

SPLITTING OF LOWER ENERGY LEVELS IN A QUANTUM DOUBLE WELL IN A MAGNETIC FIELD AND TUNNELING OF WAVE PACKETS IN NANOWIRES

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We consider the problem of the splitting of lower eigenvalues of the two-dimensional Schrödinger operator with a double-well-type potential in the presence of a homogeneous magnetic field. The main result is the observation that the partial Fourier transformation takes the operator under study to a Schrödinger-type operator with a (new) double-well-type potential but already without any magnetic field. We use this observation to investigate the influence of the magnetic field on the tunneling effects. We discuss two methods for calculating the splitting of lower eigenvalues: based on the instanton and based on the so-called libration. We use the obtained result to study the tunneling of wave packets in parallel quantum nanowires in a constant magnetic field.

Keywords: Schrödinger operator, double-well-type potential, homogeneous magnetic field, tunneling, double quantum wire, wave packet

1. Introduction

We consider the problem of the splitting of lower eigenvalues of the Schrödinger operator on the plane (y, z) with a double-well-type potential

$$V(y, z) = v_1(y) + \frac{\omega_2^2 z^2}{2}, \quad (1)$$

where $v_1(y)$ is a function of the form of a “one-dimensional double well” with two nondegenerate points $y = \pm a$ of global minimum (e.g., $v_1 = \omega_1^2(y^2 - a^2)^2/8a^2$), and in the presence of a homogeneous magnetic field directed perpendicularly to the plane (y, z) . The corresponding Schrödinger operator in the Landau gauge has the form

$$\hat{H} = -\frac{\hbar^2}{2} \frac{\partial^2}{\partial y^2} + \frac{1}{2} \left(-i\hbar \frac{\partial}{\partial z} - by \right)^2 + V(y, z). \quad (2)$$

(The vector potential is $\mathbf{A}(x) = (0, 0, by)$.) We are interested in the asymptotic behavior of the lowest eigenvalues of this operator for $\hbar \ll 1$. In the absence of a magnetic field and in the case of a general potential $V(y, z)$ that does not allow applying the variable separation method, this problem (of a quantum particle in a double potential well) has been studied sufficiently well and is widely represented in the literature (see, e.g., [1], [2]). The asymptotic behavior of the lower energy levels has a regular character, and their asymptotic expansion in a power series in the parameter \hbar can easily be obtained using the

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oscillatory approximation in a neighborhood of each of the wells. But because the wells are symmetric, the spectral levels in such a power-law asymptotic approximation with an arbitrary accuracy in \hbar are (at least) doubly degenerate. This degeneration can be removed by taking tunneling effects into account, and an exponentially small splitting (in \hbar) of energy levels determined by the formula $\Delta E = \mathcal{A}(\hbar)e^{-\mathcal{J}/\hbar}$ is obtained.

Sufficiently effective formulas for the phase \mathcal{J} based on some trajectories of the Hamiltonian system with the “tunnel” Hamiltonian $p^2/2 - V(x)$ ($p = (p_y, p_z)$ and $x = (y, z)$ hereafter in this section) can be found in the literature (see, e.g., [1]), and effective asymptotic formulas for the amplitude $\mathcal{A}(\hbar)$ were given in [2], [3] (also see [4]). In the presence of a magnetic field, the behavior of the lower part of the spectrum of the operator \widehat{H} still has a regular character, the lower-energy states can also be determined using the oscillatory approximation, and the asymptotic formulas also give a power-law degeneration of the corresponding eigenvalues. They also differ from each other by an exponentially small value, but the methods for calculating their splitting, which were developed in the works listed above, do not work in the situation with a magnetic field. The reason is that the tunneling effects were described by using the asymptotic expansions of the WKB method with “purely imaginary phases” $\varphi(x)e^{-S(x)/\hbar}$, where $S(x)$ is real-valued and $S(x) \geq 0$. Substituting such a function in the equation $\widehat{H}\psi = E\psi$ and then equating the coefficients of \hbar to the zeroth power, we obtain the Hamilton–Jacobi equation with the “tunnel” Hamiltonian $-p^2/2 + V(x)$ (or with a more convenient Hamiltonian $p^2/2 - V(x)$), which differs in the sign of p^2 from the “standard classical” Hamiltonian $p^2/2 - V(x)$ but still remains *real-valued*. In the presence of a magnetic field, the corresponding Hamiltonian becomes complex-valued and is equal to $(-ip - A(x))^2/2 + V(x)$ independently of the gauge, and the methods proposed in the above-cited papers hence in principle cannot be directly used.

Our main result is the observation (Sec. 2) that the spectral problem for the operator \widehat{H} is reducible to the spectral problem for the Schrödinger operator with a double-well-type potential but already without any magnetic field, at least in the example under study. This observation permits obtaining formulas for the splitting of lower energy levels of the initial magnetic Schrödinger operator. In Sec. 3, we discuss algorithms for calculating this splitting and estimate the influence of the magnetic field on the splitting. In Sec. 4, we consider an example of wave-packet propagation along a double “quantum” wire in the presence of a homogeneous magnetic field as an application. In the plane orthogonal to such a double wire, the potential of confining forces has the form of a double potential well. This leads to tunneling of the propagating wave packets between the two wires. We use the splitting formula to derive formulas for the time of the wave-packet propagation from one wire into the other with the magnetic field taken into account.

2. Transition from the quantum double well in a magnetic field to the double well without any magnetic field

We first show how the magnetic potential can be “eliminated” in the case under study. We apply the (partial) Fourier transformation in z defined by

$$\tilde{\psi}(y, p_z) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(y, z) e^{-i\omega_2 p_z z/\hbar} dz.$$

We introduce the new “mixed” variables $x_1 = y$ and $x_2 = p_z$. The operator \widehat{H} (see formula (2)) in this representation then becomes

$$\widehat{H}' = \frac{\widehat{p}_1^2}{2} + \frac{\widehat{p}_2^2}{2} + v_1(x_1) + \frac{(\omega_2 x_2 - b x_1)^2}{2}, \quad (3)$$

where the operators $\widehat{p}_1 = -i\hbar\partial/\partial x_1$ and $\widehat{p}_2 = -i\hbar\partial/\partial x_2$ correspond to the previous operator $-i\hbar\partial/\partial y$ and the operator of multiplication by $-\omega_2 z$. The sum of the last two terms in (3) is a function of the new

coordinates \mathbf{x}' and is here denoted by

$$\tilde{V} = v_1(x_1) + \frac{(\omega_2 x_2 - b x_1)^2}{2}.$$

The magnetic field now enters the operator \hat{H}' only as a parameter of the potential \tilde{V} , “preserving” its invariance under the sign reversal $x_{1,2} \rightarrow -x_{1,2}$. Its minimums are located at the points $(x_1, x_2) = (a, ba/\omega_2)$ and $(x_1, x_2) = -(a, ba/\omega_2)$, where $a > 0$ denotes the minimum of v_1 . *In the case under study, the spectral problem for the operator \hat{H} with a magnetic field thus reduces to the well-known eigenvalue problem in the double well without a magnetic field.*

3. Formulas for lower states and the quasidegeneration splitting

The eigenfunctions of operator (3) corresponding to lower energy levels can be constructed with an exponential accuracy, for example, using the Maslov tunnel canonical operator (see [1]). The spectrum of operator (3) has a regular character near the “well bottom,” and the asymptotic expansions of the corresponding states as $h \rightarrow 0$ can be calculated sufficiently explicitly.

1. The lower states are “asymptotically degenerate” as $h \rightarrow 0$, i.e., they can be decomposed into pairs with exponentially thin splitting of energy levels. We let χ_n^+ and χ_n^- denote such a pair; the states here are labeled by quantum numbers (double index) as $n = (n_1, n_2)$, $n_i = 0, 1, 2, \dots$. The corresponding eigenvalues are denoted by ε_n^\pm .

