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PROPAGATION OF GAUSSIAN WAVE PACKETS IN THIN PERIODIC QUANTUM WAVEGUIDES WITH A NONLOCAL NONLINEARITY

J. Brüning,* S. Yu. Dobrokhotov,† R. V. Nekrasov,† and A. I. Shafarevich†

We consider the nonlinear Schrödinger equation with an integral Hartree-type nonlinearity in a thin quantum waveguide and study the propagation of Gaussian wave packets localized in the spatial variables. In the case of periodically varying waveguide walls, we establish the relation between the behavior of wave packets and the spectral properties of the auxiliary periodic problem for the one-dimensional Schrödinger equation. We show that for a positive value of the nonlinearity parameter, the integral nonlinearity prevents the packet from spreading as it propagates. In addition, we find situations such that the packet is strongly focused periodically in time and space.

Keywords: nonstationary Schrödinger equation with an integral nonlinearity, thin tube, Gaussian wave packet, localization

1. Introduction

The solutions of the quantum mechanics equations modeling electron transport in thin-tube-type domains (*quantum waveguides*) recently became interesting because of the developments in nanotechnologies. The motion in the directions normal to the tube axis is constrained either by a rapidly increasing potential (the "soft wall" model) or by the boundary conditions (the "rigid wall" model). It is clear from physical considerations that the particle (or quasiparticle) dynamics in thin quantum waveguides must be spatially one-dimensional and the original three-dimensional equation can be reduced to a set of one-dimensional Schrödinger-type equations on the tube axis. Maslov accurately proved this fact in the model situation in 1958 [1]. Such a reduction for a wide region of quantum states was accurately performed in [2] for an original (linear) equation describing the quantum motion of charged particles with spin in a thin waveguide placed in magnetic and electric fields.

The Schrödinger-type equations with a potential independent of the electron position derived in [2] (also see [3]), just as any linear Schrödinger equations, have only localized propagating solutions inevitably spreading as they propagate through the entire waveguide length. The nonspreading of localized solutions (the ballistic transport in strongly extensive waveguides) can thus occur only if the nonlinear effects are taken into account.

Numerous models in which the solutions do not change their shape at all (solitons) are well known in the nonlinear theory. Asymptotic solutions with this property were constructed in [4], [5] for the Hartree-type equation (with a nonlocal nonlinear interaction) in the three-dimensional Euclidean space:

$$i\hbar\frac{\partial}{\partial t}\Psi=\widehat{\mathcal{H}}\Psi,\qquad \widehat{\mathcal{H}}=-\frac{\hbar^2}{2m}\Delta+\mathbf{v}_{\mathrm{int}}(\mathbf{r})+\int_{\mathbb{R}^3}G(\mathbf{r},\mathbf{r}')\big|\Psi(\mathbf{r}',t)\big|^2\,d\mathbf{r}',\quad \mathbf{r}\in\mathbb{R}^3,\tag{1}$$

*Humboldt University, Berlin, Germany, e-mail: bruening@mathematik.hu-berlin.de.

†Institute for Problems of Mechanics, RAS, Moscow, Russia, e-mail: dobr@ipmnet.ru, logno@rambler.ru, shafar@mech.math.msu.su.

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where $\Psi(\mathbf{r},t)$ is the unknown wave function (the quantum state), $\hbar$ and m are physical constants (the Planck constant and the effective mass), and the nonlinear potential kernel G and the potential $\mathbf{v}_{\rm int}$ are smooth functions. We show that for a potential $\mathbf{v}_{\rm int}$ rapidly increasing in the direction transverse to the waveguide axis ("confinement potential"), this equation (considered in a thin tube, i.e., in a quantum waveguide) has solutions with the same property of nonspreading.

The nonlinear potential $\int_{\mathbb{R}^3} G(\mathbf{r},\mathbf{r'})\big|\Psi(\mathbf{r'})\big|^2\,d\mathbf{r'}$ takes account of possible tube deformations under the action of the electron or of the possible self-action of electrons (i.e., it is the effective potential of a self-consistent field in the one-particle approximation). The same term in the case of the Bose–Einstein condensate generalizes the Gross–Pitaevskii equation to the case of a nonlocal nonlinear interaction. If the transverse waveguide dimensions vary periodically along its axis, then the asymptotic solutions thus constructed in a rough approximation can also be used to model the propagation of intermolecular excitations along long molecular chains (cf. [6]).

This paper is organized as follows. In Sec. 2, we formulate the problem statement in an appropriate curvilinear coordinate system with the problem parameters taken into account. In Sec. 3, we present formulas for the Gaussian wave packet propagating in thin nonlinear waveguides with a general structure. The case where the waveguide walls have a periodic structure and the packet properties are related to the periodic Sturm–Liouville problem is studied in detail in Sec. 4. Section 5 is auxiliary; there, we use the adiabatic approximation to reduce the original three-dimensional equation to the one-dimensional equation on the tube axis.

2. Statement of the problem in curvilinear coordinates and characteristic quantities

It is convenient to seek special localized solutions in appropriate curvilinear coordinates. These curvilinear coordinates (the longitudinal coordinate x and the transverse coordinates $\mathbf{y}=(y_1,y_2)$) are determined in the vicinity of the tube as follows. We assume that the tube axis is an infinite curve γ (we thus neglect the boundary effects, i.e., the effects of the wave packet emission and absorption at the two ends of the real tube). We assume that the curve γ is given by the equation $\mathbf{r}=\mathbf{R}(x)$, $\mathbf{r}\in\mathbb{R}^3$, $x\in\mathbb{R}$, where $\mathbf{R}(x)$ is a smooth vector function and x is a natural parameter on the curve γ, i.e., it is the curve length measured from a fixed point on γ. The orthonormal basis triple $\{\mathbf{v}=\dot{\mathbf{R}},\mathbf{n}_1,\mathbf{n}_2\}$ can be introduced at all points of the curve γ. Rotating $\mathbf{n}_1(x),\mathbf{n}_2(x)$ by the angle $\int_0^x \dot{\mathbf{n}}_1(x)\cdot\mathbf{n}_2(x)\,dx$ about the velocity vector $\mathbf{v}(x)$, we construct the vectors $\mathbf{n}'_1(x)$ and $\mathbf{n}'_2(x)$, where the dot over a symbol denotes differentiation with respect to x and the dot between vectors denotes their scalar product in $\mathbb{R}^3$. Then the curvilinear coordinates (x,y_1,y_2) introduced by the relation $\mathbf{r}=\mathbf{R}(x)+\mathbf{y}(x,y_1,y_2)$, where $\mathbf{y}(x,y_1,y_2)=y_1\mathbf{n}_1{}'(x)+y_2\mathbf{n}_2{}'(x)$, and uniquely determined in a neighborhood of γ are orthogonal. The metric in these coordinates has the form

$$g_{ij}=\begin{pmatrix} g_{11} & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix},\qquad g_{11}(x,\mathbf{y})=\big(1-k(x)y_n\big)^2,\qquad y_n=y_1\cos\theta-y_2\sin\theta,$$

where $\theta=\theta(x)$ is the angle between the normal vector and the vector $\mathbf{n}'_1$ and $k(x)$ is the curvature of γ. We therefore have the expression for the operator Δ

$$\Delta=\frac{1}{\sqrt{g}}\frac{\partial}{\partial x^j}g^{ij}\sqrt{g}\,\frac{\partial}{\partial x^i}=\frac{1}{\sqrt{g}}\frac{\partial}{\partial x}\frac{1}{\sqrt{g}}\frac{\partial}{\partial x}+\frac{1}{\sqrt{g}}\frac{\partial}{\partial y_1}\sqrt{g}\,\frac{\partial}{\partial y_1}+\frac{1}{\sqrt{g}}\frac{\partial}{\partial y_2}\sqrt{g}\,\frac{\partial}{\partial y_2},\qquad (2)$$

where $g=\det g_{ij}\equiv g_{11}(x,\mathbf{y})>0$ is the squared density of the volume measure.

We assume that the tube is sufficiently thin such that it lies in the domain where the coordinates are well defined. Because the scales along and across the tube are distinct, the problem contains a small parameter $\mu = d/l \ll 1$, where d is the characteristic tube dimension, the waveguide cross section is not necessarily circular, simply connected, and constant, and l is the characteristic waveguide length (l is also of the order of the length of the waveguide part under study).

We also assume that the characteristic scale of variations in the kernel G is much larger than the waveguide diameter (more precisely, it is of the order of l). Therefore, the nonlinear potential does not play any role in confining the particle in the interior of the waveguide; the particle is confined by the potential $\mathbf{v}_{\mathrm{int}}$. To confine the particle in the interior of the waveguide, the confinement potential must have the form of a potential well in the direction transverse to the tube axis such that its value outside the waveguide cross section must be sufficiently larger than the total energy of the particle (the subbarrier penetration into the exterior of the waveguide is then small and the wave function $\Psi \to 0$ with increasing distance from the waveguide axis).

We consider a smooth tubular neighborhood Γ of the waveguide that is sufficiently wide (its diameter strongly exceeds the waveguide diameter) and sufficiently narrow such that the coordinates x and $\mathbf{y}$ remain well defined. Because the wave function outside any neighborhood of the curve γ is exponentially small as $\mu \to 0$ (see formula (15) for the asymptotic expansion below), multiplying by the cutoff function concentrated in the interior of the domain Γ changes it by $O(\mu^\infty)$. Therefore, the following condition does not affect the asymptotic expansion of the wave function as $\mu \to 0$: the function Ψ is zero outside the domain Γ, i.e.,

$$\Psi|_{\mathbb{R}^3\setminus\Gamma} = 0. \tag{3}$$

Because of this condition, we need not consider the ambiguity of the coordinates x and $\mathbf{y}$.

