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Spectral Series of the Schrödinger Operator in Thin Waveguides with Periodic Structure, I Adiabatic Approximation and Semiclassical Asymptotics in the 2D Case

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Abstract. Asymptotic formulas for the eigenvalues (energy levels) of the 2D and 3D stationary Schrödinger operators describing the states of a quantum particle in the waveguide formed by soft walls characterized by a periodic parabolic confinement potential slowly varying along the waveguide axis are presented. The formulas are derived by a unified procedure based on adiabatic approximation and are illustrated in the first part of this paper by an example of a 2D straight waveguide. This waveguide can be used for simulating some effects in nanostructures and can be viewed as a simple linear model describing electronic transport in a long molecule consisting of so-called "sites." The accuracy of the obtained asymptotic eigenvalues and the possibility of using the adiabatic approximation are discussed. Examples of quantum states with large energies to which the adiabatic approximation does not apply are given.

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INTRODUCTION

In this paper, we construct asymptotic solutions to the spectral problem for thin quantum waveguides with so-called "soft walls" described by a periodic parabolic confinement potential slowly varying along the waveguide axis. We apply a unified procedure based on the version of adiabatic approximation suggested in [17, 6–9] and in closed form in [34, 38] for a wide class of multi-dimensional problems in various fields of mathematical and theoretical physics as well as on the semiclassical approach. It is divided into the following two steps: (1) the so-called operator separation of variables ("generalized adiabatic principle") reducing the original equation to differential or pseudodifferential equations of smaller dimension; (2) the construction of various asymptotic solutions of the simplified equations.

The goal of this paper is to obtain asymptotic formulas for the eigenvalues (energy levels) of the 2D and 3D stationary Schrödinger operators describing the states of a quantum particle in a waveguide formed by soft walls described above. In some sense, one can view this paper as a specific implementation of the above-mentioned general adiabatic approach. We illustrate the main ideas and formulas in the first part of this paper considering a 2D straight waveguide. This waveguide can be used for the simulation of some nanostructure effects which do not appear in regular waveguides [42, 13, 20, 40, 28]. On the other hand, such a quantum waveguide can be viewed as a simple linear model describing electronic transport in a long molecule consisting of so-called "sites" [26]. We derive a 1D "effective spectral problem for the longitudinal motion" of the quantum particle and then find semiclassical solutions of the equation, which correspond to various wave modes and quantum energy levels. We show that if the confinement potential changes varies only slightly, then there exist so-called slow modes which satisfy a "limit" 1D equation similar to the equations obtained and discussed in [29, 24, 12, 21, 31, 28, 43]. We also give some estimates of the accuracy of the asymptotic eigenvalues constructed with the use of the adiabatic approximation. Finally, we present examples of quantum states with large energies (we call them "superexcited modes"), where the adiabatic approximation is not applicable. Using these examples and methods in [30, 2, 41], we describe one possible mechanism of destruction of the adiabatic approximation.

The second, main part of our paper, is focused on the consideration of a 3D toric waveguide subjected to the action of a magnetic field.

1. OPERATOR SEPARATION OF VARIABLES FOR A STRAIT WAVEGUIDE

We study stationary states $\Psi(x,y)\exp(-i\frac{\mathcal{E}}{\hbar}t)$ describing the quantum motion of a particle with mass m and energy $\mathcal{E}=\text{const}$ in a straight 2D plane waveguide with periodic soft walls. Here $\hbar$ is the Plank constant and t is time. We assume that the characteristic width of the waveguide is d and its period is L. The so-called soft walls (e.g., see [12, 24, 28]) are described by the parabolic confinement potential

$$\frac{2\pi^2\hbar}{md^2}\Omega^2(x)y^2,$$

where $\Omega(x)$ is a smooth 2π-periodic function. We introduce dimensionless variables x and y with scales $L/(2\pi)$ and $d/(2\pi)$, respectively; the coordinate x-axis is taken along the longitudinal direction of the waveguide, and the y-axis is orthogonal to the x-axis. We assume that the "adiabatic parameter" $\mu=d/L$ is the main small parameter of the problem.

The wave function $\Psi(x,y)$ satisfies the 2D equation

$$\hat{\mathcal{H}}\Psi(x,y,\mu)=E\Psi(x,y,\mu), \tag{1.1}$$

where $E=\frac{4\pi^2h^2}{md^2}\mathcal{E}$ is the energy eigenvalue and $\hat{\mathcal{H}}$ is the Schrödinger operator

$$\hat{\mathcal{H}}\equiv\frac{1}{2}\left[-\mu^2\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}+\Omega^2(x)y^2\right]. \tag{1.2}$$

Imposing the Born–Karman periodicity conditions

$$\Psi(x+2\pi,y,\mu)=\Psi(x,y,\mu), \tag{1.3}$$

we consider the spectral problem for E and $\Psi(x,y,\mu)\in L_2(\mathbb{S}_x\times\mathbb{R}_y)$, where the cylinder $\mathbb{S}_x\times\mathbb{R}_y$ is the configuration space.

Taking into account the smoothness of the function $\Omega(x)$, we can use the adiabatic approximation for solving the 2D singularly perturbed problem (1.1)–(1.3). As we said before, we use the so-called generalized method of separation of variables (the generalized adiabatic principle) [6–9, 38] based on operator methods [33]. We seek approximate solutions to the spectral problem (1.1)–(1.3) in the form

$$\Psi(x,y,\mu)=\hat{\chi}\psi(x,\mu). \tag{1.4}$$

Here $\hat{\chi}=\chi(-i\mu\overset{1}{\partial}/\partial x,\overset{2}{x},y,\mu)$ is a pseudodifferential operator with symbol $\chi(p,x,y,\mu)$, and the function $\psi(x,\mu)$ is a solution of the 1D spectral problem

$$\hat{\mathcal{L}}\psi(x,\mu)=E\psi(x,\mu),\qquad \psi(x+2\pi,\mu)=\psi(x,\mu),\qquad \psi\in L_2(S_x), \tag{1.5}$$

where

$$\hat{\mathcal{L}}=\mathcal{L}(-i\mu\overset{1}{\partial}/\partial x,\overset{2}{x},\mu) \tag{1.5$'$}$$

is a pseudodifferential operator with symbol $\mathcal{L}(p,x,\mu)$. We use Feynman's notation [33, 35], and so the operator $-i\mu\partial/\partial x$ acts first and the operator $\hat{x}=x$ acts second in the expressions

$$\hat{\chi}=\chi(-i\mu\overset{1}{\partial}/\partial x,\overset{2}{x},y,\mu)\quad\text{and}\quad\hat{\mathcal{L}}=\mathcal{L}(-i\mu\overset{1}{\partial}/\partial x,\overset{2}{x},\mu).$$

Note that Eq. (1.5$'$) is known in quantum mechanics as *Peierls substitution* [39, 27], and the operator $\hat{\mathcal{L}}$ is called the *effective adiabatic Hamiltonian*. (Sometimes, this name is used only for its leading term.) The representation of Ψ in the form (1.4) and Eqs. (1.5) and (1.5$'$) form a basis of the "generalized adiabatic principle."

The main difference between (1.4) and standard forms of adiabatic approximation is that χ in (1.4) is not a *function* but an *operator*. The problem is now to obtain the symbols $\mathcal{L}$ and χ.

The substitution of (1.4) and (1.5) into (1.1) gives the operator equation

$$\hat{\mathcal{H}}\hat{\chi} = \hat{\chi}\hat{\mathcal{L}} \tag{1.6}$$

for the operators $\hat{\chi}$ and $\hat{\mathcal{L}}$.

According to the approach in [32, 6–8], we introduce the operator-valued symbol

$$\mathcal{H}(p, x, -i\partial/\partial y, y)$$

for the Schrödinger operator

$$\hat{\mathcal{H}} = \mathcal{H}(-i\mu\overset{1}{\partial}/\partial x, \overset{2}{x}, -i\partial/\partial y, y),$$

the symbol $\chi(p, x, y, \mu)$ for

$$\hat{\chi} = \chi(-i\mu\overset{1}{\partial}/\partial x, \overset{2}{x}, y, \mu),$$

and the symbol $\mathcal{L}(p, x, \mu)$ for the *effective adiabatic Hamiltonian*

$$\hat{\mathcal{L}} = \mathcal{L}(-i\mu\overset{1}{\partial}/\partial x, \overset{2}{x}, \mu).$$

Then, from the operator equation (1.6), we derive the equation [33]

$$\mathcal{H}(p - i\mu\overset{1}{\partial}/\partial x, \overset{2}{x}, -i\partial/\partial y, y)\ \chi(p, x, y, \mu) = \chi(p - i\mu\overset{1}{\partial}/\partial x, \overset{2}{x}, y, \mu)\ \mathcal{L}(p, x, \mu) \tag{1.7}$$

for the symbols $\chi(p, x, y, \mu)$ and $\mathcal{L}(p, x, \mu)$.