2. The values ε_n^\pm with small numbers $n = (n_1, n_2)$ can be calculated with an exponential accuracy in the oscillatory approximation near the minimum of the potential \tilde{V} (more precisely, at one of its two minimums, but the levels corresponding to different wells coincide because the wells are symmetric to each other):

$$\varepsilon_n^\pm = h\omega_1' \left(n_1 + \frac{1}{2} \right) + h\omega_2' \left(n_2 + \frac{1}{2} \right) + o(h), \quad (4)$$

where $\omega_1' > 0$, $\omega_2' > 0$,

$$\omega_{1,2}^{\prime 2} = \frac{1}{2} (b^2 + \omega_1^2 + \omega_2^2 \mp \sqrt{(b^2 + \omega_1^2 + \omega_2^2)^2 - 4\omega_1^2\omega_2^2}), \quad (5)$$

and we introduce the notation $\omega_1 = v_1'(a)$. The perturbation theory permits calculating corrections to formula (4), but we do not need them. In what follows, we restrict ourself to the *lowest-energy states*, i.e., to the case where $n_1 = n_2 = 0$ and omit the index $n = 0$.

3. The asymptotic behavior of the eigenfunctions is determined with a power-law accuracy by the superposition of the functions χ_{left} and χ_{right} corresponding to the oscillatory approximation in the first and second wells of the potential \tilde{V} :

$$\begin{aligned} \chi_0^+ &= \chi_{\text{left}} + \chi_{\text{right}} + O(h), & \chi_0^- &= \chi_{\text{left}} - \chi_{\text{right}} + O(h), \\ \chi_{\text{left}} &= C e^{-(\omega_1' y_-^2 + \omega_2' z_-^2)/2h}, & \chi_{\text{right}} &= C e^{-(\omega_1' y_+^2 + \omega_2' z_+^2)/2h}, \end{aligned} \quad (6)$$

where y_\pm and z_\pm are orthogonal coordinates in the respective neighborhoods of $(a, ba/\omega_2)$ and $(-a, -ba/\omega_2)$ where the quadratic forms of the potential \tilde{V} are diagonal,

$$V = \frac{\omega_1'^2}{2} y_\pm^2 + \frac{\omega_2'^2}{2} z_\pm^2 + O((y_\pm^2 + z_\pm^2)^{3/2}),$$

and $C = 1/\sqrt{\pi\omega_1\omega_2 h}$ is the normalization coefficient. These coordinates can be calculated by the formulas

$$y_\pm = (x_1 \mp a) \cos \phi + (x_2 \mp ab/\omega_2) \sin \phi, \quad z_\pm = -(x_1 \mp a) \sin \phi + (x_2 \mp ab/\omega_2) \cos \phi,$$

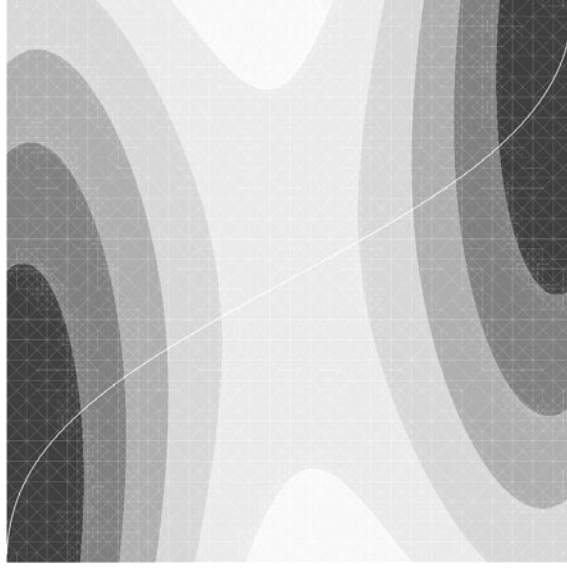


Fig. 1. Instanton on the background of level lines of the potential $\tilde{V}(x_1, x_2)$.

where

$$\tan \phi = -\frac{2b\omega_2}{b^2 + \omega_1^2 - \omega_2^2 - \sqrt{(b^2 + \omega_1^2 + \omega_2^2)^2 - 4\omega_1^2\omega_2^2}}.$$

The eigenvalues ε^\pm corresponding to functions (6) have equal power-law expansions in h in any perturbation order and differ by an exponentially small expression:

$$\varepsilon^- - \varepsilon^+ = \mathcal{A}(h)e^{-\mathcal{J}(h)/h}(1 + O(h)). \quad (7)$$

The asymptotic representation for (7) is not unique; there are at least two methods and two formulas for calculating $\mathcal{J}(h)$ and $\mathcal{A}(h)$. We describe both methods for completeness. The first method (we call it method A) is based on using the instanton (a singular trajectory) connecting two vertices of the inverted potential. The second method (we call it method B) is based on using the libration, i.e., a periodic trajectory of the Hamiltonian system with inverted potential with some energy \tilde{E} .

The phase $\mathcal{J}(h)$ in the first formula was calculated in many works (including [1]). Sufficiently explicit formulas for the amplitude $\mathcal{A}(h)$ based on the trajectories of the linear Hamiltonian system (system of variational equations) were obtained in [2]. Formulas for $\mathcal{J}(h)$ and $\mathcal{A}(h)$ in the second case (method B) were derived in [3] (also see [4]).

Method A. The process of calculating the splitting of the lowest two levels by the “instanton” formula can be divided into the following steps.

Step 1. Calculating the instanton action: the exponent $\mathcal{J}(h)$ in this case is independent of h , and we let S denote it. The quantity S is calculated along the trajectory $X(t) = (x_1(t), x_2(t))$ connecting (in infinite time) the points of unstable equilibrium in the Newtonian system with the inverted potential $-\tilde{V}(x_1, x_2)$. Namely,

$$S = \int_{-\infty}^{+\infty} \left(\frac{|\dot{X}(t)|^2}{2} + \tilde{V}(X(t)) \right) dt \quad (8)$$

is the action along the trajectory $X(t) = (x_1(t), x_2(t))$ connecting the maximum points of the inverted

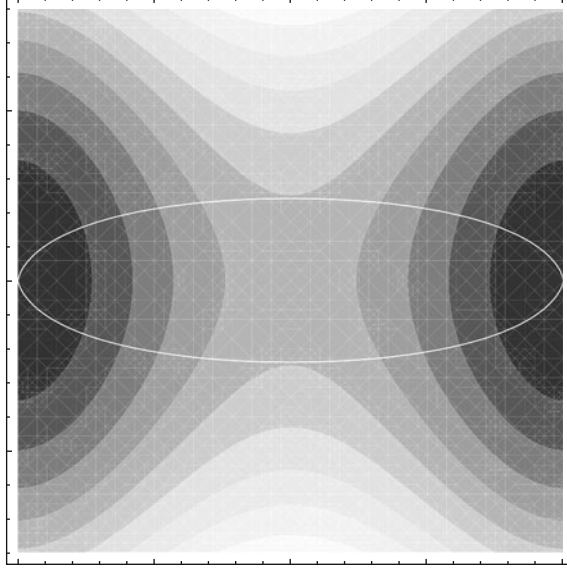


Fig. 2. Both instantons in the initial coordinates on the background of level lines of the potential $V(y, z)$.

potential \tilde{V} and is a solution of the Newton equation

$$\begin{aligned}\ddot{x}_1 &= \frac{\partial \tilde{V}}{\partial x_1} = v'_1(x_1) + \omega_2(\omega_2 x_2 - b x_1), \\ \ddot{x}_2 &= \frac{\partial \tilde{V}}{\partial x_2} = -b(\omega_2 x_2 - b x_1).\end{aligned}\tag{9}$$