After the parameters l and d are introduced, the left-hand side of Eq. (1) can be reduced to the dimensionless form with the distinct scales along and across the tube taken into account. For this, we multiply it by $\varepsilon_\perp^{-1} = md^2/\hbar^2$, change the scales $x \to \tilde{x} = x/l$ and $\mathbf{y} \to \tilde{\mathbf{y}} = \mathbf{y}/d$, introduce the dimensionless time $\tilde{t} = \hbar t/(lmd)$ (the unit velocity in these units is associated with the velocity $\hbar/(md)$, which is the characteristic longitudinal velocity of the space-localized solutions presented below), and then change $\Psi \to \widetilde{\Psi} = \sqrt[4]{g}\,\Psi$, $\sqrt[4]{g} = \sqrt{1-\mu k(x)\tilde{y}_n}$. Equation (1) with (3) taken into account then becomes

$$i\mu\frac{\partial\widetilde{\Psi}}{\partial\tilde{t}} = \widetilde{\mathcal{H}}\widetilde{\Psi}, \qquad \widetilde{\Psi}|_{\mathbb{R}^3\setminus\Gamma} = 0,$$

$$\widetilde{\mathcal{H}} = -\frac{\mu^2}{2\sqrt[4]{g}}\frac{\partial}{\partial\tilde{x}}\frac{1}{\sqrt{g}}\frac{\partial}{\partial\tilde{x}}\frac{1}{\sqrt[4]{g}} - \frac{1}{2}\Delta_{\tilde{y}} + U(\tilde{x},\tilde{\mathbf{y}},\mu) + \int_{\mathbb{R}^3}\widetilde{G}(\tilde{x},\tilde{\mathbf{y}},\tilde{x}',\tilde{\mathbf{y}}',\mu)\big|\widetilde{\Psi}(\tilde{x}',\tilde{\mathbf{y}}')\big|^2\,d\tilde{x}'\,d\tilde{\mathbf{y}}',$$

where

$$\Delta_{\tilde{y}} = \frac{\partial^2}{\partial\tilde{y}_1^2} + \frac{\partial^2}{\partial\tilde{y}_2^2}, \qquad U(\tilde{x},\tilde{\mathbf{y}},\mu) = v_{\mathrm{int}}(\tilde{x},\tilde{\mathbf{y}}) + \frac{1}{2\sqrt[4]{g}}\frac{\partial}{\partial\tilde{y}_n}\frac{1}{\sqrt{g}}\frac{\partial}{\partial\tilde{y}_n}\frac{1}{\sqrt[4]{g}},$$

$$v_{\mathrm{int}}(\tilde{x},\tilde{\mathbf{y}}) = \frac{\mathbf{v}_{\mathrm{int}}(x,\mathbf{y})}{\varepsilon_\perp}, \qquad \widetilde{G}(\tilde{x},\tilde{\mathbf{y}},\tilde{x}',\tilde{\mathbf{y}}',\mu) = \frac{V}{\varepsilon_\perp}G(l\tilde{x},l\mu\tilde{\mathbf{y}},l\tilde{x}',l\mu\tilde{\mathbf{y}}'), \qquad V = ld^2.$$

It is easy to see that because $g = 1 + O(\mu)$, the second term in the penultimate formula generated by the two last terms in (2) is of the order $\mathrm{O}(\mu^2)$. The potential confines the particle in the interior of the domain, where $|\tilde{\mathbf{y}}|^2 \le 1$, and its higher-order term $v_{\mathrm{int}} = \mathbf{v}_{\mathrm{int}}(x,\mathbf{y})/\varepsilon_\perp$ in the transverse direction hence has the form of a potential well whose depth is no less than $O(1)$. This implies that the order of the confinement potential $\mathbf{v}_{\mathrm{int}}$ is no less than that of $\varepsilon_\perp = \hbar^2/(md^2)$. The problem also contains a nonlinear potential, but because the characteristic scale of variations in the kernel G is of the order l, its dependence on the transverse variable is sufficiently weak, and we have the expansion

$$\widetilde{G}(\tilde{x},\tilde{\mathbf{y}},\tilde{x}',\tilde{\mathbf{y}}',\mu) = G_0(\tilde{x},\tilde{x}') + \mu G_1(\tilde{x},\tilde{\mathbf{y}},\tilde{x}',\tilde{\mathbf{y}}') + \cdots + O(\mu^N), \tag{4}$$

where

$$G_0(\tilde{x},\tilde{x}') = \frac{V}{\varepsilon_\perp} G(l\tilde{x}, 0, l\tilde{x}', 0)$$

and it is assumed that $G_0 \sim 1$, i.e., the nonlinear kernel G is of the order of $\varepsilon_\perp/V$, and

$$G_1(\tilde{x},\tilde{\mathbf{y}},\tilde{x}',\tilde{\mathbf{y}}') = G_{11}(\tilde{x},\tilde{x}')\tilde{y}_1 + G_{12}(\tilde{x},\tilde{x}')\tilde{y}_2 + G'_{11}(\tilde{x},\tilde{x}')\tilde{y}'_1 + G'_{12}(\tilde{x},\tilde{x}')\tilde{y}'_2,$$

$$G_{1i}(\tilde{x},\tilde{x}') = l\frac{V}{\varepsilon_\perp}\frac{\partial G}{\partial y_i}(l\tilde{x},0,l\tilde{x}',0), \qquad G'_{1i}(\tilde{x},\tilde{x}') = l\frac{V}{\varepsilon_\perp}\frac{\partial G}{\partial y'_i}(l\tilde{x},0,l\tilde{x}',0).$$

Hereafter, we omit the tilde symbols and deal with these dimensionless variables. As a result, we obtain the equation

$$\begin{aligned} &i\mu\frac{\partial \Psi}{\partial t} = \widehat{\mathcal{H}}\Psi, \qquad \widehat{\mathcal{H}} = \widehat{H} + \int_{\mathbb{R}^3} G(x,\mathbf{y},x',\mathbf{y}',\mu)\big|\Psi(x',\mathbf{y}')\big|^2\,dx'\,d\mathbf{y}', \quad \mu \ll 1, \\ &\Psi|_{\mathbb{R}^3\setminus\Gamma} = 0, \end{aligned} \tag{5}$$

where

$$\widehat{H} = -\frac{\mu^2}{2\sqrt[4]{g}}\frac{\partial}{\partial x}\frac{1}{\sqrt{g}}\frac{\partial}{\partial x}\frac{1}{\sqrt[4]{g}} - \frac{1}{2}\Delta_y + U(x,\mathbf{y},\mu), \qquad \Delta_y = \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial y_2^2},$$

and the functions $G(x,\mathbf{y},x',\mathbf{y}',\mu)$ and $U(x,\mathbf{y},\mu)$ satisfy the following condition required by their physical meaning (see above).

Condition 1. The functions U and G are smooth in all their arguments including μ; the function G is bounded and can be represented in form (4).

Our main goal is to obtain special space-localized asymptotic solutions of Eq. (5).

3. Formulas for the wave packets

It is clear from physical considerations that studying the wave functions of the original equation localized in the direction transverse to the tube axis and corresponding to weakly excited states should asymptotically reduce to studying a spatially one-dimensional equation (on the waveguide axis). This is indeed true and is realized in the framework of the adiabatic approximation. We at once present the corresponding one-dimensional nonlinear equation and the reduction procedure itself and give the corresponding proofs below. Let $\varepsilon(x)$ be an eigenvalue, let $\chi_0(x,\mathbf{y})$ be the corresponding eigenfunction of the problem

$$-\frac{1}{2}\Delta_y\chi_0 + v_{\mathrm{int}}(x,\mathbf{y})\chi_0 = \varepsilon(x)\chi_0, \quad \|\chi_0\|_y \equiv 1, \quad \operatorname{Im}\chi_0 \equiv 0, \tag{6}$$

and let the following conditions be satisfied.

Condition 2. The eigenvalue $\varepsilon(x)$ is nondegenerate for all x, and $\varepsilon(x)$ is a smooth function.

Condition 3. The relation $\langle y_i\rangle_y \equiv 0$ holds.[1]

[1]Apparently, we can always obtain this relation by a small shift (of the order μ) of the curve γ; this relation is required to simplify the formulas. But if this condition is not satisfied, then the braces in (7) contain the additional term $\mu\hat{\mathcal{L}}_1\big(\overset{2}{x}, -i\mu\overset{1}{\frac{\partial}{\partial x}}[\phi]\big)$, where $\hat{\mathcal{L}}$ is the pseudodifferential operator described in Sec. 5 below.

