp} u^*(y) + \frac{1}{2} u^{*''}(y) \Big) + u^{*'}(y) \Big(\varepsilon_{\perp} u(y) + \frac{1}{2} u^{''}(y) \Big) \mathrm{d}y \\ &= -\int_{-\infty}^{\infty} \Big(\varepsilon_{\perp} u^*(y) u(y) + \frac{1}{2} u^{*'}(y) u'(y) \Big)' \mathrm{d}y = \frac{1}{2} (|u'(-\infty)|^2 - |u'(\infty)|^2) = 0, \end{split}$$

since the function u vanishes at infinity together with the derivative.

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REFERENCES

- V. V. Belov, S. Yu. Dobrokhotov, and T. Ya. Tudorovskiy, "Asymptotic Solutions to Nonrelativistic Equations in Curved Nanotubes, I. Reduction to Spatially One-Dimensional Equations," Teoret. Mat. Fiz. 141 (2), 267–303 (2004) [Theoret. and Math. Phys. 141 (2), 1562–1592 (2004)].
- V. V. Belov, S. Yu. Dobrokhotov, and T. Ya. Tudorovskiy, "Operator Separation of Variables for Adiabatic Problems in Quantum and Wave Mechanics," J. Engng. Math. 55 (1–4), 183–237 (2006).
- V. V. Belov, S. Yu. Dobrokhotov, V. P. Maslov, and T. Ya. Tudorovskiy, "Generalized Adiabatic Principle for Electron Dynamics in Curved Nanostructures," Uspekhi Fiz. Nauk 175 (9), 1004–1010 (2005) [Physics-Uspekhi 48 (9), 962–968 (2005)].
- 4. M. C. Gutzwiller, Chaos in Classical and Quantum Mechanics (Springer-Verlag, New York, 1990).
- L. V. Berland and S. Yu. Dobrokhotov, "Operator Separation of Variables in Problems on Short-Wave Asymptotic for Differential Equations with Rapidly Oscillating Coefficients," Dokl. Akad. Nauk SSSR 296, 80–84 (1987) [Sov. Phys. Doklady 32 (9), 714–716 (1987)].
- 6. M. Born and J. R. Oppenheimer, "Zur Quantentheorie der Molekeln," Ann. Phys. 84, 457–484 (1927).
- 7. M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Clarendon Press, Oxford University Press, New York, 1954).
- J. Brüning, S. Dobrokhotov, S. Sekerzh-Zenkovich, and T. Tudorovskii, "Spectral Series of the Schrödinger Operator in Thin Waveguides with Periodic Structure, I. Adiabatic Approximation and Semiclassical Asymptotics in the 2D Case," Russ. J. Math. Phys. 13 (4), 380–396 (2006).

