

SPLITTING OF THE LOWEST ENERGY LEVELS OF THE SCHRÖDINGER  
EQUATION AND ASYMPTOTIC BEHAVIOR OF THE FUNDAMENTAL SOLUTION  
OF THE EQUATION  $h u_t = h^2 \Delta u / 2 - V(x)u$

S. Yu. Dobrokhotov, V. N. Kolokol'tsov,  
and V. P. Maslov

For the equation  $h \partial u / \partial t = h^2 \Delta u / 2 - V(x)u$  with positive potential  $V(x)$ , global exponential asymptotic behavior of the fundamental solution is obtained by the method of the tunnel canonical operator. In the case of a potential with degenerate points of global minimum, the behavior of the solutions to the Cauchy problem is investigated at times of order  $t = h^{-(1+\kappa)}$ ,  $\kappa > 0$ . The developed theory is used to obtain exponential asymptotics of the lowest eigenfunctions of the Schrödinger operator  $-h^2 \Delta / 2 - V(x)$  and to estimate the tunnel effect.

1. Introduction

This paper, which develops ideas of [1-5], is devoted to the  $h \rightarrow 0$  asymptotic behavior of different Cauchy problems for the parabolic equation

$$h \frac{\partial u}{\partial t} = \frac{1}{2} h^2 \Delta u - V(x)u, \quad x \in \mathbf{R}^n, \quad (1.1)$$

with smooth potential  $V(x)$  and the investigation of tunnel effects for the lowest energy states in the spectral problem for the Schrödinger equation

$$-1/2 h^2 \Delta u + V(x)u = Eu, \quad u \in L_2(\mathbf{R}^n). \quad (1.2)$$

In the second case, it is assumed that  $V(x) \geq 0$  and that there is a finite number of points at which  $V$  vanishes.

In probability theory and quantum mechanics there are interesting problems that are based on the same mathematical constructions. These are problems of large deviations and tunnel effects for the lowest energy states. From the point of view of specialists on differential equations, they are characterized by the presence of a small parameter  $h$  and exponential smallness with respect to  $h$  of the corresponding solutions at almost all points of the configuration space. The connection between such problems arises from the following elementary and well-known considerations. Consider Eq. (1.1). Suppose the potential  $V(x)$  is a non-negative function that increases as  $|x| \rightarrow \infty$ . Then the spectrum of the operator  $-1/2 h^2 \Delta + V(x)$  in  $Z_2(\mathbf{R}^n)$  is discrete, and if we denote by  $\{\psi_k\}$  and  $\{E_k\}$  the corresponding orthonormalized eigenfunctions and eigenvalues, then for the solution of the Cauchy problem (1.1),  $u|_{t=0} = u_0(x)$ , we have the formula

$$u = \sum_{k=0}^{\infty} c_k e^{-E_k t / h} \psi_k, \quad c_k = (\psi_k, u_0) = \int_{\mathbf{R}^n} \psi_k u_0 dx. \quad (1.3)$$

If the Fourier coefficient  $c_0 \neq 0$ , then multiplying the expansion for the function  $u$  by  $e^{E_0 t / h}$  and letting  $t$  tend to  $\infty$ , we obtain

$$\psi_0 = \lim_{t \rightarrow \infty} (u e^{E_0 t / h}) / (u_0, \psi). \quad (1.4)$$

It is on this formula and its analogs that the connection between the Cauchy problem for the time-dependent equation (1.1) and the spectral problem (1.2) is based. It is clear that the solution of the Cauchy problem for Eq. (1.1), like the solution of the problem (1.4), can be found only in exceptional cases, and for arbitrary potential  $V(x)$  analytic expressions can be obtained only asymptotically. Under the assumption that  $V(x) \geq 0$ , the

fundamental solution for  $t > 0$  of the Cauchy problem  $u|_{t=0} = \delta(x-\xi)$  for Eq. (1.1) and the eigenfunctions of the problem (1.2) corresponding to eigenvalues  $E(h) \rightarrow 0$  as  $h \rightarrow 0$  are exponentially small as  $h \rightarrow 0$  at almost all points of the configuration space and are given almost everywhere by the expressions

$$u = h^{-n/2} e^{-S(x,t)/h} (\varphi(x,t) + O(h)), \quad t > \delta > 0, \quad (1.5)$$

$$\psi = h^{-n/2} e^{-S(x)/h} (\varphi(x) + O(h)), \quad (1.6)$$

where  $S, \varphi$  are continuous functions,  $S \geq 0$ .

The absence of oscillations in the asymptotic behavior of the fundamental solution is a characteristic of the tunnel-type equations introduced and investigated by one of the authors of this paper in [1-3]. Besides the parabolic equation (1.1), these equations also include the Kolmogorov-Feller equation, some equations in the theory of viscoelastic media (Voigt model), the system of linearized Navier-Stokes equations, etc. For some of them, for example, the parabolic equation and the Kolmogorov-Feller equation, Varadhan [7] and Borovkov obtained logarithmic asymptotic behaviors  $\lim_{h \rightarrow 0} h \ln u$  (see [8]) or asymptotic

behaviors of the form (1.5); however, this was under the assumption that there are no focal points in the asymptotics.

One of the main results of this paper is the proof of the fact that the constructed asymptotics are valid not only at the "standard" times for asymptotic theory,  $t \sim O(1)$  (as  $h \rightarrow 0$ ) but also at "very large" times  $t \sim h^{-1-\alpha}$ ,  $1 > \alpha > 0$ . It is this result that allows us to make a rigorous transition from the asymptotic behavior of the fundamental solution of Eq. (1.1) to asymptotic behaviors of eigenfunctions of the Schrödinger operator that enable us to pick up the tunnel effects.

Let us explain this in more detail. Suppose that  $\xi$  is a nondegenerate point of minimum of the potential  $V(x)$ ,  $V(0) = 0$ . Then, since the potential  $V$  in the neighborhood of  $\xi$  can be approximated by the potential of a harmonic oscillator,  $V_{\text{osp}} = \langle x - \xi, \frac{\partial^2 V(\xi)}{\partial x^2} (x - \xi) \rangle$ , we can find a series of asymptotic eigenfunctions and eigenvalues of the original operator  $-\frac{1}{2}h^2\Delta + V(x)$ , and their leading terms will be identical to the eigenfunctions and eigenvalues of the quantum harmonic oscillator. In particular, the lowest eigenvalue and corresponding (asymptotic) eigenfunction have the form

$$E_0 \cong \frac{h}{2} \sum_{j=1}^n \omega_j, \quad \psi_0 \cong \frac{1}{(\pi h)^{n/4} \sqrt{\omega_1 \dots \omega_n}} e^{-S(x)/h}, \quad S = \frac{1}{2} \left\langle x - \xi, \sqrt{\frac{\partial^2 V}{\partial x^2}(\xi)} (x - \xi) \right\rangle, \quad (1.7)$$

where  $\omega_1, \dots, \omega_n > 0$ ;  $\omega_j^2$  are the eigenvalues of the matrix  $\partial^2 V(\xi) / \partial x^2$ .

The expressions (1.7), as approximations for the eigenfunctions and eigenvalues of the operator  $-\frac{1}{2}h^2\Delta + V(x)$ , have long and productively been used in physics problems, but accurate arguments that bring out the connection between the eigenfunctions and eigenvalues of the quantum harmonic oscillator and the operator  $-\frac{1}{2}h^2\Delta + V(x)$  were given in a recent study by Simon [9]. For completeness, we also give here the corresponding investigations (Sec. 7) that differ somewhat from [9] and are based on the variational principle. Note that despite the exponential decrease of the function  $\psi_0$  (1.7) this formula has only a power-law asymptotic behavior with respect to  $h$  for the genuine eigenfunctions of the operator  $-\frac{1}{2}h^2\Delta + V(x)$ , and this is quite insufficient if we want to obtain the tunnel effects.

Suppose the potential  $V(x)$  is symmetric (either with respect to the point  $x = 0$ , or with respect to some plane) and has two points of global minimum  $\xi_{\pm}$ . Then near the minimal eigenvalue  $E_0$  of the operator  $-\frac{1}{2}h^2\Delta + V(x)$  there is an eigenvalue  $E_1$  that differs from  $E_0$  by an amount exponentially small in the parameter  $h$ . We have the expressions

$$E_0 = \frac{h}{2} \sum_{j=1}^n \omega_j + O(h^2), \quad E_1 = \frac{h}{2} \sum_{j=1}^n \omega_j + O(h^2), \quad E_2 - E_1 = A \exp\left(-\frac{1}{h} \int_{\xi_-}^{\xi_+} p \, dx\right). \quad (1.8)$$

Here,  $p(t) = \dot{X}$ ,  $x = X(t)$  is the trajectory of the Newtonian system

$$\ddot{x} = -V_x \quad (1.9)$$

that connects the points  $\xi_-$  and  $\xi_+$ :  $x(\mp\infty) = \xi_{\mp}$  (if there are several such trajectories, then on the right-hand side we take the minimum over all trajectories). The function  $A(h)$  can also be found in terms of the solutions  $X(t)$  and variational systems with respect to

(1.9). The trajectory  $X(t)$  is called an instanton. Note that it is determined from a Newtonian system that differs from the ordinary classical system corresponding to the quantum problem (1.2),  $\ddot{x} = -V_x$ , by reversal in the sign of the potential  $V$  or transition from the real time  $t$  to the "imaginary" time  $it$ . Formula (1.8) first appeared in the book [5] and in [10-11] (in these last, only the argument of the exponential was calculated) and was then actively used in quantum field theory. The bulk of this work related either to the one-dimensional case  $x \in \mathbb{R}^1$  (see [11-16]) or the infinite-dimensional (continuum) case (see the review in [17]). An accurate justification in the  $n$ -dimensional case appeared in [2,18] and then in a somewhat more general situation in [19]. A stimulating role in the appearance of the studies [18,19] was played by Witten's elegant paper [20], which uncovered deep connections between certain problems of physics and mathematics.

Our first aim in this paper is to expound in more detail, sometimes differently and in a more general situation, the results of [2]; in particular, we derive (1.8), including an expression for  $A$  (absent in [18]). Our derivation, which is based on the asymptotics "at large times" of the fundamental solution of Eq. (1.1), is quite different from the methods of [18], which are based on Feynman integrals and the Agmon metric.

We describe the key points of the paper and the main heuristic arguments.

1. In Sec. 2, we give the asymptotic behavior of the fundamental solution of the parabolic equation for small  $t$ . Generalizing the construction of the WKB solutions and the exact fundamental solution  $V = \exp[-(x-\xi)^2/2th]/(\pi\hbar t)^{n/2}$  of the parabolic equation  $V_t = \hbar\Delta V$ , we seek a solution of (1.1) in the form

$$u = \frac{1}{(\pi\hbar)^{n/2}} e^{-S(x,t)/\hbar} (\varphi_0(x,t) + \hbar\varphi_1(x,t) + \dots).$$

The standard procedure of the WKB method (or zeroth method) leads to the Hamilton-Jacobi equations  $S_t + (\nabla S)^2/2 - V(x) = 0$  (but, by virtue of the purely imaginary action  $-iS$  they have "inverted" potential  $V$ ) and the transport equation  $\varphi_{0t} + \nabla S \nabla \varphi_0 + \Delta S \varphi_0/2 = 0$ . The initial conditions for  $S$  and  $\varphi_0$  are chosen from the condition  $u \rightarrow \delta(x - \xi)$  as  $t \rightarrow 0$  and with allowance for the formula for  $V$  have the form  $S|_{t=0} \rightarrow (x-\xi)^2/2t$ ,  $\varphi_0|_{t=0} \rightarrow t^{-n/2}$ . The corresponding solutions  $S$  and  $\varphi$  can be expressed in terms of the solutions of the variational problem and trajectories of the Newtonian system (1.9). For the difference between the exact solution and the asymptotic behavior  $u|_{\text{in}} = e^{-S/\hbar}\varphi/(\pi\hbar)^{n/2}$  we obtain an estimate that is important for what follows:

$$|u - u|_{\text{in}}| = e^{-S/\hbar}\varphi O(\hbar^3).$$

2. The global asymptotic behavior of the fundamental solution of Eq. (1.1) (with allowance for focal points) is given by means of the tunnel canonical operator, which is constructed in Sec. 3. Here, we give a geometric approach to the studied asymptotics (Lagrangian manifolds). There is the well-known difficulty in constructing the asymptotic behavior of  $u$  at large  $t$  due to the appearance of focal points, this leading, in particular, to the appearance of regions in the configuration space in which the function  $S$  becomes multiply valued. One of the important considerations in "tunnel" problems is that, in contrast to "ordinary" semiclassical asymptotics, only one term contributes to the result. It is the one corresponding to the branch of the function  $S(x, t)$  that at the given point  $x$  takes minimal value compared with the other branches of  $S$ .

3. In Sec. 4, we give a global construction of the asymptotics of the fundamental solution of Eq. (1.1). In Sec. 5, we prove one of the central propositions of the paper — a theorem which establishes the validity of the obtained asymptotics at "very large" times  $t \sim \hbar^{-(1+\kappa)}$ ,  $1 > \kappa > 0$ . This proof is based on repeated application of Laplace's method and makes essential use of (1.10). Here, we give solutions of special Cauchy problems for Eq. (1.1) (large deviation problems), which are then used in the spectral problem (1.2).

4. The transition from the solutions of the Cauchy problem for the time-dependent equation (1.1) to the solutions (1.2) is based (Sec. 6), as we have already noted, on formula (1.4), in which we take in place of infinitely large times values of the time  $t = \hbar^{-(1+\kappa)}$ . This is sufficient for, on the one hand, to omit from the eigenfunction expansion all the functions except those corresponding to eigenvalues in a neighborhood  $O(\hbar^2)$  of the

lowest energy value of the harmonic oscillator,  $E_0 = \frac{\hbar}{2} \sum_{j=1}^n \omega_j$ , and, on the other, to go to the

limit  $t \rightarrow \infty$  in the leading term of the asymptotic behavior  $e^{-S(x,t)/h}\varphi(x,t)$  of the fundamental solution. This procedure, which takes into account the existence in the problem of the two large parameters  $t$  and  $1/h$ , leads to determination of the asymptotic behaviors of the necessary eigenfunctions of the operator  $-\frac{1}{2}h^2\Delta + V(x)$ . The use of these functions in the expressions for the splitting of the lowest energy values, which are analogous to those in Chap. 8 of [21], gives formula (1.8) and analogous expressions for a large number of wells.

In Sec. 7, analogous results are obtained for the case when the configuration space is a torus, in particular, a circle. In Sec. 8, we analyze some examples, and in Sec. 9, as already noted, we justify the use of the oscillator approximation. Finally, since in our arguments we use very special estimates of the Laplace method, which are not found in standard treatises, we give in Sec. 10 the Laplace method with corresponding estimates.

## 2. Asymptotics in the Small of the Fundamental

### Solution of the Cauchy Problem for the Heat

#### Conduction Equation with Potential

We consider the equation

$$h \frac{\partial u}{\partial t} = \frac{h^2}{2} \Delta u - V(x)u, \quad x \in \mathbb{R}^n, \quad t \geq 0, \quad (2.1)$$

where  $h$  is a positive parameter,  $\Delta$  is the Laplacian, and the potential  $V(x)$  is a sufficiently smooth non-negative function with bounded matrix of second derivatives:

$$\left\| \frac{\partial^2 V}{\partial x_i \partial x_j} \right\| \leq C \quad \text{for all } x \in \mathbb{R}^n \text{ and fixed } C.$$

We construct the  $h \rightarrow 0$  asymptotics of the fundamental solution of the Cauchy problem for this equation, i.e., a solution  $u(t, x) = u(t, x, \xi, h)$  that satisfies the initial condition

$$u(t, x, \xi, h) = \delta(x - \xi). \quad (2.2)$$

We first find this asymptotic behavior at small times  $t$ . For this, we need some estimates and identities satisfied by the solutions of the variational system for the Newtonian equations.

We define the Hamiltonian  $H(x, p) = p^2/2 - V(x)$  and denote by  $X(t, x, p)$ ,  $P(t, x, p)$  the solutions of the Hamiltonian system

$$\dot{x} = p, \quad \dot{p} = -\frac{\partial V}{\partial x} \quad (2.3)$$

with initial condition  $X(0, x, p) = x$ ,  $P(0, x, p) = p$ . By virtue of the conditions given on  $V$ , these solutions are defined, as is well known [3,13], for all  $t$ .

We shall need the following well-known (see, for example, [6]) proposition. There exists a  $t_0$  sufficiently small that  $\det \partial X / \partial p \neq 0$  for all  $t \leq t_0$ , and for all  $x, \xi \in \mathbb{R}^n$  there exists and is unique a solution of the Hamiltonian system (2.3) with boundary conditions  $X(0) = \xi$ ,  $X(t) = x$ . At the same time, on this curve there is realized a minimal value of the functional

$$\int_0^t \left( \frac{1}{2} \dot{y}^2(\tau) + V(y(\tau)) \right) d\tau, \quad (2.4)$$

which is defined on continuous piecewise smooth curves with fixed ends  $y(0) = \xi$ ,  $y(t) = x$ . We denote the minimal value of the functional (2.4) by  $S(t, x, \xi)$ .

We introduce  $p_0(t, x, \xi)$ , a momentum such that  $X(t, \xi, p_0(t, x, \xi)) = x$ , and Jacobian

$$J(t, x, \xi) = \det \frac{\partial X}{\partial p}(t, \xi, p_0(t, x, \xi)).$$

We formulate the main result of this section (see also [23-25]).

**THEOREM 1.** If  $V(x)$  has bounded, in  $\mathbb{R}^n$ , derivatives of fourth order, then for  $t \in (0, t_0)$  the solution to the problem (2.1)-(2.2) has the form

$$u(t, x, \xi, h) = (2\pi h)^{-n/2} J(t, x, \xi)^{-1/2} \exp\left\{-\frac{1}{h} S(t, x, \xi)\right\} (1 + O(ht^3)), \quad (2.5)$$

where  $O(ht^3)$  uniformly with respect to all  $x, \xi \in \mathbb{R}^n$ .

If  $V$  possesses derivatives of order higher than the fourth, then the function  $O(ht^3)$  in (2.5) still remains a function of the form  $O(ht^3)$  after differentiation with respect to  $x$  or  $\xi$ .

If  $V(x)$  is infinitely differentiable, then for every  $M \in \mathbb{N}$

$$u(t, x, \xi, h) = (2\pi h)^{-n/2} J(t, x, \xi)^{-1/2} \exp\left\{-\frac{1}{h} S(t, x, \xi)\right\} \times \\ (1 + h\psi_1 + h^2\psi_2 + \dots + h^M\psi_M + O(h^{M+1}t^{M+3})), \quad (2.6)$$

where the functions  $\psi_j$  are defined by the recursion relations

$$\psi_j(t, x, \xi) = \frac{1}{2} \int_0^t J^{1/2} \Delta(\psi_{j-1} J^{-1/2}) d\tau \quad (2.7)$$

(here  $\psi_0 \equiv 1$ , the integral is taken along the trajectory  $X(\tau, \xi, p_0(t, x, \xi))$ , and the Laplacian is applied to the argument  $x$ ) and satisfies the estimates  $\psi_j = O(t^{j+2})$ ,  $j \geq 1$ .

We first prove some helpful auxiliary propositions. In the space of continuous matrix-valued functions on the interval  $[0, t]$  we define linear operators  $G_1, G_2$  by the formulas

$$(G_1 F)(t) = \int_0^t \left( \int_0^\tau V_{xx}''(s) F(s) ds \right) d\tau, \quad (G_2 F)(t) = \int_0^t \left( V_{xx}''(\tau) \int_0^\tau F(s) ds \right) d\tau.$$

**LEMMA 1.** The norms of the operators  $G_1, G_2$  are bounded above by  $t^2 C/2$  and for small  $t \leq t_0$  do not exceed unity. For these  $t$ , the derivatives of the solutions of the system (2.3) with respect to the initial data are given by

$$\frac{\partial X}{\partial x}(t, x, p) = (\text{Id} - G_1)^{-1} E = (\text{Id} + G_1 + G_1^2 + \dots) E, \\ \frac{\partial X}{\partial p}(t, x, p) = (\text{Id} - G_1)^{-1} t E, \quad \frac{\partial P}{\partial p}(t, x, p) = (\text{Id} - G_2)^{-1} E, \\ \frac{\partial P}{\partial x}(t, x, p) = (\text{Id} - G_2)^{-1} \int_0^t V_{xx}''(\tau) d\tau.$$

Here,  $E$  is the unit  $n \times n$  matrix, and  $\text{Id}$  is the identity operator. In particular,

$$\frac{\partial X}{\partial p}(t, x, p) = t(E + O(t^2)), \quad \frac{\partial P}{\partial p}(t, x, p) = E + O(t^2), \quad (2.8)$$

where  $O(t^2)$  uniformly with respect to all  $t \leq t_0$ ;  $x, p \in \mathbb{R}^n$ .

The proof follows from the standard [26] representation of the solution of the variational system

$$A = \begin{pmatrix} 0 & E \\ V_{xx}''(X(\tau, x, p)) & 0 \end{pmatrix} A, \quad A(0) = \begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix}$$

which is satisfied by the  $2n \times 2n$  matrix  $A(t) = \frac{\partial(X, P)}{\partial(x, p)}$  in the form of a series of a time-ordered exponential.

We recall that the functions  $S, P, X$  satisfy the following well-known identities [3,27]:

$$\frac{\partial^2 S}{\partial x^2}(t, x, \xi) = \frac{\partial P}{\partial p}(t, \xi, p_0(t, x, \xi)) \left( \frac{\partial X}{\partial p}(t, \xi, p_0(t, x, \xi)) \right)^{-1}, \quad (2.9)$$

$$\frac{\partial^2 S}{\partial \xi^2}(t, x, \xi) = \left( \frac{\partial X}{\partial p}(t, \xi, p_0(t, x, \xi)) \right)^{-1} \frac{\partial X}{\partial x}(t, \xi, p_0(t, x, \xi)). \quad (2.10)$$

Let  $t_1 + t_2 \leq t_0$ . We introduce the function  $f(\eta) = S(t_1, x, \eta) + S(t_2, \eta, \xi)$ . We denote

$$\bar{\eta} = X(t_2, \xi, p_0(t_1+t_2, x, \xi)), \quad \bar{p}_\eta = P(t_2, \xi, p_0(t_1+t_2, x, \xi)), \quad p_0 = p_0(t_1+t_2, x, \xi) = p_0(t_2, \bar{\eta}, \xi).$$

**LEMMA 2.** The following matrix equation holds:

$$\frac{\partial X}{\partial p}(t_1+t_2, \xi, p_0) = \frac{\partial X}{\partial p}(t_1, \bar{\eta}, \bar{p}_\eta) f'' \frac{\partial X}{\partial p}(t_2, \bar{\eta}, \xi). \quad (2.11)$$

In particular,

$$\det f'' = J(t_1+t_2, x, \xi) J^{-1}(t_1, x, \bar{\eta}) J^{-1}(t_2, \bar{\eta}, \xi). \quad (2.12)$$

**Proof.** We represent the mapping  $X(t_1 + t_2, \xi, p)$  as a composition of mappings:  $(\xi, p) \rightarrow (\eta = X(t_2, \xi, p), p_\eta = P(t_2, \xi, p))$  and  $(\eta, p_\eta) \rightarrow X(t_1, \eta, p_\eta)$ . Then

$$\frac{\partial X}{\partial p}(t_1+t_2, \xi, p) = \frac{\partial X}{\partial p}(t_1, \eta, p_\eta) \frac{\partial X}{\partial p}(t_2, \xi, p) + \frac{\partial X}{\partial p}(t_1, \eta, p_\eta) \frac{\partial P}{\partial p}(t_2, \xi, p).$$

For  $p = p_0$  we have  $\eta = \bar{\eta}$ ,  $p_\eta = \bar{p}_\eta$ . Substituting in the last expression the values of  $\partial X/\partial x$  and  $\partial P/\partial p$  expressed in terms of  $\frac{\partial^2 S}{\partial x^2}(t_1, x, \eta)$  and, respectively,  $\frac{\partial^2 S}{\partial \xi^2}(t_2, \eta, \xi)$  by means of the identities (2.9) and (2.10), we obtain (2.11), which is what we needed to prove.