Here, we introduce the notation

$$\| \cdot \|_y = \int_{\mathbb{R}^2} | \cdot |^2 \, d\mathbf{y}, \qquad \langle \cdot \rangle_y = \int_{\mathbb{R}^2} \overline{\chi}_0 \cdot \chi_0 \, d\mathbf{y}.$$

Then the reduced spatially one-dimensional equation has the form

$$\left\{ -i\mu \frac{\partial}{\partial t} - \frac{\mu^2}{2} \frac{\partial^2}{\partial x^2} + \varepsilon(x) + \int_{\mathbb{R}} G_0(x, x') \big|\phi(x', t, \mu)\big|^2 \, dx' \right\} \phi(x, t, \mu) = 0. \tag{7}$$

If ϕ is a solution of the reduced equation satisfying some appropriate conditions (we present them below), then the asymptotic solution of the original equation corresponding to ϕ is reconstructed from the formula

$$\Psi(x, \mathbf{y}, t, \mu) = \chi_0(x, \mathbf{y}) \phi(x, \mu, t) \big(1 + O(\mu)\big).$$

For greater clarity, we consider the situation in which the soft walls of the waveguide are modeled by the parabolic confinement potential

$$v_{\mathrm{int}}(x, y_1, y_2) = \frac{\Omega_1^2(x) y_1^2}{2} + \frac{\Omega_2^2(x) y_2^2}{2},$$

where $\Omega_j(x)$ are smooth positive functions. The dependence of Ω_j on x means that the transverse waveguide dimensions can vary smoothly along the tube axis. Problem (6) corresponds to the two-dimensional harmonic oscillator, and its solutions are numbered by the two quantum numbers ν_1 and ν_2 and have the form

$$\varepsilon(x) = \varepsilon^{(\nu_1, \nu_2)}(x) = \Omega_1(x) \left(\nu_1 + \frac{1}{2} \right) + \Omega_2(x) \left(\nu_2 + \frac{1}{2} \right), \quad \nu_i = 0, 1, 2, \ldots,$$

$$\chi_0 = \chi_0^{(\nu_1, \nu_2)}(x, y_1, y_2) = \frac{\sqrt[4]{\Omega_1(x) \Omega_2(x)}}{\sqrt{\pi 2^{\nu_1} 2^{\nu_2} \nu_1! \, \nu_2!}} e^{-\Omega_1 y_1^2/2 - \Omega_2 y_2^2/2} H_{\nu_1}\big(\sqrt{\Omega_1}\, y_1\big) H_{\nu_2}\big(\sqrt{\Omega_2}\, y_2\big),$$

where $H_\nu(x)$ is the νth Hermite polynomial. The value of $\varepsilon^{(\nu_1, \nu_2)}(x)$ is nondegenerate, for example, for the ground state $\nu_1 = 0$, $\nu_2 = 0$ and for any arbitrary ν_1 and ν_2 if $\Omega_1(x)/\Omega_2(x) = \mathrm{const} = r$, where r is an irrational number.

For Eq. (7), we consider the Cauchy problem with the initial wave function localized in a neighborhood of the point $x = X_0$:

$$\phi|_{t=0} = A e^{i P_0 (x - X_0)/\mu} e^{i (x - X_0)^2 B_0 / (2\mu)}, \tag{8}$$

where P_0 is a real number (parameter), B_0 is a complex number (parameter), $\operatorname{Im} B_0 > 0$, and the normalization constant A is chosen from the condition

$$\|\phi\|^2_{L_2(\mathbb{R})} = \int_{\mathbb{R}} \big|\phi(x)\big|^2 \, dx = 1$$

and is equal to

$$A = A(\mu, B_0) = \sqrt[4]{\frac{\operatorname{Im} B_0}{\pi \mu}}.$$

This problem corresponds to the Cauchy problem with special initial data for the original three-dimensional equation (5)

$$\Psi|_{t=0} = A e^{i P_0 (x - X_0)/\mu} e^{i (x - X_0)^2 B_0 / (2\mu)} \chi_0(x, \mathbf{y}). \tag{9}$$

The function $\Psi|_{t=0}$ also satisfies the normalization condition $\|\Psi\|^2_{L_2(\mathbb{R}^3)} = 1$. According to [4], the asymptotic solution of problem (7), (8) is expressed in terms of the solutions $\bigl(X(t), P(t)\bigr)$ of the nonlinear system

$$\dot X = P, \qquad \dot P = -\varepsilon'(X) - \frac{\partial G_0}{\partial x}(X, X), \qquad P|_{t=0} = P_0, \qquad X|_{t=0} = X_0, \tag{10}$$

and the solutions $\bigl(C(t), B(t)\bigr)$ of the linear system

$$\dot C = B, \qquad \dot B = -\varepsilon''(X(t))C - \frac{\partial^2 G_0}{\partial x^2}(X(t), X(t))C, \qquad B|_{t=0} = B_0, \qquad C|_{t=0} = 1. \tag{11}$$

It is well known [7] and can be easily verified that

$$\frac{d}{dt}(\overline{C}B - \overline{B}C) = 0, \qquad \overline{C}B - \overline{B}C = \mathrm{const} = 2i \operatorname{Im} B_0 \neq 0; \tag{12}$$

the functions B and C are therefore nonzero at all points t.

The asymptotic expansion has the form

$$\phi(x, t, \mu) = \frac{A(\mu, B_0)}{\sqrt{C(t)}} \exp\biggl\{\frac{i}{\mu}\biggl[S(t, \mu) + P(t)\bigl(x - X(t)\bigr) + \frac{\bigl(x - X(t)\bigr)^2 BC^{-1}(t)}{2}\biggr]\biggr\}\bigl(1 + O\bigl(\sqrt{\mu}\,\bigr)\bigr), \tag{13}$$

where[2]

$$S(t, \mu) = \int_0^t \biggl\{\frac{P^2(\tau)}{2} - \varepsilon\bigl(X(\tau)\bigr) - G_0\bigl(X(\tau), X(\tau)\bigr) - \frac{\mu\bigl|C(\tau)\bigr|^2}{4 \operatorname{Im} B_0}\frac{\partial^2 G_0}{\partial x'^2}\bigl(X(\tau), X(\tau)\bigr)\biggr\}\, d\tau.$$

For the squared amplitude of solutions (13) up to $O\bigl(\sqrt[4]{\mu}\,\bigr)$, we have

$$\bigl|\phi(x, t, \mu)\bigr|^2 = \frac{A^2}{\bigl|C(t)\bigr|} e^{-(x - X(t))^2 \operatorname{Im}(BC^{-1}(t))/\mu} = \frac{A^2}{\bigl|C(t)\bigr|} e^{-\pi A^4 |C(t)|^{-2}(x - X(t))^2}, \tag{14}$$

where the second relation holds because of (12). This expression depends on x as the Gaussian normalized exponential. Its amplitude is $A^2(\mu, B_0)/|C(t)| = \sqrt{\operatorname{Im} B_0/(\pi\mu)}\,|C(t)|$, and its width (just as the width of packet (13)) is determined as $|C(t)|/A^2(\mu, B_0) \sim \sqrt{\mu/\operatorname{Im} B_0}\,|C(t)|$.

The following assertion is one of the central results in this paper.

Theorem. *Let conditions* 1–3 *be satisfied. Then the function*

$$\Psi(x, \mathbf{y}, t) = \chi_0(x, \mathbf{y})\phi(x, t, \mu) \tag{15}$$

is the leading term of the formal asymptotic solution $\operatorname{mod} O(\mu^{3/2})$ *of problem* (5), (9), *where* $O(\mu^{3/2})$ *is understood in the sense of* $C(\Gamma)$*- or* $L_2(\Gamma)$*-estimates uniform on any* μ*-independent time interval.*

The proof and the formulas for the corrections are given in Sec. 5.

[2]We write the minus sign in the last term of this expression to correct the misprint in formula (1.18) in [4].

4. Wave packets in periodic structures: The nonspreading of packets and "superlocalization"

Both the initial conditions $\phi_0(x,\mu) = \phi(x,0,\mu)$ and the solutions $\phi(x,t,\mu)$ have the shape of normalized Gaussian wave packets localized near the point $x = X(t)$. Such asymptotic expansions hold for dimensionless time intervals of the order of unity (i.e., for time intervals independent of μ), and if there are no turning points, then this suffices for propagation through the entire waveguide length $\sim l$. The width $\sqrt{\mu/\operatorname{Im} B_0}\,|C(t)| \sim |C(t)|$ and the amplitude $A^2(\mu, B_0)/|C(t)| \sim 1/|C(t)|$ of packets (13) generally vary with time. It is well known that such packets necessarily spread in the linear case $G \equiv 0$ (cf. the situation described in case 1 below).

An interesting and important fact is that the Gaussian packets can propagate without spreading in the nonlinear case. Moreover, they can periodically compress along the axis x, and this compression is accompanied by an increase in their amplitude. We illustrate this fact with an example of a waveguide consisting of several repeating parts. Then $\varepsilon(x)$ is a periodic function with the period a. We also assume that the kernel is translation-invariant and symmetric: $G_0(x,x') = G_0(|x-x'|)$. Because $G_0(x,x')$ is a smooth function, we have $\partial G_0(x,x)/\partial x = 0$ and $\partial^2 G_0(x,x)/\partial x^2 = \varkappa = \text{const}$.

After the variable P is excluded, system (10) then becomes the Newton equation of motion of a particle in the a-periodic potential $\varepsilon(x)$:

$$\ddot{X} = -\varepsilon'(X), \qquad \dot{X}|_{t=0} = P_0, \qquad X|_{t=0} = X_0. \tag{16}$$

This particle can propagate through the entire tube only if the energy satisfies the condition

$$E = \frac{\dot{X}^2}{2} + \varepsilon(X) = \frac{P_0^2}{2} + \varepsilon(X_0) > \max \varepsilon(x). \tag{17}$$

Without loss of generality, we assume that $X_0 = 0$. We make this assumption to simplify the notation in what follows. As is known, $X(t, P_0)$ can then be found by inverting the integral

$$t = \int_0^{X(t,P_0)} \frac{dx}{\sqrt{2\big(E - \varepsilon(x)\big)}}.$$

After the variable B is excluded, system (11) reduces to the equation

$$-\ddot{C} - \varepsilon''\big(X(t,P_0)\big)C = \varkappa C, \qquad C|_{t=0} = 1, \qquad \dot{C}|_{t=0} = B_0, \tag{18}$$

where the coefficient $\varepsilon''\big(X(t,P_0)\big)$ depends periodically on the time t. The time period corresponds to particle translation by the potential period a and is equal to

$$T = T(P_0) = \int_0^a \frac{dx}{\sqrt{2\big(E - \varepsilon(x)\big)}}.$$

The behavior of $C(t)$ depends significantly on the parameters $\varkappa$ and P_0. We first fix the initial momentum P_0 of the packet; then (18) becomes the one-dimensional spectral problem for the periodic Sturm–Liouville operator (the one-dimensional Schrödinger equation) with the potential $-\varepsilon''\big(X(t,P_0)\big)$ and the spectral parameter $\varkappa$. It is well known [8] that the value line of $\varkappa$ splits into the spectral bands $[\varkappa_n^-, \varkappa_n^+]$ and gaps $(\varkappa_{n-1}^+, \varkappa_n^-)$, $n = 1, 2, \dots$, where

$$\varkappa_0^+ = -\infty < \min \varepsilon''(x) < \varkappa_1^- < \varkappa_1^+ \le \varkappa_2^- < \dots < \varkappa_n^+ \le \varkappa_{n+1}^- < \varkappa_{n+1}^+ \le \dots.$$

The quantities $\varkappa_j^\pm$ generally depend on P_0. We have the following cases illustrated in Figs. 1– 4.