To solve the last equation, one can use perturbation techniques. The operator-valued symbol $\mathcal{H}(p - i\mu\partial/\partial x, x, -i\partial/\partial y, y)$ is written in the form

$$\mathcal{H}(p - i\mu\partial/\partial x, x, -i\partial/\partial y, y) = \mathcal{H}_0(p, x, -i\partial/\partial y, y) + \mu p\Big(-i\frac{\partial}{\partial x}\Big) + \frac{\mu^2}{2}\Big(-i\frac{\partial}{\partial x}\Big)^2, \tag{1.8}$$

where

$$\mathcal{H}_0(p, x, -i\partial/\partial y, y) = -\frac{1}{2}\frac{\partial^2}{\partial y^2} + \frac{\Omega^2(x)}{2}y^2 + \frac{p^2}{2}, \tag{1.9}$$

and solutions of (1.7) are sought in the form of asymptotic series

$$\chi(p, x, y, \mu) = \chi_0(p, x, y) + \mu\chi_1(p, x, y) + \mu^2\chi_2(p, x, y) + \cdots, \tag{1.10}$$

$$\mathcal{L}(p, x, \mu) = \mathcal{L}_0(p, x) + \mu\mathcal{L}_1(p, x) + \mu^2\mathcal{L}_2(p, x) + \cdots. \tag{1.11}$$

The periodicity condition (1.3) requires that

$$\chi_j(p, x + 2\pi, y) = \chi_j(p, x, y), \quad j = 0, 1, \ldots, \qquad \psi(x + 2\pi, \mu) = \psi(x, \mu). \tag{1.12}$$

By substituting (1.8)–(1.11) into (1.7) and by matching the coefficients of like powers of μ, one successively obtains spectral problems for the symbols $\chi_0(p, x, y)$ and $\mathcal{L}_0(p, x)$, $\chi_1(p, x, y)$ and $\mathcal{L}_1(p, x)$, $\chi_2(p, x, y)$ and $\mathcal{L}_2(p, x)$, etc. After the desired number J of terms in the expansions (1.10) and (1.11) has been found, the approximate value of $\hat{\mathcal{L}}(p, x, \mu)$ is substituted into the spectral problem (1.5) for the eigenvalues of the energy E and eigenfunctions $\psi(x, \mu)$.

As will be clear in the following sections, to formally obtain the asymptotic formulas for E, one has to find the first two terms in the expansions (1.10), (1.11); to justify these formulas, one should also calculate the term $\mathcal{L}_2^{(\nu)}(p, x)$ in (1.11).

In the spectral problem for the symbols $\chi_j(p,x,y)$ and $\mathcal{L}_j(p,x)$, the symbol $\chi_j(p,x,y)$ is regarded as an unknown function of y belonging to $L_2(R_y)$ and parametrically depending on p and x. The symbol $\mathcal{L}_j(p,x)$ is regarded in this problem as an unknown constant and is determined from the condition of solvability of the problem for $\chi_j(p,x,y)$. When constructing the successive spectral problem for the symbols $\chi_{j+1}(p,x,y)$ and $\mathcal{L}_{j+1}(p,x)$, one takes into account the explicit dependence of $\chi_j(p,x,y)$ and $\mathcal{L}_j(p,x)$ on p and x.

Equating the terms of the order of μ^0 in (1.7) gives the spectral problem for $\chi_0(p,x,y)$ and $\mathcal{L}_1(p,x)$:

$$\mathcal{H}_0(p,x,-i\partial/\partial y,y)\chi_0(p,x,y)=\mathcal{L}_0(p,x)\chi_0(p,x,y),\quad \chi_0\in L^2(R_y). \tag{1.13}$$

The last problem can be written in view of (1.9) as

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial y^2}+\frac{\Omega^2(x)}{2}y^2\right]\chi_0(p,x,y)=v_{\text{eff}}\chi_0(p,x,y),\quad v_{\text{eff}}\equiv\mathcal{L}_0(p,x)-\frac{p^2}{2},\quad \chi_0\in L_2(R_y), \tag{1.14}$$

where p and x are considered as constants.

The eigenvalues and normalized eigenfunctions of (1.14) are

$$\begin{aligned} v_{\text{eff}}^{(\nu)}(x)&=\Omega(x)\Big(\nu+\frac{1}{2}\Big),\qquad \nu=0,1,2,\dots,\\ \chi_0^{(\nu)}(x,y)&=\left[\frac{\Omega(x)}{\pi}\right]^{1/4}\frac{1}{\sqrt{2^\nu\nu!}}\exp\Big(-\frac{\eta^2}{2}\Big)H_\nu(\eta),\qquad \eta=\sqrt{\Omega(x)}y, \end{aligned} \tag{1.15}$$

where $H_\nu(\eta)$ is the νth Hermite polynomial of the argument η. Thus

$$\mathcal{L}_0^{(\nu)}=\frac{p^2}{2}+v_{\text{eff}}^{(\nu)}(x). \tag{1.16}$$

The number ν in (1.15) is called the "transverse quantum number." We choose and fix some ν, which should be of the order of unity for the adiabatic approximation to apply.

It should be noted that the symbol $\chi_0^{(\nu)}(x,y)$ is a function of x,y. Hence the operator $\hat{\chi}_0^{(\nu)}$ generated by this symbol is simply the operator of multiplication by a function of x,y.

As will be clear in the following sections, to formally obtain the asymptotic formulas for E, one has to find terms of the order of μ in the expansions (1.10) and (1.11); to justify these formulas, one should also calculate the term $\mathcal{L}_2^{(\nu)}(p,x)$ in (1.11).

Equating the terms of the order of μ^1 in (1.7) gives the following problem for $\chi_1^{(\nu)}(p,x,y)$ and $\mathcal{L}_1^{(\nu)}(p,x)$:

$$\begin{aligned} &\mathcal{H}_0(p,x,-i\partial/\partial y,y)\chi_1^{(\nu)}(p,x,y)-\mathcal{L}_0^{(\nu)}(p,x)\chi_1^{(\nu)}(p,x,y)\\ &\qquad=\mathcal{L}_1^{(\nu)}(p,x)\chi_0^{(\nu)}(x,y)+p\left(i\frac{\partial}{\partial x}\right)\chi_0^{(\nu)}(x,y),\qquad \chi_1^{(\nu)}\in L^2(R_y). \end{aligned} \tag{1.17}$$

The last problem can be rewritten in view of (1.9) as

$$\begin{aligned} &\left[-\frac{1}{2}\frac{\partial^2}{\partial y^2}+\frac{\Omega^2(x)}{2}y^2\right]\chi_1^{(\nu)}(p,x,y)\\ &\quad=\left[\mathcal{L}_0^{(\nu)}(p,x)-\frac{p^2}{2}\right]\chi_1^{(\nu)}(p,x,y)+\mathcal{L}_1^{(\nu)}(p,x)\chi_0^{(\nu)}(x,y)+ip\frac{\partial\chi_0^{(\nu)}(x,y)}{\partial x},\qquad \chi_1^{(\nu)}\in L_2(R_y), \end{aligned}$$

or, once $\partial\chi_0^{(\nu)}(x,y)/\partial x$ has been computed, as

$$\Big[-\frac{1}{2}\frac{\partial^2}{\partial y^2}+\frac{\Omega^2(x)}{2}y^2\Big]\chi_1^{(\nu)}(p,x,y)$$
$$=\left[\mathcal{L}_0^{(\nu)}(p,x)-\frac{p^2}{2}\right]\chi_1^{(\nu)}(p,x,y)+\mathcal{L}_1^{(\nu)}(p,x)\chi_0^{(\nu)}(x,y)+ipg^\nu(x,y),\qquad \chi_1^{(\nu)}\in L_2(R_y),$$
$$g^\nu(x,y)=\frac{1}{4}\left(\frac{\Omega'}{\Omega}\right)(\sqrt{(\nu+2)(\nu+1)}\chi_0^{\nu+2}+\sqrt{\nu(\nu-1)}\chi_0^{\nu-2}),\qquad \Omega'=\frac{d\Omega}{dx}, \tag{1.18}$$

where p and x are regarded as constants.

Since the system of functions $\chi_0^{(l)}(p,x,y)$, $l=1,2,\dots$, is complete in $L_2(R_y)$ and the function $\chi_0^{(\nu)}(x,y)$ satisfies the homogeneous equation (1.14), from (1.18) we obtain

$$\mathcal{L}_1^{(\nu)}(p,x)=0,\qquad \chi_1^{(\nu)}(p,x,y)=ipg^\nu(x,y). \tag{1.19}$$

Note that the symbol $\chi_1^{(\nu)}(p,x,y)$ contains the variable p, which corresponds to the differential operator $-i\mu\partial/\partial x$, as one of its arguments. Hence the operator $\hat\chi_1^{(\nu)}$ generated by this symbol is an operator rather than a function, as was the case with $\hat\chi_0^{(\nu)}$.