Such a trajectory is known as an instanton (see Fig. 1). In the phase space $(x_1, x_2, p_1 = \dot{x}_1, p_2 = \dot{x}_2)$, such a trajectory has two components as the preimage on the plane (x_1, x_2) , and these components differ in the direction of motion (from the first bottom to the second and conversely). The projection of this trajectory on the plane (x_1, p_2) permits considering the instanton in the initial coordinates $(y = x_1, z = p_2/\omega_2)$ (see Fig. 2). System (9) in such coordinates has the form

$$\ddot{y} = v'_1(y) - b\dot{z}, \quad \ddot{z} = \omega_2^2 z - b\dot{y}.$$

Action (8) can be calculated using the Hamilton least action principle for minimizing functional (8) on the continuous curves connecting the points $(a, ab/\omega_2)$ and $(-a, ab/\omega_2)$ (vertices of the potential $-\tilde{V}$). Because the instanton symmetric parts contribute equally to (8) before and after the trajectory passes through the saddle point $(0, 0)$, we consider only one half and then replace the time t with the new time $\tau = e^{-t}$ (to eliminate the unboundedness of t). We write this as

$$S = 2 \int_0^{+\infty} \left(\frac{|\dot{X}(t)|^2}{2} + \tilde{V}(X(t)) \right) dt = 2 \int_0^1 \left(\frac{|\dot{X}(\tau)|^2}{2} \tau + \frac{\tilde{V}(X(\tau))}{\tau} \right) d\tau.$$

Numerical calculations of minimums of this functional for different values of the magnetic field showed the dependence on the magnetic field: *the action S increases as the magnetic field increases* (Fig. 3). This result can be explained as follows. As the magnetic field increases, the distance between the instanton

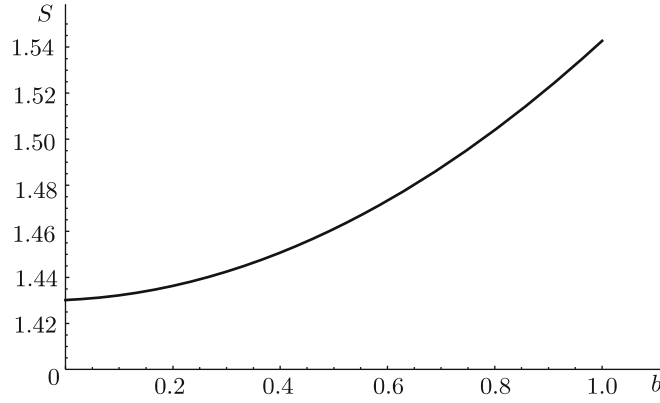


Fig. 3. Dependence of the instanton action as a function of the magnetic field value when the other parameters are fixed ($a = \omega_1 = \omega_2 = 1$).

endpoints $x' = (a, ba/\omega_2)$ and $-x' = (-a, -ba/\omega_2)$ also increases, while its maximum and minimum (and hence the characteristic) pulses remain unchanged: $p_{\min} = 0$, $p_{\max} = \sqrt{2\tilde{V}(0,0)}$. On the other hand, the action S (the Maupertuis action) can be represented as $\int_{-x'}^{x'} p dx \approx |x'|p_{\max}$.

Step 2. To calculate the pre-exponential factor (splitting amplitude)

$$\mathcal{A} = \frac{4}{\sqrt{\pi}} \sqrt{\omega'_1 \omega'_2 h} |\dot{X}(0)| \frac{1}{(Cn, n)} \frac{1}{J},$$

we must calculate the following factors.

Step 2a. The factor $\sqrt{\omega'_1 \omega'_2 h}$: direct calculations show that $\omega'_1 \omega'_2 = \omega_1 \omega_2$ (see formula (5)). Hence, $\sqrt{\omega'_1 \omega'_2 h}$ is independent of the magnetic field and is determined only by the characteristics of the initial potential V and the smallness of h .

Step 2b. The factor $|\dot{X}(0)|$ is equal to the instanton velocity at the saddle point of the potential $-\tilde{V}(x_1, x_2)$, which coincides with the midpoint of the instanton. It follows from the energy conservation law written for the midpoint and endpoints of the instanton that $|\dot{X}(0)|^2/2 - \tilde{V}(0,0) = 0$. The factor $|\dot{X}(0)| = \sqrt{2v_1(0)}$ is hence also independent of the magnetic field and is determined only by the characteristics of the initial potential V (this is $|\dot{X}(0)| = \omega_1 a/2$ for a model potential of the form $v_1 = \omega_1^2 (y^2 - a^2)^2/8a^2$).

Step 2c. The factor $J^{-1} = \lim_{t \rightarrow \infty} e^{(\omega'_1 + \omega'_2)t} \det Z(t)$ is determined by the solution of the system of variational equations for the trajectory $X(t)$. The 2×2 matrix $Z(t)$ solves the problem

$$\ddot{Z}_{ij}(t) = \sum_{k=1}^2 \frac{\partial^2 \tilde{V}}{\partial x_i \partial x_k} \Big|_{x=X(t)} Z_{kj}(t), \quad Z(0) = E, \quad Z(\infty) = 0, \quad (10)$$

where E is the 2×2 unit matrix. To calculate this factor, we must first find a solution of Eq. (10), which can be obtained by the least action principle. For this, we must use its generalization to the case of the unknown matrix-valued function

$$Z(\tau) = \text{Arg} \min_{Z(\tau) \in C([0,1])^4} \text{Tr} \int_0^1 \tau \frac{\dot{Z} \dot{Z}^T}{2} + \frac{Z \tilde{V}(X(\tau)) Z^T}{\tau} d\tau, \quad Z(0) = 0, \quad Z(1) = E.$$

After the minimum of this functional is determined, we obtain the limit

$$J^{-1} = \lim_{t \rightarrow \infty} e^{(\omega'_1 + \omega'_2)t} \det Z(t).$$

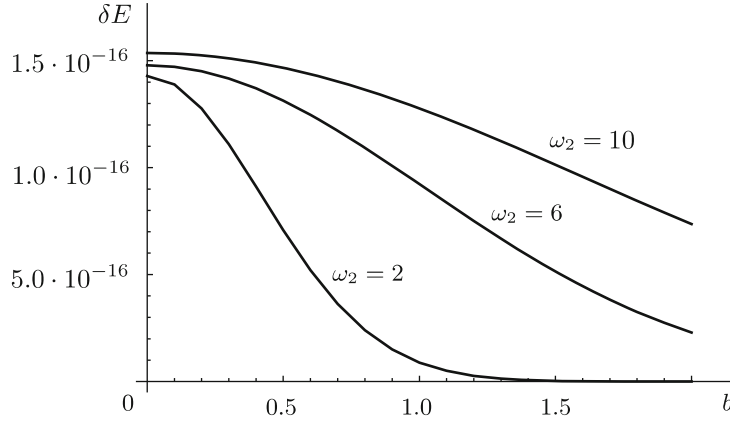


Fig. 4. The splitting $\delta E = \varepsilon^- - \varepsilon^+$ as a function of the parameter b for different values of the parameter ω_2 and for $\omega_1 = 6$, $a = 1$, $h = 0.1$.

Step 2d. The factor (Cn, n) can be obtained from the unit vector n normal to $|\dot{X}(0)|$ and the matrix $C = \dot{Z}(0)$, where $Z(t)$ are solutions of the system of variational equations (see Step 2c). But it is more convenient to calculate this matrix by the relation

$$C = \left. \frac{\partial p}{\partial x} \right|_{p=\dot{X}(0)} = \frac{\partial^2 S_1}{\partial x^2},$$

where the function S_1 satisfies the equation

$$S_1(x_1, x_2) = \min_{\mathcal{X}(\tau) \in C([0,1])} \int_0^1 \tau \frac{|\dot{\mathcal{X}}(\tau)|^2}{2} + \frac{\tilde{V}(\mathcal{X}(\tau))}{\tau} d\tau,$$

$$\mathcal{X}(0) = \left(a, \frac{ab}{\omega_2} \right), \quad \mathcal{X}(1) = (x_1, x_2).$$

The corresponding factor can therefore be calculated by a method similar to the method used in the calculations in Step 1. Correspondingly, we have the 2×2 matrix $C = \partial^2 S_1 / \partial x^2 = \partial p / \partial x|_{p=\dot{X}(0)}$.