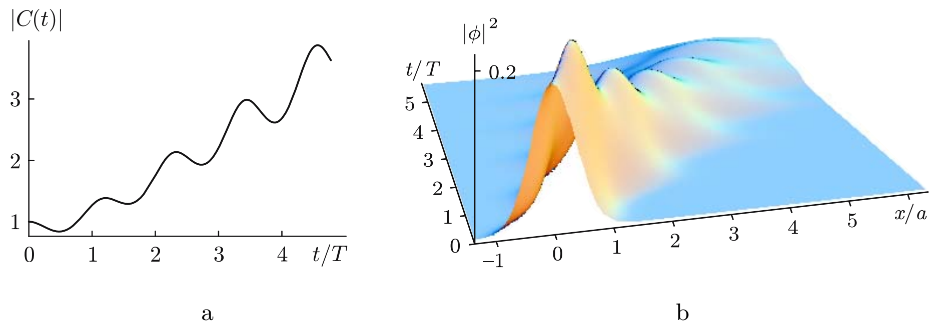

Fig. 1. Graphs of the functions $|C(t)|$ and $|\phi(x,t)|^2$ for $\varepsilon(x) = 0.1\cos x$, $P_0 = 0.75$, $\varkappa = 0$, and $B_0 = i/10$.

Case 1: $\varkappa = \varkappa_n^{\pm}$. The points $\varkappa = \varkappa_n^{\pm}$ are called the band boundaries if the gaps separating them are nondegenerate. They are associated with the following basis of solutions of linear equation (18):

$$C_1(t) = g(t), \qquad C_2(t) = tg(t) + q(t), \tag{19}$$

where $g(t)$ and $q(t)$ are some T-periodic or antiperiodic functions.

We note that for $\varkappa = 0$, Eq. (18) has a T-periodic solution $C_1(t) = \dot{X} = g(t)$ that is nonzero for all t according to (17). By the Liouville formula, the second linearly independent solution is equal to $\dot{X}\int \dot{X}^{-2}dt$ and can hence be represented in the form $C_2(t) = tg(t) + q(t)$. Therefore, $\varkappa = 0$ is certainly a band endpoint. Moreover, because $C_1(t)$ is nonzero only at the left endpoint of the first (leftmost) band [8], we have $\varkappa_1^- = 0$ for all P_0, i.e., $\varkappa = 0$ is the left endpoint of the first band. It follows from this that there is a significant difference in the behavior of wave packets for $\varkappa \le 0$ and $\varkappa > 0$.

Because $B(t) = \dot{C}(t) \ne 0$ and the derivative of the periodic function $g(t)$ is necessarily zero at some point, $C(t)$ cannot be a periodic function, i.e., if $C(t) = \alpha_1 C_1(t) + \alpha_2 C_2(t)$, then $\alpha_2 \ne 0$. For $\varkappa = 0$, the function $g(t)$ is nonzero, and the term $\alpha_2 C_2$ becomes the leading term for large t. Therefore, the wave packet necessarily spreads: its width $|C(t)|/A^2$ increases proportionally to t, and the squared amplitude decreases as $1/t$. The case $\varkappa = 0$ corresponds to the linear Schrödinger equation. Therefore, the Gaussian wave packets necessarily spread in time and space in the linear case, which, of course, is well known (see Fig. 1).

We now describe the behavior of wave packets for other $\varkappa_n^{\pm}$.

Case 2: $\varkappa \in (\varkappa_n^-, \varkappa_n^+)$. If $\varkappa \in (\varkappa_n^-, \varkappa_n^+)$, then the point $\varkappa$ lies in the interior of one of the bands (of stability of Eq. (18)). Then the basis of solutions consists of the two quasiperiodic functions

$$C_1(t) = g(t)e^{i\lambda t}, \qquad C_2(t) = \overline{g(t)}e^{-i\lambda t},$$

where $\lambda > 0$ is a quasimomentum and $g(t)$ is a T-periodic function. Therefore,

$$C(t) = a_1 g(t)e^{i\lambda t} + a_2\overline{g(t)}e^{-i\lambda t}$$

is also a quasiperiodic function. It follows from this that the wave packet *does not spread with time*, and its width $\sqrt{\mu}\,|C(t)|/A^2$ and amplitude $A/\sqrt[4]{\mu}\,\sqrt{|C|}$ pulse quasiperiodically (see Fig. 2):

$$0 < C_{\inf} \le \bigl|C(t)\bigr| \le C_{\sup} < \infty.$$

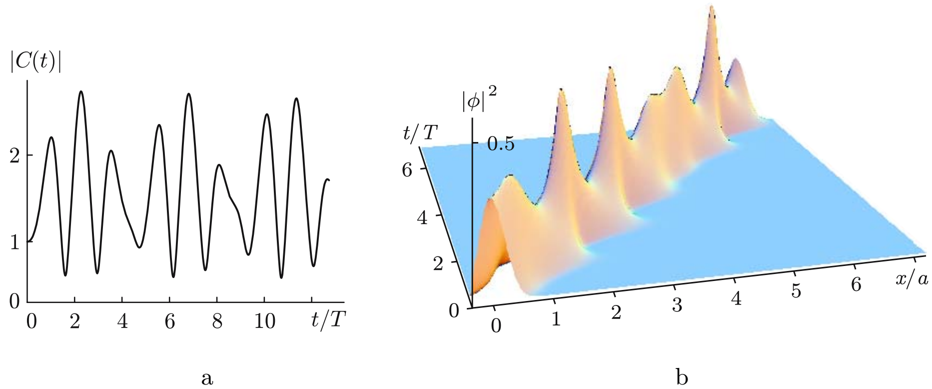

Fig. 2. The same as in Fig. 1 but for $\varkappa = 0.1$ (the band) and $B_0 = i/3$.

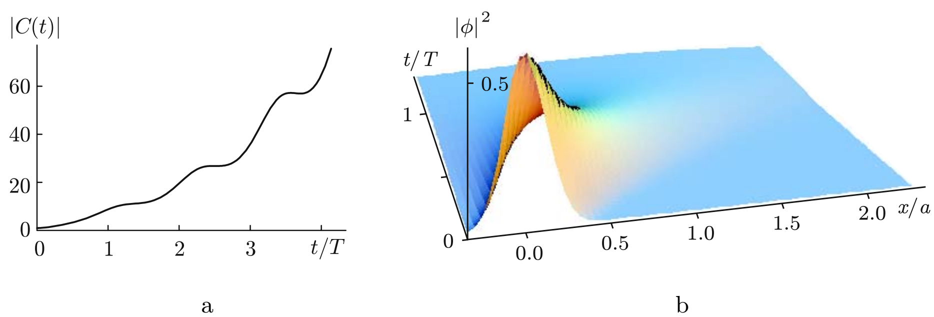

Fig. 3. The same as in Fig. 1 but for $\varkappa = -0.01$ and $B_0 = i$.

Case 3: $\boldsymbol{\varkappa \in (\varkappa_{n-1}^{+}, \varkappa_{n}^{-})}$. If $\varkappa \in (\varkappa_{n-1}^{+}, \varkappa_{n}^{-})$, then the point $\varkappa$ lies in the interior of one of the gaps (a region of instability of Eq. (18)). The basis of solutions of Eq. (18) can then be composed of the functions (also see [9]) $g(t)\cos\bigl(nt/2 + \Phi(t)\bigr)e^{\lambda t}$ and $g(t)\sin\bigl(nt/2 + \Phi(t)\bigr)e^{-\lambda t}$, where $\lambda > 0$ is the Floquet exponent, $n = 0, 1, 2, \dots$ are the gap numbers, and $g(t)$ and $\Phi(t)$ are T-periodic functions, $|g(t)| > 0$. Then

$$C(t) = g(t)\left(a\cos\left(\frac{nt}{2} + \Phi(t)\right)e^{\lambda t} + b\sin\left(\frac{nt}{2} + \Phi(t)\right)e^{-\lambda t}\right), \quad \lambda > 0. \tag{20}$$

We must here distinguish the case $n = 0$, which corresponds to $\varkappa < 0$. Then the coefficients of $e^{\pm\lambda t}$ in formula (20) cannot be zero, the term containing $e^{-\lambda t}$ becomes small compared with the term containing $e^{\lambda t}$, and $C(t) \sim e^{\lambda t}$. This means that the wave packets spread exponentially fast for $\varkappa < 0$, i.e., significantly faster than in the linear case (see Fig. 3).

In the other gaps ($n \geq 1$), the packet mainly spreads exponentially, but there exist instants t_k such that $nt/2 + \Phi(t) = \pi/2 + \pi k$. Then $C(t_k) = g(nt_k/2)e^{-\lambda t_k}$, and the packet again becomes localized such that the degree of localization increases exponentially in both x and t. We thus have a wave packet "superlocalization" that is periodic in time and space (see Fig. 4).[3]

Case 4. A similar situation occurs for the band endpoints $\varkappa_n$ other than $\varkappa = 0$. The function $g(t)$ has $n-1$ zeros at the points $\varkappa_n^{-}$ on the period $[0, T)$, and it has n zeros at the points $\varkappa_n^{+}$. The packet mainly

[3] This effect is possibly destroyed with time already in the framework of our model (5) and even of (7) because the corrections that were neglected in (13) become essential in the case of strong spreading and can prevent the already spread packet from localizing once again.