Equating the terms of the order of μ^2 in (1.7) gives a nonhomogeneous problem for $\chi_2^{(\nu)}(p,x,y)$ and $\mathcal{L}_2^{(\nu)}(p,x)$. This problem can be solved by the same method as problems (1.13) and (1.17), which gives

$$\mathcal{L}_2^{(\nu)}(0,x)=\frac{1}{8}\left(\frac{\Omega'}{\Omega}\right)^2(3\nu^2+5\nu+3). \tag{1.20}$$

We give the value of $\mathcal{L}_2^{(\nu)}(p,x)$ at $p=0$, because, as will be discussed below, to construct the main term of the asymptotic formulas, it suffices to find $\mathcal{L}_2^{(\nu)}(0,x)$.

2. SHORT WAVES AND SEMICLASSICAL ASYMPTOTICS FOR THE EQUATION OF LONGITUDINAL MOTION

Consider Eq. (1.5) with the *effective Hamiltonian* $\hat{\mathcal{L}}=\mathcal{L}(-i\mu\overset{1}{\partial}/\partial x,\overset{2}{x},\mu)$. By (1.11), (1.15), and (1.19), for the symbol $\mathcal{L}(p,x,\mu)$ of this operator, we have the asymptotic formulas

$$\mathcal{L}_{[2]}^{(\nu)}(p,x)=\frac{p^2}{2}+v_{\text{eff}}^{(\nu)}(x)+\mu^2\mathcal{L}_2^{(\nu)}(0,x), \tag{2.1}$$

where $v_{\text{eff}}^{(\nu)}(x)$ and $\mathcal{L}_2^{(\nu)}(p,x)$ are defined by (1.14) and (1.20), respectively.

We assign indexes ν and n to the function ψ in (1.5), where ν is the transverse quantum number and n is the longitudinal quantum number, which will be defined below. Then, from (1.5) and (2.1), we have the spectral problem

$$\Big[-\frac{\mu^2}{2}\frac{\partial^2}{\partial x^2}+v_{\text{eff}}^{(\nu)}(x)+\mu^2\mathcal{L}_2^{(\nu)}(0,x)\Big]\psi^{(\nu,n)}=E^{(\nu,n)}\psi^{(\nu,n)},$$
$$\psi^{(\nu,n)}(x+2\pi)=\psi^{(\nu,n)}(x),\qquad \psi^{(\nu,n)}\in L_2(S_x) \tag{2.2}$$

for $\psi^{(\nu,n)}$.

We refer to (2.2) as the *effective equation of adiabatic motion*.

Let us discuss the asymptotic behavior of the spectrum of the Sturm–Liouville problem (2.2) as $\mu\to 0$ on the interval $-\pi\leqslant x\leqslant\pi$. We assume that $\Omega(x)$ (and hence $v_{\text{eff}}^{(\nu)}(x)$) is analytic on this

interval and has only one nondegenerate point $x_{\min}$ of minimum; we denote $V^{(\nu)}_{\min} = v^{(\nu)}_{\text{eff}}(x_{\min})$. Then there exists only one global point $x_{\max} \in [\pi, \pi]$) for $v^{(\nu)}_{\text{eff}}(x)$ of maximum; we put $V^{(\nu)}_{\max} = v^{(\nu)}_{\text{eff}}(x_{\max})$. To simplify the discussion, we assume momentarily that $\mathcal{L}^{(\nu)}_2(p,x)\big|_{p=0} = 0$. This simplified problem was studied in many monographs and papers (e.g., see [22, 11, 25]). Let us briefly recall the most important results. The spectrum of eigenvalues E is discrete, so that n is a positive integer. The distance $O(\mu)$ between eigenvalues located under some energy level $E > V^{(\nu)}_{\min}$ is, generally speaking, $O(\mu)$; this means that the number of eigenvalues increases as μ tends to zero, and n is allowed to be large. The spectrum of E can be divided into four domains.

1. Lowest under-barrier region. Consider the eigenvalues $E^{(\nu,n)}$ located above and very close to $V^{(\nu)}_{\min}$. This means that $n\mu$ is small enough. To describe the eigenvalues and eigenfunctions in this case, one can use the harmonic oscillator approximation and obtain

$$E^{(\nu,n)} = v^{(\nu)}_{\text{eff}}(x) + \mu\Big(n+\frac{1}{2}\Big)\omega_0 + O(\mu^2), \quad \omega_0 = \sqrt{2\frac{\partial^2 v^{(\nu)}_{\text{eff}}}{\partial x^2}(x_{\min})} = \sqrt{2\Big(\nu+\frac{1}{2}\Big)\frac{\partial^2\Omega}{\partial x^2}(x_{\min})}. \tag{2.3}$$

The wave functions are localized in a neighborhood of the point $x_{\min}$ and have the form

$$\psi^{\nu n}(x) = C^n \exp(-\xi^2/2) H_n(\xi), \qquad \xi = \sqrt{\omega_0}(x - x_{\min}), \tag{2.4}$$

where C^n is the normalizing constant.

The number n corresponds to the number of oscillations on the interval $[-\pi, \pi]$.

2. Perturbed under-barrier region. Consider the eigenvalues $E^{k,n} < V^{(\nu)}_{\max} - \delta$, where δ is a small positive number. In this case, $n \sim \mu^{-1}$, and using the standard semiclassical approximation, we have

$$E^{(\nu,n)} = \mathcal{E}^{(\nu,n)}_{\text{un}} + o(\mu), \tag{2.5}$$

where $\mathcal{E}^{(\nu,n)}_{\text{un}}$ is defined by the *Bohr–Sommerfeld rule*

$$\frac{1}{\pi}\int_{x_-}^{x_+} \sqrt{2\Big[\mathcal{E}^{(\nu,n)}_{\text{un}} - v^{(\nu)}_{\text{eff}}(x)\Big]}\,dx = \mu\Big(n+\frac{1}{2}\Big) \tag{2.6}$$

where the $x_\pm$ are solutions of the equation $v^{(\nu)}_{\text{eff}}(x) = \mathcal{E}^{(\nu,n)}_{\text{un}}$. On the interval (x_-, x_+) and outside some neighborhood of the turning points x_-, x_+, the wave functions are

$$\psi^{(\nu,n)}(x) = \frac{C^{(\nu,n)}}{\big[2\big(\mathcal{E}^{(\nu,n)}_{\text{un}} - v^{(\nu)}_{\text{eff}}(x)\big)\big]^{1/4}}\left[\cos\left(\frac{1}{\mu}\int_{x_-}^{x}\sqrt{2\big[\mathcal{E}^{(\nu,n)}_{\text{un}} - v^{(\nu)}_{\text{eff}}(x)\big]}\,dx + \frac{\pi}{4}\right) + O(\mu)\right], \tag{2.7}$$

where $C^{(\nu,n)}$ is the normalizing constant. In the neighborhood of the turning points, one has to use other representations for $\psi^{(\nu,n)}(x)$, for instance, based on Airy functions or the Maslov canonical operator (e.g., see [22, 25]).

Note that one can formally obtain (2.3) from (2.6) assuming that $n\mu \ll 1$ and using the Taylor expansion. This is not the case for asymptotic formulas for the eigenfunctions. The Bohr–Sommerfeld rule (2.6) also gives the asymptotics for eigenvalues corresponding to the passage from "small" to "large" n [25, 11, 44].

Both cases 1 and 2 correspond to so-called "trapped waves" in the waveguide, which appear only in the case of a nonconstant function $\Omega(x)$. In the semiclassical approximation, the eigenfunctions $\psi^{(\nu,n)}$ of these waves are localized on a subinterval $[x_-, x_+]$ of the interval $[-\pi, \pi]$ and are exponentially small outside the interval. Thus if one considers the waveguide as an infinitely long one, then the functions $\psi^{(\nu,n)}$ can be viewed as "quasi-trapped" modes but not "true" eigenfunctions decaying as $|x_1| \to \infty$.

3. Transient layer. The eigenvalues belonging to a neighborhood of $V_{\max}^{(\nu)}$ form a transient layer. The Bohr–Sommerfeld rule does not apply to these states, and the asymptotics of eigenfunctions has a more complicated structure than that given by (2.3) or (2.5). We do not discuss this case here and refer to the papers [25, 15, 44, 36].