**LEMMA 3.**

$$\frac{\partial^2 S}{\partial x^2}(t, x, \xi) = \frac{1}{t}(E + O(t^2)), \quad (2.13)$$

$$J(t, x, \xi) = t^n(1 + O(t^2)), \quad (2.14)$$

where  $O(t)$  uniformly with respect to all  $t \leq t_0$ ,  $x, \xi \in \mathbb{R}^n$ ;

$$\frac{\partial^m J}{\partial x^{m_1} \partial \xi^{m_2}} = O(t^{n+2}), \quad m = m_1 + m_2, \quad (2.15)$$

$$\frac{\partial^{(m+2)}}{\partial x^{m+2}} S(t, x, \xi) = O(t) \quad (2.16)$$

for the  $m \geq 1$  for which there exist continuous derivatives of  $V$  of order  $m + 2$ , and  $O(t^{n+2})$  and  $O(t)$  uniformly with respect to  $x, \xi$  in any compact set (and uniformly with respect to all  $x, \xi \in \mathbb{R}^n$  if the corresponding derivatives of the function  $V$  are bounded in  $\mathbb{R}^n$ ).

The proof follows from the formulas of Lemma 1 and the identity (2.9).

Note that from (2.13) we obtain the equation

$$S(t, x, \xi) = \frac{(x-\xi)^2}{2t}(1 + O(t^2)) + S(t, \xi, \xi) + \left( \frac{\partial S}{\partial x}(t, \xi, \xi), x-\xi \right),$$

and therefore

$$S(t, x, \xi) = \frac{(x-\xi)^2}{2t}(1 + O(t^2)) + O(t)(1 + \|x-\xi\|), \quad (2.17)$$

where  $O(t)$  uniformly with respect to  $\xi$  in any compact set and all  $x \in \mathbb{R}^n$ .

**Proof of Theorem 1.** Consider the function

$$G(t, x, \xi, h) = (2\pi h)^{-n/2} \varphi(t, x, \xi) \exp\left\{-\frac{1}{h} S(t, x, \xi)\right\}, \quad (2.18)$$

where  $\varphi = J^{-1/2}$ . We obtain directly from the estimates (2.14) and (2.17) that  $\lim_{h \rightarrow 0} G(t, x, \xi, h) = \delta(x-\xi)$ , i.e.,  $G$  satisfies the initial condition (2.2). It is well known [27] that  $S(t, x, \xi)$  satisfies the Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t} + \frac{1}{2} \left( \frac{\partial S}{\partial x} \right)^2 - V(x) = 0,$$

and the function  $\varphi = J^{-1/2}$  satisfies the transport equation

$$\frac{\partial \varphi}{\partial t} + \frac{\partial \varphi}{\partial x} \frac{\partial S}{\partial x} + \frac{1}{2} \varphi \Delta S = 0.$$

Substituting  $G$  in (2.1) and differentiating, we obtain

$$\left[ h \frac{\partial}{\partial t} - \left( \frac{h^2}{2} \Delta - V(x) \right) \right] G = -h^2 F,$$

where

$$F = \frac{1}{2} (2\pi h)^{-n/2} \Delta \varphi \exp \left\{ -\frac{1}{h} S(t, x, \xi) \right\}. \quad (2.19)$$

It follows from the estimates (2.15) that  $\Delta \varphi = O(t^2) \varphi$ , and hence

$$F(t, x, \xi, h) = O(t^2) G. \quad (2.20)$$

Thus,  $G$  is a formal asymptotic solution of the problem (2.1)-(2.2).

We show that the exact solution of the problem (2.1)-(2.2) can be represented in the form of the convergent series

$$u(t, x, \xi, h) = G(t, x, \xi, h) + \sum_{k=0}^{\infty} h^{k+1} \int_0^t \int_{\mathbb{R}^n} G(t-\tau, x, \eta, h) \mathbf{F}^k(\tau, \eta, \xi, h) d\eta d\tau, \quad (2.21)$$

where  $\mathbf{F}^k$  is the  $k$ -th power of the integral operator  $\mathbf{F}$ , which is defined by the kernel  $\mathbf{F}$  in accordance with

$$(\mathbf{F}\psi)(t, x, \xi, h) = \int_0^t \int_{\mathbb{R}^n} F(t-\tau, x, \eta, h) \psi(\tau, \eta, \xi, h) d\eta d\tau.$$

It is easy to show that the series is well defined for small  $h$  and gives a function of the form  $G(t, x, \xi, h)(1 + O(ht^3))$ , where  $O(ht^3)$  uniformly with respect to all  $x, \xi$  in any compact set and all  $t \leq t_0$ . For this, it is necessary to estimate successively the results of applying the operators  $\mathbf{F}$  by means of Lemma 10 (from Sec. 10), using at the same time the identity (2.12), the estimates from Lemma 3, and the estimate

$$\int_{\mathbb{R}^n} \exp \{ -S(t-\tau, x, \eta) - S(\tau, \eta, \xi) + S(t, x, \xi) \} d\eta = O(1) \left( \frac{\pi \tau (t-\tau)}{t} \right)^{n/2},$$

which follows from the fact that the expression in the curly brackets does not exceed

$O(1) \left( \frac{1}{\tau} + \frac{1}{t-\tau} \right) (\eta - \eta_0)^2$ . The required asymptotic properties of the derivatives of the function  $u$  can be verified in the same way. To verify that (2.21) determines a solution of Eq. (2.1), we note that

$$\left[ h \frac{\partial}{\partial t} - \left( \frac{h^2}{2} \Delta - V(x) \right) \right] \mathbf{F}G = -h^2 \mathbf{F}F + hF,$$

and therefore

$$\left[ h \frac{\partial}{\partial t} - \left( \frac{h^2}{2} \Delta - V(x) \right) \right] u = -h^2 F - \sum_{k=1}^{\infty} h^{k+2} \mathbf{F}^k F + \sum_{k=0}^{\infty} h^{k+2} \mathbf{F}^k F = 0.$$

Thus, the representation (2.21) has been proved.

To obtain the expression (2.6), we first find a formal asymptotic WKB solution to the problem (2.1)-(2.2) of the necessary accuracy. This is done in the usual manner (as, for example, for the Schrödinger equation in [27]), and this gives formulas (2.7). The further demonstration is exactly as before.

### 3. Tunnel Canonical Operator

The global exponential asymptotic behavior of the Green's function of Eq. (2.1) is determined by the tunnel canonical operator introduced below. We use facts from symplectic geometry and the theory of Lagrangian manifolds; these can be found, for example, in [27].

We recall that the simply connected manifold  $\Lambda$  in a  $2n$ -dimensional phase space  $\mathbb{R}^{2n} = \mathbb{R}_x^n \times \mathbb{R}_p^n : \Lambda = \{ r(\alpha) = (p(r(\alpha)), x(r(\alpha))) \}$ ,  $\alpha \rightarrow r(\alpha)$ , is said to be Lagrangian if on it the Lagrange brackets vanish or, which is the same thing, if on  $\Lambda$  there is defined a function

$$S(r) = \int_{r_0}^r p dx, \quad r \in \Lambda,$$

where the integral is taken along any curve lying on  $\Lambda$  ( $r_0$  is a fixed point of  $\Lambda$ ). Suppose the function  $S(r)$  is non-negative. Then we shall call  $S(r)$  the entropy of the manifold  $\Lambda$ .

Suppose on  $\Lambda$  there is defined a measure  $d\mu = \mu(\alpha)d\alpha$ . We call the function  $J = \det \frac{\partial x}{\partial \alpha} \mu(\alpha)$  the Jacobian on  $\Lambda$ . We recall that the point  $r$  on  $\Lambda$  is called a focal (singular) point if  $J = 0$ ; otherwise it is nonsingular. In what follows, we shall assume that if the focal point  $\tilde{r}$  is a zero of the entropy  $S$  then  $\tilde{r}$  is an isolated zero of  $S$ .

We call  $r$  an inessential point of  $\Lambda$  if there exists another point  $r' \in \Lambda$  with the same projection onto  $\mathbf{R}_x^n$  and such that the entropy at it is less than at  $r$ .

We construct an operator  $K$ , which carries functions on  $\Lambda$  to functions defined on  $\mathbf{R}_x^n$ . It is this operator that will determine the global asymptotic behavior of the fundamental solution of Eq. (2.1) and some other solutions of it.

We first define the action of the tunnel operator in the neighborhood of nonsingular points of  $\Lambda$ .

Suppose  $\Omega$  is a nonsingular chart on  $\Lambda$ , i.e., a chart such that the Jacobian  $J$  is nonvanishing for all points of  $\Omega$ . We denote by  $D \subset \mathbf{R}_x^n$  the set  $\pi_x(\Omega^c)$ , where  $\pi_x$  is the natural projection from  $\mathbf{R}^{2n}$  to  $\mathbf{R}_x^n$ ,  $\Omega^c$  is the closure of the set of essential points of the region  $\Omega$ , and by  $D^\gamma \subset \mathbf{R}_x^n$  the  $\gamma$  neighborhood of the set  $D$ , i.e., the neighborhood such that  $|x - x'| \geq \gamma$  for all  $x \in \mathbf{R}_x^n \setminus D^\gamma$ ,  $x' \in D$ . We introduce a smooth function  $\theta(x, \gamma)$  that is equal to unity for  $x \in D^\gamma$  and zero for  $x \in \mathbf{R}_x^n \setminus D^{2\gamma}$ . Let  $\varphi(r, h) \in C_0^\infty(\Omega) \forall h \geq 0$  (smooth function of compact support). We define the operator  $K(\Omega)$  by

$$(K(\Omega)\varphi)(x) = |J^\gamma|^{-1/2} \exp\left\{-\frac{1}{h} S^\gamma\right\} \varphi(r(x), h) \theta(x, \gamma), \quad (3.1)$$

where  $r(x) \in \Lambda$  solves the system  $x = x(r)$ , and  $J^\gamma$  and  $S^\gamma$  are smooth functions equal to  $J$  and  $S$  on  $D$ . Of course, the function  $K(\Omega)\varphi$  depends on  $\gamma$ ,  $\theta(x, \gamma)$ , and the ways in which  $J$  and  $S$  are extended to  $J^\gamma$  and  $S^\gamma$ .

At the singular points, the expression (3.1) has singularities, and it cannot be used in calculating the asymptotic solutions. In the neighborhood of singular points, we shall use other expressions based on a choice of coordinates different from  $(p, x)$  in the phase space.

Namely, let  $I$  be a certain set of indices in  $\{1, \dots, n\}$ ,  $H_I = \frac{1}{2} \sum_{j \in I} p_j^2$ ,  $g_{H_I}^{-\sigma}$  is the phase-space shift during time  $\sigma$  along the trajectory of the Hamiltonian flow with Hamiltonian  $-H_I$ . Let  $\sigma > 0$  be so small that the region  $g_{H_I}^{-\sigma} \Omega$  is still projected in a single-valued manner onto  $\mathbf{R}_x^n$ , so that as coordinates on  $g_{H_I}^{-\sigma} \Omega$ , whose points we shall denote by  $r^\sigma$ , we can take the projections  $x(r^\sigma)$  of its points on  $\mathbf{R}_x^n$ :  $x_I(r^\sigma) = x_I(r) - \sigma p_I$ ,  $x_{\bar{I}}(r^\sigma) = x_{\bar{I}}(r)$ . Here  $x_i = (x_{j_1}, \dots, x_{j_n})$ ,  $j_i \in I$ ;  $x_{\bar{i}} = (x_{j_{h+1}}, \dots, x_{j_n})$ ,  $j_{h+1} \in \bar{I}$ ;  $\bar{I} = \{1, \dots, n\} \setminus I$ ,  $x = (x_I, x_{\bar{I}})$  determine the projections of the points of  $\Omega$  onto  $\mathbf{R}_x^n$ ,  $(p_I, p_{\bar{I}})$  are the projections of the points of  $\Omega$  onto  $\mathbf{R}_p^n$ . As the Lagrangian manifold is displaced along the trajectories of the Hamiltonian flow its entropy and Jacobian are transformed in a natural (from the point of view of Hamiltonian mechanics) manner:

$$S(r^\sigma) = S(r) + \int_0^\sigma (p dx + H_I dt),$$

where the integral is taken along trajectories that connect the initial point  $r$  on  $\Omega$  and the displaced  $r^\sigma(r)$ ,

$$J(r^\sigma(r)) = \mu(\alpha) \det \frac{\partial x(r^\sigma)}{\partial \alpha}.$$

In the given case

$$S(r^\sigma(r)) = S(r) - \frac{\sigma}{2} p_I^2(r), \quad J(r^\sigma(r)) = J(r) \det \frac{\partial x(r^\sigma)}{\partial x(r)} = J(r) \det \left( E - \sigma \frac{\partial^2 S_I}{\partial x_I^2} \right),$$



since in nonsingular charts, as is well known, the coordinates  $p$  and  $x$  are connected by the equation  $p = \partial S / \partial x$ .

In the new coordinates  $x_I(r^\sigma), x_I(r^\sigma)$  we can again write down the expression (3.1), but this formula will give a new function. To "compensate" the transition to the new coordinates in the phase space, we correct this new function, by applying to it the resolving operator  $\exp\{-\sigma \hat{H}_I\}$  of the Cauchy problem for the  $k$ -dimensional heat conduction equations. This operation leads to definition of the "inverted" local operator  $\tilde{K}(\Omega)$ :

$$\begin{aligned} (\tilde{K}(\Omega)\varphi)(x) &= \exp\{-\sigma \hat{H}_I\} (K(g_{H_I}^{-\sigma}\Omega)\varphi)(x) \equiv \\ &= (2\pi h\sigma)^{-k/2} \int_{\mathbb{R}^k} \exp\left\{-\frac{|\eta - x_I|^2}{2h\sigma}\right\} (K(g_{H_I}^{-\sigma}\Omega)\varphi)|_{x_I=\eta} d\eta \end{aligned} \quad (3.2)$$

(the function  $\varphi$  on  $g_{H_I}^{-\sigma}\Omega$  is determined by its values on  $\Omega$ :  $\varphi(r^\sigma) = \varphi(r)$ , the essential points on  $g_{H_I}^{-\sigma}\Omega$  are assumed to be the images of the essential points in  $\Omega$ ).

**LEMMA 4.** Let  $\varphi$  and  $\tilde{\varphi}$  be smooth functions of compact support on  $\Omega$  such that at the essential points of the chart  $\Omega$  the difference  $\varphi(r, h) - \tilde{\varphi}(r, h)$  has order  $O(h)$ . Then at the points  $x \in \Omega^\circ$

$$(\tilde{K}(\Omega)\tilde{\varphi})(x) = K(\Omega)(\varphi + O(h))(x).$$

**Proof.** By the definition of  $K(g_{H_I}^{-\sigma}\Omega)$

$$\begin{aligned} (\tilde{K}(\Omega)\tilde{\varphi})(x) &= (2\pi h\sigma)^{-k/2} \int_{\mathbb{R}^k} \exp\left\{-\frac{|\eta - x_I|^2}{2h\sigma}\right\} \times \\ & \times \left[ \exp\left\{-\frac{1}{h}\left(S - \frac{\sigma}{2} p_I^2\right)(r^\sigma)\right\} \theta(x, \gamma) \varphi(r^\sigma(x)) J(r^\sigma(x))^{-1/2} \det \frac{\partial x(r^\sigma)}{\partial x(r)} \right] \Big|_{x_I(r^\sigma)=\eta} d\eta. \end{aligned} \quad (3.3)$$

Here  $\theta(x, h)$  is a smooth function of compact support equal to unity in a  $\gamma$  neighborhood of  $\pi_x(g_{H_I}^{-\sigma}\Omega)^\circ$ . To calculate this integral, we use the Laplace method. For this we find the point  $\eta$  at which the derivative of the pre-exponential vanishes:

$$\begin{aligned} \bar{S} &= \frac{(\eta - x_I)^2}{2\sigma} + \left(S - \frac{\sigma}{2} p_I^2\right)(r^\sigma) \Big|_{x_I(r^\sigma)=\eta}, \\ \frac{\partial \bar{S}}{\partial \eta} &= \frac{\eta - x_I}{\sigma} + \left[ \frac{\partial S}{\partial x_I} \left(E - \frac{\sigma}{2} \frac{\partial p_I}{\partial x_I}\right) \left(\frac{\partial x_I(r^\sigma)}{\partial x_I(r)}\right)^{-1} \right] \Big|_{x_I(r^\sigma)=\eta} = \frac{\eta - x_I}{\sigma} + \frac{\partial S}{\partial x_I}(r^\sigma) \Big|_{x_I(r^\sigma)=\eta}. \end{aligned} \quad (3.4)$$

From the condition of vanishing of this expression, we find

$$\eta = x_I + \sigma \frac{\partial S}{\partial x_I}(r^\sigma) \Big|_{x_I(r^\sigma)=\eta},$$

and hence for  $x \in \pi_x \Omega$  there exists a unique  $\eta$  that satisfies this equation:  $\eta(x) = x_I(r^\sigma(r(x)))$ .

We calculate the second derivative of the pre-exponential:

$$\begin{aligned} \frac{\partial^2 \bar{S}}{\partial \eta^2} &= \frac{1}{\sigma} + \frac{\partial^2 S}{\partial x_I^2}(r^\sigma) \left(\frac{\partial x_I(r^\sigma)}{\partial x_I(r)}\right)^{-1} \Big|_{x_I(r^\sigma)=\eta} = \\ &= \frac{1}{\sigma} \left(\frac{\partial x(r^\sigma)}{\partial x(r)} + \frac{\partial^2 S}{\partial x_I^2}(r^\sigma) \sigma\right) \left(\frac{\partial x_I(r^\sigma)}{\partial x_I(r)}\right)^{-1} \Big|_{x_I(r^\sigma)=\eta} = \frac{1}{\sigma} \left(\frac{\partial x(r^\sigma)}{\partial x(r)}\right)^{-1} \Big|_{x_I(r^\sigma)=\eta}, \end{aligned}$$

since

$$\frac{\partial x(r^\sigma)}{\partial x(r)} = E - \sigma \frac{\partial^2 S}{\partial x_I^2}$$

whence, in particular, it follows that  $\eta(x)$  is a nondegenerate minimum point of  $\bar{S}(\eta)$ . Substituting the critical value of  $\eta(x)$  in the expression (3.4) for  $\bar{S}$ , we immediately find  $\bar{S}(\eta(x)) = S(x)$ . We now have everything ready to write down the asymptotic behavior of the integral (3.3) by the Laplace method (for  $x \in \pi_x(\Omega^\circ)$ ):

$$\begin{aligned} (\tilde{K}(\Omega)\varphi)(x) &= (2\pi h\sigma)^{-k/2} (2\pi h)^{k/2} \exp\left\{-\frac{1}{h} S\right\} \times \\ & \times \left(\sigma^k \det \left(\frac{\partial x(r^\sigma)}{\partial x(r)}\right)\right)^{1/2} \theta(x(r^\sigma(r(x))), \gamma) J(r(x))^{-1/2} \det \left(\frac{\partial x(r)}{\partial x(r^\sigma)}\right)^{1/2} (\tilde{\varphi}(r(x)) + O(h)). \end{aligned}$$

After obvious cancellations, we obtain

$$\tilde{K}(\Omega)\tilde{\varphi}(x)=\theta(x(r^\sigma(r(x))),\gamma)(\tilde{\varphi}(r(x))+O(h))J(r(x))^{-1/2}\exp\left\{-\frac{1}{h}S\right\},$$

i.e., at the points  $x\in\Omega^c$

$$\tilde{K}(\Omega)\tilde{\varphi}=K(\Omega)(\varphi+O(h)),$$

as we needed to prove.

This lemma suggests a way of defining a local operator in the neighborhood of a singular point. As is known from symplectic geometry (see [3,27]), in the neighborhood of any such point  $r$  on  $\Lambda$  there exist focal coordinates  $(p_I, x_{\bar{I}})$ , where  $I\subset\{1, \dots, n\}$ ,  $\bar{I}=\{1, \dots, n\}\setminus I$ ,  $(p_I, x_{\bar{I}})$  are sets of projections of the points of  $\Lambda$  onto the corresponding coordinate axes in  $\mathbf{R}^{2n}$ , and the least possible power  $|I|$  of the set  $I$  is equal to the corank of the matrix  $\partial x(r)/\partial \alpha$ . It is readily seen that for any singular point there exists a neighborhood  $\Omega$  in  $\Lambda$  with focal coordinates  $(p_I, x_{\bar{I}})$  and number  $\sigma > 0$  such that the transformation  $\Omega \rightarrow g_{HI}^{-\sigma}\Omega$  carries it to a position in which it is uniquely projected onto  $\mathbf{R}_x^n$ , and the function  $\tilde{S}(\eta)$  of the form (3.4) is non-negative for  $x\in\pi_x\Omega$ . For such a neighborhood  $\Omega$  we define a local tunnel operator in accordance with (3.2). As in the lemma, we can prove that the operator defined in this way is invariant (in the same sense as in the lemma) with respect to the magnitude of  $\sigma$  and its direction specified by the set  $I$ , and also the other parameters that occur in its definition. The global tunnel operator is determined by a resolution of the identity in the same way as for an ordinary canonical operator [27],

namely, we choose a canonical atlas of charts on  $\Lambda: \Lambda = \bigcup_{j=1}^{\infty} \Omega_j$ , such that to each singular

chart  $\Omega_j$  there correspond focal coordinates  $(p_I, x_{\bar{I}})$  and number  $\sigma_j$  satisfying the conditions listed above and necessary for definition of the local operator  $K(\Omega_j)$ ; let  $\{e_j(r)\}$  be the resolution of the identity on  $\Lambda$  corresponding to the chosen atlas. Then the tunnel canonical operator is defined as the mapping  $C_0^\infty(\Lambda \times [0, 1]) \rightarrow C^\infty(\mathbf{R}_x^n[0, 1])$  by the formula

$$K\varphi = \sum_j K(\Omega_j)(e_j\varphi).$$

We introduce equivalence ratios on  $C^\infty(\mathbf{R}_x^n)$ : the functions  $g, h \in C^\infty(\mathbf{R}_x^n)$  are equivalent if  $g - h$  belongs to the space of functions of the form  $K\varphi$ , where  $\varphi$  is  $O(h)$  in  $\pi_x(\Lambda^c)$  (this subspace is well defined and does not depend on the parameters that specify  $K$ ). Note that for functions that do not vanish on  $\pi_x(\Lambda^c)$  and have the form  $K\varphi$  and  $K\psi$  in the image of  $K$  this equivalence is equivalent to the equation  $K\varphi/K\psi=1+O(h)$ . We denote by  $\Phi$  the corresponding factor space. From the arguments we have given, the lemma, and its analog for singular charts we conclude that the following theorem holds.

**THEOREM 2.** The tunnel canonical operator

$$K: C_0^\infty(\Lambda \times [0, 1]) \rightarrow \Phi$$

does not depend on the choice of the canonical atlas, the resolution of the identity, and the parameters  $\sigma$  and  $\gamma$  that define the local operator.