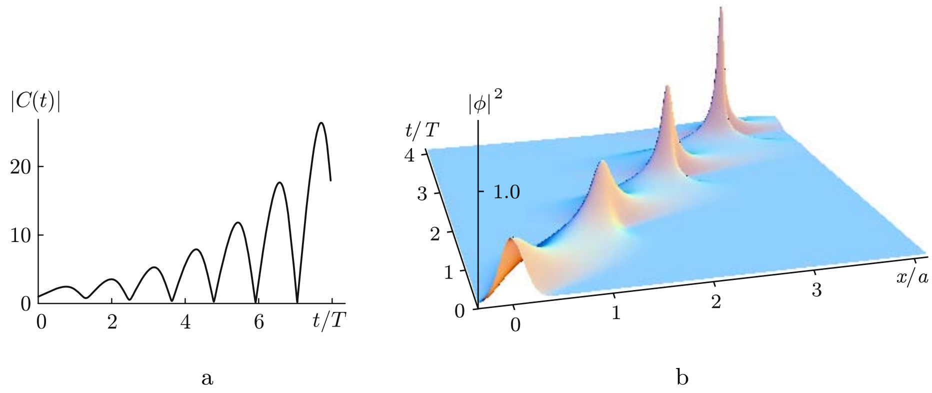

Fig. 4. The same as in Fig. 1 but for $\varkappa = 0.2$ (the gap) and $B_0 = i$.

spreads exponentially, but it again localizes but without any increase in amplitude at the points t_k, where $g(t) = 0$.

The calculations illustrated by Figs. 1–4 were performed for the potential $\varepsilon(x) = 0.1\cos x$ and the initial condition $P_0 = 0.75$ ($X_0 = 0$, $C_0 = 1$). Therefore, $a = 2\pi$ and $T \simeq 7.29$. The wave packet propagation is shown by the behavior of the amplitude $|\phi(x,t)|^2$ (see formula (14)). Because the width of such packets $|C(t)|^2/A^2 = \sqrt{\mu}\,|C(t)|^2/\sqrt{\operatorname{Im} B_0}$ is proportional to $\sqrt{\mu}$ and $\mu \ll 1$, it is difficult to visualize their propagation over distances of the order of unity. We therefore set $\mu = 1$ in these figures, and the surface must be imagined to be more localized in the spatial coordinate (i.e., compressed by the factor $\sqrt{\mu}$). We also chose the parameter B_0 to make the picture more illustrative; its value is presented under each of the figures.

It is sometimes reasonable to assume that the value of $\varkappa$ is fixed and analyze the character of the behavior of $C(t)$ depending on the other parameters, for example, on the initial momenta P_0. Such parameters are contained in Eq. (18) already not as spectral parameters but as some more complicated parameters. For reasonable values of the parameters, the alteration of cases 1–4 as these parameters vary continuously also has the form of a band structure. This fact is demonstrated in Fig. 5 on the plane of the parameters $\varkappa$ and P_0. In particular, for $\varkappa > 0$, the band structure in $P_0 > P_{\min} + \delta$, where $P_{\min} = \sqrt{2\max\varepsilon(x) - 2\varepsilon(X_0)}$ and $\delta > 0$, contains finitely many bands such that the first band starts at $P_0 > P_{\min} + \delta$ and the upper band ranges to $+\infty$. This follows from an analysis of problem (18) and can also be seen in Fig. 5 by choosing an arbitrary value of $\varkappa$.

5. Reduction to the spatially one-dimensional equation

We now show that finding semiclassical-type asymptotic solutions of the original spatially three-dimensional equation that are localized in the direction transverse to the tube axis reduces (in the "generalized adiabatic approximation") to solving a spatially one-dimensional equation similar to the original equation. It is well known (and can be easily verified) that the norm of the function Ψ satisfying Eq. (5) is preserved in time. Following [2], we seek solutions of Eq. (5) in the form

$$\Psi = \widehat{\chi}\phi(x,\mu,t), \qquad \widehat{\chi} = \chi\biggl(\overset{2}{x}, -i\mu\frac{\overset{1}{\partial}}{\partial x}, \mathbf{y}, [\phi], \mu\biggr)$$

such that

$$\|\Psi\|^2 = \int_{\mathbb{R}^3} |\widehat{\chi}\phi|^2(x,\mathbf{y})\,dx\,d\mathbf{y} = 1, \qquad \|\phi\|^2 = \int_{\mathbb{R}} \bigl|\phi(x)\bigr|^2\,dx = 1 \tag{21}$$

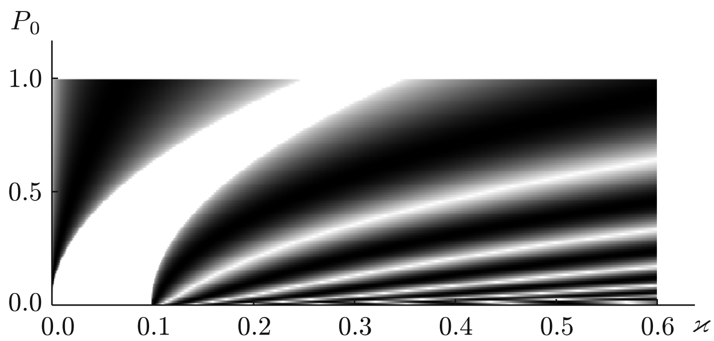

Fig. 5. The shape of the band structure on the plane of the parameters $(\varkappa, P_0)$ for $\varepsilon(x) = 0.1\cos x$, $P_0 > P_{\min} = 0$, and $\varkappa \geq 0$. The band regions are shaded, and the gap regions are the white strips.

for all t and $\phi(x, \mu, t)$ is the solution of the one-dimensional Hartree-type equation

$$i\mu\phi_t = \hat{\mathcal{L}}\phi, \qquad \hat{\mathcal{L}} = \mathcal{L}\Big(\overset{2}{x}, -i\mu\frac{\overset{1}{\partial}}{\partial x}, [\phi], \mu\Big). \tag{22}$$

Here, $\hat{\chi}$ and $\hat{\mathcal{L}}$ are some pseudodifferential operators whose symbols $\chi(x, p, \mathbf{y}, [\phi], \mu)$ and $\mathcal{L}(x, p, [\phi], \mu)$ generally depend on the function ϕ. Hereafter, the digits 1 and 2 over the operators denote the order of action of the operators x and $-i\mu\,\partial/\partial x$ (in particular, the differentiation operator in (22) acts first); the hat over a function (symbol) denotes the corresponding μ-pseudodifferential operator (see [10] for the strict definition and the properties of μ-pseudodifferential operators).

Just the symbols χ and $\mathcal{L}$ must be determined to reduce initial equation (5) to one-dimensional equation (22). Then Eq. (5) necessarily implies the chain of relations

$$\widehat{\chi}\hat{\mathcal{L}}\phi = i\mu\widehat{\chi}\phi_t = i\mu\Psi'_t = \widehat{\mathcal{H}}\Psi = \widehat{\mathcal{H}}\widehat{\chi}\phi.$$

A sufficient condition for them to hold is the relation

$$\widehat{\chi}\hat{\mathcal{L}} = \widehat{\mathcal{H}}\widehat{\chi}. \tag{23}$$

A sufficient condition for the normalization is the requirement that the function ϕ be normalized and the operator $\widehat{\chi}$ be unitary:

$$\int_{\mathbb{R}^2} \widehat{\chi}^*(y)\widehat{\chi}(y)\,dy = E. \tag{24}$$

We use the following relations[4] to pass from operators to their symbols:

1. The symbol of the product of two operators $A\big(\overset{2}{x}, -i\mu\overset{1}{\partial}/\partial x, \mu\big)B\big(\overset{2}{x}, -i\mu\overset{1}{\partial}/\partial x, \mu\big)$ is expressed in terms of their symbols as $A\big(\overset{2}{x}, p - i\mu\overset{1}{\partial}/\partial x, \mu\big)B(x, p, \mu)$.

2. The symbol of the operator $A^*\big(\overset{2}{x}, -i\mu\overset{1}{\partial}/\partial x, \mu\big)$ adjoint to the operator $A(\overset{2}{x}, -i\mu\overset{1}{\partial}/\partial x, \mu)$ is expressed in terms of its symbol as $A^*(x, p, \mu) = \bar{A}\big(\overset{1}{x}, p + i\mu\overset{2}{\partial}/\partial x, \mu\big)1$.

[4] These formulas for pseudodifferential operators were accurately derived, and the conditions on their symbols were described in [10]. These formulas can be easily verified for the symbols polynomial in p, i.e., for the differential operators to which our operators finally belong.

Relation (23) then leads to the equation

$$
\begin{aligned}
&\chi\Big(\overset{2}{x}, p - i\mu\frac{\overset{1}{\partial}}{\partial x}, y, [\phi], \mu\Big)\mathcal{L}\big(x, p, [\phi], \mu\big) = \\
&\qquad = \mathcal{H}\Big(\overset{2}{x}, p - i\mu\frac{\overset{1}{\partial}}{\partial x}, y, -i\frac{\partial}{\partial y}, [\widehat{\chi}\phi], \mu\Big)\chi\big(x, p, y, [\phi], \mu\big),
\end{aligned}
\tag{25}
$$

and relation (24) leads to the equation

$$
\int_{\mathbb{R}^2} \bar{\chi}\Big(\overset{1}{x}, p + i\mu\frac{\overset{2}{\partial}}{\partial x} - i\mu\frac{\partial}{\partial z}, y\Big)\chi(z, p, y)\, dy\Big|_{z=x} = 1. \tag{26}
$$

It is clear that to construct asymptotic solutions (as $\mu \to 0$) of the original problem, it suffices to present the solutions of Eqs. (25) and (26) satisfying these equations $\operatorname{mod} O(\mu^N)$ for an appropriate N. The construction of such solutions is described by the following assertion.