These formulas used to calculate S and \mathcal{A} as functions of the parameters b and ω_2 lead to the following results. The magnetic field component b increases the instanton action S and simultaneously decreases the value of the splitting of lower levels. Conversely, the parameter ω_2 decreases the value of the action (as is shown below, this parameter in the problem with wires also corresponds to the value of the magnetic field in one of the transverse directions). The action attains a certain constant value for sufficiently large values of this parameter and hence ceases to affect the splitting, while the pre-exponential factor \mathcal{A} begins to play its own role. In turn, the parameter \mathcal{A} increases as ω_2 increases. We can hence draw the following general conclusion: the splitting decreases as the parameter b (magnetic field) increases, and the splitting increases as the parameter ω_2 increases. This conclusion is illustrated by the curves in Fig. 4. Figure 5 shows the results of splitting obtained by V. Zalipaev from a numerical analysis of the corresponding Schrödinger equation.

Method B. The derivation of formulas for the phase \mathcal{J} and the amplitude \mathcal{A} is based on the following consideration (see [3] and also [4]). The geometric objects determining the asymptotic wave functions in the oscillatory approximation are “small” tori of the following form in the coordinates y_{\pm} , z_{\pm} and in the

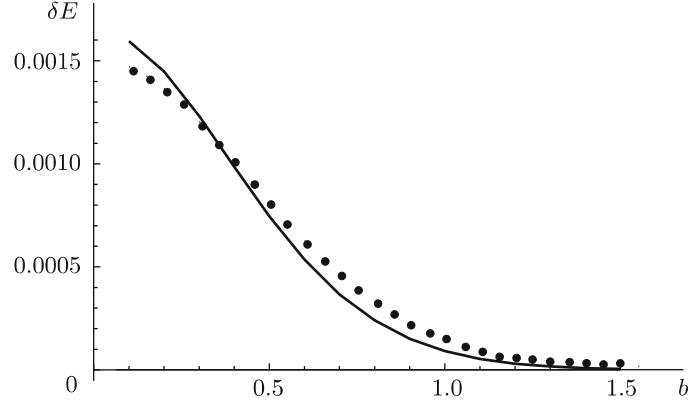


Fig. 5. The splitting $\delta E = \varepsilon^- - \varepsilon^+$ as a function of the parameter b for $\omega_2 = \omega_1 = 1$, $a = 1$, $h = 0.1$. The points were obtained numerically by the computer program `Comsol`, and the curve corresponds to calculations by instanton formula (7).

corresponding momentum coordinates $p_{y\pm}$, $p_{z\pm}$:

$$\Lambda_{\pm} = \{p_{y\pm} = -\sqrt{h\omega'_1} \sin \phi_1, p_{z\pm} = -\sqrt{h\omega'_2} \sin \phi_2, \\ y_{\pm} = \sqrt{h/\omega'_1} \cos \phi_1, z_{\pm} = \sqrt{h/\omega'_2} \cos \phi_2\}.$$

They are “almost invariant” under the action of the phase flow generated by the initial Hamiltonian $H = p^2/2 + V(x)$ and are near the minimum of V at the energy level $(h/2)(\omega'_1 + \omega'_2)$. If V is replaced with harmonic oscillator potentials, then Λ_{\pm} are the Liouville tori corresponding to quadratic Hamiltonians. The (approximate) motion along them is almost periodic because of the Hamiltonian system with Hamiltonian H . If the corresponding phase flow is denoted by g_H^t , then we obtain

$$g_H^t \Lambda_{\pm} = \{p_{y\pm} = -\sqrt{h\omega'_1} \sin(\phi_1 + \omega'_1 t), p_{z\pm} = -\sqrt{h\omega'_2} \sin(\phi_2 + \omega'_2 t), \\ y_{\pm} = \sqrt{h/\omega'_1} \cos(\phi_1 + \omega'_1 t), z_{\pm} = \sqrt{h/\omega'_2} \cos(\phi_2 + \omega'_2 t)\}.$$

The instanton is the trajectory connecting the inverted potential maximums on the limit classical energy level, while the quantum (“inverted”) level is equal to $-\mathcal{E}_0 = -(h/2)(\omega'_1 + \omega'_2) + O(h^2)$. The object that is more reasonable for determining the tunneling from the physical standpoint, is therefore the path Γ_+ connecting Λ_+ and Λ_- in the complex phase space or the path Γ_- determining the motion in the opposite direction, and we have $\mathcal{J} = \pi J(\tilde{E})$, where

$$J(\tilde{E}) = \frac{1}{2\pi} \oint \mathbf{p} d\mathbf{x} \quad (11)$$

is the action of the path (cycle) $\Gamma = \Gamma_+ + \Gamma_-$. Precisely the corresponding libration gives this cycle (one of its possible realizations), but its definition is related not to the energy level \mathcal{E}_0 but to another energy level \tilde{E} because “part of the energy” is “consumed” in the tunneling process by motions transverse to this path. Replacing the instanton action in formula (7) with the libration action implies recalculating the amplitude, which becomes simpler, $\mathcal{A} = \omega'_1 h / \sqrt{\pi e}$, and the splitting formula can be rewritten in terms of the libration as [1], [4]

$$\varepsilon_0^- - \varepsilon_0^+ = \frac{\omega'_1 h}{\sqrt{\pi e}} e^{-\pi J(\tilde{E})/h} (1 + O(h)). \quad (12)$$

We now note that $J(\tilde{E})/h$ depends on h (in terms of \tilde{E}). The following algorithm is used to calculate $J(\tilde{E})$. We consider the Hamiltonian system (with the inverted potential $-\tilde{V}$)

$$\begin{aligned} \dot{p}_1 &= \frac{\partial \tilde{V}}{\partial x_1} = v_1'(x_1) + \omega_2(\omega_2 x_2 - b x_1), & \dot{p}_2 &= \frac{\partial \tilde{V}}{\partial x_2} = -b(\omega_2 x_2 - b x_1), \\ \dot{x} &= p_1, & \dot{x}_2 &= p_2. \end{aligned} \quad (13)$$

The trajectory connecting the potential vertices (instanton) is at a nonzero and “nonquantum” energy level. The classical trajectory corresponding to the quantum problem is at a lower energy level other than $E = 0$. This periodic trajectory in the phase space is called a libration. It was shown in [5] that there is at least one such a trajectory at each energy level. We assume that there is only one such a trajectory at each energy level in our case. We let $T = T(E)$ denote its period and vary E to obtain a family of librations (periodic trajectories) smoothly depending on the parameter E and passing into the instanton solution in the limit as $E \rightarrow 0$. Instead of the parameter E , we can use the action variable

$$J = J(E) = \frac{1}{2\pi} \oint \mathbf{p} \, d\mathbf{x} \quad (14)$$

calculated along this trajectory and then parameterize librations, their periods, energy levels, etc., by this variable. We let $J^0 = J(0)$ denote the limit action (as $E \rightarrow 0$) and assume that $J \in [J^0 - \Delta, J^0)$, where Δ is a small positive number independent of h . We thus obtain a libration of the form

$$L(J) = \{p = \mathcal{P}(\Omega(J)t, J), x = \mathcal{X}(\Omega(J)t, J)\},$$

where $\Omega(J) = 2\pi/T(J)$ is the libration frequency, $H|_L = E(J)$, and $J \in [J^0 - \Delta, J^0)$. The functions $\mathcal{P}(\varphi, J)$, $\mathcal{X}(\varphi, J)$ are smooth in a given half-interval and 2π -periodic in the parameter φ .