**Remark 1.** Let  $\Lambda^0$  be a certain Lagrangian manifold in  $\mathbf{R}_x^n \times \mathbf{R}_p^n: \Lambda = \{(x, p) \in \mathbf{R}^{2n}: x = x(\alpha), p = p(\alpha), \alpha \in \mathbf{R}^n\}$  with positive measure  $d\mu(\alpha) = \mu(\alpha) d\alpha_1, \dots, d\alpha_n$  and non-negative entropy  $S_0$ , and  $H(x, p)$  be a Hamilton function such that its Lagrangian is non-negative. Then on the Lagrangian manifold  $g_H^\dagger \Lambda^0 = \Lambda^\dagger$  shifted along the characteristics of the Hamiltonian flow  $g_H^\dagger$  there are naturally defined the transported measure  $d\mu_\dagger$  and the (also non-negative) entropy  $S^\dagger$  in accordance with

$$S^\dagger(r) = S^0(r_0) + \int_0^t \left( p(\tau) \frac{\partial H}{\partial p}(\tau) - H(p(\tau), x(\tau)) \right) d\tau, \quad (3.5)$$

where  $r \in \Lambda^\dagger$  is the image of  $r_0 \in \Lambda^0$  under displacement along the solutions  $p(\tau), x(\tau)$  of the Hamiltonian system; the integral is taken along this solution. It is known [27] that the function defined in this manner on  $\Lambda^\dagger$  is the generating function of this manifold.

**Remark 2.** In some important cases the tunnel operator is defined not only on finite functions but also on all bounded (smooth) functions on  $\Lambda$ . It is readily seen that this holds when the Lagrangian manifold satisfies the additional condition of "properness":

for every  $x \in \mathbb{R}^n$  the set  $\{p \in \mathbb{R}^n : (x, p) \in \Lambda\}$  is compact. This property holds for the manifolds  $\Lambda^{t, \xi}$  introduced in what follows for  $t > 0$ ; they play a special role in the theory.

#### 4. Global Asymptotic Behavior of the Fundamental Solution and the Problem of Large Deviations

The tunnel canonical operator introduced above makes it possible to express in general form the exponential asymptotic behavior for the Green's function of the problem (2.1) at an arbitrary time.

We denote by  $\Lambda^{t, \xi}$  the Lagrangian manifold obtained by displacement of the plane  $\Lambda^{0, \xi} = \{(p, x) : x = \xi\}$  along the trajectories of the Hamiltonian system (2.3) during the time  $t$ . We assume that on  $\Lambda^{0, \xi}$  the entropy is zero and the measure in the coordinates  $p \in \mathbb{R}^n$  is unity, and that on  $\Lambda^{t, \xi}$  these objects are determined by means of the displacement (see Remark 1 above). We denote by  $K^{t, \xi}$  the tunneling canonical operator on  $\Lambda^{t, \xi}$ .

**THEOREM 3.** A. Suppose there exists a finite number  $k$  of trajectories  $X(\tau, \xi, p_j)$  that connect the points  $\xi, x$  during the time  $t$  and realize a minimum of the functional (2.4) equal to  $S(t, x, \xi)$ . Then the solution of the problem (2.1)–(2.2) at these  $t, x$  has the form

$$u(t, x, \xi, h) = (2\pi h)^{-n/2} \exp\left\{-\frac{1}{h} S(t, x, \xi)\right\} \sum_{j=1}^k J_j^{-1/2}(t, x, \xi) (1 + O(h)), \quad (4.1)$$

where  $J_j$  is the Jacobian along the trajectory  $X(\tau, \xi, p_j)$ .

B. In the general case, the solution  $u(t, x, \xi, h)$  is determined by the formula

$$u(t, x, \xi, h) = (2\pi h)^{-n/2} K^{t, \xi}(1 + O(h)). \quad (4.2)$$

**Proof.** At small  $t$ , this theorem follows directly from (2.5) and the definition of the canonical operator. For  $t \in ((m-1)t_0, mt_0]$  the solution (2.1)–(2.2) can be represented in the form

$$u(t, x, \xi, h) = G_\tau^m \delta(x - \xi) = G_\tau^{m-1} u(\tau, x, \xi, h), \quad (4.3)$$

where  $\tau = t/m \in (0, t_0]$ ,  $G_\tau^m$  is the power of the operator,

$$(G_\tau \varphi)(x, \xi, h) = \int_{\mathbb{R}} u(\tau, x, \eta, h) \varphi(\eta, \xi, h) d\eta. \quad (4.4)$$

If  $X$  is not a focal point of the manifold  $\Lambda^{t, \xi}$ , then there exists a finite number  $\tilde{r}$  of trajectories  $X_r(\tau) = X(\tau, \xi, p_r)$  of the Hamiltonian system (2.3) that connect  $\xi$  and  $x$  during the time  $t$  and realize a minimum of the entropy. It then follows from Laplace's method that to within exponentially small quantities the solution (4.3) is equal to the sum of  $\tilde{r}$  terms of the form

$$\int_{V_j^1} \dots \int_{V_j^{m-1}} u(\tau, x, \eta_1, h) \dots u(\tau, \eta_{k-1}, \xi, h) d\eta_1 \dots d\eta_{k-1}, \quad (4.5)$$

where  $V_j^\ell$  is a small neighborhood of the point  $X_j(\ell\tau)$  such that from  $\xi$  to every point of  $V_j^\ell$  there leads only one trajectory that realizes a minimum of the functional (2.4) during the time  $\ell\tau$ . In (4.3), we replace all the functions  $u$  by formal asymptotic solutions  $G$ . Then the expression (4.3) is changed by  $O(h)$ . Calculating now successively the integrals with respect to  $d\eta_\ell$ ,  $\ell = 1, \dots, k-1$ , by Laplace's method, and using the identity (2.12), we obtain (4.1).

But if  $x$  is the projection of an essential focal point, then direct application of Laplace's method to (4.3) is impossible, since the stationary points are degenerate. In this case, we use the following device. Employing Lemma 4, we write the integral kernel of the last operator in (4.3) in the form (3.2)–(3.3), where the subset  $I$  is chosen in such a way that the rotated neighborhood  $g_{HI}^{-\sigma} \Omega$  of the focal point  $r(x)$  in  $\Lambda^{t, \xi}$  is uniquely projected onto  $\mathbb{R}^n$ . Then, for  $m = 2$ , say, (4.3) can be rewritten in the form

$$u(t, x, \xi, h) = (2\pi h \sigma)^{-k/2} \int_{\mathbb{R}^k} \exp\left\{-\frac{(\eta - x_I)^2}{2h\sigma}\right\} \times$$

$$\int_{\mathbf{R}^n} \exp \left\{ -\frac{1}{h} (\mathcal{S}(r(r^\sigma)) + S(\tau, z, \xi)) \right\} \theta(x, \gamma) J^{-1/2}(r(r^\sigma(x))) J(\tau, z, \xi)^{-1/2} \Big|_{x_I(r^\sigma)=\eta} dz d\eta,$$

where

$$\mathcal{S}(r(r^\sigma)) = \left( S - \frac{\sigma}{2} \left( \frac{\partial S}{\partial x_I} \right)^2 \right) (\tau, x(r(r^\sigma(\eta, x_I))), z)$$

is the transformed phase on the manifold  $g_H^\sigma \Lambda^{\tau, \xi}$  in the neighborhood of the point  $x$ . Calculating now the integral with respect to  $z$  by Laplace's method, we obtain, as in the previous situation, (4.2). This argument completes the proof of the theorem.

The solution to the Cauchy problem of a linear equation with arbitrary initial function is given, as is well known, by the convolution of this initial function with the fundamental solution. Using this fact, we find an asymptotic expression for the solution to the problem of large deviations. This is the name given to the Cauchy problem for the equation (2.1) with initial data

$$u|_{t=0} = \varphi^0(x), \quad (4.6)$$

where  $\varphi^0(x)$  is a discontinuous function that does not vanish in a certain closed bounded region  $D_0 \subset \mathbf{R}_x^n$ ,  $\varphi^0(x) \equiv 0$  outside  $D_0$  and  $\varphi^0(x) \in C^\infty(D_0)$ , and the boundary  $\partial D_0$  is smooth. As was noted above, the solution of this problem is determined by virtue of Theorem 3 by the formula

$$u(t, x, h) = (2\pi h)^{-n/2} \int_{\mathbf{R}^n} K(1 + O(h))(t, x, \xi, h) \varphi^0(\xi) d\xi, \quad (4.7)$$

where  $K = K^{\tau, \xi}$  is the tunnel canonical operator on the family of Lagrangian manifolds  $\Lambda^{\tau, \xi}$ . We denote by  $D_t$  the projection onto  $\mathbf{R}_x^n$  of the image of the region  $\{p=0, x \in D_0\}$  under the action of the Hamiltonian flow (2.3). It can be shown that for all  $x \in \mathbf{R}_x^n$  not lying on the boundary  $\partial D_t$  of  $D$  the integral (4.7) can be calculated by Laplace's method.

**THEOREM 4.** The solution to the Cauchy problem (2.1), (4.6) has the following form:

A. For  $x \in D_t \setminus \partial D_t$

$$u(t, x, \xi, h) = K_{in}^t(\varphi^0(\xi(g_H^t(r)))) + O(h), \quad (4.8)$$

where  $K_{in}^t$  is the tunnel canonical operator constructed on the Lagrangian manifolds  $\Lambda_{in}^t = g_H^t\{p=0\}$ , the images under the action of the Hamiltonian flow of the plane  $\{p=0\}$  in  $\mathbf{R}_x^n \times \mathbf{R}_p^n$ , on which the measure and the Jacobian have unit values:  $d\mu = d\xi^1 \dots d\xi^n$ ,  $J = 1$ , and the entropy is zero, so that on  $\Lambda_{in}^t$  the Jacobian  $J = \det \frac{\partial X}{\partial \xi}(t, \xi, 0)$ , while the entropy is calculated in accordance with formula (3.5) along the solutions  $X(\tau, \xi, 0)$  of the system (2.3) with initial data  $X(0) = \xi$ ,  $P(0) = 0$ .

B. For  $x \in \mathbf{R}_x^n \setminus D_t$

$$u(t, x, h) = \left( \frac{h}{2\pi} \right)^{n/2} K_{out}^t(\rho(r)^{-1} \varphi^0(g_H^{-t}(r))) + O(h),$$

where  $K_{out}^t$  is constructed on the Lagrangian manifolds  $\Lambda_{out}^t = g_H^t \Lambda_{out}^t$ ,  $\Lambda_{out}^0 = \{p = \rho n(x), x \in \partial D_0, \rho \in \mathbf{R}^1, n(x)$  is the vector of the unit outer normal to  $\partial D_0$  at the point  $x\}$  and on  $\Lambda_{out}^0$  the entropy is zero and the Jacobian unity,  $d\mu = d\rho d\alpha_1 \dots d\alpha_{n-1}$ ;  $\alpha_1, \dots, \alpha_{n-1}$  are orthonormalized curvilinear coordinates on the manifold  $\partial D_0$  with unit metric tensor, and  $\rho(r)$  is determined by the relation  $\rho(r)n(g_H^{-t}r) = p(g_H^{-t}r)$ .

The proof is obtained by direct calculation in accordance with Laplace's method of integrals of the form

$$\int_{\mathbf{R}_\xi^n} K(\Omega_j)(e_j \varphi^0(\xi)) d\xi,$$

where  $\{\Omega_j\}$  is a canonical atlas on  $\Lambda^{\tau, \xi}$ , and in case A the point of minimum of the phase is an inner point of the region, and in case B it is a boundary point; for calculations in the neighborhood of focal points, the device from the proof of the previous theorem should be used.

## 5. Asymptotic Behavior of the Solutions at Large

Times (of Order  $h^{-(1+\kappa)}$ ,  $\kappa > 0$ )

Suppose the potential  $V(x)$  satisfies the following additional conditions:  $V(x) \rightarrow \infty$  as  $|x| \rightarrow \infty$  and  $V(x)$  vanishes only at a finite number of points (of global minimum)  $\xi_1, \dots, \xi_t$ , at which the matrix of second derivatives  $V''(x)$  is nondegenerate. We denote the eigenvalues of the matrix  $V''(\xi_k)$  by  $(\omega_j^k)^2$ :  $\omega_j^k > 0$ ,  $j = 1, \dots, n$ . Under these conditions on  $V$ , we investigate in this section the asymptotic behavior of solutions of the problems (2.1), (4.6) (or (2.1) and (2.2)) at "large" times  $t$  of order  $h^{-(1+\kappa)}$ ,  $\kappa > 0$ , and also the  $t \rightarrow \infty$  limits of their logarithmic asymptotic behaviors. First, we study some properties of the solutions of the Hamilton-Jacobi equation and the Hamiltonian system in the case of the Hamiltonian  $H = \frac{1}{2}p^2 - V(x)$  when the potential has the indicated properties.

We recall that the resulting operator of the Cauchy problem for the Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t} + \frac{1}{2} \left( \frac{\partial S}{\partial x} \right)^2 - V(x) = 0, \quad S|_{t=0} = S_0(x) \quad (5.1)$$

is the mapping  $R_t$  that associates the initial function  $S_0$  with the solution  $S = R_t S_0$  of the problem at the time  $t$ . It is well known that the resulting operator of the problem (5.1) is defined on the set of functions bounded below by the formula (see, for example, [28,29])

$$(R_t S_0)(x) = \inf_{\xi} (S_0(\xi) + S(t, x, \xi)). \quad (5.2)$$

The semigroup of nonlinear operators  $R_t$  is uniquely determined by the following properties [28,30]: a) for small  $t$  and smooth convex initial functions  $S_0(x)$  the function  $(R_t S_0)(x)$  is a classical, i.e., everywhere smooth, solution of the Cauchy problem; b) the operators  $R_t$  are continuous in a certain natural topology on the space of functions that are bounded below; c) the operators  $R_t$  commute with the operations of taking the minimum of functions and adding constants, i.e.,

$$R_t(\min(S_1, S_2)) = \min(R_t S_1, R_t S_2), \quad R_t(\lambda + S(x)) = \lambda + R_t S(x). \quad (5.3)$$

At the same time, the image  $R_t S$  of any function (bounded below) at points of differentiability satisfies the Hamilton-Jacobi equation. It follows directly from the expression (5.2) for  $R_t$  that this image for  $t > 0$  is always locally Lipschitz continuous and, therefore, almost everywhere differentiable.

We recall that the function  $S(t, x, \xi)$  in (5.2) was introduced at the beginning of Sec. 2 and denotes a lower bound of the functional

$$J(y(\cdot)) = \int_{-t}^0 (\frac{1}{2} \dot{y}^2(\tau) + V(y(\tau))) d\tau, \quad (5.4)$$

which is defined on continuous piecewise smooth curves parametrized by a segment of length  $t > 0$  with fixed ends  $y(-t) = \xi$ ,  $y(0) = x$ . It is well known that under the conditions imposed on the potential at the beginning of Sec. 2 the minimum of the functional (5.4) is always realized on a smooth curve [6]. This fact is readily deduced from the remark that since for small  $t$  (less than a certain fixed  $t_0$ ) the minimum of (5.4) is realized on a unique smooth curve; for arbitrary  $t$  the minimum with respect to piecewise smooth curves is identical to the minimum with respect to the set of piecewise smooth curves whose derivatives have not more than  $t/t_0$  discontinuities at fixed times  $kt_0$ ,  $k \in \mathbb{N}$ ,  $k \leq t/t_0$ . Note also the symmetry of the function  $S$ :  $S(t, x, y) = S(t, y, x)$  for all  $t, x, y$ . This fact follows from the invariance of Newton's system with respect to time reversal.

We introduce functions that are important for what follows:

$$S_k(x) = \inf \{S(t, x, \xi_k) : t \geq 0\}, \quad k=1, \dots, l, \quad (5.5)$$

and also their minimum

$$S(x) = \min \{S_k(x), k=1, \dots, l\}. \quad (5.6)$$

It is clear that the function  $S(t, x, \xi_k)$  for fixed  $\xi_k, x$  monotonically does not increase with respect to  $t$ , since rest at  $\xi_k$  (a zero of the potential) does not increase the value of the functional (5.4). Therefore

$$S_k(x) = \lim_{t \rightarrow \infty} S(t, x, \xi_k). \quad (5.7)$$

In addition, the functions  $S_k(x)$  are everywhere non-negative, since the functional (5.4) takes only positive values, and  $S_k(x) = 0 \Leftrightarrow x = \xi_k$ . We need above all the following facts about these functions.

**PROPOSITION 1.** The functions  $S_k(x)$ ,  $k = 1, \dots, l$ , and  $S(x)$  are fixed points of the resolving operator (5.2) of the Cauchy problem (5.1).

**PROPOSITION 2.** If  $x$  is such that

$$S_k(x) < \min_{j \neq k} (S_j(x) + S_k(\xi_j)), \quad (5.8)$$

then the limit in (5.7) is realized on a smooth curve, i.e., there exists a smooth curve  $q: (-\infty, 0] \rightarrow \mathbb{R}^n$  such that

$$S_k(x) = \int_{-\infty}^0 (1/2 \dot{q}^2(t) + V(q(t))) dt, \quad (5.9)$$

and

$$q(0) = x, \quad \lim_{t \rightarrow -\infty} q(t) = \xi_k, \quad \lim_{t \rightarrow -\infty} \dot{q}(t) = 0.$$

**Proof of Proposition 1.** From the definition (5.2) of the operator  $R_t$  and the monotonicity with respect to  $t$  of the function  $S(t, x, \xi_k)$  we obtain successively

$$R_t S_k(x) = \inf_{\xi} \inf_{\tau \geq 0} (S(\tau, \xi, \xi_k) + S(t, x, \xi)) = \inf_{\tau \geq 0} S(t + \tau, x, \xi_k) = \inf_{\tau \geq 0} S(\tau, x, \xi_k) = S_k(x).$$

It now follows from (5.3) that  $R_t$  does not change under the action of (5.3).

**Proof of Proposition 2.** We fix  $k \in \{1, \dots, l\}$ ,  $x \in \mathbb{R}^n$ , satisfying (5.8). From the above very simple properties of the functions  $S_k(x)$  and  $S(t, x, \xi)$  it follows that there exists a sequence  $\{q_m(t)\}$  of solutions of the Hamiltonian system (2.3) parametrized by time intervals  $[-T_m, 0]$  ( $T_m \rightarrow \infty$  as  $m \rightarrow \infty$ ) such that  $q(-T_m) = \xi_k$ ,  $q(0) = x$ , and on  $q_m$  a minimum of the functional (5.4) is realized, i.e.,  $J(q_m(\cdot)) = S(T_m, x, \xi_k)$ . We obtain the existence of a limiting trajectory in several stages:

A. For every  $j \neq k$  there exists a neighborhood  $U_j$  of the point  $\xi_j$  such that from a certain number (in what follows, when going over to a subsequence, we shall assume that we begin from the first) none of the trajectories  $q_m$  intersect  $U_j$ . Indeed, supposing otherwise for arbitrary  $\varepsilon$ , and using the continuity of  $S_j(x)$  (which follows from the properties of the resolving operator  $R_t$  and Proposition 1), we construct a neighborhood  $U_j$  of the point  $\xi_j$  such that in it  $S_j(y) < \varepsilon$ . By the assumption, there exist trajectories with arbitrarily large number  $m$  for which  $y_m = q_m(-t_m) \in U_j$  for some  $t_m$ . Therefore

$$S(T_m, x, \xi_k) = S(t_m, x, y_m) + S(T_m - t_m, y_m, \xi).$$

But  $S(t, x_1, x_2) \geq S_j(x_1) - S_j(x_2)$  for all  $x_1, x_2 \in \mathbb{R}^n$ ,  $j \in \{1, \dots, l\}$  (this inequality is obtained by going to the limit  $\tau \rightarrow \infty$  from the obvious inequality  $S(t, x_1, x_2) > S(t + \tau, x_1, \xi_j) - S(\tau, x_2, \xi_j)$ ). Therefore

$$S(T_m, x, \xi_k) \geq S_j(x) + S_j(\xi_k) - 2S_j(y_m) \geq S_j(x) + S_j(\xi_k) - 2\varepsilon.$$

Going to the limit  $T_m \rightarrow \infty$  and bearing in mind that  $\varepsilon$  is arbitrary we obtain

$$S_k(x) \geq S_j(x) + S_j(\xi_k),$$

which contradicts (5.8).

B. For every neighborhood  $U$  of the point  $\xi_k: x \notin U$  there exists a number  $N$  and times  $t_1 < t_0 < 0$  such that for numbers  $m > N$  the time

$$t_m(U) = \sup\{\tau : q_m(\tau) \in U\}$$

belongs to the interval  $[t_1, t_0]$ . Indeed, on the one hand, the trajectories cannot remain outside  $U$  for an infinitely long time  $t$  (since then the value of the functional on them, which is larger than  $t \cdot \min\{V(y) : y \in U, y \notin U_j, j \neq k\}$ , tends to infinity) and, on the other hand, the trajectories cannot move arbitrarily rapidly from  $x$  to  $U$ , since

$$\min_{y \in U} S(\tau, x, y) \rightarrow \infty \text{ as } \tau \rightarrow 0.$$

C. It follows directly from the arguments of B that the sequences  $t_m(U)$  and  $y_m(U) = q_m(t_m(U))$  belong to compact sets  $[t_1, t_0]$  and  $\partial U$ , respectively. Therefore, these sequences have a limit point, and, going to a subsequence, we can assume that they have a limit. Choosing an arbitrary sequence of numbers  $\varepsilon_p \rightarrow 0$ ,  $p \rightarrow \infty$  and corresponding balls  $B_p$  of radius  $\varepsilon_p$  with center at  $\xi_k$ , we construct (by the diagonal method) a sequence of trajectories  $q_m(\tau)$  such that for  $p \in \mathbb{N}$  the sequences  $t_m(B_p)$  and  $y_m(B_p)$  have limits  $t(p)$  and  $y(p)$ . Using the Arzela-Ascoli theorem, we now choose a subsequence of trajectories  $q_m(\tau)$  such that for every  $p$  the sequence of pieces of trajectories  $q_m(\tau)$ ,  $\tau \in [t(p), 0]$ , converges in the  $C^1$  topology. The limits of these pieces then form together the required limiting trajectory  $q: (-\infty, 0] \rightarrow \mathbb{R}^n$ .

COROLLARY. For all points  $x, y$  there exists the limit

$$\lim_{t \rightarrow \infty} S(t, x, y) = \min_{j, k} (S_k(x) + S_j(y) + S_k(\xi_j)). \quad (5.10)$$

Remark 3. This number is called the Agmon distance between the points  $x, y$ .

We discuss the geometrical meaning of the functions  $S_k(x)$ . Since  $z_k = (\xi_k, 0)$  is a hyperbolic nondegenerate singular point of the Hamiltonian system, there follows from the general theory [31] the existence of stretching and contracting invariant subsets  $W_k^{\text{in}}$  and  $W_k^{\text{out}}$  embedded in  $\mathbb{R}^{2n}$ . The dimension of each of them is  $n$ , since half the eigenvalues of the linear part of the Hamiltonian system in the neighborhood of  $z_k$  are positive and the other half negative. The stretching (contracting) manifold is defined as the set of points  $(x, p) \in \mathbb{R}^{2n}$  such that the trajectories of the system omitted from them tend to  $z_k$  as  $t \rightarrow -\infty$  (respectively, as  $t \rightarrow +\infty$ ). In the given case, both these manifolds are Lagrangian, since they are invariant under the action of the Hamiltonian flow, which is a group of symplectic transformations, so that the bracket of two tangent vectors at a point in, for example,  $W_k^{\text{out}}$ , is, on the one hand, invariant under the action of the flow and, on the other, tends to zero as  $t \rightarrow -\infty$  and, hence, is equal to zero.

PROPOSITION 3. In the region distinguished by the inequality (5.8), the function  $S_k(x)$  is the generating function (or entropy) of the stretching Lagrangian manifold  $W_k^{\text{out}}$  in its essential part, normalized to zero at  $z_k = (\xi_k, 0)$  (the essential part of a Lagrangian manifold was defined in Sec. 3).