4. Over-barrier region. Consider the eigenvalues $E^{(\nu,n)} > V_{\max}^{(\nu)}$. One can again use the Bohr–Sommerfeld rule to construct the asymptotics of eigenvalues. It is only necessary to take into account the fact that, modulo $O(\mu^\infty)$, each eigenvalue is doubly degenerate. This means that, as a rule, along with the eigenvalue $E_+^{(\nu,n)}$, there exists an eigenvalue $E_-^{(\nu,n)}$ such that $E_+^{(\nu,n)} = E_-^{(\nu,n)} + O(\mu^\infty)$, although sometimes the splitting between $E_+^{(\nu,n)}$ and $E_-^{(\nu,n)}$ can be zero (e.g., see [22, 19, 11]). In any case, one can write

$$E_\pm^{(\nu,n)} = \mathcal{E}_{\rm ov}^{(\nu,n)} + O(\mu^2), \qquad \frac{1}{\sqrt{2}\pi}\int_0^{2\pi}\sqrt{\mathcal{E}_{\rm ov}^{(\nu,n)} - v_{\rm eff}^{(\nu)}(x)}dx = \mu n. \tag{2.8}$$

There are no turning points on the entire real axis, and there exist global representations of the eigenfunctions:

$$\begin{aligned}
\psi_1^{(\nu,n)}(x) &= \frac{C^{(\nu,n)}}{\left[2\big(\mathcal{E}_{\rm ov}^{(\nu,n)} - v^{(\nu)}{\rm eff}(x)\big)\right]^{1/4}}\left[\cos\left(\frac{1}{\mu}\int_{x_0}^{x}\sqrt{2\left[\mathcal{E}_{\rm ov}^{(\nu,n)} - v_{\rm eff}^{(\nu,n)}(x)\right]}dx\right) + O(\mu)\right],\\
\psi_2^{(\nu,n)}(x) &= \frac{C^{(\nu,n)}}{\left[2\big(\mathcal{E}_{\rm ov}^{(\nu,n)} - v^{(\nu)}{\rm eff}(x)\big)\right]^{1/4}}\left[\sin\left(\frac{1}{\mu}\int_{x_0}^{x}\sqrt{2\left[\mathcal{E}_{\rm ov}^{(\nu,n)} - v_{\rm eff}^{(\nu)}(x)\right]}dx\right) + O(\mu)\right].
\end{aligned} \tag{2.9}$$

Here the point x_0 should be chosen in a special way (see [19]), and $C^{(\nu,n)}$ is the normalizing constant. Over the barrier, there are no focal points. We shall return to these formulas later.

Remark. We considered the wave regimes 1–4 on the basis of the 1D equation (2.2), which had been derived from the original 2D equation (1.1) with the use of the generalized adiabatic approximation. It should be noted that, at first, similar asymptotic solutions were obtained from Eq. (1.1) directly. For instance, regime 1 fits exactly into the framework of the well-known *Born–Oppenheimer method* [10]. Indeed, from the view point of this method, we have "trapped waves" in a deep potential well. Thus, lowest trapped modes are localized near the point $x_{\min}$, which immediately leads to the oscillator approximation as long as one can neglect other terms. The deepness of the potential well formally means that we can divide both sides of Eq. (2.2) by μ^2 and obtain an equation with a "high" barrier. From the physical point of view, this means that the energy of so-called "size quantization," which is an amplitude of the effective potential, is much greater than the energy of the ground state of "free" Schrödinger equation with the Born–Karman boundary condition at the distance L. In dimensional variables, this means that

$$\frac{\hbar^2}{mL^2} \ll \max(v_{\rm eff}^{(\nu)}) \sim |\Delta E_\perp| \sim \frac{\hbar^2}{md^2}.$$

Here m is the mass of a quantum particle in the waveguide. We obtain the ground state for a potential satisfying the condition

$$\frac{\hbar^2}{m\lambda^2} \sim \frac{\kappa\lambda^2}{2}, \qquad \frac{\hbar^2}{md^2} \sim \frac{\kappa L^2}{2}, \qquad \lambda \sim \sqrt{Ld},$$

where κ is the elastic coefficient.

The general approach to the construction of asymptotic eigenvalues and eigenfunctions of the original operator for the case in which $n \sim 1/\mu$ was given by Maslov [32]. Note also that although the Bohr–Sommerfeld rule works for various n (including small $n \sim 1$), there are different physical causes (and consequently different parameters) that lead to this formula. For regimes 2 and 4, the

cause is that locally one can represent the eigenfunction in a form of a "plane wave", while for regime 1, the main argument is the "weakness" of cubic and other terms in the Taylor expansion of the effective potential near the point of minimum. When passing from regimes 2 and 4 to regime 1, the wave functions are transformed from the WKB-type ("distorted plane waves") to the oscillator type. At the same time, the accuracy of spectrum determination, generally speaking, changes during the passage. Thus it is a natural result that the quantization rule that works in the limits 2, 4, and 1 also works between these regimes, while the eigenfunctions are transformed significantly.

3. ASYMPTOTIC SOLUTION OF THE EQUATION OF LONGITUDINAL MOTION FOR A WAVEGUIDE OF NEARLY CONSTANT WIDTH

The function $\Omega(x)$ describing the parabolic confinement potential was assumed in the preceding section to be a function of the variable x alone. But the procedure used in these sections applies to the more general case in which Ω also depends on the parameter μ. Consider a waveguide, important for applications, of nearly constant width for which

$$\Omega(x) = \Omega_0 + \mu^{2\alpha}\Omega_1(x), \qquad \Omega_0 = \text{const} > 0, \quad \alpha > 0. \tag{3.1}$$

In view of (1.15) and (3.1), Eq. (2.2) can we rewritten as

$$\Big[-\frac{\mu^2}{2}\frac{\partial^2}{\partial x^2} + \mu^{2\alpha}\Omega_1(x)\Big(\nu+\frac{1}{2}\Big) - \mu^2\mathcal{L}_2^{(\nu)}(0,x)\Big]\psi^{(\nu,n)} = \mu^{2\alpha}\tilde{E}^{(\nu,n)}\psi^{(\nu,n)},$$
$$\psi^{(\nu,n)}(x+2\pi) = \psi^{(\nu,n)}(x), \quad \psi^{(\nu,n)} \in L_2(S_x), \tag{3.2}$$

where

$$\tilde{E}^{(\nu,n)} = \mu^{-2\alpha}\Big[E^{(\nu,n)} - \Omega_0\Big(\nu+\frac{1}{2}\Big)\Big].$$

In (3.2), the term with $\mathcal{L}_2^{(\nu)}(p,x) = 0$ can be omitted, since it is proportional to the derivative $\Omega'(x)$ and hence, by (3.1), is of the order of $\mu^{2+2\alpha}$.

First, consider the following two cases: (1) $0 < \alpha < 1$ and (2) $\alpha = 1$. We introduce the new parameter

$$h = \mu^{1-\alpha}, \tag{3.3}$$

and rewrite (3.2) in the form

$$\Big[-\frac{h^2}{2}\frac{\partial^2}{\partial x^2} + \Omega_1(x)\Big(\nu+\frac{1}{2}\Big)\Big]\psi^{(\nu,n)} = \tilde{E}^{(\nu,n)}\psi^{(\nu,n)},$$
$$\psi^{(\nu,n)}(x+2\pi) = \psi^{(\nu,n)}(x), \qquad \psi^{(\nu,n)} \in L_2(S_x). \tag{3.4}$$

The parameter h can be viewed as the dimensionless wave length along the x-axis; we refer to it as a *semiclassical parameter*. In case 1, which can be called the "short-wave limit", all results obtained in the previous section, which were based on the semiclassical or harmonic oscillator approximation, remain valid.

In case 2, where α =1 and h =1, there is no small parameter in (3.2) and the equation cannot be analyzed asymptotically. This case can be called the "long wave limit" (or the "limiting" case). The equations corresponding to this case were obtained (in more complicated situations, e.g., with curved axis of the waveguide) and studied in the papers [29, 31, 43, 28, 21], etc. In this case, it is possible to construct so called "trapped modes" in the infinite waveguide (see [29, 31, 21, 23]).

In case 3, where $\alpha > 1$ and $h > 1$, one can treat the term $\mu^{2\alpha}\Omega_1(x)(\nu+1/2)$ in (3.2) as a small perturbation and use perturbation theory.

The *semiclassical parameter* h characterizes the "longitudinal function" $\psi^{(\nu,n)}$ and, generally speaking, is independent of μ, although the formulas for the asymptotic solution of the definitive equation depend on the relationship between μ and h.

Remark 1. The possibility of using the adiabatic approximation is ensured by the nonzero part Ω_0 of $\Omega(x,\mu)$. Actually, the correction $\mu^{2\alpha}\Omega_1(x)$ can be moved into the corrections $\mathcal{L}_1$ or even into $\mathcal{L}_2$ (for $\alpha \geqslant 2$). Also in more complicated cases, some terms from $\mathcal{L}_1$ and $\mathcal{L}_2$ could appear in the "limiting" equation.[1] We consider this situation in Part II of the present paper.