Lemma 1. *Let the function $\phi(x, t, \mu)$ have the form $\phi(x, t, \mu) = A(\mu)e^{iS(x,t)/\mu}\varphi(x, t, \mu)$, where S, $\operatorname{Im} S \geq 0$, and φ are arbitrary fixed smooth functions and $A(\mu)$ is the normalization constant. Then the functions*

$$
\mathcal{L} = \mathcal{L}_0 + \mu\mathcal{L}_1, \qquad \chi = \chi_0 + \mu\chi_1,
$$

where $\mathcal{L}_0$, χ_0, χ_1, and $\mathcal{L}_1$ are defined by formulas (36), (37), (42), *and* (43), *satisfy Eqs.* (25) *and* (26) *up to $O(\mu^2)$. The estimate is uniform on arbitrary bounded domains of the space and time coordinates and the variable p, i.e., the discrepancy does not exceed $C\mu^2$, where C depends only on the functions S and φ and on the choice of the bounded range of the coordinates in the extended phase space.*

Proof. We seek the symbols $\mathcal{L}$ and χ among the smooth functions such that the following expansions hold on the semiclassical functions ϕ (for example, on the functions of the form $\phi(x, t, \mu) = A(\mu)e^{iS(x,t)/\mu}\varphi(x, t, \mu)$):

$$
\begin{aligned}
&\chi\big(x, p, y, [\phi], \mu\big) = \chi_0\big(x, p, y, [\phi]\big) + \mu\chi_1\big(x, p, y, [\phi]\big) + \cdots + O(\mu^N), \\
&\mathcal{L}\big(x, p, [\phi], \mu\big) = \mathcal{L}_0\big(x, p, [\phi]\big) + \mu\mathcal{L}_1\big(x, p, [\phi]\big) + \cdots + O(\mu^N), \\
&\chi\Big(\overset{2}{x}, p - i\mu\frac{\overset{1}{\partial}}{\partial x}, y, [\phi], \mu\Big)\mathcal{L}\big(x, p, [\phi], \mu\big) = \chi_0\big(x, p, y, [\phi]\big)\mathcal{L}_0\big(x, p, [\phi]\big) + \\
&\qquad + \mu\Big[\chi_1\big(x, p, y, [\phi]\big)\mathcal{L}_0\big(x, p, [\phi]\big) - \\
&\qquad - i\frac{\partial\chi_0}{\partial p}\big(x, p, y, [\phi]\big)\frac{\partial\mathcal{L}_0}{\partial x}\big(x, p, [\phi]\big) + \\
&\qquad + \chi_0\big(x, p, y, [\phi]\big)\mathcal{L}_1\big(x, p, [\phi]\big)\Big] + \cdots + O(\mu^N),
\end{aligned}
\tag{27}
$$

where the estimate $O(\mu^N)$ is uniform in any bounded range of the space, time, and momentum variables. After the symbols are calculated, we can easily see that these estimates are indeed satisfied.

The right-hand side of relation (25) can be represented similarly to (27). For this, we write the expansion of the symbol

$$\mathcal{H}\biggl(x, p, y, -i\frac{\partial}{\partial y}, \mu, [\widehat{\chi}\phi]\biggr) = H\biggl(x, p, y, -i\frac{\partial}{\partial y}, \mu\biggr) + \mathcal{G}\bigl(x, \mathbf{y}, [\widehat{\chi}\phi], \mu\bigr)$$

of the initially given operator $\widehat{\mathcal{H}}$. We obtain the expansion of the linear term

$$H\biggl(x, p, \mathbf{y}, -i\frac{\partial}{\partial \mathbf{y}}, \mu\biggr) = H_0 + \mu H_1 + \cdots + O(\mu^N), \tag{28}$$

where

$$H_0 = \frac{p^2}{2} + v_{\mathrm{int}}(x, \mathbf{y}) + \frac{\Delta_y}{2}, \qquad \Delta_y = \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial y_2^2}, \qquad H_1(x, p, y) = k(x) y_n p^2,$$

and H_0 differs from the subsequent terms by its dependence on $-i\partial/\partial\mathbf{y}$ (the so-called operator-valued symbol). The expansion of the nonlinear term $\mathcal{G}(x, \mathbf{y}, [\widehat{\chi}\phi], \mu)$

$$\begin{aligned}
&\int_{\mathbb{R}^3} G(x, \mathbf{y}, x', \mathbf{y}', \mu)\bigl(\widehat{\chi}\phi(x', \mathbf{y}', \mu)\bigr)\overline{\widehat{\chi}\phi(x', \mathbf{y}', \mu)}\, dx'\, d\mathbf{y}' = \\
&\qquad = \int_{\mathbb{R}} \overline{\phi(x', \mu)}\biggl(\int_{\mathbb{R}^2} \widehat{\chi}^* G(x, \mathbf{y}, x', \mathbf{y}', \mu)\widehat{\chi}\, d\mathbf{y}'\biggr)\phi(x', \mu)\, dx' = \\
&\qquad = \mathcal{G}_0\bigl(x, [\chi_0], [\phi]\bigr) + \mu\bigl(\mathcal{G}_1\bigl(x, [\chi_0], [\chi_1], [\phi]\bigr) + \mathcal{G}_1^y\bigl(x, \mathbf{y}, [\chi_0], [\phi]\bigr)\bigr) + \cdots + O(\mu^N)
\end{aligned} \tag{29}$$

is obtained by using the relations presented after formula (24):

$$\begin{aligned}
\mathcal{G}_0\bigl(x, [\chi_0], [\phi]\bigr) = {}& \int_{\mathbb{R}} \overline{\phi(x', \mu)} G_0(x, x') \times \\
& \times \biggl(\int_{\mathbb{R}^2} \widehat{\overline{\chi_0(x', p', y')}\chi_0}(x', p', y')\, d\mathbf{y}'\biggr)\phi(x', \mu)\, dx',
\end{aligned} \tag{30}$$

$$\begin{aligned}
\mathcal{G}_j\bigl(x, [\chi_0], [\chi_j], [\phi]\bigr) = {}& 2\int_{\mathbb{R}} \overline{\phi(x', \mu)} G_0(x, x') \times \\
& \times \biggl(\mathrm{Re} \int_{\mathbb{R}^2} \widehat{\overline{\chi_j(x', p', \mathbf{y}')}\chi_0}(x', p', \mathbf{y}')\, d\mathbf{y}'\biggr)\phi(x', \mu)\, dx',
\end{aligned} \tag{31}$$

$$\begin{aligned}
\mathcal{G}_1^y\bigl(x, \mathbf{y}, [\widehat{\chi}_0\phi]\bigr) = {}& \int_{\mathbb{R}} \overline{\phi(x', \mu)} \times \\
& \times \biggl(\int_{\mathbb{R}^2} G_1(x, x', \mathbf{y}, \mathbf{y}')\widehat{\overline{\chi_0(x', p', y')}\chi_0}(x', p', y')\, d\mathbf{y}'\biggr)\phi(x', \mu)\, dx' + \\
& + i\int_{\mathbb{R}} \overline{\phi(x', \mu)}\biggl(\frac{\partial}{\partial x'}\int_{\mathbb{R}^2} \widehat{\frac{\partial\overline{\chi_0(x', p', y')}}{\partial p'} G_0(x, x')\chi_0}(x', p', y')\, d\mathbf{y}'\biggr)\phi(x', \mu)\, dx', \quad \ldots
\end{aligned} \tag{32}$$

The expressions for $\mathcal{G}_j^y(x, y, [\chi_0], [\chi_1], \ldots, [\chi_{j-1}], [\phi])$ are very complicated, and we do not use them later.

The left-hand side of relation (29) with $G \equiv 1$ for the function $\Psi = \hat{\chi}\psi$ is equal to its norm. Therefore, we automatically have the expansion for the left-hand side of unitary condition (24). We rewrite this condition as relations for the symbols $\chi_i(x, p, \mathbf{y})$:

$$\int_{\mathbb{R}^2} \overline{\chi}_0(x, p, \mathbf{y})\chi_0(x, p, \mathbf{y})\, d\mathbf{y} \equiv (\chi_0, \chi_0)_y = 1,$$

$$\operatorname{Re}\int_{\mathbb{R}^2} \overline{\chi}_j(x, p, \mathbf{y})\chi_0(x, p, \mathbf{y})\, d\mathbf{y} \equiv \operatorname{Re}(\chi_0, \chi_j)_y = R_j(x, p),$$

where R_j is determined in terms of $\chi_0, \ldots, \chi_{j-1}$, in particular,

$$R_1(x, p) = i\frac{\partial}{\partial x}\int_{\mathbb{R}^2} \chi_0 \frac{\partial \overline{\chi}_0}{\partial p}\, d\mathbf{y}. \tag{33}$$

Because the answer obtained below is nonunique, we supplement these relations with the conditions $\operatorname{Im}\chi_0 = 0$ and $\operatorname{Im}(\chi_0, \chi_j) = 0$. As a result, we have

$$\begin{aligned} &\int_{\mathbb{R}^2} \overline{\chi}_0(x, p, \mathbf{y})\chi_0(x, p, \mathbf{y})\, d\mathbf{y} \equiv (\chi_0, \chi_0)_y = 1, \qquad \operatorname{Im}\chi_0 = 0, \\ &\int_{\mathbb{R}^2} \overline{\chi}_j(x, p, \mathbf{y})\chi_0(x, p, \mathbf{y})\, d\mathbf{y} \equiv (\chi_0, \chi_j)_y = R_j(x, p). \end{aligned} \tag{34}$$

We then substitute expansions (27)–(29) in Eq. (25) and obtain a relation whose terms are of different orders in μ. We successively consider this relation for the terms of different orders in the system with the corresponding relation from (34) and obtain a recursive chain of linear systems that allows determining all terms of the expansions of $\mathcal{L}$ and χ (see similar calculations for $G \equiv 0$ in [2]).