The motion governed by system (13) in a neighborhood of $L(J)$ in the phase space is determined by the corresponding system of variational equations. The basis of its solutions can be composed of the following functions. Two solutions are $(\dot{\mathcal{P}}, \dot{\mathcal{X}})$, $(\partial\mathcal{P}/\partial J + (\partial\Omega/\partial J)(\partial\mathcal{P}/\partial\Omega), \partial\mathcal{X}/\partial J + (\partial\Omega/\partial J)(\partial\mathcal{X}/\partial\Omega))$. According to the Floquet–Lyapunov theory, the other two solutions can be represented as the Floquet solutions

$$W(t) = \mathcal{W}(\Omega(J)t, J)e^{\pm\beta(J)t}, \quad Z(t) = \mathcal{Z}(\Omega(J)t, J)e^{\pm\beta(J)t}, \quad (15)$$

where the functions $\mathcal{Z}(\varphi, J)$ for $J \in [J^0 - \Delta, J^0)$ are smooth vector functions 2π -periodic in the angle argument φ and $\beta(J) > 0$ is the Floquet exponent.

We note that the libration is an unstable closed trajectory and the Floquet exponents take purely real values in this case. The (approximate) equation for $J(\tilde{E})$ becomes

$$E(J(\tilde{E})) - \frac{1}{2}\beta(J(\tilde{E}))h = -\frac{h}{2}(\omega_1' + \omega_2'). \quad (16)$$

In practical calculations, it is convenient first to determine the energy $\tilde{E} = E(J(\tilde{E}))$ by rewriting the preceding equation in a form suitable for the iteration method:

$$\tilde{E} = \frac{1}{2}\tilde{\beta}(\tilde{E})h - \frac{h}{2}(\omega_1' + \omega_2'). \quad (17)$$

The algorithm for calculating $J(\tilde{E})$ hence consists of the following steps.

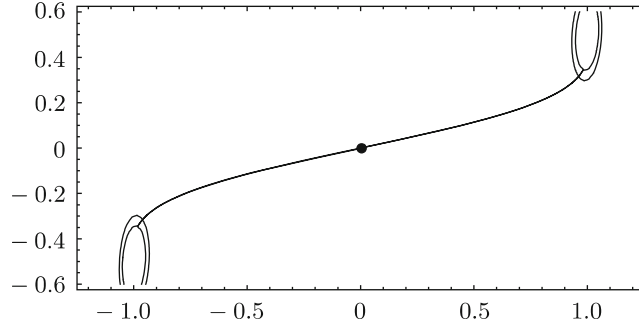


Fig. 6. Libration in the coordinates (x_1, x_2) and the two energy levels $E = E_0$ (outside) and $\tilde{E} = E_0 + \beta(\tilde{E})h/2$ (inside) corresponding to the libration energy.

Step 1. We construct the zeroth-order approximation E^0 of the solution of Eq. (17) omitting $(1/2)\tilde{\beta}(\tilde{E})h$ or $(1/2)\tilde{\beta}(\tilde{E})h - (h/2)\omega'_2$ in its right-hand side. We construct the libration (closed trajectory) corresponding to this energy. The possibility of using the least action principle in Hamiltonian form to seek this trajectory is nonobvious here because its final position in space and time is unknown (its period is not known in advance). Because of the symmetry, we know that it passes through the origin. We therefore choose the initial conditions $\dot{x}_1(0)$ and $\dot{x}_2(0)$ at the point

$$x_1(0) = 0, \quad x_2(0) = 0, \quad \frac{1}{2}(\dot{x}_1(0))^2 + \frac{1}{2}(\dot{x}_2(0))^2 = -E^0,$$

by using the “shooting” method and starting from the requirement that the trajectory must completely return to the initial position. This step is sufficiently laborious because the trajectory is unstable and its period is unknown.

Step 2. We further construct a sequence E^1, E^2, \dots (and the corresponding librations) converging sufficiently fast to \tilde{E} :

$$E^0 = -\frac{1}{2}\omega'_1 h - \frac{1}{2}\omega'_2 h, \quad E^{n+1} = E^n + \frac{1}{2}\tilde{\beta}(E_n)h.$$

This step is easy if the first step is already completed.

Step 3. We can then easily calculate $J(\tilde{E})$ by formula (14).

The libration pattern typical of such problems and corresponding to the required energy level \tilde{E} in the configuration space of the mixed momentum–coordinate representation (x_1, x_2) is shown in Fig. 6.

Comparing the two calculation methods described above (A and B) shows that they are completely consistent. Formulas (7) and (16) are compared using the logarithmic scale multiplied by h :

$$J_0(h) - h \log \sqrt{h} = S - Ch + O(h^2),$$

where we take

$$C = \log \left(4\sqrt{\omega'_1 \omega'_2} |\dot{X}(0)| \frac{1}{(Cn, n)} J^{-1} \right) - \log \left(\frac{\omega'_1}{\sqrt{e}} \right).$$

The typical result of comparing at a point in the parameter space $(a, b, \omega_1, \omega_2)$ is shown in Fig. 7.

4. Quantum double well in a magnetic field in special three-dimensional cases

We discuss the conditions under which the situation based on the Fourier transformation and leading from the Schrödinger operator in a magnetic field to the Schrödinger operator without a magnetic field can

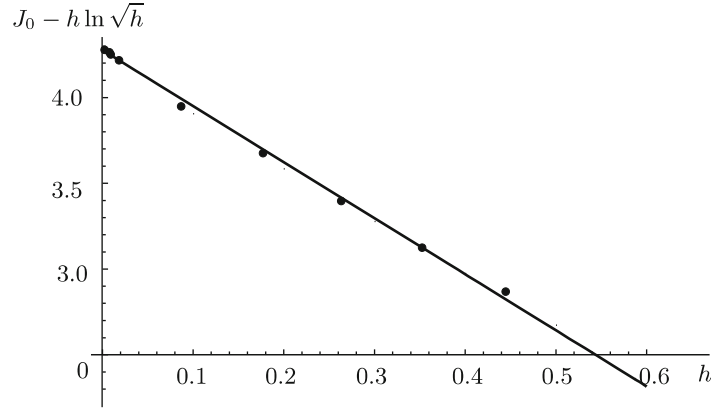


Fig. 7. Graph of the functions $J_0 - h \log \sqrt{h}$ (points) and $S - Ch$ (straight line).

be realized in the three-dimensional case. We consider the potential $V(x_1, x_2, x_3)$ of the form

$$V(x_1, x_2, x_3) = v_1(x_1) + \frac{\omega_2^2 x_2^2}{2} + \frac{\omega_3^2 x_3^2}{2},$$

where $v_1(x_1)$ is a one-dimensional double-well-type potential.

We show that the corresponding spectral equation for Schrödinger operator (2) is reducible to the spectral problem for the Schrödinger equation with the double-well potential but without any magnetic field in the cases where

1. the magnetic field is perpendicular to the axis Ox_1 or
2. the magnetic field coincides with the direction of the axis Ox_1 or
3. the magnetic field is directed arbitrarily but $\omega_2 = \omega_3$.