Proof. The generating function of the manifold  $W_k^{\text{out}}$ , normalized to zero at  $z_k$  is given by

$$\sigma(z) = \int_{z_k}^z p dq,$$

where the integral is taken along any curve in  $W_k^{\text{out}}$  that connects  $z_k$  and  $z = (x, p)$ . Choosing as such a curve the trajectory  $z(t) = (x(t), p(t))$  of the Hamiltonian system with boundary conditions  $z(-\infty) = z_k$ ,  $z(0) = z$  (such a definition exists in accordance with the definition of  $W_k^{\text{out}}$ ), we see that

$$\sigma(z) = \int_{-\infty}^0 \left( \frac{1}{2} \dot{x}^2(t) + V(x(t)) \right) dt.$$

Therefore, in the essential part of  $W_k^{\text{out}}$  we have  $\sigma(z) = S_k(x)$ , as we needed to prove. From this in particular there follows smoothness of  $S_k(x)$  in the neighborhood of the point  $\xi_k$ . Note also that in Proposition 2 we have essentially proved the existence of an invariant stretching manifold in the given case.

PROPOSITION 4. On  $W_k^{\text{out}}$  there is defined the smooth measure  $d\mu$ , which is related to the Hamiltonian flow by the condition

$$d\mu(z_t) = \exp\left(\sum_{j=1}^n \omega_j^k t\right) d\mu(z_0), \quad (5.11)$$

where  $z_t$  is the image of  $z_0 \in W_k^{\text{out}}$  under the action of the flow (2.3).

Proof. The existence of this measure follows from the theory of normal forms of systems of ordinary differential equations in the neighborhood of isolated attractive (or repulsive) fixed points applied to the flow (2.3) on  $W_k^{\text{out}}$ . Indeed, in the nonresonance case, i.e., when every number  $\omega_j^k$  (we recall that  $(\omega_j^k)^2$  are eigenvalues of the matrix  $V''(\xi_k)$ )

is different from any linear combination of the form  $\sum_{i \neq j} v_i \omega_i^h$ , where  $v_i$  are natural numbers

such that  $\sum_{i \neq j} v_i \geq 2$ , the system (2.3) on  $W_k^{\text{out}}$  is in accordance with [22] linearizable, i.e., in a small neighborhood of the singular point on  $W_k^{\text{out}}$  there exist coordinates  $\mu = (\mu_1, \dots, \mu_n)$  that depend smoothly on  $(x, p)$  and in which the system (2.3) has the linear form

$$\mu_j(t) = \exp\{\omega_j^h t\} \mu_j(0), \quad j=1, \dots, n.$$

Then obviously

$$\det \frac{\partial \mu(t)}{\partial \mu(0)} = \exp\left\{t \sum_{j=1}^n \omega_j^h\right\}. \quad (5.12)$$

Therefore, the coordinates  $\mu$  determine in the neighborhood of the fixed point a measure  $d\mu$  on  $W_k^{\text{out}}$  that satisfies (5.11). It is clear that this measure can be naturally extended to a measure on the whole of  $W_k^{\text{out}}$  with retention of (5.11). In the case when resonance relations are present, the system cannot be linearized even locally by a smooth transformation (in this situation, a linearizing transformation can be chosen in general only in the class of nonsmooth homeomorphisms [22,31]). However, there always exists a polynomial normal Poincaré form [32]. It is easy to show that the coordinates  $\mu$  specifying this form satisfy as before (5.12) and, hence, determine the necessary measure satisfying (5.11).

It is clear that the measure on  $W_k^{\text{out}}$  with condition (5.11) is uniquely defined up to a constant factor. We shall find it convenient to choose a measure  $\mu$  that, besides (5.11), satisfies the following normalization: at a fixed point  $z = (\xi_k, 0)$

$$\det \left( \frac{\partial \mu}{\partial x} \right) = 1. \quad (5.13)$$

Remark 4. If  $V$  is analytic, then the coordinates  $\mu$  can be calculated by means of Dirichlet series, the coefficients of which are found from recursion relations [2,5].

At the nonsingular points of  $W_k^{\text{out}}$  we now define the Jacobian

$$J_k = \det \left( \frac{\partial x}{\partial \mu} \right). \quad (5.14)$$

We denote by  $D^k$  the neighborhood of the point  $\xi_k$  distinguished by the inequalities

$$S_k(x) \leq \min \{S_j(x), j \neq k\} \quad (5.15)$$

(obviously  $x \in D^k$  satisfies (5.8)). Let  $\Omega^k$  be a smooth Lagrangian manifold with edge such that  $\Omega^k \subset W_k^{\text{out}}$ ,  $\Omega^k$  contains all essential points of  $W_k^{\text{out}}$  projected to a certain  $\gamma$  neighborhood of the region  $D^k$  ( $\gamma$  is an arbitrary small positive parameter) and does not contain points above a  $2\gamma$  neighborhood of  $D^k$ . We denote by  $K_{st}^k$  the tunnel canonical operator constructed from  $\Omega^k$  with the phase  $S_k$  and Jacobian  $J_k$  above introduced on it. This operator will play the main part in the following constructions.

We turn to the Cauchy problem (2.1), (4.6).

PROPOSITION 5. Suppose the potential  $V$  satisfies the conditions listed at the beginning of the section, the initial function  $\varphi^0$  in (4.6) is the characteristic function of the bounded region  $D$  with smooth boundary

$$u|_{t=0} = \varphi^0(x) = \begin{cases} 1, & x \in D, \\ 0, & x \notin D. \end{cases} \quad (5.16)$$

and all  $\xi_1, \dots, \xi_k$  belong to the interior of  $D$ . Then at all points  $x \in \mathbb{R}^n$  there exists a limit as  $t \rightarrow \infty$  of the first term of the logarithmic asymptotic behavior of the solution to the problem (2.1), (5.16). This limit does not depend on  $D_0$  and has the form

$$\lim_{t \rightarrow \infty} \lim_{h \rightarrow 0} (h \ln u) = -S(x). \quad (5.17)$$

Proof. It follows from Theorem 4 that

$$\lim_{h \rightarrow 0} (h \ln u) = -\sigma(t, x),$$



where

$$\sigma(t, x) = \int_0^t \left( \frac{1}{2} \dot{y}^2(\tau) + V(y(\tau)) \right) d\tau, \quad (5.18)$$

$y(\tau) = X(\tau, \xi(t, x), p_0(t, x))$  is the trajectory of the Hamiltonian (Newtonian) system (2.3) that connects the points  $\xi(t, x)$  and  $x$  and satisfies the conditions: a)  $\dot{y}|_{\tau=0} = 0$ , if  $x \in D_i \setminus \partial D_i$  (then  $\xi(x, t) \in \text{int } D_i$ ); b) the vector  $\dot{y}|_{\tau=0}$  is normal to the boundary  $\partial D_0$  at the point  $\xi(t, x)$  if  $x \in \mathbb{R}^n \setminus D_i$  (then  $\xi(t, x) \in \partial D_0$ ). By  $y(\tau)$  we understand a trajectory that satisfies one of these conditions and realizes a minimum of the functional (5.4).

It follows from the definitions that

$$0 \leq \sigma(t, x) \leq \min_k S(t, x, \xi_k),$$

and hence

$$\overline{\lim} \sigma(t, x) \leq S(x). \quad (5.19)$$

We denote by  $\tilde{\xi}(t, x)$  the point on the trajectory  $y(\tau)$  that specifies  $\sigma(t, x)$  in accordance with (5.18) at which the function  $V(x)$  has a minimum; we denote by  $\tilde{t}$  the time for which  $y(\tilde{t}) = \tilde{\xi}(t, x)$ . Obviously  $\sigma(t, x) \geq tV(\tilde{\xi}(t, x))$ . Therefore, as  $t \rightarrow \infty$  the point  $\tilde{\xi}(t, x)$  tends to a certain point  $\xi_k$  of global minimum of  $V(x)$  and, hence, in particular

$$\lim_{t \rightarrow \infty} S(t, \tilde{\xi}(t, x), \xi_k) = 0.$$

Hence and from the relations

$$\begin{aligned} S(t, \tilde{\xi}(t, x), \xi_k) + \sigma(t, x) &= S(t, \tilde{\xi}(t, x), \xi_k) + \\ &\left( \int_0^{\tilde{t}} + \int_{\tilde{t}}^t \right) \left[ \frac{1}{2} \dot{y}^2(\tau) + V(y(\tau)) \right] d\tau \geq S_k(2t - \tilde{t}, x, \xi_k) \geq S_k(x) \end{aligned}$$

we obtain the inequality

$$\overline{\lim}_{t \rightarrow \infty} \sigma(t, x) \geq S_k(x) \geq S(x). \quad (5.20)$$

The inequalities (5.19) and (5.20) prove Proposition 5.

In exactly the same way, using the Corollary to Proposition 2, it is possible to obtain the limit of the first term of the logarithmic asymptotic behavior of the fundamental solution to the Cauchy problems for Eq. (2.1).

**PROPOSITION 6.** Under the conditions formulated on the potential

$$\lim_{t \rightarrow \infty} \lim_{h \rightarrow 0} (h \ln u(t, x, \xi, h)) = - \min_{j, k} (S_k(x) + S_j(y) + S_j(\xi_j)),$$

where  $u(t, x, \xi, h)$  is the solution to the problem (2.1)-(2.2).

**PROPOSITION 7.** Under the conditions of Proposition 5,  $x \in \text{int } D^k$

$$\lim_{t \rightarrow \infty} \left[ \exp \left( \frac{t}{2} \sum_{j=1}^n \omega_j^k \right) u_0 \right] = K_{st}^k (1 + O(h)), \quad (5.21)$$

where  $u_0$  is the leading term in the exponential asymptotic behavior of the problem (2.1), (5.16), and  $K_{st}^k$  is the tunnel operator on  $\Omega^k$  introduced above.

**COROLLARY.** If for all  $k = 1, \dots, \ell$  the sums  $\sum_{j=1}^n \omega_j^k$  are the same and equal to  $\mathcal{E}$ , then

$$\lim_{t \rightarrow \infty} \exp \left\{ \frac{t}{2} \mathcal{E} \right\} u_0 = \sum_{k=1}^{\ell} K_{st}^k (1 + O(h)). \quad (5.22)$$

**Proof of Proposition 7.** In accordance with Proposition 5, for each  $x$  and sufficiently large  $t$  the solution to the problem (2.1), (5.16) will be expressed by formula (4.8) of Theorem 3. At the same time, if  $x \in D^k$  is the projection of only nonsingular essential points

of the manifold  $\Omega^k$  (of course, then a finite number of them), then for sufficiently large  $t$  there will over  $x$  be only nonsingular essential points of the manifold  $\Lambda_{\text{In}}^t$  determining the tunnel operator  $K_{\text{In}}^t$  in (4.8). In this case, we shall have at  $x$  nonvanishing Jacobians

$J(t) = \det \frac{\partial X}{\partial x}(t)$ , which occur in the expression for  $K_{\text{In}}^t$ , and the Jacobian  $\partial x / \partial \mu$  in the formula for  $K_{\text{St}}^k$ . Since then the manifold  $\Omega^k$  can be locally diffeomorphically projected onto  $\mathbf{R}^n$  along all points of the trajectory connecting  $z_k = (\xi_k, 0)$  and  $z = (x, p) \in \Omega^k$ , it follows that

$$\frac{\partial X}{\partial x}(t) = \frac{\partial x}{\partial \mu}(X(t)) \frac{\partial \mu}{\partial \mu_0}(t) \frac{\partial \mu}{\partial x}(X(0)).$$

Hence, taking into account (5.12)–(5.13) we obtain

$$\det \frac{\partial X}{\partial x}(t) = \det \frac{\partial x}{\partial \mu} \exp \left\{ t \sum_{j=1}^n \omega_j^h \right\} (1 + O(t^{-1})). \quad (5.23)$$

From (5.23) and Proposition 5 we obtain (5.21) for the nonsingular points of  $\Omega^k$ . In the case of a singular essential point it is necessary to use a device analogous to the one employed at the end of the proof of Theorem 3.

We have investigated for  $t = h^{-(1+\kappa)}$  the leading term in the exponential asymptotic behavior of the solution of the problem (2.1), (5.16). However, as is clear from the introduction (see also Sec. 6), for applications to the theory of the lowest levels of a Schrödinger operator it is necessary to know the behavior of the solution (and not only the leading term) of the problem (2.1), (5.16) at large times  $t$  of order  $h^{-(1+\kappa)}$ ,  $\kappa > 0$ . The corresponding theorem formulated below is one of the main results of this paper. In all that follows in this section we assume that the sums  $\sum_{j=1}^n \omega_j^h$  are the same for all  $k = 1, \dots, \ell$ .

**THEOREM 5.** The solution  $u(t, x, h)$  to the Cauchy problem (2.1), (5.16) for  $t = h^{-(1+\kappa)}$ ,  $\kappa > 0$  and  $h \rightarrow 0$  has the form

$$u = \exp \left\{ -\frac{t}{2} \mathcal{E} \right\} \sum_{k=1}^l K_{\text{St}}^k (1 + O(h)), \quad (5.24)$$

where  $O(h)$  uniformly with respect to  $x$  and  $\kappa$  in any compact set.

**Proof.** We consider only the case of a point  $x \in \text{int } D^h$  that is the projection of nonsingular real points of  $\Omega^k$ . We shall then consider the case of a singular point in the usual way, i.e., using the device from the end of the proof of Theorem 3. As we have already noted, for sufficiently large  $t$  the solution  $u(t, x, h)$  is determined by a formula of the type (4.8), and the corresponding points on  $\Lambda_{\text{In}}^t$  are also nonsingular). At the same time,  $u(t, x, h)$  can be expressed in the form

$$u(t, x, h) = (2\pi h)^{-n/2} \int_{D_0} u(t, x, \xi, h) d\xi,$$

where the fundamental solution  $u(t, x, \xi, h)$  is determined by formula (4.3).

The basic idea is that the number  $m$  of iterations in (4.3) should be taken above what is minimally necessary, i.e., not the integral part of  $t/t_0$  but somewhat larger. This makes it possible to use the fact that for small times  $t$  the correction in formula (2.5) in Theorem 1 has the form  $O(ht^3)$ , and not simply  $O(h)$ . Thus, we shall choose the number of iterations of order  $m = t^{1+\alpha}$ , where  $\alpha > 0$  (more precisely, of course, we take the integral part of  $t^{1+\alpha}$ ). Then the time of one iteration  $\tau$  in (4.3) will be of order

$$\tau = t/t^{(1+\alpha)} = t^{-\alpha} = h^{\alpha(1+\kappa)}. \quad (5.25)$$

Let  $q_r(\tau)$ ,  $\tau \in (-\infty, 0]$ ,  $r \leq \tilde{r}$ , be a finite set of trajectories connecting  $\xi_k$  and  $x$  during infinite time on which the limiting phase  $S_k(x)$  is realized (see Proposition 2). We choose a small  $\varepsilon$  such that at large  $t$  in an  $\varepsilon$  neighborhood of each trajectory  $q_r$  there exists a unique trajectory connecting  $\xi_k$  and  $x$  during time  $t$ .

Then the fundamental solution will be equal to the sum of  $\tilde{r}$  terms of the form (4.5) with balls of radius  $\varepsilon$  as  $V_j$  up to an exponentially small remainder. However, it is

necessary to show that this remainder is small uniformly in  $t$  and  $m$ . We first consider the expression (4.5), where  $u(t, x, \xi, h)$  is of the form (2.5) and  $V_j$  is a ball of radius  $\varepsilon$ . We shall calculate the integrals in (4.3) successively, applying to each integral Laplace's method with estimate of accuracy (10.12) (this result is deferred to Sec. 10 in order not to interrupt the exposition). From the estimate of the coefficient  $\alpha(h)$  of  $h$  in the remainder of formula (10.12) and the estimates for the derivatives of the Jacobian and the phase at small  $\tau$  (see Sec. 2) it can be seen that the first three terms in the estimate for  $\alpha(h)$  have the form  $O(\tau^3)f(x_0)$ . Choosing a suitable  $\delta$ , we achieve the same for the penultimate term.

To estimate the last term in (10.12), it is necessary to know how to estimate integrals of the form

$$\int_{V_j} \exp\left\{-\frac{1}{h}[S(T, x, \eta_j) + S(\tau, \eta_j, \eta) - S(T + \tau, x, \eta)]\right\} d\eta_j, \quad (5.26)$$

where  $T = k\tau$  for some  $k < m$ . But by virtue of the choice of the neighborhoods  $V_j$  the function  $S(T, x, \eta_j)$  is convex with respect to  $\eta_j$  in  $V_j$ . At the same time, for the second derivative of the function  $S(\tau, \eta_j, \eta)$  we have the estimate (2.13), so that the expression in the curly brackets in (5.26) does not exceed

$$-\frac{1}{h\tau}(1+O(\tau))(\eta_j - \eta_j^0)^2.$$

Therefore, the integral (5.26) is bounded below by

$$[2\pi h\tau(1+O(\tau))]^{n/2}. \quad (5.27)$$

Thus, each application of Laplace's method (each iteration) will add to the leading term of the asymptotic behavior a factor of the form  $(1 + O(h\tau^3))$ . Thus, the complete integral (4.5) will differ from its leading term of the asymptotic behavior by a factor

$$\gamma(h) = \underbrace{(1 + O(h\tau^3)) \dots (1 + O(h\tau^3))}_m.$$

The deviation of  $\gamma(h)$  from unity can therefore be estimated by  $(1 + Ch\tau^3)^m - 1$ , where  $C$  is a constant and, hence, with allowance for

$$|\gamma(h) - 1| \leq (1 + Ch^{1+3\alpha(1+\kappa)})^{h^{-(1+\kappa)(1+\alpha)}} - 1 = \exp\{h^{-(1+\kappa)(1+\alpha)} \ln(1 + Ch^{1+3\alpha(1+\kappa)})\} - 1 = \\ \exp\{O(h^{1+3\alpha(1+\kappa) - (1+\kappa)(1+\alpha)})\} - 1 = O(h^{1+(1+\kappa)(2\alpha-1)}),$$

this expression has the form  $O(h)$  for  $\alpha > \frac{1}{2}$ .

We now estimate the difference between the expression (4.3) and the sum  $\tilde{r}$  of terms of the form (4.5), which in what follows we shall call the main part of the expression (4.3). We first explain what is the difficulty in obtaining the necessary estimate. It is clear that the minimum of the phase in the case of integration over the exterior of  $\varepsilon$  tubes of the trajectories  $q_r(\tau)$  is greater than  $S_k(x)$  by a certain amount  $\Delta$ , so that when the integral over the exterior of the  $\varepsilon$  tubes is calculated a factor  $\exp\{-\Delta/h\}$ , which is absent in the main term, appears. However, each application of the operator  $G_\tau$  in (4.3) adds a factor  $(2\pi h)^{-n/2}$ , so that after  $m$  iterations we obtain a coefficient  $(2\pi h)^{-mn/2}$ , which is not "knocked out" by the factor  $\exp\{-\Delta/h\}$  for  $m$  of order  $h^{1+\kappa}$ ,  $\kappa > 0$ . In the case of  $m$  fixed or of order  $h^{1-\kappa}$ ,  $\kappa > 0$ , the expression  $(2\pi h)^{-mn/2}$  is small compared with  $\exp\{-\Delta/h\}$ , and therefore in this situation the exponential smallness of the deviation of (4.3) from its main part is obvious, and this was used by us in the proof of Theorem 3. Here, however, we need a more accurate discussion.

Nondegeneracy of the matrix of second derivatives of the potential in the neighborhood of points of global minimum has as a consequence the following fact: For every point  $\xi_k$  there exists a neighborhood  $U_k \ni \xi_k$  such that for all  $x, y \in U_k$  and any  $t$  there exists a unique trajectory of the Newtonian system that connects  $x$  and  $y$  in time  $t$ , lies in  $U_k$ , and realizes a minimum of the functional (5.4); at the same time, the function  $S(t, x, y)$  is smooth and convex with respect to each of the arguments  $x, y \in U_k$  separately for all  $t$ . We first estimate the deviations of (4.3) from its main part for a point  $x$  in the neighborhood  $U_k$ . In this case, the trajectory  $q_\tau(\tau)$  that joins  $\xi_k$  and  $x$  over an infinite time interval is unique. The integral over the exterior of its  $\varepsilon$  tube can be represented as a sum of integrals over the set  $\tilde{U}_k$ , the complement of this  $\varepsilon$  tube in  $U_k$ , and over the exterior of  $U_k$ . More precisely, the first integral  $I_1$  is taken over the set of the  $\eta_1, \dots, \eta_m$  that

all belong to  $U_k$  with at least one of them lying outside the  $\varepsilon$  tube of the trajectory  $q(\tau)$ , while the second integral  $I_2$  is taken over the set of  $\eta_1, \dots, \eta_m$  for which at least one lies outside  $U_k$ . The integral  $I_1$  can be estimated in exactly the same way as in the estimate of the integral over the interior of the  $\varepsilon$  tubes of the limiting trajectories, since the convexity of  $S(t, x, y)$  for  $x, y \in U_k$  means that integrals of the type (5.26) over  $U_k$  can be estimated by the expressions (5.27). The integral  $I_2$  can be represented as a sum of  $m$  integrals over the sets  $\Omega_1, \dots, \Omega_m$ , where

$$\Omega_j = \{\eta_1, \dots, \eta_{j-1} \in U_k; \eta_j \notin U_k; \eta_{j+1}, \dots, \eta_m \in \mathbb{R}^n\}.$$

The integral over each  $\Omega_j$  is exponentially small compared with the main term. To see this, it is necessary to integrate over  $\eta_1, \dots, \eta_{j-1}$  in accordance with the preceding scheme, and then obtain for the resulting phase

$$S(j\tau, \eta_j, \xi) + S(\tau, \eta_{j+1}, \eta_j) + \dots + S(\tau, x, \eta_m) - S(t, x, \xi)$$

a lower bound in terms of the expression

$$\Delta + \frac{(\eta_{j+1} - \eta_j)^2}{2\tau} + \dots + \frac{(x - \eta_m)^2}{2\tau},$$

where  $\Delta > 0$  is the lower bound for the expression  $S(j\tau, \eta_j, \xi) - S(t, x, \xi)$  (for example,  $\Delta = \min_{y \in U_k} S_k(y) - S_k(x)$ ). As a result, we obtain a sum of  $m = h^{-(1+\kappa)(1+\alpha)}$  expressions that are exponentially small with respect to  $h$ , and the sum itself is therefore also exponentially small.

When  $x \notin U_k$ , we use the following arguments. For large times  $t$ , almost all critical points  $\eta_j^0$  of the phase are in  $U_k$ , except for a small number of points of order  $h^\alpha$ . Therefore, for  $\alpha < 1$  their number has the order  $h^{1-\kappa}$ ,  $\kappa' > 0$ . As was noted above, for  $h^{1-\kappa'}$  critical points the estimate is trivial, and for the remaining integrals we repeat the arguments applied in the case  $x \in U_k$ . Thus, the parameter  $\alpha$  introduced at the beginning of the proof must be chosen in the interval  $(\frac{1}{2}, 1)$ . This last argument completes the proof of Theorem 5.

The following theorem is proved in exactly the same way.

**THEOREM 6.** Under the assumptions of Theorem 5, the solution  $u_k(t, x, h)$  of the Cauchy problem for Eq. (2.1) with initial condition

$$u_k(0, x, h) = \chi_{V^\kappa}(x), \quad (5.28)$$

where  $\chi_{V^\kappa}(x)$  is the characteristic function of the closed neighborhood  $V^\kappa \subset \text{int } D^k$  of just the one point  $\xi_k$ , has for  $t = h^{-(1+\kappa)}$ ,  $\kappa > 0$  and  $h \rightarrow 0$  the form

$$u_k = e^{-\frac{t}{2} \mathcal{E}} K_k(1 + O(h)) = \exp\left\{-\frac{\mathcal{E}}{2} h^{-(1+\kappa)}\right\} K_k(1 + O(h)), \quad (5.29)$$

up to terms that are exponentially small in the limit  $h \rightarrow 0$  compared with the function (5.24).