Using our approach, we "serve" this whole situation "free of charge," although sometimes exceeding the accuracy; it is only necessary to take into account these terms correctly. It is possible to prove that, in our example, the functions $\mathcal{L}_j$ are polynomial in p, but sometimes this is not the case. (We consider this situation in Part II of this paper.) Moreover, sometimes it is impossible to find explicit formulas even for $\mathcal{L}_0$. On the other hand, for $h \gg \mu$, the passage to Eq. (3.4) from Eq. (2.2) is similar to the replacement of the quantum "adiabatic" momentum $\hat{p} = -i\mu\frac{\partial}{\partial x}$ by the quantum "semiclassical" momentum $\hat{p}_h = \frac{h}{\mu}\hat{p} = -ih\frac{\partial}{\partial x}$ (along with the renormalization of energy). Assume that we consider solutions of Eq. (3.4) such that $\hat{p}_h\psi^{\nu n} = O(1)$. Then we can say that instead of functions (symbols of operators) $\mathcal{L}(p,x,\mu)$ or $\mathcal{L}_0(p,x)$, $\mathcal{L}_1(p,x)$, etc., in formulas (1.16), (1.19), (1.20), etc., we have $\mathcal{L}(\frac{\mu}{h}p_h,x,\mu)$, $\mathcal{L}_0(\frac{\mu}{h}p_h,x)$, $\mathcal{L}_1(\frac{\mu}{h}p_h,x)$, etc. with bounded p_h. Thus we can replace $\mathcal{L}_0(p,x)$, $\mathcal{L}_1(p,x)$, etc. by their Taylor or even asymptotic expansions with respect to the small parameter μ/h or the small "adiabatic" momentum p and use regular perturbation theory to construct these functions as well as the functions (symbols) χ_j. It is this fact that underlies homogenization theory, some version of averaging, some approaches in solid state physics, etc. (see [7] and the bibliography therein).

Remark 2. For two potentials with different α_1 and α_2 at the same energy level, we have $n_1/n_2 \sim \mu^{\alpha_1-\alpha_2}$. Thus for a "softer potential," there are more levels lying under a certain energy level.

4. ACCURACY OF ASYMPTOTIC EXPANSIONS

In this section, we discuss the accuracy of the asymptotic expansions and the minimum reasonable number of their terms.

Since we construct not an asymptotic eigenvalue but a subsequence of eigenvalues or an *asymptotic spectral series*, it is convenient to give the following formal definition of such a series.

Definition. We say that a subsequence of asymptotic eigenvalues (spectral series) is *reasonable* if the possible error of an asymptotic eigenvalue is less than the minimum distance between the closest eigenvalues in the series.

We estimate the minimum number J of terms in the expansions (1.10) and (1.11) necessary to construct a reasonable spectral series.

Suppose that, using the method in Section 2, we have found the terms $\mathcal{L}_j^{(\nu)}(p,x,\mu)$ and $\chi_j^{(\nu)}(p,x,y,\mu)$, $j = 0,1,\dots,J$, in the expansions (1.11) and (1.10). Denote

$$\mathcal{L}_{[J]}^{(\nu)}(p,x,\mu) = \sum_{j=0}^{J}\mu^j\mathcal{L}_j^{(\nu)}(p,x), \qquad \chi_{[J]}^{(\nu)}(p,x,y,\mu) = \sum_{j=0}^{J}\mu^j\chi_j^{(\nu)}(p,x,y), \tag{4.1}$$

and denote by $\hat{\chi}_{[J]}^{(\nu)}$ and $\hat{\mathcal{L}}_{[J]}^{(\nu)}$ the operators generated by the symbols $\chi_{[J]}^{(\nu)}(p,x,y,\mu)$ and $\mathcal{L}_{[J]}^{(\nu)}(p,x,\mu)$.

Let the functions $\psi_{\mathrm{as}}^{(\nu,n)}$ and numbers $E_{\mathrm{as}}^{(\nu,n)}$ be approximate solutions of the spectral problem (1.5) with the asymptotic effective Hamiltonian $\hat{\mathcal{L}}_{[J]}^{(\nu)}$. Then $\psi_{\mathrm{as}}^{(\nu,n)}$ satisfy the equation

$$(\hat{\mathcal{L}}_{[J]}^{(\nu)} - E_{\mathrm{as}}^{(\nu,n)})\psi_{\mathrm{as}}^{(\nu,n)}(x) = f_{[J+1]}(x), \tag{4.2}$$

where the difference $f_{[J+1]}(x)$ between the exact and approximate solutions of (4.2) depends on the number J, the quantum numbers ν and n, and also on the values of the parameters μ and h. To simplify the notation, we do not show this dependence.

[1] In this Example 1 according to (1.19), (1.20), $\mathcal{L}_1 = 0$ and for $\alpha = 1$ $\mathcal{L}_2 = O(\mu^4)$.

Proposition 1. *Denote*

$$\Psi_{\rm as}^{(\nu,n)} \equiv \hat{\chi}_{[J]}^{(\nu)} \psi_{\rm as}^{(\nu,n)}. \tag{4.3}$$

Then $\Psi_{\rm as}^{(\nu,n)}$ *satisfies the equation*

$$\left[\hat{\mathcal{H}} - E_{\rm as}^{(\nu,n)}\right] \Psi_{\rm as}^{(\nu,n)} = \mu^{J+1} \hat{\mathcal{F}}_{[J+1]}^{(\nu)} \psi_{\rm as}^{(\nu,n)} + \hat{\chi}_J^{(\nu)} f_{[J+1]}, \tag{4.4}$$

where $\hat{\mathcal{F}}_{[J]}^{(\nu)}$ *is an operator whose symbol regularly depends on* μ*.*

Proof. The substitution of (1.10) and (1.11) into (1.6) gives

$$\hat{\mathcal{H}} \hat{\chi}_J^{(\nu)} - \hat{\chi}_{[J]}^{(\nu)} \hat{\mathcal{L}}_{[J]}^{(\nu)} = \mu^{J+1} \hat{\mathcal{F}}_{[J+1]}^{(\nu)}, \tag{4.5}$$

where $\hat{\mathcal{F}}_{[J]}^{(\nu)}$ is an operator whose symbol regularly depends on μ.

Now, taking into account (4.3) and (4.2), we have

$$\begin{aligned}\left[\hat{\mathcal{H}} - E_{\rm as}^{(\nu,n)}\right] \Psi_{\rm as}^{(\nu,n)} &= \left[\hat{\mathcal{H}} - E_{\rm as}^{(\nu,n)}\right] \hat{\chi}_{[J]}^{(\nu)} \hat{\psi}_{\rm as}^{(\nu,n)} \\ &= \left[\hat{\mathcal{H}} \hat{\chi}_{[J]}^{(\nu)} - \hat{\chi}_{[J]}^{(\nu)} \hat{\mathcal{L}}_{(\nu)}^{\nu}\right] \psi_{\rm as}^{(\nu,n)} + \hat{\chi}_{[J]}^{(\nu)} f_{[J+1]} = \mu^{J+1} \hat{\mathcal{F}}_{[J]}^{(\nu)} \psi_{\rm as}^{(\nu,n)} + \hat{\chi}_{[J]}^{(\nu)} f_{([J+1]}. \end{aligned} \tag{4.6}$$

Proposition 2. *Let* $\hat{A}$ *be a self-adjoint operator acting in an appropriate Hilbert space with some norm* $\|\cdot\|$*, and let a function* φ *with norm* $\|\varphi\| = 1$ *satisfy the equation*

$$\hat{A}\varphi = \lambda\varphi + f, \tag{4.7}$$

where λ *is any number and* f *is any function. Then the distance between the spectrum of* $\hat{A}$ *and* λ *does not exceed* $\|f\|$*. If the spectrum of* $\hat{A}$ *is discrete, then this means that there exists at least one eigenvalue* $\tilde{\lambda}$ *of the operator* $\hat{A}$ *such that* $\tilde{\lambda} - \lambda = \|f\|$*. Thus if one finds a solution* φ *of the equation* $\hat{A}\varphi = \lambda\varphi + f$ *with the discrepancy* f*,* $\|f\| = O(\varepsilon)$*, then* λ *approximates the eigenvalue* $\tilde{\lambda}$ *of the operator* $\hat{A}$ *modulo* $f = O(\varepsilon)$ *(see* [37]*).*

It follows from Proposition 2 that different asymptotic eigenvalues λ^i and λ^j of the spectral series approximate different points of the spectrum if

$$\min_{i \neq j} |\lambda^i - \lambda^j| \gg \|f\|. \tag{4.8}$$

An application of (4.8) and (4.4) leads to the following assertion.

Proposition 3. *Let* $E_J^{(\nu,n\pm1)}$ *be the asymptotic eigenvalue closest to* $E_J^{(\nu,n)}$*. The spectral series* $E_J^{(\nu,n)}$ *is reasonable provided that*

$$|E_J^{(\nu,n\pm1)} - E_J^{(\nu,n)}| \gg \|\mu^{k+1} \hat{\mathcal{F}}_{[J]}^{(\nu)} \psi_{\rm as}^{(\nu,n)} + \hat{\chi}_{[J]}^{(\nu)} f_{[J]}\|. \tag{4.9}$$

We point out that the above considerations are valid *without any assumptions* about the structure of $(\psi_{\rm as}^{(\nu,n)}, E_{\rm as}^{(\nu,n)})$. Therefore, one can see that (2.2) *does not guarantee* the validity of (4.9).

Consider the case in which $(\psi_{\rm as}^{(\nu,n)}, E_{\rm as}^{(\nu,n)})$ are obtained by the semiclassical approximation. Recall that $|\partial\psi_{\rm as}^{(\nu,n)}/\partial x| \sim h^{-1}$ in this case. Let us apply these estimates to asymptotic solutions constructed above for the spectral problem (1.1).