5.1. Calculation of the symbols $\mathcal{L}_0$ and χ_0. Collecting the zeroth-order terms in μ, we obtain the so-called problem for the transverse mode:

$$\begin{aligned} &\Big(-\frac{1}{2}\Delta_y + v_{\text{int}}(x, \mathbf{y})\Big)\chi_0\big(x, p, \mathbf{y}, [\phi]\big) = \\ &\qquad = \chi_0\big(x, p, \mathbf{y}, [\phi]\big)\Big(\mathcal{L}_0\big(x, p, [\phi]\big) - \frac{p^2}{2} - \mathcal{G}_0\big(x, [\chi_0\phi]\big)\Big), \\ &(\chi_0, \chi_0)_y = 1, \qquad \operatorname{Im}\chi_0 = 0. \end{aligned} \tag{35}$$

We assume that the kernel of the self-adjoint operator $-\Delta_y/2 + v_{\text{int}}(x, \mathbf{y}) - \varepsilon(x)$ is one-dimensional, i.e., $\varepsilon(x)$ is a nondegenerate eigenvalue of the operator $-\Delta_y/2 + v_{\text{int}}(x, \mathbf{y})$. Then, for the eigenvalue $\varepsilon(x)$ chosen above, the equation obtained for χ_0 and $\mathcal{L}_0$ can be solved uniquely (χ_0 is generally determined up to the sign):

$$\mathcal{L}_0\big(x, p, [\phi]\big) = \frac{p^2}{2} + \varepsilon(x) + \int_{\mathbb{R}} G_0(x, x')\big|\phi(x')\big|^2\, dx', \tag{36}$$

where $\varepsilon(x)$ and $\chi_0\big(x, p, \mathbf{y}, [\phi]\big)$ are the eigenvalue and the eigenfunction of the spectral problem

$$\begin{aligned} &-\frac{1}{2}\Delta_y\chi_0\big(x, p, \mathbf{y}, [\phi]\big) + v_{\text{int}}(x, \mathbf{y})\chi_0\big(x, p, \mathbf{y}, [\phi]\big) = \varepsilon(x)\chi_0\big(x, p, \mathbf{y}, [\phi]\big), \\ &\|\chi_0\|_y \equiv 1, \quad \operatorname{Im}\chi_0 \equiv 0. \end{aligned} \tag{37}$$

Under such a choice, the function χ_0 is independent of p and ϕ, i.e., $\widehat{\chi}_0$ is the linear operator of multiplication by a function (by the transverse mode). The expressions containing $\partial\chi_0/\partial p$ can therefore be simplified in what follows.

5.2. Calculations of the corrections. We collect the terms with μ^j, $j = 1, 2, \dots$, and obtain the inhomogeneous equations for χ_j and L_j:

$$\begin{aligned} &\Big(-\frac{1}{2}\Delta_y + v_{\text{int}}(x,\mathbf{y}) - \varepsilon(x)\Big)\chi_j = F_j - H_j\chi_0 + \chi_0(\mathcal{L}_j - \mathcal{G}_j), \\ &(\chi_0, \chi_j)_y = R_j, \end{aligned} \tag{38}$$

where the functions $F_j = F_j(x, \mathbf{y}, p, [\phi])$ are determined by the preliminarily calculated $\chi_0, \dots, \chi_{j-1}$ and $\mathcal{L}_0, \dots, \mathcal{L}_{j-1}$, in particular,

$$F_1(x, \mathbf{y}, p, [\phi]) = i\bigg(\frac{\partial H_0}{\partial p}\frac{\partial \chi_0}{\partial x} - \frac{\partial \mathcal{L}_0}{\partial x}\frac{\partial \chi_0}{\partial p}\bigg) - \mathcal{G}_1^y\chi_0 = ip\frac{\partial \chi_0}{\partial x} - \mathcal{G}_1^y\chi_0. \tag{39}$$

The left-hand side of the first equation in (38) is orthogonal to χ_0 because χ_0 is the kernel of the self-adjoint operator $-\Delta_y/2 + v_{\text{int}}(x,\mathbf{y}) - \varepsilon(x)$. To solve (38), we must therefore prove that the right-hand side of this equation is orthogonal to the kernel χ_0:

$$\mathcal{L}_j\big(x, p, [\phi]\big) = \langle \chi_0, H_j\chi_0\rangle_y - \langle \chi_0, F_j\rangle_y + \mathcal{G}_j\big(x, [\chi_0], [\chi_j], [\phi]\big). \tag{40}$$

This relation does not permit determining L_j until χ_j is found, but it strongly simplifies Eq. (38). Indeed, we substitute (40) in (38) and obtain the linear system of equations for χ_j:

$$\begin{aligned} &\Big(-\frac{1}{2}\Delta_y + v_{\text{int}}(x,\mathbf{y}) - \varepsilon(x)\Big)\chi_j = F_j - H_j\chi_0 - \langle \chi_0, F_j\rangle_y + \langle \chi_0, H_j\chi_0\rangle_y, \\ &(\chi_0, \chi_j)_y = R_j. \end{aligned} \tag{41}$$

System (41) has a unique solution χ_j. Proceeding by induction on j, we can easily show that χ_j is a polynomial in the variable p. We substitute this solution in the right-hand side of (40) and find $\mathcal{L}_j$. In particular, for $\mathcal{L}_1$ and χ_1, we have

$$\begin{aligned} &\Big(-\frac{1}{2}\Delta_y + v_{\text{int}}(x,\mathbf{y}) - \varepsilon(x)\Big)\chi_1 = F_1 - H_1\chi_0 - \langle \chi_0, F_1\rangle_y + \langle \chi_0, H_1\chi_0\rangle_y, \\ &(\chi_0, \chi_1)_y = 0, \end{aligned} \tag{42}$$

the second relation implies that $\mathcal{G}_1 = 0$, and hence (40) has the form

$$\mathcal{L}_1\big(x, p, [\phi]\big) = \langle \chi_0, H_1\chi_0\rangle_y + \langle \chi_0, \mathcal{G}_1^y\chi_0\rangle_y. \tag{43}$$

To complete the proof of Lemma 1, it remains to substitute $\mathcal{L} = \mathcal{L}_0 + \mu\mathcal{L}_1$ and $\chi = \chi_0 + \mu\chi_1$ in expression (25), omit the zeroth- and first-order terms in μ (they cancel, which, for example, follows from the derivation procedure), transfer the remaining terms to the right-hand side of the relation, and estimate the discrepancy thus obtained.

The description of asymptotic solutions of the original problem is based on the following assertion, which follows readily from Lemma 1.

Lemma 2. *Let a function of the form* $\phi(x,t,\mu)=A(\mu)e^{iS(x,t)/\mu}\varphi(x,t,\mu)$ *satisfy reduced equation* (22) *with the obtained symbol* $\mathcal{L}=\mathcal{L}_0+\mu\mathcal{L}_1$ *generally with a discrepancy of the form* $\mu^\alpha A(\mu)e^{i\widetilde{S}(x,t)/\mu}\widetilde{\varphi}(x,t,\mu)$, $\alpha>1$. *Then the function*

$$\Psi(x,\mathbf{y},t,\mu)=\big(\chi_0(x,\mathbf{y})+\mu\widehat{\chi}_1\big)\phi(x,t,\mu)$$

satisfies Eq. (5) *up to a discrepancy in the norm of* $L_2(\Gamma)$ *not exceeding* $O(\mu^\beta)=o(\mu)$, *where* $\beta=\min(\alpha,2)$.

5.3. Construction of localized wave packets for the reduced equation. To complete the proof of the theorem, it remains to show that function (13) satisfies reduced equation (22) with the desired accuracy. We note that if Condition 3 (see Sec. 3) is satisfied, then $\mathcal{L}_1=0$, and Eq. (22) has form (7). The propagation of localized wave packets asymptotically satisfying Eq. (7) was studied in [4], where the solutions were given up to any power of the small parameter; in the leading term, these solutions are determined by formula (13). Using the constructions proposed in [4], we can easily determine the form of the discrepancy of such solutions.

Lemma 3. *Functions* (13) *satisfy Eq.* (7) *up to a discrepancy of the form* $\mu^{3/2}A(\mu)e^{iS(x,t,\mu)/\mu}\widetilde{\varphi}(x,t,\mu)$, *where* S *and* $\widetilde{\varphi}$ *are smooth functions.*

It follows from Lemmas 2 and 3 that the function

$$\Psi(x,\mathbf{y},t)=\big(\chi_0(x,\mathbf{y})+\mu\widehat{\chi}_1\big)\phi(x,t,\mu)$$

is a formally asymptotic solution $\operatorname{mod} O(\mu^{3/2})$ of original problem (5), which completes the proof of the theorem.

5.4. An example of calculations of the symbols $\mathcal{L}_0$, $\mathcal{L}_1$, χ_0, and χ_1. We consider the situation in which the confinement potential has the form

$$v_{\mathrm{int}}(x,y_1,y_2)=\frac{\Omega_1^2(x)y_1^2}{2}+\frac{\Omega_2^2(x)y_2^2}{2}.$$

Then problem (37) corresponds to the two-dimensional harmonic oscillator, and its solutions are numbered by the two quantum numbers ν_1 and ν_2 and have the form

$$\varepsilon(x)=\varepsilon^{(\nu_1,\nu_2)}(x)=\Omega_1(x)\left(\nu_1+\frac{1}{2}\right)+\Omega_2(x)\left(\nu_2+\frac{1}{2}\right),\quad \nu_i=0,1,2,\dots,$$

$$\chi_0=\chi_0^{(\nu_1,\nu_2)}(x,y_1,y_2)=$$
$$=\frac{\sqrt[4]{\Omega_1(x)\Omega_2(x)}}{\sqrt{\pi 2^{\nu_1}2^{\nu_2}\nu_1!\,\nu_2!}}\exp\left(-\frac{\Omega_1 y_1^2}{2}-\frac{\Omega_2 y_2^2}{2}\right)H_{\nu_1}\big(\sqrt{\Omega_1(x)}\,y_1\big)H_{\nu_2}\big(\sqrt{\Omega_2(x)}\,y_2\big),$$

where $H_\nu(x)$ is the νth Hermite polynomial. The function $\mathcal{L}_0$ is determined by formula (36).