## 6. Exponential Asymptotic Behavior of the Lowest Levels of Schrödinger Operators

We consider the time-independent Schrödinger equation

$$\hat{H}\psi = E\psi, \quad \psi \in L_2(\mathbb{R}^n), \quad x \in \mathbb{R}^n, \quad (6.1)$$

where

$$\hat{H} = -\frac{\hbar^2}{2} \Delta + V(x), \quad (6.2)$$

and the potential  $V(x)$  satisfies the conditions imposed on it at the beginning of Sec. 5.

We shall also assume that  $\mathcal{E} = \sum_{j=1}^n \omega_j^k$  does not depend on the point  $\xi_k$  and, therefore,

Theorems 5 and 6 hold. It is well known [33] that for a potential  $V$  that increases at infinity the spectrum of the operator (6.2) is discrete. Because  $V(x)$  is non-negative, the spectrum is, in addition, non-negative. In addition, by virtue of the localization principle under the assumptions that have been made the power-law asymptotic behavior of

the lowest energy levels of  $\hat{H}$  is determined solely by the behavior of  $V(x)$  in the neighborhood of the minima  $\xi_1, \dots, \xi_\ell$ . In particular,  $\hat{H}$  has precisely  $\ell$  eigenvalues  $E_1, \dots, E_\ell$  of the form  $1/2h(\mathcal{E} + O(h))$ , while for all the higher levels  $E$  the inequality  $E/h - \mathcal{E}/2 \geq C > 0$  holds with a certain constant  $C$ . The proofs of these facts can be found, for example, in [9] (see also Sec. 9). We denote by  $\psi_j$  the eigenfunctions of the operator  $\hat{H}$ ,  $j = 1, \dots, \ell$ , corresponding to  $E_j$ .

To construct the exponential asymptotic behaviors of the functions  $\psi_j$ , it is convenient to introduce the space  $\Phi$ , which is defined as the factor space of  $L_2(\mathbf{R}^n)$  with respect to the subspace

$$P = \left\{ f \in L_2(\mathbf{R}^n) : f = \sum_{j=1}^{\ell} K_j(O(h)) \right\},$$

where the tunnel operators  $K_j$  are the same as in Theorems 5 and 6. For brevity, we shall also denote by  $K_j$  the projections of functions of the form  $K_j(1 + O(h))$  in  $\Phi$ . The arguments that follow are based on Theorem 7:

**THEOREM 7.** Two  $\ell$ -dimensional vector spaces generated by functions  $K_j$ ,  $j = 1, \dots, \ell$  and, respectively, the projections of the eigenfunctions  $\psi_j$  in  $\Phi$  are identical. In particular, for all  $j = 1, \dots, \ell$

$$\psi_j = \sum_{i=1}^{\ell} C_i(h) K_i$$

up to functions in  $P$ ;  $C_i(h)$  are certain coefficients.

**Proof.** Let  $u_k(t, x, h)$  be solutions of the heat conduction equation (2.1) with initial condition  $u_k(0, x, h)$  of the form (5.28). If

$$u_k(0, x, h) = \sum_{j=1}^{\infty} \alpha_j \psi_j(x)$$

is an expansion of the initial condition in a series in eigenfunctions of the operator  $\hat{H}$ , then

$$u_k(t, x, h) = \sum_{j=1}^{\infty} \alpha_j e^{-tE_j/h} \psi_j(x),$$

is obviously a series expansion of the solution  $u_k(t, x, h)$ . Let  $t = h^{-(1+\kappa)}$ . Substituting (5.29) on the left-hand side and multiplying by  $\exp\{t\mathcal{E}/2\}$ , we obtain

$$K_k(1 + O(h)) = \sum_{j=1}^{\infty} \exp\{-h^{1+\kappa}(E_j/h - \mathcal{E}/2)\} \psi_j.$$

From the properties of the eigenvalues noted above it follows that we can, taking any compact set in  $\mathbf{R}^n$ , choose  $\kappa > 0$  such that for  $x$  in the compact set all terms with  $j > \ell$  are in the space  $P$  and, hence, in  $\Phi$

$$K_k = \sum_{j=1}^{\ell} \beta_j(h) \psi_j.$$

Theorem 7 follows from this fact and the linear independence of the functions  $K_j$ .

Particularly interesting problems are those in which tunnel effects are important from the point of view of the physics, i.e., problems in which the potential  $V(x)$  has a certain symmetry. In this case, the coefficients  $C_j(h)$  in Theorem 7 can usually be calculated explicitly. We consider two such situations.

**PROPOSITION 8.** Suppose  $V(x)$  has only two minima:

$$\xi_1 = (|\xi_1|, 0, \dots, 0), \quad \xi_2 = (-|\xi_1|, 0, \dots, 0),$$

and that  $V(x)$  is even with respect to the first coordinate:  $V(R(x)) = V(x)$ , where  $R(x_1, x_2, \dots, x_n) = (-x_1, x_2, \dots, x_n)$  is the reflection with respect to the hyperplane  $\{x_1 = 0\}$ . Then (up to functions in  $P$ )

$$\psi_1 = C(\hbar) (K_1 + K_2), \quad (6.3)$$

$$\psi_2 = C(\hbar) (K_1 - K_2), \quad (6.4)$$

$$C(\hbar) = (\hbar\pi)^{-n/4} (\omega_1 \dots \omega_n)^{1/4}, \quad (6.5)$$

where  $\omega_j = \omega_j^1 = \omega_j^2$ .

Proof. We shall assume that  $E_1 \neq E_2$  (if  $E_1 = E_2$ , then the entire two-dimensional space spanned by  $K_1$  and  $K_2$  is an eigenspace for  $\hat{H}$  with eigenvalue  $E_1 = E_2$ , and therefore the eigenfunctions can be taken, for example, in the form (6.3) and (6.4), and the proposition is already proved; however, it will be shown below that in reality  $E_1 \neq E_2$ ). Because  $V(x)$  is even, it follows that if  $\psi(x)$  is an eigenfunction of  $\hat{H}$  with eigenvalue  $E$ , then so is  $\psi(R(x))$  with the same eigenvalue. However, both the eigenspaces corresponding to  $E_1$  and  $E_2$  are one dimensional. Therefore  $\psi_1(R(x)) = \alpha_1 \psi_1(x)$ ,  $\psi_2(R(x)) = \alpha_2 \psi_2(x)$ , where  $\alpha_1$  and  $\alpha_2$  are certain complex constants with modulus equal to unity. But it is obvious from the construction of  $K_1$ ,  $K_2$  (see Sec. 5) that  $K_1(R(x)) = K_2(x)$ , from which it immediately follows that  $\alpha_{1,2} = \pm 1$ , and (6.3) and (6.4) hold. A formula for  $C(\hbar)$  follows from the normalization condition:  $\|\psi_j\| = 1$ , and Laplace's method should be used to calculate the norms of the functions  $K_1$  and  $K_2$ .

PROPOSITION 9. Suppose  $V(x)$  has three minima  $\xi_1$ ,  $\xi_2$ ,  $\xi_3$  in the plane  $\{x_3 = x_4 = \dots = x_n = 0\}$  and that  $V(x)$  is invariant with respect to the rotation  $R$  of this plane through  $120^\circ$ :  $V(R(x)) = V(x)$ , from which in particular  $\xi_2 = R(\xi_1)$ ,  $\xi_3 = R(\xi_2)$ . In this case the one-dimensional eigenspace of the lowest energy  $E_1$  is generated by the function

$$\psi_1 = C(\hbar) (K_1 + K_2 + K_3), \quad (6.6)$$

and the two other levels are equal:  $E_2 = E_3$ , their eigenspace consisting of functions  $\psi = C_1(\hbar)K_1 + C_2(\hbar)K_2 + C_3(\hbar)K_3$  that satisfy the condition  $C_1(\hbar) + C_2(\hbar) + C_3(\hbar) = 0$ ; in other words, it is generated by the functions  $\psi_{ij} = K_i - K_j$ , where  $i, j = 1, 2, 3$ .

Proof. As in Proposition 8, it is sufficient to make the assumption that not all the levels  $E_1$ ,  $E_2$ ,  $E_3$  coincide. Then there necessarily exists a one-dimensional eigenspace (among the three lowest levels). From symmetry considerations, as above, we find that the eigenfunction  $\psi_1$  of this one-dimensional subspace satisfies the condition  $\psi_1(R(x)) = \psi_1(x)\alpha$ , where  $|\alpha| = 1$ . Since the transformation  $R$  generates a cyclic group of transformations of order 3, i.e.,  $R(R(R(x))) = x$ , it is obvious that  $\alpha^3 = 1$ . Finally, bearing in mind that the eigenfunctions of  $\hat{H}$  can be assumed to be real, and that the transformation  $R$  preserves the reality, we find that  $\alpha = 1$ , from which (6.6) follows. We now consider the two-dimensional eigenspace. For it, the functions  $\psi(x)$  and  $\tilde{\psi}(x) = \psi(R(x))$  form a basis. Therefore  $\tilde{\tilde{\psi}}(x) = \tilde{\psi}(R(x))$  is a linear combination of them:  $\tilde{\tilde{\psi}} = \alpha\psi + \beta\tilde{\psi}$ . Replacing in this equation  $x$  by  $R(x)$ , we obtain  $\psi = \alpha\tilde{\tilde{\psi}} + \beta\tilde{\psi}$ . Substituting in this equation the previous one, we obtain  $(1 - \alpha\beta)\psi = (\alpha + \beta^2)\tilde{\psi}$ , whence  $1 - \alpha\beta = 0$ ,  $\alpha + \beta^2 = 0$ . It follows from these equations that  $\beta^3 = -1$ , and we again conclude from the reality arguments that  $\beta = -1$  and, hence, also  $\alpha = -1$ . Therefore  $\tilde{\tilde{\psi}} = -(\psi + \tilde{\psi})$ . For the function  $\psi = C_1(\hbar)K_1 + C_2(\hbar)K_2 + C_3(\hbar)K_3$  this condition is equivalent to the equation  $C_1(\hbar) + C_2(\hbar) + C_3(\hbar) = 0$  as we needed to prove.

Following [2], we now calculate the exponentially small (with respect to the parameter  $\hbar$ ) distance between the lowest energy levels  $E_1$  and  $E_2$  in the case of a potential  $V(x)$  with two symmetric minima, i.e., under the conditions of Proposition 8 (the arguments for the case of Proposition 9 are similar). We multiply Eq. (6.1) for  $\psi_1$  of the form (6.3) by  $\psi_2$  of the form (6.4), and Eq. (6.1) for  $\psi_2$  by  $\psi_1$  and subtract one of these relations from the other. We then integrate the result over a certain region  $D$  with smooth boundary. We obtain

$$-\int_D \frac{\hbar^2}{2} (\psi_1 \Delta \psi_2 - \psi_2 \Delta \psi_1) dx = (E_2 - E_1) \int_D \psi_1 \psi_2 dx, \quad (6.7)$$

and integrating the left-hand side of this equation by Green's formula we find

$$E_2 - E_1 = -\frac{\hbar^2}{2} \int \left( \psi_1 \frac{\partial \psi_2}{\partial n} - \psi_2 \frac{\partial \psi_1}{\partial n} \right) ds / \int_D \psi_1 \psi_2 dx, \quad (6.8)$$

where  $\partial/\partial n$  is the derivative along the outer normal  $n$  to the boundary  $\partial D$ .

As the region  $D$  we take  $D^1$  (see Sec. 5), which in this case,  $V(x)$  being even, coincides

with the half-space  $\{x_1 \geq 0\}$ . We substitute (6.3) and (6.4) in (6.8) and calculate the denominator on the right-hand side of (6.8) by Laplace's method:

$$\int_{D_1} \psi_1 \psi_2 dx = C(h)^2 \int_{D_1} (K_1^2 - K_2^2) dx = C(h)^2 \int_{D_1} K_1^2 dx (1 + O(h)) = \frac{1}{2} (1 + O(h)) \|\psi_1\|^2 = \frac{1}{2} + O(h).$$

We obtain

$$E_2 - E_1 = 2h^2 C(h)^2 (1 + O(h)) \int_{\partial D^1} \left( K_1 \frac{\partial K_2}{\partial n} - K_2 \frac{\partial K_1}{\partial n} \right) ds. \quad (6.9)$$

To calculate this integral by Laplace's method, we first assume that there exists a unique nondegenerate point  $y_0$  of global minimum of the function  $S_1(x)|_{\partial D^1}$  ( $S_k, J_k$  are the entropy and Jacobian on the manifolds  $\Omega^k$  introduced in Sec. 5). The integrand in (6.9) in the neighborhood of  $y_0$  over  $\partial D^1$  is

$$J_1^{-1/2} \exp\{-S_1/h\} \frac{\partial}{\partial n} (J_2^{-1/2} \exp\{-S_2/h\}) - J_2^{-1/2} \exp\{-S_2/h\} \frac{\partial}{\partial n} (J_1^{-1/2} \exp\{-S_1/h\}) = \\ \frac{1}{h} (1 + O(h)) (J_1 J_2)^{-1/2} \left( \frac{\partial S_1}{\partial n} - \frac{\partial S_2}{\partial n} \right) \exp\left\{-\frac{1}{h} (S_1 + S_2)\right\};$$

and because  $V(x)$  is even, so that  $S_1(R(x)) = S_2(x)$ ,  $J_1(R(x)) = J_2(x)$ , the expression in which we are interested is equal to

$$\frac{2}{h} J_1^{-1} \exp\left\{-\frac{2}{h} S_1\right\} \frac{\partial S_1}{\partial n} (1 + O(h)).$$

Therefore, calculating the  $(n-1)$ -dimensional integral in (6.9) by Laplace's method, we find that

$$E_2 - E_1 = 4hC(h)^2 (1 + O(h)) (\pi h)^{(n-1)/2} J_1^{-1}(y_0) \frac{\partial S_1}{\partial n}(y_0) \exp\left\{-\frac{2}{h} S_1(y_0)\right\} (\det A)^{-1/2},$$

where  $A$  is the matrix of second derivatives of the function  $S_1|_{\partial D^1}$  with respect to the variables  $x_2, \dots, x_n$ . We now note that if  $y \in \partial D^1$  is a stationary point of the function  $S_1|_{\partial D^1}$ , then the trajectory  $q_1(\tau)$  of the Newtonian system  $\ddot{q} = V'(q)$  in Proposition 2 in Sec. 5, i.e., the trajectory such that  $q_1(-\infty) = \xi_1$ ,  $q_1(0) = y$  with the action along  $q_1(\tau)$  equal to  $S_1$ , is orthogonal to the boundary  $\partial D^1$ . By virtue of the symmetry, the trajectory  $q_2(\tau) = Rq_1(\tau)$  is also orthogonal to  $\partial D^1$ , and  $q_2(-\infty) = \xi_2$ ,  $q_2(0) = y$ . It follows from this that, first, there exists a smooth trajectory  $q(\tau)$  of the Newtonian system for which  $q(-\infty) = \xi_1$ ,  $q(+\infty) = \xi_2$ ,  $\dot{q}(-\infty) = \dot{q}(+\infty) = 0$ ,  $q(0) = y$ , and, second,

$$S_1(y) = S_2(y) = \frac{1}{2} \int_{-\infty}^{\infty} \left( \frac{1}{2} \dot{q}^2 + V(q) \right) d\tau = \frac{1}{2} \int_{-\infty}^{\infty} \dot{q}^2 d\tau, \quad (6.10)$$

since the Hamiltonian  $H$  on  $q(\tau)$  is zero. Solutions  $q(\tau)$  of the Newtonian system  $\ddot{q} = V'(q)$  satisfying the conditions  $\dot{q}(-\infty) = \dot{q}(+\infty) = 0$ ,  $q(-\infty) = \xi_1$ ,  $q(+\infty) = \xi_2$ , are called the instantons corresponding to the quantum-mechanical problem specified by the Hamiltonian  $H$ . We denote by  $S_{12}$  the minimum of the integral  $\int \dot{q}^2 d\tau$  over all instantons (in other words,  $S_{12}$  is twice the Agmon distance between the points  $\xi_1$  and  $\xi_2$ ; see the Corollary to Proposition 2 in Sec. 5 and Remark 3 after it). Substituting in (6.9) formula (6.5) for  $C(h)$  we obtain

$$E_2 - E_1 = 4\pi^{-1/2} h^{1/2} (1 + O(h)) (\omega_1 \dots \omega_n)^{1/2} J_1^{-1}(y_0) \frac{\partial S_1}{\partial n}(y_0) \det A^{-1/2} \exp\{-S_{12}/h\}. \quad (6.11)$$

If there exist several nondegenerate points of global minimum of  $S_1|_{\partial D^1}$ , then  $E_2 - E_1$  is equal to the sum of the expressions on the right-hand side of (6.11) over all such points. Note also that the derivative  $\frac{\partial S_1}{\partial n}(y_0)$  in (6.11) is the velocity modulus  $|\dot{q}(0)|$  of the instanton at the point  $y_0$ . From (6.11) in particular there follows a formula for the first term of the logarithmic asymptotic behavior of the number  $E_2 - E_1$ , which determines the splitting of the lowest energy levels of the operator  $\hat{H}$ :

$$\lim_{h \rightarrow 0} h \ln(E_2 - E_1) = -S_{12}. \quad (6.12)$$

Note that in the case when the minimum  $y_0$  of the function  $S_1|_{\partial D^1}$  is degenerate the result

of [34] can be used to calculate the first term in the logarithmic asymptotic behavior of  $E_2 - E_1$ . Therefore, in contrast to (6.11), formula (6.12) is true in the general case.

It is possible to obtain in the same way asymptotic expressions for the splitting of the lowest levels for the potential in Proposition 9, and also for other potentials with symmetry.

### 7. Tunnel Operator on a Torus and Schrödinger Equation with Periodic Potential

In this section, we briefly explain the theory of a periodic tunnel operator and its application to the construction of exponential asymptotics of the lowest eigenfunctions of Schrödinger operators with periodic potential.

Suppose the function  $V(x)$  is  $2\pi$ -periodic with respect to each coordinate. We consider the heat conduction equation

$$h \frac{\partial u}{\partial t} = \frac{h^2}{2} \Delta u - V(x)u \quad (7.1)$$

in the class of  $2\pi$ -periodic (with respect to each spatial coordinate  $x \in \mathbf{R}_x^n$ ) functions. In such a formulation, the problem is equivalent to consideration of Eq. (7.1) on the  $n$ -dimensional torus  $\mathbf{T}^n = \mathbf{R}^n / (2\pi\mathbf{Z})^n$ . The existence and uniqueness of the solution follow from the standard theorems of the theory of linear equations. The Green's function of the periodic Cauchy problem for Eq. (7.1) is defined as the periodic (with respect to  $x$ ) solution  $u^p(t, x, \xi, h)$  of the equation that satisfies the initial condition

$$u^p(0, x, \xi, h) = \sum_{N \in \mathbf{Z}^n} \delta(x - (\xi + 2\pi N)). \quad (7.2)$$

We shall assume that  $V(x)$  is sufficiently smooth, non-negative, and has on the torus  $\mathbf{T}^n$  only a finite number of zeros  $\xi_1, \dots, \xi_l$ . Then

$$u^p(t, x, \xi, h) = \sum_{N \in \mathbf{Z}^n} u(t, x, \xi + 2\pi N, h), \quad (7.3)$$

where  $u(t, x, \xi, h)$  is a nonperiodic Green's function of the form (2.5) for small  $t$  and the form (4.1) and (4.2) for all finite times. This fact follows directly from the linearity of Eq. (7.1) and the consideration that the phase  $S(t, x, \xi)$  tends to infinity for  $\xi \rightarrow \infty$  and fixed  $t, x$  (see Sec. 2), from which we obtain convergence of the series (7.3) and also the fact that in the sum (7.3) only a finite number of terms makes a real contribution to the asymptotic behavior.

Now suppose that the function  $V$  has on the torus  $\mathbf{T}^n$  only a finite number of zeros  $\xi_1, \dots, \xi_l$ , at which the matrix of second derivatives  $V''(\xi_k)$  is nondegenerate and has eigenvalues  $(\omega_j^k)^2$ ,  $\omega_j^k > 0$ ,  $j=1, \dots, n$ , and  $\mathcal{E} = \sum_{j=1}^n \omega_j^k$  does not depend on  $k$ . We shall also denote

by  $\xi_k$  the pre-images of  $\xi_k$  in the square with side  $2\pi$  in  $\mathbf{R}_x^n$ . Then it follows from the superposition principle and Theorem 6 that the solution of the periodic Cauchy problem with initial condition

$$u_k^p(0, x, h) = \sum_{N \in \mathbf{Z}^n} \chi_{V^k}(x + 2\pi N), \quad (7.4)$$

where  $\chi_{V^k}$  is the characteristic function of a small closed neighborhood  $V^k$  of the point  $\xi_k \in \mathbf{R}_x^n$ , is for  $t = h^{-(1+\nu)}$ ,  $\nu > 0$ ,  $h \rightarrow 0$ , equal to

$$u_k^p = \exp\left\{-\frac{\mathcal{E}}{2} h^{-(1+\nu)}\right\} \sum_{N \in \mathbf{Z}^n} K_{k, N} (1 + O(h)), \quad (7.5)$$

where the tunnel operators  $K_{k, N}$  are defined as in Sec. 5 (see the notation after Eq. (5.15)), but with respect to a countable set of points  $\xi_{k, N} = \xi_k + 2\pi N$ :  $k=1, \dots, l$ ,  $N \in \mathbf{Z}^n$ , the zeros of  $V(x)$  in  $\mathbf{R}_x^n$ . In particular, the region  $D_{k, N}^k$  that occurs in the definition of the operator  $K_{k, N}$  is distinguished by the inequality



$$S_{k,N}(x) \leq \min_{j,M} \{S_{j,M}(x) : (j,M) \neq (k,N)\}. \quad (7.6)$$

We consider the following Schrödinger equation on a torus:

$$\hat{H}\psi = E\psi, \quad \psi \in L_2(\mathbb{T}^n), \quad (7.7)$$

$\hat{H} = -\frac{1}{2}h^2\Delta + V(x)$ . This problem is equivalent to finding smooth solutions of Eq. (7.7) in the whole of space but with a condition of periodicity of the solution  $\psi$ . It is well known that this problem has a positive discrete spectrum. Moreover, as in the case of the Schrödinger operator in  $\mathbb{R}^n$  considered in the previous section,  $\hat{H}$  on the torus has precisely  $l$  eigenvalues  $E_1, \dots, E_l$  of the form  $\frac{1}{2}h(\mathcal{E} + O(h))$ , and for all higher levels  $E$  the inequality  $E/h - \mathcal{E}/2 \geq C > 0$  holds (see, for example, [9]).

As in the case of Theorem 7, it can be shown that the lowest eigenfunctions  $\psi_1, \dots, \psi_l$  are linear combinations

$$\psi_j = \sum_{i=1}^l C_i(h) \tilde{K}_i$$

of periodic tunnel operators

$$\tilde{K}_j = \sum_{N \in \mathbb{Z}^n} K_{j,N}.$$

Suppose  $V(x)$  has only two minima in  $\mathbb{T}^n$ , the images of the points  $\xi_1 = (|\xi_1|, 0, \dots, 0)$ ,  $\xi_2 = (-|\xi_1|, 0, \dots, 0)$  in  $\mathbb{R}^n$ ,  $|\xi_1| < 2\pi$ , and  $V(x)$  is even with respect to each coordinate. Then it is readily seen that the regions  $D^{k,N} = D^{k,0} + N$ ,  $k=1, 2$ , are parallelepipeds:

$$D^1 = \{x \in \mathbb{R}^n : x_1 \in [0, \pi], x_j \in [-\pi, \pi] \forall j \neq 1\}, \quad D^2 = \{x \in \mathbb{R}^n : x_1 \in [-\pi, 0], x_j \in [-\pi, \pi] \forall j \neq 1\}.$$

As in Proposition 8 of Sec. 6,  $\psi_1 = C(h)(\tilde{K}_1 + \tilde{K}_2)$ ,  $\psi_2 = C(h)(\tilde{K}_1 - \tilde{K}_2)$ . A specific feature of the periodic case is manifested in the calculation of the splitting  $E_2 - E_1$ . It is clear that now  $-\lim_{h \rightarrow 0} h \ln(E_2 - E_1)$  will be equal to the minimum over all instantons on the torus that

lead both from  $\xi_1$  to  $\xi_2$  and from  $\xi_1$  to  $\xi_1$ . Formula (6.11) is modified similarly in the non-degenerate case.