It is easy to verify that, as a rule, the distance between the closest eigenvalues determined by the Bohr–Sommerfeld rules (2.6) and (2.8) with parameter h is $O(h)$; thus, the distance between the closest numbers (2.3), (2.5), (2.6), and (2.8) is μ^2/h, and the discrepancy on the right hand side in Eq. (1.1) should be at least $o(\mu^2/h)$ (e.g., $O(\mu^2)$ for $h \ll 1$ and $O(\mu^3)$ and $h = 1$).

If one assumes that $\|\hat{\mathcal{F}}^{(\nu)}_{[J]}\psi^{(\nu,n)}_{\mathrm{as}}\| < C_1\|\psi^{(\nu,n)}_{\mathrm{as}}\|$ and $\|\hat{\chi}^{(\nu)}_{[J]}f_{[J]}\| < C_2\|f_{[J]}\|$, where C_1 and C_2 do not depend on any small parameters, then on the right hand side in (4.9), we will have

$$O(\mu^{J+1}) + O(\|f_{[J]}\|) = O(\mu^{J+1}) + o(\mu^2/h).$$

Thus we see that one has to put $J = 1$ for the case in which $h \ll 1$ and $J = 2$ for the case in which $h = O(1)$. These considerations fail for $\psi^{(\nu,n)}_{\mathrm{as}}$ (still with small $\|f_J\|$) such that

$$\mu^{J+1}\hat{F}^{(\nu)}_{[J]}\psi^{(\nu,n)}_{\mathrm{as}} = O(\mu^2/h).$$

In Example 1, $\hat{\mathcal{F}}^{(\nu)}_{[J]} = O(\hat{p}^{J+1})$, $\hat{\chi}^{(\nu)}_{[J]} = \sum_{j=0}^{J}\mu^j O(\hat{p}^j)$, where $h < \mu$, and hence

$$\mu^{J+1}\|\hat{\mathcal{F}}^{(\nu)}_{[J]}\psi^{\mathcal{F}}_{\mathrm{as}}\| = O\Big((\mu^2/h)^{J+1}\Big), \qquad \|\hat{\chi}^{(\nu)}f_{[J]}\| = o(\mu^2/h) + o\Big((\mu^2/h)^{J+1}\Big).$$

If $h > \mu^2$, then the discrepancy is $o(\mu^2/h)$, but if $h \leqslant \mu^2$, then the discrepancy will be equal to $O\big((\mu^2/h)^{J+1}\big) \geqslant \mu^2/h$. Thus in this situation, the adiabatic approximation no longer works.

Let us illustrate this reasoning by the simplest example corresponding to the solutions (2.7); first, we give several important remarks.

Remarks. *First*, all these considerations pertain only to asymptotic eigenvalues but not to asymptotic eigenfunctions. Generally speaking, the functions constructed are not necessarily asymptotic to the actual eigenfunctions. That is why they are usually called "quasimodes." For instance, instead of the functions (2.7), one can take the functions

$$\begin{gathered}\psi^{(\nu,n)}_{\pm}(x) = A^{(\nu,n)}\exp\left[\frac{iS^{(\nu,n)}}{h}\right], \quad S^{(\nu,n)} = \pm\int_{x_0}^{x}\sqrt{\mathcal{E}^{(\nu,n)}_{\mathrm{ov}} - v^{(\nu)}_{\mathrm{eff}}(x)}dx,\\ A^{(\nu,n)} = \frac{C^{(\nu,n)}}{\big[\mathcal{E}^{\nu n}_{\mathrm{ov}} - v^{(\nu)}_{\mathrm{eff}}(x)\big]^{1/4}}, \quad C^{(\nu,n)} = \mathrm{const},\end{gathered} \tag{4.10}$$

which, as a rule, are not asymptotic to exact eigenfunctions of the operator (3.4) but are the asymptotics of their linear combination (2.7). It is these functions that will be used in our example. We refer the reader to [1, 37, 14, 11, 19], where this question is discussed in more detail.

Second, the smallness of the discrepancy $|f_{[J+1]}|$ in Eq. (4.2) or Eq. (2.2) does not guarantee appropriate estimates for the original problem Eq. (1.1): there exists a correction due to $\hat{\mathcal{F}}^{(\nu)}$, and it is necessary to take at least two terms in the expansion of $\chi^{(\nu)}$. This also means that, for this aim, *it does not suffice to substitute the leading asymptotic term* $\hat{\chi}^{(\nu)}_0\psi^{(\nu,n)}$ *into the original equation*; *the first correction* $\hat{\chi}^{(\nu)}_1\psi^{(\nu,n)}$ *is needed*. We return to this question at the end of this subsection.

Third, the above discussion resembles heuristic considerations and ideas. To implement them, one has to introduce appropriate Hilbert spaces, describe the domains of the operators $\hat{\mathcal{H}}$ and $\hat{\mathcal{L}}$, etc. Then one can choose one of two ways. The first way is to estimate the operators $\chi^{(\nu)}_{[J]}, \mathcal{L}^{(\nu)}_{[J]}, \hat{\mathcal{F}}^{(\nu)}_{J}$ in an appropriate scale of (Hilbert) spaces and then establish the relationship between the discrepancy f_{J+1} in Eq. (4.2) and full discrepancy in the original equation (1.1). The second way is to find the "final" function $\Psi^{(\nu,n)}_{[J]} = \hat{\chi}^{(\nu)}_{[J]}\psi^{(\nu,n}_{[J]}$ and then directly estimate the "final" discrepancy in the original equation (1.1). The choice depends on the specific situation. We illustrate the ideas of obtaining rigorous estimates by the simplest example below; some more general and complicated cases can be found, e.g., in [32, 35].

Example. Estimating of the difference between asymptotic and exact "over-barrier" eigenvalues.

Let us estimate the accuracy of the asymptotic eigenvalues found by our method for the waveguide considered in Section 4 under the assumption that $\alpha > 1$, i.e., for the "over-barrier" region of the spectrum. For the operator on the left-hand side in (2.2), we take the asymptotic eigenvalues in the form

$$E^{(\nu,n)} = \Omega_0(\nu + 1/2) + \mu^{2\alpha}\mathcal{E}_{\rm ov}^{(\nu,n)} \equiv \Omega_0(\nu + 1/2) + \Big(\frac{\mu}{h}\Big)^2\mathcal{E}_{\rm ov}^{(\nu,n)}, \tag{4.11}$$

where $\mathcal{E}_{\rm ov}^{(\nu,n)}$ is determined from the Bohr–Sommerfeld rule (2.8) with parameter h instead of μ, and the asymptotic eigenfunctions in the form of quasimodes $\psi_{\pm}^{(\nu,n)}(x)$ in (4.10).

The substitution of $\psi_{\pm}^{(\nu,n)}(x)$ into (3.4) gives

$$\Big[-\frac{h^2}{2}\frac{\partial^2}{\partial x^2} + \Omega_1(x)\Big(\nu + \frac{1}{2}\Big) - \mathcal{E}_{\rm ov}^{(\nu,n)}\Big]\psi^{(\nu,n)} = h^2 f_{[1]}^{(n)}, \tag{4.12}$$

where the discrepancy $f_{[1]}^{(n)}$ is

$$f_{[1]}^{(n)} = -\frac{1}{2}\exp\Big[\frac{iS^{(\nu,n)}}{h}\Big]\frac{\partial^2 A^{(\nu,n)}}{\partial x^2}. \tag{4.13}$$

Hence, by Proposition 1, there exists an exact eigenvalue $\tilde{E}^{(\nu,n)}$ of the operator given by the formula $-\frac{h^2}{2}\frac{\partial^2}{\partial x^2} + \Omega_1(x)(\nu + 1/2)$ such that $\tilde{E}^{(\nu,n)} - \mathcal{E}_{\rm ov}^{(\nu,n)} = O(h^2)$. But, as we mentioned above, it does not suffice to say that the value $\mathcal{E}_{\rm ov}^{(\nu,n)}$ approximates some eigenvalue of the full original operator. Let us take $k = 1$ in formulas (4.4). Then

$$F_{[1]}^{(\nu)} = \Big[\frac{\partial g^{(\nu)}}{\partial x}p^2 - \frac{1}{2}\frac{\partial^2\chi_0^{(\nu)}}{\partial x^2} - g^{(\nu)}\Omega'(x)\Big(\nu + \frac{1}{2}\Big)\Big]. \tag{4.14}$$

According to formulas (1.10) and (1.18), the functions (4.10) give the quasimodes $\Psi_{\pm}^{(\nu,n)}$ of the original equations in the form

$$\begin{aligned}\Psi_{\pm}^{(\nu,n)} &= \Big(\chi_0^{(\nu)}(x,y) + \mu\chi_1^{(\nu)}(-i\mu\overset{1}{\partial}/\partial x, \overset{2}{x}, y)\Big)\psi_{\pm}^{(\nu,n)}(x)\\ &= \exp\Big(\frac{iS^{(\nu,n)}}{h}\Big)\Big(\chi_0^{(\nu)}(x,y) + \frac{i\mu^2}{h}p^{(\nu,n)}g^{(\nu)}(x,y)\Big)A^{(\nu,n)} + \mu^2\exp\Big(\frac{iS^{(\nu,n)}}{h}\Big)\frac{\partial A^{(\nu,n)}}{\partial x}g_1(x,y).\end{aligned} \tag{4.15}$$