- V. S. Buslaev and M. V. Buslaeva, "Singularity of the Green Function of the Nonstationary Schrödinger Equation," Funktsional. Anal. i Prilozhen. **32** (2), 80–83 (1998) [Funct. Anal. Appl. **32** (2), 132–134 (1998)].
- A. V. Chaplik, "Quasi-Classical Wave Function of a System with Many Degrees of Freedom," Zh. Eksper. Teoret. Fiz. 43, 84–86 (1963) [Soviet Phys. JETP 16, 61–62 (1963)].
- L. A. Chernozatonskii, E. G. Gal'pern, N. R. Serebryanaya, and I. V. Stankevich, "Polymers of Single-Wall Nanotubes: Geometry, Diffraction Patterns, and Electronic Spectrum Modeling," AIP Conf. Proc. 486, Ed. by H. Kuzmany, J. Fink, M. Mehring, and S. Roth (New York, 1999), p. 284.
- R. C. T. da Costa, "Quantum Mechanics of a Constrained Particle," Phys. Rev. A 23 (4), 1982–1987 (1981).
- G. F. Dell'Antonio and L. Tenuta, "Semiclassical Analisys of Constrained Quantum Systems," arXiv: math-ph/0312034 1, 11 (2003).
- S. Yu. Dobrokhotov, "Maslov's Methods in the Linearized Theory of Gravitational Waves on a Liquid Surface," Dokl. Akad. Nauk SSSR 269 (1), 76–80 (1983) [Sov. Phys. Doklady 28, 229–231 (1983)].
- S. Yu. Dobrokhotov and A. I. Shafarevich, "Semiclassical Quantization of Invariant Isotropic Manifolds of Hamiltonian Systems," in *Topological Methods in the Theory of Hamiltonian Systems* (Faktorial, Moscow, 1998).
- 16. A.V. Eletskii, "Carbon Nanotubes and Their Emission Properties," Uspekhi Phys. Nauk **172** (4), (2002).
- 17. M.V. Entin and L.I. Magarill, "Spin-Orbit Interaction of Electrons on a Curved Surface," Phys. Rev. B 64, 085330 (2001).
- P. Duclos and P. Exner, "Curvature-Induced Bound States in Quantum Waveguides in Two and Three Dimensions," Rev. Math. Phys. 7, 73–102 (1995).
- 19. V. Gantmakher and Y. Levinson, *Carrier Scattering in Metals and Semiconductors* (North-Holland, Amsterdam, 1987).
- 20. H. Jensen and H. Koppe, "Quantum Mechanics with Constraints," Ann. Phys. 269, 77–104 (1971).
- M. V. Karasev, "New Global Asymptotics and Anomalies in the Problem of Quantization of an Adiabatic Invariant," Funktsional. Anal. i Prilozhen. 24 (2), 24–36 (1990) [Funct. Anal. Appl. 24 (2), 104–114 (1990)].
- E. M. Lifshits and L. P. Pitaevsky, *Statistical Physics*, Part 2: *Condensed State Theory* (Pergamon Press, New York; Oxford–Elmford, 1980).
- L. I. Magarill and M. V. Entin, "Electrons in Curvilinear Quantum Wire," Zh. Éxper. Teoret. Fiz. 123 (4), 867–876 (2003).
- 24. M. V. Karasev and V. P. Maslov, Russian Math. Surveys 39, 133–205 (1984).
- 25. V. P. Maslov, "Asymptotics of Eigenfunctions of the Equation $\Delta u + k^2 u = 0$ with Boundary Conditions on Equidistant Curves and the Scattering of Electromagnetic Waves in a Waveguide," Dokl. Akad. Nauk SSSR **123** (4), 631 (1958).
- 26. V. P. Maslov, Perturbation Theory and Asymptotic Methods (MGU, Moscow, 1965).
- V. P. Maslov, The Complex WKB Method for Nonlinear Equations (Nauka, Moscow, 1977); English transl.: The Complex WKB Method for Nonlinear Equations. I. Linear Theory (Birkhäuser, Basel– Boston–Berlin, 1994).
- 28. V. P. Maslov, Operational Methods (Nauka, Moscow, 1973).
- V. P. Maslov and M. V. Fedoryuk, Semiclassical Approximation in Quantum Mechanics (Reidel, Dordrecht, 1981).
- V. P. Maslov, Mathematical Aspects of Integral Optics (MIEM, Moscow, 1983); Journal version: Russ. J. Math. Phys. 8 (1), 83–180; (2), 180–238 (2001).
- G. Panatti, H. Spohn, and S. Teufel, "Effective Dynamics for Bloch Electrons: Peierls Substitution and Beyond," Comm. Math. Phys. 242 (3), 547–578 (2003).
- 32. R. E. Peierls, Quantum Theory of Solids (Interscience, New York, 1960).
- N. A. Poklonski, E. F. Kislyakov, G. G. Fedoruk, and S. A. Virko, "Model of an Electron Structure of the Metal Doped Carbon Nanotube," Fiz. Tverd. Tela 42 (10), 1911–1914 (2000).
- R. Saito, G. Dresselhaus, and M.S. Dresselhaus, *Physical Properties of Carbon Nanotubes* (Imperial College Press, London, 1998).
- P. C. Schuster and R. L. Jaffe, "Quantum Mechanics on Manifolds Embedded in Euclidean Space," Ann. Physics 307, 132 (2003).