We next calculate $\mathcal{L}_1$ and χ_1. To calculate $\mathcal{G}_1^y$ by formula (32) and then the right-hand side of Eq. (42), we use the specific form of the terms G_1 and H_1 in expansions (4) and (28):

$$
\begin{aligned}
\mathcal{G}_1^y &= \frac{1}{\sqrt{2\Omega_1}}\big(\sqrt{\nu_1+1}\,\chi_0^{\nu_1+1,\nu_2} + \sqrt{\nu_1}\,\chi_0^{\nu_1-1,\nu_2}\big)\int_{\mathbb{R}} G_{11}(x,x')\big|\phi(x')\big|^2\,dx' + \\
&\quad + \frac{1}{\sqrt{2\Omega_2}}\big(\sqrt{\nu_2+1}\,\chi_0^{\nu_1,\nu_2+1} + \sqrt{\nu_2}\,\chi_0^{\nu_1,\nu_2-1}\big)\int_{\mathbb{R}} G_{12}(x,x')\big|\phi(x')\big|^2\,dx',\\
F_1 &= ip\frac{1}{4}\frac{\Omega_1'}{\Omega_1}\big(-\sqrt{(\nu_1+2)(\nu_1+1)}\,\chi_0^{\nu_1+2,\nu_2} + \sqrt{\nu_1(\nu_1-1)}\,\chi_0^{\nu_1-2,\nu_2}\big) + \\
&\quad + ip\frac{1}{4}\frac{\Omega_2'}{\Omega_2}\big(-\sqrt{(\nu_2+2)(\nu_2+1)}\,\chi_0^{\nu_1,\nu_2+2} + \sqrt{\nu_2(\nu_2-1)}\,\chi_0^{\nu_1,\nu_2-2}\big) - \mathcal{G}_1^y,\\
H_1(x,p,y)\chi_0^{\nu_1,\nu_2} &= k'(x)p^2 y_n \chi_0^{\nu_1,\nu_2} = \\
&= \frac{\cos\theta}{\sqrt{2\Omega_1}}k'(x)p^2\big(\sqrt{\nu_1+1}\,\chi_0^{\nu_1+1,\nu_2} + \sqrt{\nu_1}\,\chi_0^{\nu_1-1,\nu_2}\big) - \\
&\quad - \frac{\sin\theta}{\sqrt{2\Omega_2}}k'(x)p^2\big(\sqrt{\nu_2+1}\,\chi_0^{\nu_1,\nu_2+1} + \sqrt{\nu_2}\,\chi_0^{\nu_1,\nu_2-1}\big),\\
\langle \mathcal{G}_1^y, \chi_0^{\nu_1,\nu_2}\rangle_y &= 0, \qquad \langle F_1, \chi_0^{\nu_1,\nu_2}\rangle_y = 0, \qquad \langle H_1\chi_0^{\nu_1,\nu_2}, \chi_0^{\nu_1,\nu_2}\rangle_y = 0,
\end{aligned}
\tag{44}
$$

where the first three relations can be obtained using the well-known formulas for the Hermite polynomials

$$
xH_\nu(x) = \frac{1}{2}\big(H_{\nu+1}(x) + 2\nu H_{\nu-1}(x)\big), \qquad \frac{\partial H_\nu}{\partial x} = 2\nu H_{\nu-1},
$$

and the next three relations easily follow, for example, from the orthogonality of the system of functions $\chi_0^{\nu_1,\nu_2}$ and the first two relations.

As a result, the equation for χ_1 becomes

$$
\begin{aligned}
\Big(-\frac{1}{2}\Delta_y + v_{\mathrm{int}}(x,\mathbf{y}) - \varepsilon^{\nu_1,\nu_2}(x)\Big)\chi_1^{\nu_1,\nu_2} &= A_{\nu_1+2,\nu_2}\chi_0^{\nu_1+2,\nu_2} + A_{\nu_1+1,\nu_2}\chi_0^{\nu_1+1,\nu_2} + \\
&\quad + A_{\nu_1-1,\nu_2}\chi_0^{\nu_1-1,\nu_2} + A_{\nu_1-2,\nu_2}\chi_0^{\nu_1-2,\nu_2} + \\
&\quad + A_{\nu_1,\nu_2+2}\chi_0^{\nu_1,\nu_2+2} + A_{\nu_1,\nu_2+1}\chi_0^{\nu_1,\nu_2+1} + \\
&\quad + A_{\nu_1,\nu_2-1}\chi_0^{\nu_1,\nu_2-1} + A_{\nu_1,\nu_2-2}\chi_0^{\nu_1,\nu_2-2},
\end{aligned}
\tag{45}
$$

$$
(\chi_0^{\nu_1,\nu_2}, \chi_1^{\nu_1,\nu_2}) = 0,
$$

where the coefficients $A_{i,j} = A_{i,j}\big(x,p,[\phi]\big)$ are equal to

$$
A_{\nu_1+2,\nu_2} = -\frac{i\sqrt{(\nu_1+2)(\nu_1+1)}}{4}\frac{\Omega_1'(x)}{\Omega_1(x)}p, \qquad A_{\nu_1,\nu_2+2} = -\frac{i\sqrt{(\nu_2+2)(\nu_2+1)}}{4}\frac{\Omega_2'(x)}{\Omega_2(x)}p,
$$

$$
A_{\nu_1-2,\nu_2} = \frac{i\sqrt{(\nu_1+1)\nu_1}}{4}\frac{\Omega_1'(x)}{\Omega_1(x)}p, \qquad A_{\nu_1,\nu_2-2} = -\frac{i\sqrt{(\nu_2+1)\nu_2}}{4}\frac{\Omega_2'(x)}{\Omega_2(x)}p,
$$

$$A_{\nu_1+1,\nu_2} = \frac{\sqrt{\nu_1+1}}{\sqrt{2\Omega_1(x)}}\Big(k'(x)p^2\cos\theta - \int_{\mathbb{R}} G_{11}(x,x')\big|\phi(x')\big|^2\,dx'\Big),$$

$$A_{\nu_1-1,\nu_2} = \frac{\sqrt{\nu_1}}{\sqrt{2\Omega_1(x)}}\Big(k'(x)p^2\cos\theta - \int_{\mathbb{R}} G_{11}(x,x')\big|\phi(x')\big|^2\,dx'\Big),$$

$$A_{\nu_1,\nu_2+1} = -\frac{\sqrt{\nu_2+1}}{\sqrt{2\Omega_2(x)}}\Big(k'(x)p^2\sin\theta + \int_{\mathbb{R}} G_{12}(x,x')\big|\phi(x')\big|^2\,dx'\Big),$$

$$A_{\nu_1,\nu_2-1} = -\frac{\sqrt{\nu_2}}{\sqrt{2\Omega_2(x)}}\Big(k'(x)p^2\sin\theta + \int_{\mathbb{R}} G_{12}(x,x')\big|\phi(x')\big|^2\,dx'\Big).$$

It is easy to verify that the solution has the form

$$\begin{aligned}\chi_1^{\nu_1,\nu_2} = {} & B_{\nu_1+2,\nu_2}\chi_0^{\nu_1+2,\nu_2} + B_{\nu_1+1,\nu_2}\chi_0^{\nu_1+1,\nu_2} + B_{\nu_1-1,\nu_2}\chi_0^{\nu_1-1,\nu_2} + \\ & + B_{\nu_1-2,\nu_2}\chi_0^{\nu_1-2,\nu_2} + B_{\nu_1,\nu_2+2}\chi_0^{\nu_1,\nu_2+2} + B_{\nu_1,\nu_2+1}\chi_0^{\nu_1,\nu_2+1} + \\ & + B_{\nu_1,\nu_2-1}\chi_0^{\nu_1,\nu_2-1} + B_{\nu_1,\nu_2-2}\chi_0^{\nu_1,\nu_2-2},\end{aligned} \tag{46}$$

where

$$B_{i,j}(x,p) = \frac{A_{i,j}(x,p)}{\varepsilon^{\nu_1,\nu_2}(x) - \varepsilon^{i,j}(x)} = \frac{A_{i,j}(x,p)}{\Omega_1(x)(\nu_1 - i) + \Omega_2(x)(\nu_2 - j)}.$$

Formula (43) with relations (44) taken into account gives the result

$$\mathcal{L}_1 \equiv 0.$$

We note that this result also holds in a more general case of a “symmetric” confinement potential with $\langle y_i\chi_0, \chi_0\rangle_y \equiv 0$, $i = 1, 2$. The higher-order terms $\mathcal{L}_j$ and χ_j, $j > 1$, can also be calculated.

6. Conclusion

We now list the main results obtained in this paper. For the nonlinear equation describing a quantum particle in a thin waveguide with an integral Hartree-type potential, we constructed asymptotically localized solutions that have the shape of Gaussian wave packets. We analyzed the character of such solutions with an example of a waveguide with periodically varying walls and compared it with the case of a linear waveguide. We found three essentially different regimes of behavior of these asymptotic expansions, namely, spreading, pulsation, and periodic superlocalization (focusing). We showed that these regimes are related to the spectral characteristics of an auxiliary one-dimensional periodic spectral problem for the Sturm–Liouville operator.

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