Here $p^{(\nu,n)} = \frac{\partial S^{(\nu,n)}}{\partial x}$ and $g^{(\nu)}(x,y)$ is defined in Eq. (1.18). Likewise,

$$\begin{aligned}\hat{F}_{[J]}^{(\nu)}\psi_{\pm}^{(\nu,n)} &= \Big[-\mu^2\frac{\partial g^{(\nu)}}{\partial x}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2\chi_0^{(\nu)}}{\partial x^2} - g^{(\nu)}\Omega'(x)\Big(\nu + \frac{1}{2}\Big)\Big]\exp\Big(\frac{iS^{(\nu,n)}}{h}\Big)A^{(\nu,n)}\\ &= \Big[\frac{\partial g^{(\nu)}}{\partial x}\Big(\frac{\mu^2}{h^2}(p^{(\nu,n)})^2A^{(\nu,n)} + 2i\frac{\mu^2}{h}p^{(\nu,n)}\frac{\partial A^{(\nu,n)}}{\partial x} + i\frac{\mu^2}{h}\frac{\partial p^{(\nu,n)}}{\partial x}A^{(\nu,n)} - \mu^2\frac{\partial^2 A^{(\nu,n)}}{\partial x^2}\Big)\\ &\quad + \Big(-\frac{1}{2}\frac{\partial^2\chi_0^{(\nu)}}{\partial x^2} - g^{(\nu)}\Omega'(x)\Big(\nu + \frac{1}{2}\Big)\Big)A^{(\nu,n)}\Big]\exp\Big(\frac{iS^{(\nu,n)}}{h}\Big),\end{aligned} \tag{4.16}$$

$$\hat{\chi}_1^{(\nu)}f_{[J]} = \Big[-\frac{\mu^2}{2}\Big(\chi_0^{(\nu)}(x,y) + \frac{i\mu^2}{h}p^{(\nu,n)}g^{(\nu)}(x,y)\Big)\frac{\partial^2 A^{(\nu,n)}}{\partial x^2} - \frac{\mu^4}{2}\frac{\partial^3 A^{(\nu,n)}}{\partial x^3}g_1(x,y)\Big]\exp\Big(\frac{iS^{(\nu,n)}}{h}\Big). \tag{4.17}$$

Thus the substitution of the function $\Psi^{(\nu,n)}$ into Eq. (1.1) gives

$$\left(\widehat{\mathcal{H}} - E^{(\nu,n)}\right)\Psi_{\pm}^{(\nu,n)} = \left[\mu^2 R_1(x,y) + \frac{\mu^4}{h^2}R_1(x,y) + \frac{\mu^4}{h}R_3(x,y) + \mu^4 R_4(x,y)\right]\exp\left(\frac{iS^{(\nu,n)}}{h}\right), \quad (4.18)$$

where R_j are smooth functions decaying at the rate of a Gaussian exponent as $|y| \to \infty$.

Hence the L_2-norm of the right hand side is equal to $O(\mu^2) + O(\mu^4/h^2)$. Now it is easy to find the limit of the adiabatic approximation. On the one hand, $\Psi^{(\nu,n)} = \Psi_0^{(\nu,n)} + O(\mu^2/h)$, where $\Psi_0^{\nu n} = \chi_0^{(\nu)}(x,y)\psi^{(\nu,n)}(x)$. Thus the correction $O(\mu^2/h)$ to the function $\Psi_0^{(\nu,n)}$ is small if $\mu^2 \gg h$. Only then we can say that the function $\Psi_0^{(\nu,n)}$ is the *leading term* of the asymptotic solution $\Psi^{\nu n}$. On the other hand, we have the same result from the estimate of the right-hand side in (4.18). Indeed, if $\mu^2 \gg h$, then the L_2-norm of the right-hand side is equal to $o(\mu)$, and by Proposition 1, we desire the existence of an exact eigenvalue $\tilde{E}^{\nu n}$ such that $\tilde{E}^{(\nu,n)} = E^{(\nu,n)} + o(\mu)$. If $h = O(\mu^2)$ or $h\mu^2 \gg \mu^2$, then the distance between the asymptotic eigenvalues $E^{(\nu,n)}$ and $E^{(\nu,(n\pm1))}$ is $O(\mu^2/h)$, which is less than the correction $O(\mu^2/h)$, and the adiabatic approximation works no longer. Actually, the study of the situation $h = O(\mu^2)$, corresponding to "superexcited states," is one the main goals of this paper; we consider this situation in the next section.

Remark. We again point out that the adiabatic approximation permits one to construct some ("regular" in the example considered, see the next subsection) part of spectrum of the operator $\hat{\mathcal{H}}$. Thus the natural question arises: do the described adiabatic and semiclassical approaches allow one to find all eigenvalues lying below some fixed energy $E^{(\nu',n')}$? This question is not trivial (e.g., see [14]) even for our simple example. We can only say that the answer seems to be "yes"; at least physicists usually believe so. Assuming that the answer is in the positive for the operator $\hat{\mathcal{H}}$ in Eq. (1.1), let us find the so-called density of low states.

The density of states plays an important role in solid state physics and also in nanophysics [42]. Since we have a "regular" structure of the spectrum near its bottom, one can obtain simple formulas for the density. For the given "subband" corresponding to the effective Hamiltonian with number ν, we have

(1) $dn/dE \sim 1/\mu^{1+\alpha}$ for low-lying states.

(2) $dn/dE \sim 1/(\mu\sqrt{E})$ for ultrashort modes.

Let us also repeat that in practice the parameters μ and h are numbers and the relation (3.1) is rather artificial. Thus it is possible to include some parts of the power μ^α in the potential (or other coefficients) of the original equation and relate it to the "canonical" cases mentioned in Section 1.

Conclusions. From the above considerations, we can make the following conclusions.

1. To obtain the main asymptotic formulas for the eigenvalues of energy E for a thin quantum waveguide, one should find the first three terms $\mathcal{L}_0^{(\nu)}(p,x)$, $\mathcal{L}_1^{(\nu)}(p,x)$, and $\mathcal{L}_2^{(\nu)}(0,x)$ in the expansion (1.11), where the last term $\mathcal{L}_2^{(\nu)}(0,x)$ is calculated at $p = 0$ and is needed in the long-wave approximation.

2. To reconstruct the main part of the operator $\hat{\chi}^{(\nu)}$, one should find the first three terms $\chi_0^{(\nu)}(p,x,y)$, $\chi_1^{(\nu)}(p,x,y)$, and $\chi_2^{(\nu)}(0,x,y)$ in the expansion (1.10) of its symbol, where the last term $\chi_2^{(\nu)}(0,x,y)$ is calculated at $p = 0$ and is needed in the long-wave approximation.

It should also be noted that although the effective equation (3.2), (3.4) of adiabatic motion can be analyzed for $h \sim 1/n$ as small as desired, its solutions cannot sometimes be used in the construction of the asymptotic solution of the original equation (1.1). One of these cases corresponds to the situation in which the term $\mu\chi_1^{(\nu)}$ in the expansion (1.10) is of the order of the term $\chi_0^{(\nu)}$, so that the expansion (1.10) is unusable. This case will be considered in the next section.

5. SUPEREXCITED STATES, THE ORIGIN OF INSTABILITY, AND FERMI ACCELERATION

The WKB approximation can be applied to Eq. (2.2) not only for $n \sim 1/\mu$ (as was done above) but also for $n \gg 1/\mu$, e.g., for $n = 1/\mu^{3/2}$. Since $\mathcal{E}_{\text{ov}}^{(\nu,n)} \gg v_{\text{eff}}^{(\nu)}(x)$ in these cases, one can apply

formulas (4.10) and then, using the Taylor expansion, obtain

$$\mathcal{E}^{(\nu,n)}_{\mathrm{ov}} = (n\mu)^2 + \Omega^{\mathrm{av}}\Big(\nu+\frac{1}{2}\Big) + \Big((\mu n)^{-2}\Big), \qquad \Omega^{\mathrm{av}} = \frac{1}{2\pi}\int_0^{2\pi}\Omega(x)dx, \tag{5.1}$$

$$\begin{aligned}
\Psi^{(\nu,n)}_{+}(x) &\simeq \frac{\Omega^{1/4}(x)}{\pi^{3/4}\sqrt{2^k k!}}\cos(nx)\exp\Big(-\frac{\Omega(x)y^2}{2}\Big)H_\nu(\sqrt{\Omega(x)}y),\\
\Psi^{(\nu,n)}_{-}(x) &\simeq \frac{\Omega^{1/4}(x)}{\pi^{3/4}\sqrt{2^k k!}}\sin(nx)\exp\Big(-\frac{\Omega(x)y^2}{2}\Big)H_\nu(\sqrt{\Omega(x)}y).
\end{aligned} \tag{5.2}$$

To obtain this formula, one can also use a version of the Born approximation for the construction of eigenvalues and eigenfunctions [10]. Now the problem is in the precision of adaptability of formula (1.4) as well as the adiabatic approximation in general for these numbers n. Let us analyze the first correction $\mu\hat{\chi}^{(\nu)}\psi^{(\nu,n)}$ from this point of view. It is easily seen that $p \sim n\mu$. Thus we readily find that, starting from $n = 1/\mu^2$, the term $\mu\hat{\chi}^{(\nu)}\psi^{(\nu,n)} = O(1)$ is not the correction to the leading term of the asymptotic solution of the original equation in spite of the fact that the function $\psi\nu n$ is an asymptotic solution of Eq. (2.2).