In case 1, it is necessary to realize the gauge $A(x) = (0, b_3 x_1, -b_2 x_1)$ of the vector potential and perform the Fourier h -transformation in the variables x_2 and x_3 . In case 2, it is necessary to choose $A(x) = (0, -b_1 x_3, b_1 x_2)$ and perform the Fourier h -transformation in the variables x_2 and x_3 . In case 3, the symmetry of the potential V with respect to the axis Ox_1 allows assuming that $b_3 = 0$. We choose the potential in the form $A(x) = (b_2 x_3, 0, b_1 x_2)$, perform a partial Fourier h -transformation in the variable x_3 , and obtain the representation for the Schrödinger operator

$$\widehat{H}' = (\widehat{p}_1 - b_2 \widehat{p}_3')^2 + \widehat{p}_2^2 + \frac{\omega_3^2 \widehat{p}_3'}{2} + v_1(x_1) + \frac{\omega_2^2 x_2^2}{2} + (x_3' - b_1 x_2)^2.$$

After an appropriate linear change of the coordinates x_1 , x_2 , and x_3' , this operator again takes the “non-magnetic” form $\widehat{H} = \widehat{p}^2/2 + \widetilde{V}(x)$.

5. Tunneling of wave packets in quantum nanowires

5.1. Wave packets in a solitary quantum wire in a homogeneous magnetic field. The quantum waveguide (“solitary quantum wire”) in the three-dimensional space with coordinates (x, y, z) , directed along the axis Ox , with “soft walls” in the transverse cross section, and placed in a constant magnetic field \mathbf{B} with the components $(b_x, b_y, 0)$ is modeled by the Schrödinger operator

$$\widehat{\mathcal{H}} = \frac{1}{2} \left(-ih \frac{\partial}{\partial x} - b_y z \right)^2 - \frac{h^2}{2} \frac{\partial^2}{\partial y^2} + \frac{1}{2} \left(-ih \frac{\partial}{\partial z} - b_x y \right)^2 + U(y, z).$$

Here, $U = (\omega^2/2)(y^2 + z^2)$ is the potential of parabolic confinement (see [6]) with the frequency ω . We choose the coordinates y and z to satisfy the condition $b_z = 0$ and choose the gauge such that the potential \mathbf{A} of the magnetic field \mathbf{B} is independent of x : $\mathbf{A} = (b_y z, 0, b_x y)$.

We consider the problem of the propagation of a Gaussian beam in such a waveguide. The corresponding wave function $\Psi(x, y, z, t)$ satisfies the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi = \hat{\mathcal{H}} \Psi. \quad (18)$$

We first consider the well-known solution obtained without any magnetic field (for $b_x = b_y = b_z = 0$). It can be easily obtained by the method of separation of variables and has the form of a Gaussian “small cap” traveling along the axis x and spreading in this direction:

$$\Psi^0(r, t) = f(t, x) \chi^0(y, z), \quad \chi^0(y, z) = e^{-\omega(y^2+z^2)/2\hbar}, \quad (19)$$

$$f(t, x) = \frac{Ae^{-iE_0 t/\hbar}}{\sqrt{\alpha + it}} e^{-(x-Pt)^2/2\hbar(\alpha+it)} e^{ixP/\hbar} e^{-iP^2 t/2\hbar}, \quad E_0 = \omega\hbar, \quad (20)$$

where α is a positive parameter characterizing the “cap” width at the time $t = 0$ and the parameter A is the amplitude.

The solution generalizing (19) and (20) to the case with a magnetic field ($b_x \neq 0, b_z \neq 0$) has the form

$$\Psi^0(x, y, z, t) = \frac{C}{\sqrt{g(t)}} e^{iS(t)/\hbar} e^{i/h\langle P(t), r-R(t) \rangle} e^{i/(2\hbar)\langle r-R(t), Q(t)(r-R(t)) \rangle}, \quad (21)$$

where C is a constant, r is a column vector with the components (x, y, z) , and the vector-valued functions $P(t) = (P_x(t), P_y(t), P_z(t))$ and $R(t) = (X(t), Y(t), Z(t))$, the functions $S(t)$ and $g(t)$, and the 3×3 matrix-valued function $Q(t)$ are defined by the relations

$$\begin{aligned} P_x(t) &= P = \text{const}, & P_y(t) &= 0, & P_z(t) &= 0, \\ X(t) &= \frac{P\omega^2}{\omega_y^2} t, & Y(t) &= 0, & Z(t) &= \text{const} = \frac{Pb_y}{\omega_y^2}, \\ S(t) &= \frac{P^2 t \omega^2}{2 \omega_y^2} + \frac{\hbar}{2} \beta, & g(t) &= \frac{b_y^2 \beta}{\omega_y^3 (\omega + \omega_y)} + \mu(t), & \mu(t) &= \alpha + it \frac{\omega^2}{\omega_y^2}, \\ Q(t) &= \frac{\beta}{(\omega + \omega_y) g(t)} \begin{pmatrix} i \frac{\omega + \omega_y}{\beta} & i \frac{b_x b_y}{\omega_y \beta} & \frac{b_y}{\omega_y} \\ i \frac{b_x b_y}{\omega_y \beta} & i \left(\frac{b_y^2 (\omega_x^2 + \omega \omega_y)}{\omega_y^3 \beta} + \omega \mu(t) \right) & -\frac{b_x \omega_y}{\beta} \mu(t) \\ \frac{b_y}{\omega_y} & -\frac{b_x \omega_y}{\beta} \mu(t) & i \omega_y \mu(t) \end{pmatrix} \end{aligned} \quad (22)$$

with the notation $\omega_y^2 = b_y^2 + \omega^2$, $\omega_x^2 = b_x^2 + \omega^2$, and

$$\beta = \sqrt{\frac{\omega_x^2 + \omega_y^2 + \sqrt{(\omega_x^2 + \omega_y^2)^2 - 4\omega^2 \omega_y^2}}{2}} + \sqrt{\frac{\omega_x^2 + \omega_y^2 - \sqrt{(\omega_x^2 + \omega_y^2)^2 - 4\omega^2 \omega_y^2}}{2}}.$$

This solution can be obtained by different methods, in particular, by using the Maslov complex germ theory (see [7]), but it is convenient for us to obtain this solution by the partial Fourier transformation in the variable x . Namely, for the function

$$\tilde{\Psi}^0(p_x, y, z, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi^0(x, y, z, t) e^{-ip_x x/\hbar} dx,$$

we have the equation

$$ih \frac{\partial \tilde{\Psi}^0}{\partial t} = \hat{\mathcal{H}} \tilde{\Psi}^0, \quad (23)$$

$$\begin{aligned} \hat{\mathcal{H}} &= -\frac{\hbar^2}{2} \frac{\partial^2}{\partial y^2} + \frac{1}{2} \left(-ih \frac{\partial}{\partial z} - b_x y \right)^2 + \frac{1}{2} (p_x - b_y z)^2 + \frac{\omega^2}{2} (y^2 + z^2) = \\ &= -\frac{\hbar^2}{2} \frac{\partial^2}{\partial y^2} + \frac{1}{2} \left(-ih \frac{\partial}{\partial z'} - b_x y \right)^2 + \frac{1}{2} \omega^2 y^2 + \frac{1}{2} \omega_y^2 z'^2 + \frac{1}{2} \frac{\omega^2 p_x^2}{\omega_y^2}, \end{aligned} \quad (24)$$

where

$$z' = z - \frac{b_y p_x}{\omega_y^2}. \quad (25)$$

The solution of this equation corresponding to (21) can be obtained by the method of separation of variables and subsequent application of the well-known Darwin–Fock (model) formulas for the harmonic oscillator in a magnetic field (or using the Maslov complex germ theory [7]). The solution has the form

$$\tilde{\Psi}(p_x, y, z, t) = C e^{-\alpha(p_x - P)^2/2\hbar} e^{-i\mathcal{E}_0(p_x)t/\hbar} \tilde{\chi}(p_x, y, z), \quad (26)$$

where

$$\mathcal{E}_0(p_x) = \frac{1}{2} \frac{\omega^2 p_x^2}{\omega_y^2} + \frac{\hbar}{2} \beta, \quad \tilde{\chi}(p_x, y, z) = \exp \left[\frac{i}{\hbar} \left(\frac{1}{2} \langle r_{\perp} - R_{\perp}, q(r_{\perp} - R_{\perp}) \rangle \right) \right] \quad (27)$$

are the least eigenvalue and the corresponding eigenfunctions of the operator $\hat{\mathcal{H}}$. In the last formula, we have

$$r_{\perp} = \begin{pmatrix} y \\ z \end{pmatrix}, \quad R_{\perp} = \begin{pmatrix} 0 \\ \frac{p_x b_y}{\omega_y^2} \end{pmatrix}, \quad q = \frac{1}{\omega + \omega_y} \begin{pmatrix} i\omega\beta & -b_x \omega_y \\ -b_x \omega_y & i\omega_y \beta \end{pmatrix}.$$