It is well known (see, for example, [35,36]) that investigation of the spectrum of the Schrödinger equation (7.7) with periodic  $V(x)$  (but, of course, now without the requirement of periodicity of the solution  $\psi$ ) reduces in a certain sense to the solution of different problems on the torus. We illustrate this thesis by applying the results obtained above to the investigation of the one-dimensional Schrödinger equation

$$-\frac{1}{2}h\psi''(x) + V(x)\psi(x) = E\psi(x) \quad (7.8)$$

on the line  $x \in \mathbb{R}^1$  with non-negative even periodic potential  $V(x + 2\pi) = V(x)$  that has in the interval  $[0, 2\pi]$  a unique minimum at  $\xi = \pi$ . It is known that the spectrum of this problem is absolutely continuous and consists of a countable set of intervals  $[\alpha_1, \alpha_2] \cup [\alpha_3, \alpha_4] \cup \dots$  lying on the half-line  $\mathbb{R}_+$ . At the same time,  $\alpha_{2j-1}$  (respectively,  $\alpha_{2j}$ ) is the  $j$ -th eigenvalue of the operator

$$\hat{H}\psi = -\frac{h^2}{2}\psi''(x) + V(x)\psi(x)$$

on the line with periodic condition  $\psi(x + 2\pi) = \psi(x)$  (respectively, with antiperiodic boundary condition  $\psi(x + 2\pi) = -\psi(x)$ ). These facts are proved, for example, in [35]. It obviously follows from this that  $\alpha_1$  and  $\alpha_2$  are the lowest levels of the operator  $\hat{H}$  defined on the doubled circle, i.e., the calculation of the width of the first allowed band  $[\alpha_1, \alpha_2]$  of the spectrum reduces to calculation of the splitting of the lowest discrete levels for the operator on a circle with potential with two minima. The solution of this problem is described above. Therefore

$$\lim_{h \rightarrow 0} h \ln(\alpha_2 - \alpha_1) = -S_{1,2}, \quad (7.9)$$

where  $S_{1,2}$  is the minimum of the action over the instantons (i.e., the solutions of the equation  $\ddot{q} = V'(q)$  with boundary conditions  $q(-\infty) = \xi$ ,  $q(+\infty) = -\xi$ ). This formula is well known in the physics literature [17,37]. Our methods also enable us to calculate the linear term in the exponential asymptotic behavior of the width of the band  $[\alpha_1, \alpha_2]$  in

accordance with a formula analogous to (6.11). The condition of nondegeneracy, required for fulfillment of (6.11), is satisfied automatically in the one-dimensional case. As region D, we take the interval  $[0, 2\pi]$ , so that formula (6.9) in the one-dimensional periodic case gives

$$\alpha_2 - \alpha_1 = 2h^2 C(h)^2 (1 + O(h)) (\bar{K}_1 \bar{K}_2' - \bar{K}_2 \bar{K}_1') |_0^{2\pi},$$

whence

$$\alpha_2 - \alpha_1 = 8\sqrt{h} (1 + O(h)) \pi^{-1/2} J_1^{-1} (V''(\pi))^{1/2} \dot{y}(\pi) \exp\left\{-\frac{2}{h} S_1(\pi)\right\}, \quad (7.10)$$

where  $\dot{y}(\pi)$  is the velocity at the point  $\pi$  of the instanton leading from  $-\pi$  to  $\pi$ .

## 8. Examples

1. We consider the Schrödinger equation (6.1) with potential  $V(x_1, \dots, x_n)$  having two symmetric wells:

$$V = \frac{\alpha}{2} \sum_{k=1}^n (x_k - x_{k-1})^2 + \frac{\beta}{4} \sum_{k=1}^n (x_k - \xi)^2 (x_k + \xi)^2.$$

Here  $\alpha > 0$ ,  $\beta > 0$ ,  $\xi > 0$  are parameters,  $x_0 \stackrel{\text{def}}{=} x_n$ . It is obvious that  $V(x) \geq 0$ ,  $V(x) \rightarrow \infty$  as  $|x| \rightarrow \infty$ , and  $V(x)$  satisfies the condition  $V(-x) = V(x)$  and has only two points of global minimum:  $x^\pm = \pm(\xi, \xi, \dots, \xi)$ . We find the eigenvalues  $\omega_m^2$  of the matrix  $\partial^2 V / \partial x_i \partial x_j$ . The equations for their determination have the form

$$-\alpha(z_{k+1} - 2z_k + z_{k-1}) + 2\beta\xi^2 z_k = \omega^2 z_k, \quad k=1, \dots, n, \quad z_0 = z_n.$$

Their solutions are well known and give the following sets of eigenfunctions and eigenvalues (see, for example, [38]):

$$\omega_m^2 = 4\alpha \sin^2 \frac{\pi}{n} m + 2\beta\xi^2, \quad (z_m)_k = \frac{1}{\sqrt{h}} \exp\left\{i \frac{2\pi}{h} mk\right\}, \quad m=0, 1, \dots, n-1.$$

Thus, the formula for the lowest energy states is

$$E_0^\pm = \frac{h}{2} \sum_{m=0}^{n-1} \sqrt{4\alpha \sin^2 \frac{\pi}{n} m + 2\beta\xi^2 + O(h^2)}.$$

We calculate the splitting  $\Delta = E^+ - E^-$ . We find an instanton solution from the Newtonian system:

$$\ddot{x}_k = \beta(x_k^3 - x_k \xi) - \alpha(x_{k+1} - 2x_k + x_{k-1}), \quad x_k|_{t=-\infty} = -\xi, \quad x_k|_{t=\infty} = \xi, \quad k=1, \dots, n.$$

One of the solutions (possibly unique) has the form

$$x_1 = x_2 = \dots = x_n = \sqrt{\xi} \operatorname{th}(\sqrt{\beta\xi} t / \sqrt{2}).$$

We show that this solution ensures a minimum of the integral

$$2S = \min_{x_k(t)} \int_{-\infty}^{\infty} \left( \frac{\dot{x}^2}{2} + V(x(t)) \right) dt, \quad x_k(-\infty) = -\xi, \quad x_k(\infty) = \xi, \quad k=1, \dots, n.$$

Indeed, it is obvious that

$$\begin{aligned} 2S &= \min_{x_k(\pm\infty) = \pm\xi} \sum_{k=1}^n \int_{-\infty}^{\infty} \left[ \frac{\dot{x}_k^2}{2} + \frac{\alpha}{2} (x_k - x_{k-1})^2 + \frac{\beta}{4} (x_k + \xi)^2 (x_k - \xi)^2 \right] d\tau \geq \\ &\quad \min_{x_k(\pm\infty) = \pm\xi} \sum_{k=1}^n \int_{-\infty}^{\infty} \left[ \frac{\dot{x}_k^2}{2} + \frac{\beta}{4} (x_k + \xi)^2 (x_k - \xi)^2 \right] d\tau = \\ &\quad \sum_{k=1}^n \min_{x_k(\pm\infty) = \pm\xi} \int_{-\infty}^{\infty} \left[ \frac{\dot{x}_k^2}{2} + \frac{\beta}{4} (x_k + \xi)^2 (x_k - \xi)^2 \right] d\tau = \end{aligned}$$

$$n \min_{\substack{q(t) \\ q(\pm\infty)=\pm\xi}} \int_{-\infty}^{\infty} \left[ \dot{q}^2 + \frac{\beta}{4} (q + \xi)^2 (q - \xi)^2 \right] d\tau.$$

The last minimum is attained on the solution  $q = \sqrt{\xi} \tanh(\sqrt{\beta\xi}t/\sqrt{2})$  of the system  $\ddot{q} = \beta(q^3 - \xi q)$ . Note that at the same time  $2S$  is equal to the last expression in this chain only in the case of vanishing of all the  $x_k(t)$ , which ensures the necessary proposition. We calculate  $2S$ . By virtue of the equations  $\dot{x}^2 = V(x(t))$  and  $\dot{q}^2 = \beta(q - \xi)^2 (q + \xi)^2 / 4$

$$2S = n \int_{-\infty}^{\infty} \dot{q}^2 dt = \frac{\sqrt{\beta}h}{2} \int_{-\xi}^{\xi} (\xi - x)(\xi + x) dx = \frac{2n\sqrt{\beta}\xi^3}{3}.$$

Thus

$$E_1 - E_0 = A \exp\left\{-\frac{2n\sqrt{\beta}\xi^3}{3h}\right\}.$$

This formula can be readily extended to the Schrödinger equation with potential

$$V = \sum_{k=1}^n \alpha_k (x_k - x_{k-1})^2 + \frac{\beta}{4} \sum_{k=1}^n u(x_k),$$

where  $\alpha_k > 0$ , and  $u(z)$  is an even function that increases as  $|x| \rightarrow \infty$  and has two nondegenerate points of global minimum.

2. We consider one further example — the Schrödinger equation for the hydrogen ion. We note first that the theory presented in the previous sections can also be applied under weaker restrictions on the potential  $V$ . Namely, the potential  $V$  can have several isolated singular points and need not increase as  $|x| \rightarrow \infty$ . An example of such a situation is considered in this subsection.

This problem, which admits separation of the variables, has been investigated in many studies; in particular, semiclassical asymptotic behaviors were obtained in [39] for high-energy states. Here, we obtain series of eigenvalues and their splitting, for the obtaining of which the method of [39] does not apply. The potential has the form

$$V = -\left( \frac{\alpha}{\sqrt{x^2 + y^2 + (z-a)^2}} + \frac{\alpha}{\sqrt{x^2 + y^2 + (z+a)^2}} \right),$$

where  $\alpha, a$  are dimensionless physical constants, and  $\pm a$  determine the points on the  $z$  axis at which the atoms are situated. We express the problem in cylindrical coordinates  $\rho, \varphi, z$  and take into account the azimuthal symmetry, representing the wave function in the form  $e^{im\varphi}\psi(\rho, z)$  ( $m$  is an integer):

$$-\frac{\hbar^2}{2} \left( \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} + \frac{\partial^2}{\partial z^2} \right) \psi + V_1 \psi = E \psi,$$

$$V_1(\rho, z) = \frac{p_\varphi^2}{2\rho^2} - \alpha \left\{ \frac{1}{\sqrt{\rho^2 + (z-a)^2}} + \frac{1}{\sqrt{\rho^2 + (z+a)^2}} \right\}, \quad p_\varphi = m\hbar.$$

It is readily seen that the potential  $V_1$  is bounded below for  $p_\varphi \geq \text{const}$ . In addition, it is easy to show (see below) that it has two points of global minimum if  $p_\varphi^2 \leq 8\alpha a / 3\sqrt{3}$ . Thus, we can apply the above scheme to this problem. It is more convenient to make the calculations in the special coordinates  $\sigma, \tau, \varphi$  (prolate ellipsoid of revolution),  $\sigma \geq 1 \geq \tau \geq -1$ ,  $\varphi \in [0, 2\pi]$ , which are related to the cylindrical coordinates by the formulas  $z = a\sigma\tau$ ,  $\varphi = \varphi$ ,  $\rho^2 = a^2(\sigma^2 - 1)(1 - \tau^2)$ . In these coordinates, we obtain for the function  $\psi$  the problem

$$-\frac{\hbar^2}{\sigma^2 - \tau^2} \left( \frac{\partial}{\partial \sigma} (\sigma^2 - 1) \frac{\partial}{\partial \sigma} + \frac{\partial}{\partial \tau} (1 - \tau^2) \frac{\partial}{\partial \tau} \right) \psi + V_{\text{eff}} \psi = 2a^2 E \psi, \quad (8.1)$$

where

$$V_{\text{eff}} = \frac{1}{\sigma^2 - \tau^2} \left[ p_\varphi^2 \left( \frac{1}{\sigma^2 - 1} + \frac{1}{1 - \tau^2} \right) - 4\alpha\sigma \right],$$

$p_\varphi = m\hbar$ . In what follows, we assume that  $m \sim 1/h$  (essentially, the large number  $m$  is a parameter in the investigated problem). The potential  $V_{\text{eff}}$  has two symmetric points of

local minimum, which are found by equating to zero the derivatives  $\partial V_{\text{eff}}/\partial \tau$ ,  $\partial V_{\text{eff}}/\partial \sigma$ . As a result of straightforward but lengthy calculations we find that the points of global minimum  $\tau_{\pm}$  and  $\sigma_0$  and the value  $\mathcal{E} = -V_{\text{eff}}(\tau_{\pm}, \sigma_0)$  are determined as follows. The point  $\sigma_0$  is found as root of the equation (it is readily seen that the root exists and is unique)

$$\sigma^3 = \frac{a\alpha}{4p_\phi^2}(\sigma^2+1)^2(\sigma^2-1).$$

The value of  $\mathcal{E}$  and the points  $\tau_{\pm}$  can be expressed in terms of  $\sigma_0$  by the formulas

$$\mathcal{E} = \mathcal{E}(|p_\phi|) = |p_\phi| \frac{1}{(\sigma_0^2-1)^2} + \frac{2\alpha}{|p_\phi|^2\sigma_0}, \quad \tau_{\pm} = \pm \sqrt{1 - \frac{p_\phi}{\sqrt{\mathcal{E}}}}.$$

We now set  $\tilde{E} = 2a^2E + \mathcal{E}$ ,  $\tilde{V}_{\text{eff}} = V_{\text{eff}} + \mathcal{E}$ , and then Eq. (8.1) takes the form

$$-\frac{\hbar^2}{\sigma^2-\tau^2} \left( \frac{\partial}{\partial \sigma}(\sigma^2-1) \frac{\partial}{\partial \sigma} + \frac{\partial}{\partial \tau}(1-\tau^2) \frac{\partial}{\partial \tau} \right) \psi + \tilde{V}_{\text{eff}} \psi = \tilde{E} \psi. \quad (8.2)$$

At the same time  $\tilde{V}_{\text{eff}} \geq 0$ . We apply the oscillator approximation. With allowance for the fact that in Eq. (8.2) the derivatives have variable coefficients the frequencies  $\omega_j$  are determined as eigenvalues of the matrix (see [5])

$$\mathcal{H} = \begin{pmatrix} -H_{xp} & -H_{xx} \\ H_{pp} & H_{px} \end{pmatrix},$$

which is formed from the derivatives  $\partial^2 H/\partial p_i \partial p_j$ ,  $\partial^2 H/\partial p_i \partial x_j$ ,  $\partial^2 H/\partial x_i \partial x_j$  calculated at the points  $\sigma = \sigma_0$ ,  $\tau = \tau_{\pm}$ . Here  $p_1 = p_\sigma$ ,  $p_2 = p_\tau$ ,  $x_1 = \sigma$ ,  $x_2 = \tau$  and  $H$  is the "tunnel" Hamiltonian

$$H = \frac{1}{\sigma^2-\tau^2} (p_\sigma^2(\sigma^2-1) + p_\tau^2(1-\tau^2)) - \tilde{V}_{\text{eff}}.$$

As a result of simple but lengthy calculations we find

$$\omega_1 = \frac{|p_\phi| (3\sigma_0^2-1) \sqrt{3\sigma_0^4-2\sigma_0^2+3}}{\sigma_0(\sigma_0^2-1)(\sigma_0^4-1)}, \quad \omega_2 = \frac{|p_\phi| (3\sigma_0^2-1) \sqrt{(3\sigma_0^2-1)(3-\sigma_0^2)}}{\sigma_0(\sigma_0^2-1)(\sigma_0^4-1)}.$$

Thus, the required eigenvalues of the problem (8.2) have the form

$$\tilde{E}_{0,1} = \frac{1}{2}(\hbar\omega_1 + \hbar\omega_2) + O(\hbar^2).$$

In the classical limit, these eigenvalues correspond to motion of electrons in the circles determined by the equations  $\sigma = \sigma_0$ ,  $\tau = \tau_{\pm}$ . We find the splitting by using Eqs. (6.11). We have

$$-\hbar \ln(\tilde{E}_1 - \tilde{E}_0) = \int_{\xi_-}^{\xi_+} p dx + O(\hbar),$$

where  $\xi_{\pm} = (\sigma_0, \tau_{\pm})$ . Analyzing the Hamiltonian system to determine the instanton solution, the solution satisfying the conditions  $p_\tau = 0$ ,  $\sigma = \sigma_0$ ,  $\tau = \tau_{\mp}$  for  $t \rightarrow \mp\infty$ , we can readily show that the minimum is attained on solutions for which  $p_\sigma \equiv 0$ ,  $\sigma = \sigma_0$ . Thus

$$\int_{\xi_-}^{\xi_+} p dx = \int_{\tau_-}^{\tau_+} p_\tau d\tau,$$

and it is convenient to replace the parameter  $t$  by the parameter  $\tau$ . Using the law of energy conservation, we find as a result of simple calculations

$$p_\tau = |p_\phi| \frac{\tau_+^2 - \tau^2}{(1-\tau^2)(1-\tau_+^2)}.$$

Hence

$$\int_{\tau_-}^{\tau_+} p_\tau d\tau = 2\tau_+ \sqrt{\mathcal{E}} + |p_\phi| \ln \frac{1-\tau_+}{1+\tau_+},$$

and finally we have the series of eigenfunctions of the original problem:

$$E_{0,1}^m = -\frac{1}{2a^2} \mathcal{E}_m + \frac{1}{2a^2} (\hbar\omega_1 + \hbar\omega_2) + O(\hbar^2), \quad -\hbar \ln(E_0^m - E_1^m) \approx |p_\phi| \ln \frac{1-\tau_+}{1+\tau_+} + 2\tau_+ \sqrt{\mathcal{E}_m} + O(\hbar),$$

where  $p_\sigma = mh$  and  $\mathcal{E}_m = \mathcal{E}(mh)$ .

9. Power-Law Asymptotic Behavior of the Eigenfunctions of the Operator  $-\hbar^2\Delta/2 + V(x)$  Concentrated in the Region of Minima of the Potential

In this section, we consider the spectral problem for the following Schrödinger equation with small parameter  $h$ :

$$\hat{H}\psi \stackrel{\text{def}}{=} -\frac{1}{2}h^2\Delta\psi + V(x)\psi = E\psi, \quad x \in \mathbb{R}^n, \quad \psi \in L_2(\mathbb{R}^n), \quad (9.1)$$

with smooth potential  $V(x)$  that satisfies

- 1)  $V(x) \geq 0$ ;
- 2)  $V(x)$  increases as  $|x| \rightarrow \infty$ ;

then (see [33]) the spectrum of the operator  $\hat{H}$  is discrete;

3) one of the two following conditions is satisfied: 3')  $V(x)$  has one point of global minimum  $(\xi^0)$ ; 3'')  $V(x)$  has two points of global minimum  $(\xi^1$  and  $\xi^2)$ .

In case 3'),  $V(\xi^0) = 0$  and  $V(x) > 0$  for  $x \neq \xi$ , and in case 3'')  $V(\xi^1) = V(\xi^2) = 0$  and  $V(x) > 0$  for  $x \neq \xi^1$  and  $x \neq \xi^2$ . In addition, we assume the points  $\xi^0$  or  $\xi^{1,2}$  are non-degenerate points of minimum, i.e., that the matrices

$$A_k = \frac{1}{2} \left\| \left\| \frac{\partial^2 V}{\partial x_i \partial x_j}(\xi^k) \right\| \right\|, \quad k=0 \quad \text{or} \quad k=1,2,$$

are strictly positive. Up to times of higher order, the potential  $V(x)$  in the neighborhoods of the points of minimum is equal to harmonic oscillator potentials:

$$V_{\text{osc}} = \frac{1}{2} \langle x - \xi^k, A^k(x - \xi^k) \rangle,$$

$k = 0$  or  $k = 1, 2$ . The eigenfunctions and eigenvalues of the corresponding Schrödinger operators  $-\hbar^2\Delta/2 + V_{\text{osc}}^k$  are well known. The minimal eigenvalue  $\mathcal{E}_k$  of each of these operators is not degenerate and has the form

$$\mathcal{E}_k = \frac{\hbar}{2} \sum_{j=1}^n \omega_j^k, \quad k=0 \quad \text{or} \quad k=1,2. \quad (9.2)$$

where  $(\omega_j^k)^2$ ,  $j = 1, \dots, n$ , are the eigenvalues of the matrix  $A^k$ ,  $\omega_j^k > 0$ . They correspond to eigenfunctions (normalized to 1 in  $L_2(\mathbb{R}^n)$ )

$$\varphi_k = \frac{\exp\left(-\frac{1}{2\hbar} \langle (x - \xi^k), \sqrt{A^k}(x - \xi^k) \rangle\right)}{(2\pi\hbar\omega_1^k \dots \omega_n^k)^{1/4}}. \quad (9.3)$$

Here and in all that follows, we denote the norm in  $L_2(\mathbb{R}^n)$  of the functions  $\varphi$  by  $\|\varphi\|$ .

In this section, for completeness of the exposition we reproduce the proof of the following well-known and rather transparent fact (see the Introduction): The minimal eigenvalue and the corresponding eigenfunction of the original spectral problem (9.1) are well approximated by the eigenvalue and eigenfunction of the harmonic oscillator. Namely, we prove the following propositions.

**THEOREM 8.** Suppose the potential  $V(x)$  satisfies the conditions 1, 2, 3':

a) let  $E_0$  be the minimal eigenvalue and  $\psi_0$  the corresponding eigenfunction, and  $\psi_0$  be real valued,  $\|\psi_0\| = 1$ . Then there exists  $\epsilon > 0$  such that

$$E_0 = \mathcal{E} + O(h^{1+\delta}), \quad \|\varphi_0 - \psi_0\| = O(h^\delta);$$

b) suppose the real-valued  $\varphi$  satisfies the equation

$$\hat{H}\varphi = E\varphi + f(x), \quad \|\varphi\| = 1, \quad (9.4)$$

where  $E$  and  $f$  are such that

$$E = \mathcal{E}_0 + O(h^{1+\delta}), \quad \|f\| = O(h^\delta), \quad \delta > 0;$$

then

$$\|\varphi - \varphi^0\| = O(h^\mu), \quad \mu = \max(\delta/2, 1/5). \quad (9.5)$$

**THEOREM 9.** Suppose the potential  $V(x)$  satisfies the conditions 1, 2, 3", and  $E_0$  is the minimal eigenvalue of the operator  $\hat{H}$ . Then: a)  $E_0 = \mathcal{E} + O(h^{1+\delta})$ , where  $\mathcal{E} = \min(\mathcal{E}_1, \mathcal{E}_2)$ ,  $0 < \delta < 1/5$ ; b) if  $\mathcal{E}_1 \neq \mathcal{E}_2$ , for example,  $\mathcal{E}_2 > \mathcal{E}_1$ , then for any real-valued solution of Eq. (9.4) in which  $E = \mathcal{E}_1 + O(h^{1+\delta})$  and  $\|f\| = O(h^\delta)$ , we have

$$\|\varphi - \varphi^1\| = O(h^\delta). \quad (9.6)$$

If  $\mathcal{E}_1 = \mathcal{E}_2$ , then for any real-valued solution of Eq. (9.5) there exist constants  $\alpha_1$  and  $\alpha_2$  such that

$$\|\varphi - \alpha_1 \varphi^1 - \alpha_2 \varphi^2\| = O(h^\mu), \quad \mu = \max(\delta/2, 1/5). \quad (9.7)$$

These propositions are fairly well known in the physics literature and show that in the case of a potential  $V$  with one point of global minimum (one well) or two asymmetric wells the smallest eigenvalue of the operator  $\hat{H}$  is separated from the following eigenvalues by an amount  $\sim O(h)$ . But if the wells are symmetric or "almost symmetric," i.e., the quadratic parts of the potential  $V$  in the neighborhood of the points of minimum can be reduced to the same form by means of orthogonal transformations, then in a neighborhood of the minimal eigenvalue measuring  $h^{1+\delta}$  there is a further eigenvalue.