Consider this situation in detail for the original equation (1.1). It is convenient to use the parameter $h = \mu^2$, put $x_1 = x$, $x_2 = \mu y$ from the very beginning, and rewrite Eq. (1.1) in the form

$$\hat{\mathcal{H}}\Psi \equiv \frac{1}{2}\left[-h^2\frac{\partial^2}{\partial x_1^2} - h^2\frac{\partial^2}{\partial x_2^2} + \Omega^2(x_1)\eta^2\right]\Psi = hE^{(\nu,n)}\Psi^{(\nu,n)}, \qquad \Psi^{(\nu,n)}(x_1+2\pi,x_2) = \Psi^{(\nu,n)}(x_1,x_2), \tag{5.3}$$

where $E^{(\nu,n)}$ is the same as in Eq. (1.1).

The classical Hamiltonian (or symbol), corresponding to the "h"-differential operator in (5.3) has the form

$$H = \frac{1}{2}\big(p_1^2 + p_2^2 + \Omega(x_1)x_2^2\big). \tag{5.4}$$

Generally speaking, the Hamiltonian system

$$\begin{aligned}
\dot{x}_1 &= p_1, \qquad \dot{p}_1 = -\frac{1}{2}\Omega_1'(x_1)x_2^2,\\
\dot{x}_2 &= p_2, \qquad \dot{p}_2 = -\Omega(x_1)x_2
\end{aligned}$$

corresponding to (5.4) is not integrable, and, as we mentioned before, it is impossible to find an analytical description of the spectrum not only exactly but also asymptotically. But in the phase space, this Hamiltonian system has the family of (exact) trajectories $\Gamma = (p_1 = P_1 \equiv q = \mathrm{const}, x_1 = X_1 \equiv qt, p_2 = 0, x_2 = 0)$ with the projection $x_2 = 0$, which is the waveguide axis parametrized by the parameter q. Thus, using the methods in [34, 2, 41, 5], one can try to construct the series of eigenfunctions and eigenvalues of the operator (5.4) localized in a neighborhood of the line $x_2 = 0$ and corresponding to the trajectories Γ. Following [34], it is necessary to write out the variational system for the complex functions $Z = \delta x_1$ and $W = \delta p_1$ describing the corrections to the trajectory Γ:

$$\dot{Z} = W, \qquad \dot{W} = -\Omega^2(X_1)Z, \quad X_1 = qt. \tag{5.5}$$

This system has periodic coefficients and therefore can be studied by methods of Floquet–Lyapunov theory. According to [34, 41], one can construct the above-mentioned asymptotic eigenfunction if system (5.5) is stable. This is equivalent to the assumption that (5.5) has Floquet solutions

$$W = W_0(X_1)\exp(i\beta t), \qquad Z = Z_0(X_1)\exp(i\beta t), \qquad \bar{W}^0Z^0 - W^0\bar{Z}^0 = 2i,$$

where the Floquet index $\beta(q)$ is real and $W(x_1)$ and $Z(x_1)$ are 2π-periodic functions of x_1. Let us assume that the stability condition holds. The functions $W_0(x_1)$ and $Z_0(x_1)$, as well as the Floquet

index $\beta(q)$, are not uniquely determined, and we fix them in the following way. The complex-valued function $Z_0(x_1)$ vanishes nowhere. Thus one can define a continuous branch $\Theta(x_1) = \operatorname{Arg} Z_0(x_1)$ of its argument for $x_1 \in (-\infty, \infty)$, $\operatorname{Arg} Z_0(0) = 0$. We choose the function Z_0 in such a way that $\operatorname{Arg} Z_0(x_1 + 2\pi) - \operatorname{Arg} Z_0(x_1) = 0$. This condition also determines $\beta(q)$:

$$\beta(q) = \frac{q}{2\pi} \operatorname{Arg} Z|_t^{t+2\pi/q}.$$

To find the asymptotic eigenvalues, one has to quantize the parameter q (i.e., the trajectory Γ) using the Bohr–Sommerfeld rule $\frac{1}{2\pi}\int p dx = nh$, where n is any integer, which gives $q = q^n = nh$. Then the asymptotic eigenvalues can be written as a sum of the kinetic energy $(q^n)^2/2 = (nh)^2/2$ and the "Floquet correction" $h\beta(p_1^n)(\nu + 1/2)$,

$$hE^{(\nu,n)} = \frac{(nh)^2}{2} + h\beta(q_1^n)(\nu + 1/2) + O(h^2).$$

Turning back to notation in Section 2, we have $q^n = n\sqrt{\mu}$ and

$$E^{(\nu,n)} = \frac{(n\mu)^2}{2} + \beta(q^n)(\nu + 1/2) + O(\mu^2). \tag{5.6}$$

The corresponding asymptotic eigenfunctions are

$$\begin{aligned}
\Psi_+^{(\nu,n)} &= \frac{1}{\sqrt{R}} \cos\left(nx_1 + \frac{nx_2^2}{2\mu^{3/2}R}\, \frac{\partial R}{\partial x_1}(x_1) - \Big(\nu + \frac{1}{2}\Big)\Theta(x_1)\right) \exp\Big(- \frac{x_2^2}{2\mu^2 R^2(x_1)}\Big) H_\nu\Big(\frac{x_2}{\mu R}\Big), \\
\Psi_-^{(\nu,n)} &= \frac{1}{\sqrt{R}} \sin\left(nx_1 + \frac{nx_2^2}{2\mu^{3/2}R}\, \frac{\partial R}{\partial x_1}(x_1) - \Big(\nu + \frac{1}{2}\Big)\Theta(x_1)\right) \exp\Big(- \frac{x_2^2}{2\mu^2 R^2(x_1)}\Big) H_\nu\Big(\frac{x_2}{\mu R}\Big),
\end{aligned} \tag{5.7}$$

where $R(x_1) = |Z_0|(x_1)$.

The form (5.6) of the asymptotic eigenvalues is very similar to the expression (5.7); it seems that one only needs to change the "average" frequency Ω^{av} by the Floquet number β. But there exists a big difference between these formulas. First, the dependence on $\Omega(x)$ is more complicated in the second case than the averaging in the first one, and in contrast to Ω^{av}, β depends on the frequency q^n. The second difference is much more important: for frequencies q^n belonging to some gaps on the axis $p_1 = q$, the classical motion along the waveguide axis becomes unstable and formulas (5.7) fail. Since the classical trajectories in these gaps are unstable, we interpret this fact as *the destruction of adiabatic approximation corresponding to the regular quantum motion and the passage to chaotic behavior*.

Let us compare the behavior of the asymptotic eigenfunctions (5.2) and (5.7). Consider them on the cross-section $x_1 = \text{const}$ of the waveguide. The functions (5.2) depend on the variable frequency $\Omega(x_1)$ locally: the dependence of eigenfunctions $\Psi_\pm^{(\nu,n)}$ in the normal direction does not "feel" the behavior of $\Omega(x_1)$ at points x_1 different from r. In the second case, (5.7), the dependence of eigenfunctions $\Psi_\pm^{(\nu,n)}$ in normal direction "feels" the dependence $\Omega(x_1)$ (via the variational system) on x_1 *along the entire waveguide*.

It seems to be true that the length of the gaps increases together with q (or the longitudinal energy), and finally the bands of stability become very small and disappear; this means that, for high longitudinal energy, the quantum waveguide displays *chaotic behavior*.

One can interpret this situation as follows. Consider the motion of a classical particle near the waveguide axis. If one chooses the system of coordinates related to the particle coordinate on the x_1-axis, then the dependence of $\Omega(x_1)$ on x_1 means the presence of "rapidly oscillating" walls, and for "superexcited" states the frequency of "transverse" oscillations has the same order as the "longitudinal" frequency.

This problem is well known in classical mechanics [45]. First it was considered by Fermi; therefore the possible acceleration of the particle in such a problem is called "Fermi acceleration." So it is natural to say that the appearance of instability gaps for Eq. (5.5) is caused by an analog of Fermi acceleration and hence, in this example, the Fermi acceleration destroys the regular spectrum and the adiabatic approximation.

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