We note that the variable p_x in formula (26) is contained only in the (complex) phase and this phase depends on p_x quadratically. To obtain the function Ψ^0 in (x, y, z) , we must therefore calculate the integral

$$\Psi^0 = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \tilde{\Psi}^0(p_x, y, z, t) e^{ip_x x/\hbar} dp_x \quad (28)$$

exactly, and this leads to formula (21). We stress that the wave-packet representation in form (26) (and (28)) is useful from the standpoint of the problem of the wave-packet propagation in two parallel quantum wires.

If the coordinate y is shifted in the potential U by a distance $\pm a$, i.e., if the problem with the potential $U = (\omega^2/2)((y \pm a)^2 + z^2)$ is considered, then not only the argument of the corresponding wave functions changes, but also a new phase factor appears in these functions. Namely, the function $\Psi^0(x, y, z, t)$ is replaced with $e^{\pm iab_x z/\hbar} \Psi^0(x, y \pm a, z, t)$, and the function $\tilde{\Psi}(p_x, y, z, t)$ is replaced with $e^{\pm iab_x z/\hbar} \tilde{\Psi}(p_x, y, z, t)$.

5.2. Wave packets in parallel quantum wires in a homogeneous magnetic field. We now consider the case where there are two close parallel quantum wires (waveguides) and a wave packet propagates in one of them. In this case, it is natural to assume that the confinement potential in the variables y and z has the form

$$V = \frac{1}{8a^2}\omega^2(y^2 - a^2)^2 + \frac{1}{2}\omega^2 z^2.$$

The term $\omega_1^2(y^2 - a^2)^2/8$ in the potential V has the form of a double potential well in the direction y and determines a potential barrier between the two wires.

It is clear that if the wires are rather far from each other, then they can be considered separately, the oscillatory approximation can be used, and the packets behave independently in each of the wires. The potential V in a neighborhood of the points $(y = -a, z = 0)$ and $(y = a, z = 0)$ can be represented as

$$V = \frac{1}{2}\omega^2(y \pm a)^2 + \frac{1}{2}\omega^2 z^2 + O(y \pm a)^3.$$

We consider only the case where the packet propagates in the left wire.

We first consider the case without any magnetic field. The corresponding approximate wave function Ψ_{appr} of the Schrödinger equation

$$ih \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \Psi + V(y, z) \Psi$$

then has form (19), (20) with the shifted argument $y \rightarrow y + a$ and $\Psi_{\text{appr}} = f(x, t) \chi^0(x, y + a, z)$, where $f(x, t)$ is defined in (20). But for large times (in dimensionless variables of the order $1/\hbar$ and higher), this approximation begins to deviate from the exact answer and becomes significant when the wave packet is tunneling from one wire to the other. Because the confinement potential is symmetric, the function χ^0 can be represented as

$$\chi^0(x, y + a, z) \approx \frac{1}{2}(\chi^+ + \chi^-),$$

where χ^+ and χ^- are the even and odd eigenfunctions corresponding to the two minimum eigenvalues E^\pm of the operator $(\hbar^2/2)(\partial^2/\partial y^2 + \partial^2/\partial z^2)\Psi + V(y, z)$:

$$E^\pm = \hbar\omega + O(\hbar^2), \quad \Delta E = E^- - E^+ = \frac{\omega \hbar}{\sqrt{\pi e}} e^{-\pi J(\omega \hbar/2)/\hbar} (1 + O(\hbar)).$$

The exact solution of the Cauchy problem for the Schrödinger equation then has the form

$$\Psi = \frac{f(t, x)}{2} (\chi^+ e^{-itE^+/\hbar} + \chi^- e^{-itE^-/\hbar}) = \frac{f(t, x)}{2} e^{-itE^+/\hbar} (\chi^+ + \chi^- e^{-it\Delta E/\hbar}).$$

At the instant $t = T \equiv \pi \hbar / \Delta E$, the wave function Ψ becomes

$$\Psi = f(T) e^{-iT E^+/\hbar} \frac{\chi^+ - \chi^-}{2} \approx f(T) e^{-iT E^+/\hbar} \chi^0(x, y - a, z),$$

and the wave packet therefore moves from the “left” wire into the “right” wire.

We now consider a similar problem in the case where two parallel wires are placed in a magnetic field with the components (b_x, b_y, b_z) . We choose a gauge such that the vector potential has the coordinates $(b_y z - b_z y, 0, b_x y)$. It is convenient to consider such a situation directly for the Schrödinger equation in the mixed (p_x, y, z) representation for the function $\tilde{\Psi}(p_x, y, z, t)$,

$$ih \frac{\partial \tilde{\Psi}}{\partial t} = \hat{\mathcal{H}}^w, \quad \hat{\mathcal{H}}^w = \left(-\frac{\hbar^2}{2} \frac{\partial^2}{\partial y^2} + \frac{1}{2} \left(-ih \frac{\partial}{\partial z} - b_x y \right)^2 + W \right) \tilde{\Psi}, \quad (29)$$

$$W = \frac{1}{2}(p_x - b_y z + b_z y)^2 + \frac{1}{8a^2}\omega^2(y^2 - a^2)^2 + \frac{1}{2}\omega^2 z^2.$$

We first show that the presence of the longitudinal component b_z of the magnetic field destroys the “double-well” symmetry. More precisely, the potential has the form of a double or single well as $b_z \neq 0$. We obtain the local minimums of the potential W :

$$\begin{aligned}\frac{\partial W}{\partial y} &= b_z(p_x - b_y z + b_z y) + \frac{1}{8a^2} \omega^2 (y^2 - a^2) y = 0, \\ \frac{\partial W}{\partial z} &= -b_y(p_x - b_y z + b_z y) + \omega^2 z = 0.\end{aligned}$$

We express z from the second relation and obtain the straight line $z = b_y(p_x + b_z y)/(\omega^2 + b_y^2)$ passing through the points of minimums of the potential $W(y, z)$. We use this relation to replace z in the potential $W(y, z)$ and obtain the value of the potential on this line

$$\frac{1}{2} \frac{\omega^2}{\omega^2 + b_y^2} (p_x + b_z y)^2 + \frac{1}{8a^2} \omega^2 (y^2 - a^2)^2.$$

This implies that the symmetry of the potential is violated for $b_z \neq 0$. (An exception is the point $p_x = 0$, which does not play any role in studying the wave-packet propagation.) Because the symmetry is violated, the supports of the eigenfunctions of $\widehat{\mathcal{H}}^w$ are localized in a neighborhood of either the left or the right well, and the wave packet hence has the same property.