Despite the transparency of the formulated propositions, their proofs require some calculations. The main idea of the proof (somewhat different from [9]) consists of using the variational principle and taking into account the fact that solutions of Eqs. (9.1) and (9.4) corresponding to low energies,  $E \sim O(h)$  are localized in the neighborhood of the bottom of the well (or wells) in the potential. It is more complicated to prove Theorem 9 (for two points of minimum of  $V$ ), and precisely this proof we give. The proof of Theorem 8 is similar to that of Theorem 9, and we omit it. Theorem 9 is proved by the following sequence of lemmas. In all that follows we shall denote by  $C_j$  constants that do not depend on  $h$ .

We first prove assertion a). Thus, we assume that the conditions 1, 2, 3" hold.

**LEMMA 5.** For the smallest eigenvalue  $E_0$  of the operator  $\hat{H}$  the following estimate holds (see (9.2)):

$$E_0 \leq \min(\mathcal{E}_1, \mathcal{E}_2) (1 + C_1 h^\delta). \quad (9.8)$$

**Proof.** For any  $\varphi$  in the domain of definition of  $\hat{H}$

$$E_0 \leq (\varphi, \hat{H}\varphi) / \|\varphi\|^2.$$

We introduce a smooth "cutting off" function  $e(y)$ ;  $y \in \mathbb{R}$ :  $e(y) = 1$  for  $|y| < 1$ ;  $e(y) = 0$  for  $|y| > 2$ . As  $\varphi$  we choose the function  $\psi = e(|x - \xi^j|) \varphi^j$ . The calculation of  $(\psi, \hat{H}\psi)$  and  $(\psi^*, \psi)$  by Laplace's method leads directly to the inequality (9.8).

Let  $\varepsilon$  be a certain number in the interval  $(0, \frac{1}{2})$ . We denote by  $\Omega_1^\varepsilon$  and  $\Omega_2^\varepsilon$  neighborhoods of the points  $\xi^1$  and  $\xi^2$  of radius  $h^\varepsilon$ :  $\Omega_j^\varepsilon = \{x \in \mathbb{R}^n : |x - \xi^j| < h^\varepsilon\}$ ,  $j=1, 2$ , and by  $\Omega_3^\varepsilon$  the region of points that lie outside  $\Omega_1^\varepsilon, \Omega_2^\varepsilon$ :

$$\Omega_3^\varepsilon = \mathbb{R}^n \setminus (\Omega_1^\varepsilon \cup \Omega_2^\varepsilon).$$

We denote by  $\mathcal{F}$  the functional

$$\mathcal{F}(\varphi) = \int_{\mathbb{R}^n} \left( \frac{h^2}{2} |\nabla \varphi|^2 + V(x) |\varphi|^2 \right) dx. \quad (9.9)$$

**LEMMA 6** (Localization of eigenfunctions). Let  $\varphi \in L_2(\mathbb{R}^n)$ ,  $\|\varphi\| = 1$  and  $\mathcal{F}(\varphi) \leq C_2 h$ . Then

$$\int_{\Omega_3^\varepsilon} |\varphi|^2 dx \leq C_3 h^{1-2\varepsilon}. \quad (9.9')$$

**Proof.** We have

$$\mathcal{F}(\varphi) \geq \int_{\Omega_3^\varepsilon} V(x) |\varphi|^2 dx \geq \min_{x \in \Omega_3^\varepsilon} V(x) \cdot \int_{\Omega_3^\varepsilon} |\varphi|^2 dx.$$

By virtue of the condition on the potential,  $\min_{\Omega_3^{\xi}} V(x)$  is attained on the boundary of the balls  $\Omega_1^{\xi}$  and  $\Omega_2^{\xi}$ , where obviously  $V(x) \geq C_4 h^{2\varepsilon}$ ,  $C_4 > 0$ . From this we obtain the required

$$\frac{C_2}{C_4} h^{1-2\varepsilon} \int_{\Omega_3^{\xi}} |\varphi|^2 dx.$$

We now consider the variational problem for functions  $\varphi$  defined in the balls  $\bar{\Omega}_1^{\xi}$  and  $\bar{\Omega}_2^{\xi}$  that is determined by the operators for harmonic oscillators,

$$F_j(\varphi) = \int_{\Omega_j^{\xi}} \left( \frac{h^2}{2} |\nabla \varphi|^2 + V_{\text{osc}}^j |\varphi|^2 \right) dx, \quad \varphi \in L_2(\bar{\Omega}_j^{\xi}), \quad \|\varphi\|_{L_2(\bar{\Omega}_j^{\xi})} = 1. \quad (9.10)$$

We denote by  $\tilde{\mathcal{E}}_j$  the minimum of the functional  $F_j$  and  $\tilde{\mathcal{E}}_0 = \min(\tilde{\mathcal{E}}_1, \tilde{\mathcal{E}}_2)$ .

**LEMMA 7.** For the minimal eigenvalue  $E_0$  of the problem (9.1) we have

$$E_0 \geq \tilde{\mathcal{E}}_0 (1 + \kappa_1) + \kappa_2, \quad (9.11)$$

where

$$\kappa_1 = O(h^{2\varepsilon}), \quad \kappa_2 = O(h^{2\varepsilon}). \quad (9.12)$$

**Proof.** As trial function in the functional  $\mathcal{F}$  (9.9) we take a function  $\varphi$  satisfying the assumptions of Lemma 6 (such a function exists by virtue of Lemma 5). In accordance with the results of Lemma 6, we have

$$\mathcal{F}(\varphi) \geq \sum_{j=1}^2 \int_{\Omega_j^{\xi}} \left( \frac{h}{2} |\nabla \varphi|^2 + V(x) |\varphi|^2 \right) dx \geq$$

(by virtue of the expansion of  $V(x)$  in Taylor series at the points  $\xi^1$  and  $\xi^2$  and of the properties of  $V(x)$  and the balls  $\Omega_j^{\xi}$ )

$$\geq \sum_{j=1}^2 \int_{\Omega_j^{\xi}} \left( \frac{h^2}{2} |\nabla \varphi|^2 + V_{\text{osc}}^j |\varphi|^2 \right) dx - \kappa_2 \geq$$

(by virtue of Lemma 6)

$$\begin{aligned} &\geq \sum_{j=1}^2 \int_{\Omega_j^{\xi}} \left( \frac{h^2}{2} |\nabla \varphi|^2 + V_{\text{osc}}^j |\varphi|^2 \right) dx (1 + \kappa_1) \left( \sum_{j=1}^2 \int_{\Omega_j^{\xi}} |\varphi|^2 dx \right)^{-1} - \kappa_2 \geq \\ &(1 + \kappa_1) \min_{\psi_1, \psi_2} \left[ \frac{\sum_{j=1}^2 \int_{\Omega_j^{\xi}} \left( \frac{h^2}{2} |\nabla \psi_j|^2 + V_{\text{osc}}^j |\psi_j|^2 \right) dx}{\sum_{j=1}^2 \int_{\Omega_j^{\xi}} |\psi_j|^2 dx} \right] - \kappa_2. \end{aligned}$$

This minimum is calculated with respect to functions  $\psi_j \in L_2(\Omega_j^{\xi})$  and  $\kappa_1, \kappa_2$  satisfying the estimates (9.12). Denoting

$$\int_{\Omega_j^{\xi}} |\psi_j|^2 dx = \alpha_j^2,$$

we can rewrite the last expression in the form

$$(1 + \kappa_1) \min \left( \sum_{j=1}^2 \alpha_j^2 \int_{\Omega_j^{\xi}} \frac{1}{2} h^2 (\nabla \psi_j)^2 + V_{\text{osc}}^j |\psi_j|^2 dx \right) - \kappa_2,$$

where the minimum is calculated with respect to all  $\psi_j \in L_2(\Omega_j^{\xi})$ ,  $\|\psi_j\| = 1$  and  $\alpha_j \in \mathbf{R}^1$ ,  $\alpha_1^2 + \alpha_2^2 = 1$ . Obviously the last expression is equal to

$$(1 + \kappa_1) \min_{\alpha_1^2 + \alpha_2^2 = 1} (\tilde{\mathcal{E}}_1 \alpha_1^2 + \tilde{\mathcal{E}}_2 \alpha_2^2) - \kappa_2 = (1 + \kappa_1) \tilde{\mathcal{E}}_0 - \kappa_2.$$

The following lemma establishes a relation between the minimal eigenvalues of the

operators for the harmonic oscillator in the complete space  $\mathbf{R}^n$  and in the ball  $\Omega_\varepsilon^e, 0 < \varepsilon < 1/2$ .

LEMMA 8.

$$\mathcal{E}_j \geq \mathcal{E}_j(1 + \kappa_3) \equiv \frac{\hbar}{2} \left( \sum_{k=1}^n \omega_k^j \right) (1 + \kappa_3), \quad \kappa_3 = O(\hbar^{1-2\varepsilon}), \quad 0 < \varepsilon < 1/2.$$

Proof. The basic idea is that extension of the region  $\Omega_j^\varepsilon$  in the functional  $F_j$  to  $\mathbf{R}^n$  leads in the least eigenvalue merely to appearance of a factor  $(1 + \kappa_3)$ . To simplify the notation, we shall assume  $\xi^j = 0$  and omit the index  $j$ .

Consider the functional

$$F_\varepsilon(\psi) = \int_{\Omega_\varepsilon^e} \left( \frac{1}{2} \hbar^2 |\nabla \psi|^2 + V_{\text{osc}} |\psi|^2 \right) dx, \quad \|\psi\|_{L_2(\Omega_\varepsilon^e)} = 1, \quad V_{\text{osc}} = 1/2 \langle x, A^k x \rangle.$$

Suppose the minimum of  $F_\varepsilon$  is attained on the function  $\psi$ ; then  $\psi$  satisfies the Schrödinger equation

$$-1/2 \hbar^2 \Delta \psi + V_{\text{osc}} \psi = \tilde{\mathcal{E}} \psi.$$

At the same time

$$\tilde{\mathcal{E}} \leq \frac{\hbar}{2} \sum_{k=1}^n \omega_k (1 + \kappa_i), \tag{9.13}$$

where  $|\kappa_i| \leq C(N) \hbar^N$ ,  $N$  is any natural number, and  $C(N)$  is a constant. This last result is readily seen by choosing as trial function  $\psi$  in the functional  $F$  the eigenfunction  $\varphi^0$  (9.3) of the harmonic oscillator in  $\mathbf{R}^n$  and taking into account at the same time the estimate

$$\int_{|x| > \hbar^\varepsilon} \left( \frac{1}{2} \hbar^2 |\nabla \varphi|^2 + V_{\text{osc}} |\varphi|^2 \right) dx = O(\hbar^\infty)$$

for  $\varepsilon < 1/2$ .

We note further that for the function  $\psi$  there is an estimate analogous to the estimate of Lemma 6:

$$\int_{\hbar^\varepsilon/2 \leq |x| \leq \hbar^\varepsilon} |\psi|^2 dx \leq C_5 \hbar^{1-2\varepsilon}. \tag{9.14}$$

Indeed, by virtue of (9.13) we have as in Lemma 6

$$C_5 \hbar \geq \frac{1}{2} \int_{\hbar^\varepsilon/2 \leq |x| \leq \hbar^\varepsilon} V_{\text{osc}} |\psi|^2 dx \geq \frac{1}{2} \min_{|x| = \hbar^\varepsilon/2} V_{\text{osc}} \int_{\hbar^\varepsilon/2 \leq |x| \leq \hbar^\varepsilon} |\psi|^2 dx,$$

from which (9.14) follows immediately.

We derive one further auxiliary equation. Suppose  $\varphi$  satisfies the inhomogeneous Schrödinger equation

$$-1/2 \hbar^2 \Delta \varphi + V(x) \varphi = E \varphi + f,$$

where  $\Omega$  is a certain region in  $\mathbf{R}^n$ ,  $g(x, \hbar)$  is a certain function,  $\text{supp } g \in \Omega$ . We denote  $\varphi_1 = g\varphi$  and  $\varphi_2 = (1-g)\varphi$ . We consider the functional

$$\Phi_\Omega(\varphi) = \int_{\Omega} \left( \frac{\hbar^2}{2} |\nabla \varphi|^2 + V |\varphi|^2 \right) dx,$$

and then

$$\Phi_\Omega = \Phi_\Omega(\varphi_1) + \Phi_\Omega(\varphi_2) + \int_{\Omega} [g(1-g)E |\varphi|^2 + \varphi \bar{f} + \bar{\varphi} f - 2\hbar^2 (\nabla g)^2 |\varphi|^2] dx. \tag{9.15}$$

To derive (9.15), we transform the expression

$$\int_{\Omega} \left( \frac{\hbar^2}{2} (\nabla \varphi_1 \nabla \bar{\varphi}_2 + \nabla \bar{\varphi}_1 \nabla \varphi_2) + V(\varphi_1 \bar{\varphi}_2 + \bar{\varphi}_1 \varphi_2) \right) dx =$$



(integrating by parts)

$$\begin{aligned}
 &= \int_{\Omega} \left[ \frac{h^2}{2} (-\varphi_1 \Delta \bar{\varphi}_2 - \varphi_2 \Delta \bar{\varphi}_1) + V(\varphi_1 \bar{\varphi}_2 + \bar{\varphi}_1 \varphi_2) \right] dx = \\
 &\int_{\Omega} \left[ \frac{h^2}{2} (-\varphi_1 (1-g) \Delta \bar{\varphi} + 2\varphi_1 \nabla g \cdot \nabla \bar{\varphi} + \varphi_1 \Delta g \bar{\varphi} - (1-g) \bar{\varphi}_1 \Delta \varphi + \right. \\
 &\quad \left. 2\bar{\varphi}_1 \nabla g \cdot \nabla \varphi + \bar{\varphi}_1 \Delta g \varphi) + V(\varphi_1 \bar{\varphi}_2 + \bar{\varphi}_1 \varphi_2) \right] dx =
 \end{aligned}$$

(by virtue of the definition of  $\varphi_{1,2}$  and the equation for  $\varphi$ )

$$\begin{aligned}
 &= \int_{\Omega} [g(1-g)(E|\varphi|^2 + \varphi \bar{f} + \bar{\varphi} f) + h^2 \nabla(g^2) \cdot \nabla(|\varphi|^2) + 2h^2 g \Delta g |\varphi|^2] dx = \\
 &\int_{\Omega} [g(1-g)(E|\varphi|^2 + \varphi \bar{f} + \bar{\varphi} f) - 2h^2 (\nabla g)^2 |\varphi|^2] dx.
 \end{aligned}$$

From this (9.15) follows.

In (9.15) we now set  $V = V_{\text{OSC}}$ ,  $f=0$ ,  $\Omega = \Omega_\varepsilon$ ,  $g = e(|x|/2h^\varepsilon)$ ,  $\varphi = \psi$ ,  $\varphi_1 = g\psi$ ,  $E = \tilde{\mathcal{E}}$ , where  $e(y)$  is the "cutting off" function defined in Lemma 5. From (9.15)

$$F_\varepsilon(\psi) \geq \Phi_{\Omega_\varepsilon}(\varphi_1) + I, \quad (9.16)$$

where

$$I = \int_{\Omega_\varepsilon} (\mathcal{E}_0 g(1-g) |\psi|^2 - 2h^2 (\nabla g)^2 |\psi|^2) dx.$$

By virtue of the definition of  $e$ ,  $\psi$  (9.13), and (9.14),  $I$  admits the obvious estimate

$$|I| \leq C_7 h^{2-2\varepsilon} + C_8 h^{3-4\varepsilon}.$$

Further, from (9.13)

$$1 = \int_{\Omega_\varepsilon} |\psi|^2 dx = \int_{\Omega} |\psi_1|^2 dx + \int_{\Omega_\varepsilon} (1-e^2) |\psi|^2 dx = \int_{\Omega_\varepsilon} |\varphi_1|^2 dx + \kappa_5, \quad |\kappa_5| < C_9 h^{1-2\varepsilon}. \quad (9.17)$$

From (9.16) and (9.17)

$$\tilde{\mathcal{E}} \geq \frac{\int_{\Omega_\varepsilon} (1/2 h^2 |\nabla \varphi_1|^2 + V_{\text{OSC}} |\varphi_1|^2) dx}{\int_{\Omega_\varepsilon} |\varphi_1|^2 dx} (1 - \kappa_6) - \kappa_7,$$

where  $0 < \kappa_7 < C_9 h^{2-2\varepsilon} + C_{10} h^{3-4\varepsilon}$ ,  $0 < \kappa_6 < C_{11} h^{1-2\varepsilon}$ . Since  $\psi_1$  is a function of compact support, the domain of integration on the right-hand side can be replaced by  $\mathbf{R}^n$ . Since the obtained equation has a minimum, which is attained on the eigenfunction (9.3) of the harmonic oscillator in  $\mathbf{R}^n$ , we readily obtain, taking into account the inequality  $\varepsilon < \frac{1}{2}$ , the assertion of the lemma.

Combining now Lemmas 7 and 8, assuming  $1/3 < \varepsilon < 1/2$ , and choosing at the same time  $\delta = \min(3\varepsilon - 1, 1 - 2\varepsilon)$ , we obtain proposition a) of Theorem 9.

We now turn to the proof of proposition b) of Theorem 9.

Consider the functional

$$\Phi(\varphi) = \int_{\mathbf{R}^n} \left( \frac{h^2}{2} |\nabla \varphi|^2 + V_{\text{OSC}} |\varphi|^2 \right) dx, \quad \|\varphi\| = 1,$$

where  $V_{\text{OSC}}$  is the harmonic oscillator potential  $V = 1/2 \langle x, A^2 x \rangle$ ,  $\mathcal{E}_0$  is its minimal value (9.2), and  $\varphi^0$  is the eigenfunction (9.3).

**LEMMA 9.** Let  $\varphi$  be a real-valued function possessing the property

$$\Phi(\varphi) = \mathcal{E}_0(1 + O(h^\gamma)), \quad \gamma > 0. \quad (9.18)$$

Then  $\|\varphi - \varphi^0\| \leq C_{12} h^{\gamma/2}$ .

Proof. We denote by  $\psi_\nu$  the normalized eigenfunctions of the operator  $\hat{H}_{\text{osc}}$ . The system  $\{\psi_\nu\}$  forms a basis in  $L_2(\mathbf{R}^n)$ . Therefore, for  $\varphi(x, h)$  we have the decomposition  $\varphi = \sum_{\nu=0}^{\infty} a_\nu \psi_\nu$ ,  $a_\nu$  are Fourier coefficients, and at least  $a_0$  is real (since  $\mathcal{E}_0$  is not degenerate). We substitute  $\varphi$  in (9.18) and use the properties of the functions  $\psi_\nu$ . As a result, we obtain the equations

$$\sum_{\nu=0}^{\infty} E_\nu |a_\nu|^2 = E_0(1 + O(h^\delta)), \quad \sum_{\nu=0}^{\infty} |a_\nu|^2 = 1. \quad (9.19)$$

We denote by  $\mathcal{E}'$  the  $\mathcal{E}_\nu$  closest to  $\mathcal{E}_0$ :  $\mathcal{E}' = E_0 + h \min(\omega_1, \dots, \omega_n)$ . From (9.19)

$$\mathcal{E}_0 a_0^2 + \mathcal{E}' \sum_{\nu>0} |a_\nu|^2 \leq \mathcal{E}_0(1 + O(h^\gamma)).$$

It follows that  $(\mathcal{E}' - \mathcal{E}_0)(1 - a_0^2) \leq \mathcal{E}_0 \cdot O(h^\gamma)$  or  $1 - a_0^2 \leq C_{13} h^\delta/2$ , and therefore

$$\|\varphi - \varphi^0\|^2 = (1 - a_0^2)^2 + \sum_{\nu>0} |a_\nu|^2 \leq 2(1 - a_0^2) \leq C_{13} h^\gamma.$$

Now suppose the function  $\varphi$  satisfies Eq. (9.4) with  $E = \mathcal{E} + O(h^{1+\delta})$  (see Theorem 9). Then from Eq. (9.4), taking into account the estimate  $\mathcal{E} = O(h)$ , we obtain for the energy functional  $\mathcal{F}$  (9.9):  $\mathcal{F}(\varphi) \leq C_{14} h$ . Then by virtue of Lemma 6 for  $\varepsilon \in (0, 1/2)$  we have for  $\varphi$  the estimate (9.9').

We now show that we can represent the function  $\varphi$  up to terms of higher order as a sum of two terms, each of which will satisfy either the condition of Lemma 9 or be small. Using the "cutting off" function  $e(y)$  from Lemma 5, we introduce the functions  $g_j = e(|x - \xi^j|/2h^\varepsilon)$  and  $g = g_1 + g_2$ . It is clear that the supports of  $g_1$  and  $g_2$  do not intersect, and  $g^2 = g_1^2 + g_2^2$ . From the estimate (9.9') for  $\varphi$  we directly obtain the equation

$$\|\varphi g\|^2 = \|\varphi g_1\|^2 + \|\varphi g_2\|^2 = 1 - \kappa_8 h^{1-2\varepsilon}, \quad (9.20)$$

where  $\kappa_8 \leq C_{14}$ .

We calculate the functional  $\mathcal{F}$  on the function  $g\varphi$ . Integration by parts gives (cf. formula (9.15))

$$\mathcal{F}(g\varphi) = \int_{\mathbf{R}^n} \left( h^2 \frac{(\nabla g)^2 \varphi^2 - g^2 \Delta \varphi}{2} + g^2 V \varphi^2 \right) dx. \quad (9.21)$$

Using Eq. (9.4), the estimate (9.20) and the definition of  $\mathcal{E}$ , we obtain from this

$$\mathcal{F}(g\varphi) = \int_{\mathbf{R}^n} \left( g^2 (E\varphi^2 + \varphi f) + \frac{h^2}{2} (\nabla g)^2 \varphi^2 \right) dx = \mathcal{E} (1 + \kappa_9 h^{1-2\varepsilon}) + \kappa_{10} h^{1+\delta},$$

where  $\kappa_9, \kappa_{10} \leq C_{15}$ .

On the other hand, by the definition of  $g$ ,  $e$ , and the Taylor expansion of  $V$  in the neighborhood of the points  $\xi^j$  we have

$$\mathcal{F}(g\varphi) = \sum_{j=1}^2 \int_{\mathbf{R}^n} \left( \frac{h^2}{2} (\nabla (g_j \varphi))^2 + V_{\text{osc}}^j (g_j \varphi)^2 \right) dx + \kappa_{11} h^{3\varepsilon},$$

where  $|\kappa_{11}| \leq C_{16}$ .

Thus, it follows from (9.20) and (9.21) that

$$\frac{\sum_{j=1}^2 \int_{\mathbf{R}^n} \left( \frac{h^2}{2} (\nabla (g_j \varphi))^2 + V_{\text{osc}}^j (g_j \varphi)^2 \right) dx}{\|g_1 \varphi\|^2 + \|g_2 \varphi\|^2} = \frac{\mathcal{E} (1 + \kappa_9 h^{1-2\varepsilon}) + \kappa_{10} h^{1+\delta} + \kappa_{11} h^{3\varepsilon}}{1 - \kappa_8 h^{1-2\varepsilon}}.$$

Assuming  $\varepsilon \in (1/3, 1/2)$ , denoting  $\max(1 - 2\varepsilon, 3\varepsilon - 1, \delta)$  by  $\gamma$ , and, in addition,  $\alpha_j = \|g_j \varphi\| / \sqrt{\|g_1 \varphi\|^2 + \|g_2 \varphi\|^2}$ , we obtain

$$\sum_{j=1}^2 \alpha_j^2 \int_{\mathbb{R}^n} \left( \frac{h^2}{2} (\nabla \psi_j)^2 + V_{\text{osc}}^j \psi_j^2 \right) dx = \mathcal{E}_2 (1 + \kappa_{12} h^\gamma),$$

and at the same time  $\alpha_1^2 + \alpha_2^2 = 1$ ,  $|\kappa_{12}| \leq C_{15}$ .

Now, taking into account the inequalities

$$\int_{\mathbb{R}^n} \left( \frac{h^2}{2} (\nabla \psi_j)^2 + V_{\text{osc}}^j \psi_j^2 \right) dx \geq \mathcal{E}_j,$$

we find by straightforward arguments that: 1) when  $\mathcal{E}_1 < \mathcal{E}_2$ , then  $\alpha_2^2 < C_{16} h^\gamma$ ,  $\alpha_1^2 = 1 + \kappa_{13} h^\gamma$ ,  $|\kappa_{13}| < C_{16}$  and

$$\int_{\mathbb{R}^n} \left( \frac{h^2}{2} (\nabla \varphi_1)^2 + V_{\text{osc}}^1 \varphi_1^2 \right) dx = \mathcal{E}_1 (1 + \kappa_{14} h^\gamma), \quad |\kappa_{14}| < C_{17},$$

2) when  $\mathcal{E}_1 = \mathcal{E}_2$ , then

$$\int_{\mathbb{R}^n} \left( \frac{h^2}{2} (\nabla \psi_j)^2 + V_{\text{osc}}^j \psi_j^2 \right) dx = \mathcal{E}_j (1 + \kappa_4^j h^\gamma), \quad |\kappa_4^j| < C_{17}.$$

From Lemma 9 in case 1 we immediately obtain  $g\varphi = \varphi^0 + \theta^0$ , where  $\|\theta^0\| \leq C_{18} h^{1/2}$ , and in case 2  $g\varphi = \alpha_1 \varphi^1 + \alpha_2 \varphi^2 + \theta^1$ , where  $\|\theta^1\| \leq C_{18} h^{1/2}$  and  $\varphi^j$  have the form (9.3).

To complete the proof of the theorem, it now remains to note that  $\|g\varphi - \varphi\| \leq C_{19} h^{(1-2\varepsilon)/2} \leq C_{19} h^{1/2}$  and that  $\max_{1/3 < \varepsilon < 1/2} (1 - 2\varepsilon, 3\varepsilon - 1) = 2/5$ .

## 10. Laplace's Method with Estimate of the Remainder Term

We derive the formulas used in the foregoing sections by Laplace's method of calculating asymptotic integrals with accuracy estimates. Such estimates are not found in the well-known guides to this method (see, for example, [40]).

We shall investigate the  $h \rightarrow 0$  behavior of the integral

$$I(h) = \int_{\Omega} f(x) \exp\{-S(x)/h\} dx, \quad (10.1)$$

where  $\Omega$  is a region in  $\mathbb{R}^n$ ,  $h$  is a positive real parameter, the functions  $f(x)$  and  $S(x)$  are real and continuous in  $\Omega$ , and  $f(x) \geq 0$  in  $\Omega$ .

We first recall the simplest obvious estimate for  $I(h)$  [40]: if  $M \leq \inf\{S(x) : x \in \Omega\}$  and it is known that  $I(h)$  converges for  $h = h_0$ , then  $I(h)$  converges for all  $h \in (0, h_0)$  and at the same time

$$I(h) \leq \exp\{-M/h\} \exp\{M/h_0\} I(h_0). \quad (10.2)$$

To obtain a more accurate estimate, we introduce further assumptions:

a) the function  $S(x)$  attains its minimal value in  $\Omega$  at a unique point  $x_0 \in \Omega$ , and there exists a compact neighborhood  $U$  of the point  $x_0$  in  $\Omega$  such that for every convex neighborhood  $U' \subset U$  of the point  $x_0$

$$\inf\{S(x) : x \in \Omega \setminus U'\} = \min\{S(x) : x \in \partial U'\}; \quad (10.3)$$

b)  $x_0$  is a nondegenerate point of minimum of the function  $S(x)$ , i.e., the matrix  $S''(x_0)$  is positive definite;

c)  $S(x)$  is thrice continuously differentiable in  $U$ ;

d)  $I(h)$  converges for  $h = h_0$ .

We denote by  $d$  and  $D$ , respectively, the smallest eigenvalue and determinant of the matrix  $S''(x_0)$ ; let

$$\Phi = \max\{f(x) : x \in U\}, \quad C_3 = \max\{\|S'''(x)\| : x \in U\}$$

( $\|S'''(x)\|$  is the norm of  $S'''(x)$  as a polylinear functional in  $\mathbf{R}^n$ ). We fix  $\beta \in (1/3, 1/2)$  and an arbitrary  $\delta > 0$ , and set

$$U_\beta(h) = \{x \in \Omega : (S''(x_0)(x-x_0), x-x_0) \leq h^{2\beta}\}$$

(the ellipsoid  $U_\beta(h)$  is obviously contained in the ball of radius  $\sqrt{1/d}h^\beta$  in  $\Omega$  with center at  $x_0$ ).

**LEMMA 10.** Let  $h \leq h_0$  be such that  $U_\beta(h) \subset U$  and, in addition,

$$\exp\{1/2 h_0^{2\beta-1} - 1/2 h^{2\beta-1}\} \leq (2\pi h)^{n/2} h^{1+\delta}, \quad (10.4)$$

$$1/2 C_3 d^{-n/2} h^{3\beta-1} \leq 1; \quad (10.5)$$

then

$$I(h) \leq \exp\{-S(x_0)/h\} (2\pi h)^{n/2} e^{1/2} [D^{-n/2} \Phi + h^{1+\delta} I(h_0) \exp\{S(x_0)/h_0\}]. \quad (10.6)$$

**Proof.** We split the integral  $I(h)$  into the sum  $I_1(h) + I_2(h)$  of integrals over the regions  $U_\beta(h)$  and  $\Omega \setminus U_\beta(h)$ , respectively. Since the ellipsoid  $U_\beta(h)$  is obviously contained in the ball of radius  $\sqrt{1/d}h^\beta$  in  $\Omega$  with center at  $x_0$ , for  $x \in U_\beta(h)$

$$S(x) = S(x_0) + 1/2 (S''(x_0)(x-x_0), x-x_0) + \sigma(x), \quad (10.7)$$

where

$$|\sigma(x)| \leq \frac{1}{3!} C_3 d^{-n/2} h^{3\beta}, \quad (10.8)$$

and hence, by virtue of (10.5),  $|\sigma(x)|/h \leq 1/3$ , and therefore

$$I_1(h) \leq \Phi \exp\{-S(x_0)/h\} e^{1/3} \int_{U_\beta(h)} \exp\left\{-\frac{1}{2h} (S''(x_0)(x-x_0), x-x_0)\right\} dx \leq (2\pi h)^{n/2} D^{-n/2} \Phi e^{1/3} \exp\{-S(x_0)/h\}. \quad (10.9)$$

Turning to the estimate of  $I_2(h)$ , we note that in accordance with (10.3)

$$\inf\{S(x) : x \in \Omega \setminus U_\beta(h)\} = \min\{S(x) : x \in \partial U_\beta(h)\}. \quad (10.10)$$

Using now for  $x \in \partial U_\beta(h)$  the representation (10.7), we obtain from (10.8)

$$\inf\{S(x) : x \in \Omega \setminus U_\beta(h)\} \geq S(x_0) + \frac{1}{2} h^{2\beta} - \frac{1}{3!} C_3 d^{-n/2} h^{3\beta}. \quad (10.11)$$

Hence and from the general estimate (10.2) it follows that

$$I_2(h) \leq \exp\left\{-\frac{1}{h} \left(S(x_0) + \frac{1}{2} h^{2\beta} - \frac{1}{3!} C_3 d^{-n/2} h^{3\beta}\right)\right\} \exp\left\{\frac{1}{h_0} \left(S(x_0) + \frac{1}{2} h^{2\beta} - \frac{1}{3!} C_3 d^{-n/2} h^{3\beta}\right)\right\} \times \int_{\Omega \setminus U_\beta(h)} f(x) \exp\{-S(x)/h_0\} \leq \exp\{-S(x_0)/h\} \exp\{-1/2 h^{2\beta-1}\} I(h_0) e^{1/3} \exp\{S(x_0)/h_0\} \exp\{1/2 h_0^{2\beta-1}\}.$$

From the estimates obtained for  $I_1(h)$  and  $I_2(h)$  and the condition (10.4) Lemma 10 follows directly.

**THEOREM 10.** Suppose that in addition to the conditions of Lemma 10 there exist in  $U$  continuous derivatives  $f'$ ,  $f''$  of the function  $f$  and the fourth derivative of the function  $S$ . We denote by  $\Phi_1$ ,  $\Phi_2$ ,  $C_4$ , respectively, the maxima of the norms in  $U$  of the polylinear mappings  $f'(x)$ ,  $f''(x)$ ,  $S^{(4)}(x)$ . Then for  $h$  satisfying the condition of Lemma 10

$$I(h) = (2\pi h)^{n/2} D^{-n/2} (f(x_0) + \alpha(h)h) \exp\{-S(x_0)/h\}, \quad (10.12)$$

where  $\alpha(h)$  satisfies the estimate

$$|\alpha(h)| \leq 1/2 \Phi_2 d^{-1} n + 1/4 e^{1/3} \Phi C_3^2 d^{-n/2} n(n+1)(n+2) + \left(\frac{1}{4!} C_4 f(x_0) + \frac{1}{3!} C_3 \Phi_1\right) d^{-2} n(n+2) + f(x_0) (2\pi h_0)^{n/2} h^\delta + e^{1/3} D^{n/2} h^\delta \exp\{S(x_0)/h\} I(h_0).$$

**Proof.** We represent  $I(h)$  in the form

$$I(h) = \exp\{-S(x_0)/h\} (I_0(h) + I_1(h) + I_2(h) + I_3(h)),$$

where

$$\begin{aligned}
I_1(h) &= f(x_0) \int_{U_\beta(h)} \exp\left\{-\frac{1}{2h}(S''(x_0)(x-x_0), x-x_0)\right\} dx, \\
I_2(h) &= \int_{U_\beta(h)} (f(x)-f(x_0)) \exp\left\{-\frac{1}{2h}(S''(x_0)(x-x_0), x-x_0)\right\} dx, \\
I_3(h) &= \int_{U_\beta(h)} f(x) \left(\exp\left\{-\frac{\sigma(x)}{h}\right\} - 1\right) \exp\left\{-\frac{1}{2h}(S''(x_0)(x-x_0), x-x_0)\right\} dx, \\
I_4(h) &= \int_{\Omega \setminus U_\beta(h)} f(x) \exp\left\{-\frac{1}{h}(S(x)-S(x_0))\right\} dx.
\end{aligned}$$

The function  $\sigma(x)$  in the integral  $I_3$  is defined in (10.7).

We shall denote by  $B_Y(R)$  the ball of radius  $R$  in  $\mathbf{R}^n$  with center at  $y \in \mathbf{R}^n$ . As we have already noted,  $U_\beta(h) \subset B_{x_0}(\sqrt{1/d}h^\beta)$ .

We investigate the integral  $I_1(h)$ . We represent it as a difference of integrals over  $\mathbf{R}^n$  and over  $\mathbf{R}^n \setminus U_\beta(h)$ . The integral over the whole of  $\mathbf{R}^n$  is tabulated: as is well known, it is  $(2\pi h)^{n/2} D^{-1/2} f(x_0)$ . Making then in the second integral a change of the variable of integration in accordance with the formula  $\sqrt{S_0''}(x-x_0)=y$ , we obtain

$$I_1(h) = f(x_0) D^{-1/2} \left[ (2\pi h)^{n/2} + \int_{\mathbf{R}^n \setminus B_0(h^\beta)} \exp\{-\|y\|^2/2h\} dy \right].$$

For the integral here we can obtain an upper bound in accordance with formula (10.2) in terms of

$$\exp\{-1/2h^{2\beta-1} + 1/2h_0^{2\beta-1}\} \int_{\mathbf{R}^n} \exp\{-\|y\|^2/2h_0\} dy = (2\pi h_0)^{n/2} \exp\{-1/2h^{2\beta-1}\} \exp\{1/2h_0^{2\beta-1}\}.$$

As a result, using (10.4), we obtain

$$I_1(h) = (2\pi h)^{n/2} D^{-1/2} (f(x_0) + \alpha_1(h)h), \quad (10.13)$$

where

$$|\alpha_1(h)| \leq f(x_0) (2\pi h_0)^{n/2} h^\delta. \quad (10.14)$$

We turn to the integral  $I_2(h)$ . Expanding  $f(x)$  in a Taylor series to the second term and noting that the integral of an odd function over a symmetric region is equal to zero, we obtain

$$I_2 \leq \frac{1}{2} \Phi_2 \int_{U_\beta(h)} \|x-x_0\|^2 \exp\left\{-\frac{1}{2h}(S''(x_0)(x-x_0), x-x_0)\right\} dx.$$

Making the substitution  $\sqrt{S''(x_0)}(x-x_0)=y$  and noting that  $\|S''(x_0)^{-1}\|=d^{-1}$ , we arrive at the estimate

$$I_2 \leq 1/2 \Phi_2 D^{-1/2} d^{-1} \int_{B_0(h^\beta)} \|y\|^2 \exp\{-\|y\|^2/2h\} dy.$$

Using now the well-known formula

$$\int_{\mathbf{R}^n} \|y\|^k \exp\{-\|y\|^2/2h\} dy = \frac{\pi^{n/2}}{\Gamma(n/2)} \Gamma\left(\frac{n+k}{2}\right) (2h)^{(n+k)/2} \quad (10.15)$$

(which is readily derived by going over to spherical coordinates) for  $k=2$ , we obtain the estimate

$$I_2(h) \leq 1/2 \Phi_2 D^{-1/2} d^{-1} (2\pi h)^{n/2} h n. \quad (10.16)$$

We estimate the integral  $I_3(h)$ . For this it is also necessary to divide it into a sum of two integrals:  $I_3(h) = I_3'(h) + I_3''(h)$ . Here

$$I_3'(h) = \int_{U_\beta(h)} f(x) \left(\exp\left\{-\frac{\sigma(x)}{h}\right\} - 1 + \frac{\sigma(x)}{h}\right) \exp\left\{-\frac{1}{2h}(S''(x_0)(x-x_0), x-x_0)\right\} dx,$$

$$I_3''(h) = \int_{U_\beta(h)} f(x) \left( -\frac{\sigma(x)}{h} \right) \exp \left\{ -\frac{1}{2h} (S''(x_0)(x-x_0), x-x_0) \right\} dx.$$

In the proof of the lemma we obtained the estimate  $|\sigma(x)/h| \leq 1/3$ , in  $U_\beta(h)$ . Hence and from the estimate  $|\sigma(x)| \leq \frac{1}{3!} C_3 \|x-x_0\|$  it follows that

$$\begin{aligned} \exp \left\{ -\frac{\sigma(x)}{h} \right\} - 1 + \frac{\sigma(x)}{h} &= \left( -\frac{\sigma(x)}{h} \right)^2 \left( \frac{1}{2!} + \frac{1}{3!} \left( -\frac{\sigma(x)}{h} \right) + \dots \right) \leq \\ & \left| \frac{\sigma(x)}{h} \right|^2 9 \left( e^{1/3} - \frac{4}{3} \right) \leq 9e^{1/3} \left( \frac{C_3}{3!} \right)^2 \frac{\|x-x_0\|^6}{h^2} = 1/4 C_3^2 e^{1/3} \|x-x_0\|^6 h^{-2}, \end{aligned}$$

and therefore

$$I_3'(h) \leq 1/4 C_3^2 \Phi e^{1/3} h^{-2} \int_{U_\beta(h)} \|x-x_0\|^6 \exp \left\{ -\frac{1}{2h} (S''(x_0)(x-x_0), x-x_0) \right\} dx.$$

Making now, as above, the substitution  $\sqrt{S''(x_0)}(x-x_0) = y$ , we obtain

$$I_3'(h) \leq 1/4 C_3^2 \Phi e^{1/3} h^{-2} D^{-1/2} d^{-3/2} \int_{\mathbb{R}^n} \|y\|^6 \exp \{ -\|y\|^2/2h \} dx.$$

Using (10.15) for  $k = 6$ , and also the equation  $\Gamma\left(\frac{n}{2} + 3\right) = \frac{n}{2} \left(\frac{n}{2} + 1\right) \left(\frac{n}{2} + 2\right) \Gamma\left(\frac{n}{2}\right)$ , we obtain

$$I_3'(h) \leq 1/4 (2\pi h)^{n/2} D^{-1/2} \Phi C_3^2 e^{1/3} d^{-3/2} n(n+2)(n+4). \quad (10.17)$$

To estimate  $I_3''$  we note that in  $U$

$$\left| \sigma(x) - \frac{1}{3!} S'''(x_0)(x-x_0)^3 \right| \leq \frac{1}{4!} C_4 \|x-x_0\|^4.$$

Bearing in mind that the integral of an odd function over a symmetric region is zero, we have

$$\begin{aligned} I_3''(h) &= \int_{U_\beta(h)} \exp \left\{ -\frac{1}{2h} (S''(x_0)(x-x_0), x-x_0) \right\} \times \\ & \left[ f(x_0) \left( -\frac{\sigma(x)}{h} + \frac{1}{3!} \frac{1}{h} S'''(x_0)(x-x_0)^3 \right) + (f(x) - f(x_0)) \left( -\frac{\sigma(x)}{h} \right) \right] dx, \end{aligned}$$

and therefore

$$I_3''(h) \leq \int_{U_\beta(h)} \left( \frac{1}{4!} C_4 f(x_0) + \frac{1}{3!} C_3 \Phi_1 \right) \|x-x_0\|^4 h^{-1} \exp \left\{ -\frac{1}{2h} (S''(x_0)(x-x_0), x-x_0) \right\} dx.$$

Making as above the change of variable and using (10.15) for  $k = 4$ , we obtain

$$I_3''(h) \leq \left( \frac{1}{4!} C_4 f(x_0) + \frac{1}{3!} C_3 \Phi_1 \right) (2\pi h)^{n/2} D^{-1/2} d^{-2} n(n+2). \quad (10.18)$$

The integral  $I_4$  is estimated in the same way as in the proof of Lemma 10. Thus

$$I_4(h) \leq e^{1/3} (2\pi h)^{n/2} h^{1+\delta} \exp \{ S(x_0)/h_0 \} I(h_0). \quad (10.19)$$

From the estimates (10.13), (10.14), (10.16)-(10.19) we obtain Theorem 10.

**Remark 5.** If we do not require the existence of  $f''$  and  $S^{(4)}$  in  $U$ , then the formula for  $I(h)$  in Theorem 10 is changed — it will no longer be possible in general to represent the remainder term in the form  $O(h)$ , but only in the form  $O(h^{2\beta-1})$ .

**Remark 6.** Somewhat different, "more uniform with respect to the dimension" estimates of the remainder term  $\alpha(h)h$  can be obtained if one calculates the main term, not from an integral over a ball (or ellipsoid), as in our arguments, but from an integral over a cube.

## LITERATURE CITED

1. V. P. Maslov, Dokl. Akad. Nauk SSSR, 258, 1112 (1981).
2. V. P. Maslov, Tr. Mosk. Inst. Akad. Nauk SSSR, 163, 150 (1984).
3. V. P. Maslov, Perturbation Theory and Asymptotic Methods [in Russian], Moscow State University, Moscow (1965).
4. V. P. Maslov, Asymptotic Methods and Perturbation Theory [in Russian], Nauka, Moscow (1988).
5. V. P. Maslov, The Complex WKB Method in Nonlinear Equations [in Russian], Nauka, Moscow (1977).
6. V. P. Maslov, Zh. Vychisl. Mat. Mat. Fiz., No. 1 114 (1961); No. 4, 638 (1961).
7. S. R. Varadhan, Commun. Pure Appl. Math., 19, 231 (1966).
8. A. A. Borovkov, Teor. Veroyatn. Ee Primen., 12, 635 (1967).
9. B. Simon, Ann. Inst. H. Poincaré, 38, 295 (1983).
10. A. M. Polyakov, Nucl. Phys., 120, 429 (1977).
11. E. Gildener and A. Patrascigin, Phys. Rev. D, 16, 425 (1977).
12. E. M. Harrel, Commun. Math. Phys., 75, 239 (1980).
13. E. M. Harrel, Ann. Phys. (N.Y.), 119, 351 (1979).
14. G. Jona-Lasinio, L. Martinelli, and E. Scoppola, Commun. Math. Phys., 80 (1981).
15. J. M. Combes, P. Duclos, and R. Seiler, Commun. Math. Phys., 92, No. 2 (1983).
16. T. F. Pankratova, Dokl. Akad. Nauk SSSR, 276, 795 (1984).
17. R. Rajaraman, Solitons and Instantons, North-Holland, Amsterdam (1984).
18. B. Simon, Ann. Math., 120, 89 (1984).
19. B. Heffler and J. Sjöstrand, Commun. in P. D. E., 9, 337 (1984); Ann. Inst. H. Poincaré, 42, 127 (1985); Commun. in P. D. E., 13, 245 (1985); Ann. Inst. H. Poincaré, 46, 353 (1987).
20. E. Witten, J. Diff. Geom., 17, 661 (1982).
21. L. D. Landau and E. M. Lifshitz, Quantum Mechanics: Nonrelativistic Theory, 3rd ed., Pergamon Press, Oxford (1977).
22. P. Hartman, Ordinary Differential Equations, Wiley, New York (1964).
23. Yu. I. Kifer, Izv. Akad. Nauk SSSR, Ser. Mat., 38, 1091 (1974).
24. V. M. Babich, Dokl. Akad. Nauk SSSR, 289, 836 (1986).
25. S. A. Molchanov, Usp. Mat. Nauk, 30, 3 (1975).
26. V. P. Maslov, Complex Markov Chains and Feynman Path Integrals [in Russian], Nauka, Moscow (1977).
27. V. P. Maslov and M. V. Fedorov, The Semiclassical Approximation for the Equations of Quantum Mechanics [in Russian], Nauka, Moscow (1976).
28. V. N. Kolokol'tsov and V. P. Maslov, Funktsional. Analiz i Ego Prilozhen., No. 1, 1 (1989); No. 4, 53 (1989).
29. V. P. Maslov, Asymptotic Methods of Solution of Pseudodifferential Equations [in Russian], Nauka, Moscow (1987).
30. V. P. Maslov, Usp. Mat. Nauk, 42, 39 (1987).
31. J. Palis, Jr, and W. de Melo, Geometric Theory of Dynamical Systems, Springer, New York (1982).
32. S. Sternberg, Am. J. Math., 79, 809 (1957).
33. F. A. Berezin and M. A. Shubin, The Schrödinger Equation [in Russian], Moscow State University, Moscow (1983).
34. V. P. Maslov and M. V. Fedoryuk, Mat. Zametki., 30, 763 (1981).
35. E. C. Titchmarsh, Eigenfunction Expansions Associated with Second-Order Differential Equations, Vol. 2, Clarendon Press, Oxford (1958).
36. M. Reed and B. Simon, Methods of Modern Mathematical Physics, Vol. 4, Academic Press, New York (1978).
37. S. Coleman, "The uses of instantons," in: The Whys of Subnuclear Physics (ed. A. Zichichi), New York (1979), pp. 805-916.
38. O. Madelung, Theory of Solids [Russian translation], Nauka, Moscow (1980).
39. S. S. Gershtein, L. I. Ponomarev, and T. P. Puzynina, Zh. Eksp. Teor. Fiz., 48, No. 2 (1965).
40. M. V. Fedoryuk, Asymptotics, Integrals, and Series [in Russian], Nauka, Moscow (1987).