We assume that $b_z = 0$ and perform change (25) in Eq. (29). The operator $\widehat{\mathcal{H}}^w$ then becomes

$$\widehat{\mathcal{H}}^w = \left(-\frac{\hbar^2}{2} \frac{\partial^2}{\partial y^2} + \frac{1}{2} \left(-i\hbar \frac{\partial}{\partial z'} - b_x y \right)^2 + \frac{1}{8a^2} \omega^2 (y^2 - a^2) + \frac{1}{2} \omega_y^2 z'^2 \right) + \frac{1}{2} \frac{\omega^2 p_x^2}{\omega_y^2}, \quad (30)$$

and we can use the results in Sec. 2 to construct asymptotic expansions of its eigenfunctions $\chi^\pm(p_x, y, z')$ describing the two lower-energy states $\varepsilon^+ < \varepsilon^-$.

We show that in the mixed (p_x, y, z) representation, the solution $\widetilde{\Psi}$ describing the propagation of the wave packet that is in the left wire at $t = 0$ can be represented as the superposition

$$\begin{aligned}\widetilde{\Psi}(p_x, y, z, t) &= \frac{C}{2} e^{-\alpha(p_x - P)^2/2\hbar} e^{-i\omega^2 p_x^2 t/2\hbar\omega_y^2} (\chi^+(y, z') e^{-i\varepsilon^+ t/\hbar} + \chi^-(y, z') e^{-i\varepsilon^- t/\hbar}) = \\ &= \frac{C}{2} e^{-i\omega^2 p_x^2 t/2\hbar\omega_y^2} e^{-i\varepsilon^+ t/\hbar} (\chi^+(y, z') + \chi^-(y, z') e^{-i\Delta\varepsilon t/\hbar}), \quad \Delta\varepsilon = \varepsilon^- - \varepsilon^+.\end{aligned} \quad (31)$$

We assume that the functions $\chi^\pm(y, z') \pm \chi^\mp(y, z')$ near the points $(y, z) = (\pm a, 0)$ are approximated by functions (27) (with the argument shift and the phase shift taken into account). In the usual (x, y, z) representation, this solution has the form

$$\Psi(x, y, z, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \widetilde{\Psi}(p_x, y, z, t) e^{ip_x x/\hbar} dp_x. \quad (32)$$

We note that formulas (31) and (32) are exact and the ε^\pm are independent of p_x .

As in the absence of a magnetic field, the phase π is accumulated in the second term in (31) at time $T = \pi\hbar/\Delta\varepsilon$, which results in the wave packet “overflowing” from the left wire to the right wire. Such a transition can be described by the asymptotic formulas obtained in Sec. 2. We have the following formulas for ΔE and T :

$$\Delta\varepsilon = \frac{\omega'_1 \hbar}{\sqrt{\pi e}} e^{-\pi J(\widetilde{E}(h))/\hbar} (1 + O(h)), \quad T = \frac{\pi \sqrt{\pi e}}{\omega'_1} e^{\pi J(\widetilde{E}(h))/\hbar} (1 + O(h)), \quad (33)$$

where $\omega'_1 = \sqrt{\omega_x^2 + \omega_y^2} - \sqrt{(\omega_x^2 + \omega_y^2)^2 - 4\omega^2\omega_y^2}/2$ and the expression for $J(\tilde{E}(h))$ is obtained by the algorithm discussed in Sec. 2. This allows obtaining the solution Ψ for $t = 0$ and for $t = T$:

$$\begin{aligned}
\Psi(x, y, z, 0) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\alpha(p_x - P)^2/2\hbar} \frac{\chi^+(y, z') + \chi^-(y, z')}{2} e^{ip_x x/\hbar} dp_x \approx \\
&\approx \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\alpha(p_x - P)^2/2\hbar} \tilde{\chi}\left(y, z - \frac{b_y p_x}{\omega'^2}\right) e^{ip_x x/\hbar} dp_x \approx \\
&\approx e^{ib_x a z/\hbar} \Psi^0(x, y + a, z, 0), \\
\Psi(x, y, z, T) &= \frac{e^{-i\varepsilon^+ T/\hbar}}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\alpha(p_x - P)^2/2\hbar} e^{-i\omega_2^2 p_x^2 T/2\hbar(\omega_2^2 + b_y^2)} \times \\
&\quad \times \frac{\chi^+(y, z') - \chi^-(y, z')}{2} e^{ip_x x/\hbar} dp_x \approx \\
&\approx \frac{e^{-i\varepsilon^+ T/\hbar}}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\alpha(p_x - P)^2/2\hbar} e^{-i\omega_2^2 p_x^2 T/2\hbar(\omega_2^2 + b_y^2)} \times \\
&\quad \times \tilde{\chi}\left(y, z - \frac{b_y p_x}{\omega'^2}\right) e^{ip_x x/\hbar} dp_x \approx e^{-ib_x a z/\hbar} \Psi^0(x, y - a, z, T).
\end{aligned} \tag{34}$$

We say a few words about the relations between the problem parameters. The wave packet is characterized by the parameter α determining its “width” and the momentum P characterizing the frequency of spatial oscillations along the axis x and the velocity with which the packet moves along this axis. We assume that the length of quantum wires is L (in dimensionless units). Then the time of the wave packet travel through this distance is $T_1 = L\omega_y^2/P\omega^2$. The wave packet amplitude becomes

$$\begin{aligned}
&\sqrt{\left(\frac{b_y^2\beta}{\omega_y^3(\omega + \omega_y)} + \alpha\right) \left/ \left| \frac{b_y^2\beta}{\omega_y^3(\omega + \omega_y)} + \left(\alpha + iT_1\frac{\omega^2}{\omega_y^2}\right) \right| \right|} = \\
&= \sqrt{\left(\frac{b_y^2\beta}{\omega_y^3(\omega + \omega_y)} + \alpha\right) \left/ \left| \frac{b_y^2\beta}{\omega_y^3(\omega + \omega_y)} + \left(\alpha + i\frac{L}{P}\right) \right| \right|}
\end{aligned}$$

times less in this time period. For the tunneling effect to have an affect, the time T_1 must be no less than the (large) tunneling time, i.e., $T_1 \geq T$ or

$$\frac{L\omega_y^2}{P\omega^2} \geq \frac{\pi\sqrt{\pi e}}{\omega'_1} e^{\pi J(\tilde{E}(h))/\hbar} \iff J(\tilde{E}(h)) \leq \frac{\hbar}{\pi} \log\left(\frac{L\omega_y^2\omega'_1}{\pi\sqrt{\pi e}P\omega^2}\right).$$

Of course, the packet “spreading” in the variable x should not be too strong. A more detailed analysis of the relations between the parameters P , α , L , ω , b_x , b_y , and a clarifying the situation of simultaneous “not strong spreading” and tunneling will be discussed in subsequent publications. We now only note that the actual small parameter in the considerations related to tunneling is the parameter $h\omega$, and it is natural to assume that ω is a large quantity for nanowires. Moreover, the packet parameters α and P can take different values that are not related to h , ω , a , b_x , and b_y , and precisely this permits choosing appropriate parameters of the problem.

The general conclusion about the influence of the magnetic field on the tunneling effects for the wave packets is that the magnetic field either completely destroys the tunneling (if $b_z \neq 0$) or, in accordance with the conclusions in Sec. 3, decelerates the tunneling as the component b_x increases (this component corresponds to the variable b in this section) and accelerates this effect as the component b_y increases (this component increases together with the variable $\omega_y^2 = b_y^2 + \omega^2$ corresponding to ω_2^2 in the notation in Sec. 3).

6. Conclusion

We have shown that the problem of the splitting of lower levels for the Schrödinger operator with a constant magnetic field with a special double-well-type potential in the two-dimensional case is reducible to the well-studied spectral problem for the Schrödinger operator with the magnetic field appearing only as a parameter of the scalar potential. We used the methods and formulas developed for the usual Schrödinger operator in the double-well potential to calculate the exponential splitting of energy levels for the initial problem and their dependence on the magnetic field. We used the obtained formulas to analyze the effects of wave-packet tunneling in a double quantum wire (doubled quantum waveguide).

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