объединенный
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ядерных
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дубна

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L.G.Zastavenko

THE INTEGRAL REPRESENTATION OF THE ONE-DIMENSIONAL QUASICLASSICAL WAVE FUNCTION IN A VICININTY OF THE TURNING POINT (THE AIRY INTEGRAL GENERALIZATION)

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1. INTRODUCTION

In the one-dimensional quantum mechanics one has to consider a differential equation of the form

$$[-\frac{d^2}{dx^2} + F(x)]\psi = 0 , \qquad F(x) = 2(V(x) - E) . \tag{1}$$

Here E is the total energy, V(x) is the potential energy. The quasiclassical limit of quantum mechanics corresponds to a large function F(x):

$$F(x) = \lambda^2 f(x) , \qquad \lambda \to \infty . \tag{2}$$

It is convenient in this limit to transform ψ into

$$\psi = e^{-\lambda S(x)} A(x, \lambda) . \tag{3}$$

One has

$$\frac{d^2}{dx^2}[e^{-\lambda S(x)} A] = e^{-\lambda S}[\lambda^2 (\frac{dS}{dx})^2 A - \lambda [\frac{d^2S}{dx^2} + 2\frac{dS}{dx}\frac{d}{dx}]A + \frac{d^2A}{dx^2}] , \tag{4}$$

so eqs. (1), (2) give

$$(\frac{dS}{dx})^2 = f(x) , \tag{5}$$

$$(\frac{d^2S}{dx^2} + 2\frac{dS}{dx}\frac{d}{dx} - \frac{1}{\lambda}\frac{d^2}{dx^2}) A(x, \lambda) = 0 ; \tag{6}$$

substituting here

$$A(x, \lambda) = \sum_{k=0}^{\infty} A_k(x) \lambda^{-k} \tag{7}$$

we get from eq. (6)

$$(\frac{d^2S}{dx^2} + 2\frac{dS}{dx}\frac{d}{dx}) A_0(x) = 0 ,$$
$$(\frac{d^2S}{dx^2} + 2\frac{dS}{dx}\frac{d}{dx}) A_k = \frac{d^2A_{k-1}}{dx^2} , \quad k = 1, 2, 3, ... \tag{8}$$

1.1. Let the function $f(x)$ be negative within the interval

$$a < x < b \tag{9}$$

and positive outside.

The the eigenfunctions of the problem would rapidly oscillate as $\lambda \to +\infty$ inside the interval (9) and fastly decrease outside.

1.1.1. Correspondingly, one can take

$$S(x) = \int_x^a \sqrt{f(u)}\,du , \quad \frac{dS}{dx} = -\sqrt{f(x)} \tag{10}$$

for $x < a$;
then eq. (8) gives

$$A_0(x) = \frac{1}{\sqrt{-dS/dx}} = f(x)^{-1/4} . \tag{11}$$

1.1.2. In the interval (9) the function $S(x)$ is imaginary:

$$S(x) = \pm i\sigma(x) = \pm i \int_a^x \sqrt{-f(u)}\,du \tag{10a}$$

so that eqs. (3), (7) change to:

$$\psi(x, \lambda) = \sum_{k=0}^{\infty} (e^{i\lambda\sigma(x)} B_k(x) + e^{-i\lambda\sigma(x)} \bar{B}_k(x))\lambda^{-k} . \tag{3a}$$

1.1.3. We will suppose the function $f(x)$ to be regular for all real values of x.

1.2. The approximations (3), (7) and (3a) are valid only far enough from the turning point: really, eqs. (8), (11) give

$$A_0(x) \sim (a-x)^{-1/4} ,$$

$$A_1(x) \sim (a-x)^{-7/4} , \tag{12}$$

$$A_2(x) \sim (a-x)^{-13/4}$$

as $x \to a$, and expansion (7) is not valid if $\lambda(a-x)^{3/2} \ll 1$.

1.2.1. It is easy to construct the approximation of $\psi(x,\lambda)$ valid in the vicinity of the turning point, e.g., $x = a$ (ref. [1]), Mathematical Appendix, Sec. b).

Near the point $x=a$ one has

$$f(x) = C_1(x-a) + C_2(x-a)^2 + \dots , \quad C_1 < 0 . \tag{13}$$

Neglecting here all but the first terms and substituting the linear function $f(x)$ into eqs. (1), (2), one can get the solution in a form of the Airy integral

$$\tilde{\psi}(x, \lambda) = \int_C \exp\{\lambda[-\frac{p^3}{3C_1} + p(x-a)]\}dp \ . \tag{14}$$

Here C is the contour $|\arg p| = \pi/3$. The value of the integral (14) as $\lambda \to +\infty$ for $x < a$ is defined by the saddle point

$$p = p(x) = \sqrt{-C_1(a-x)} \tag{15}$$

and for $x > a$ – by the saddle points

$$p = p(x) = \pm i\sqrt{-C_1(x-a)} \ . \tag{16}$$

1.2.2. The integral representation (14) allows one to connect the quasiclassical wave function (3), (7), (10) valid for $x < a$, and the wave function (3a) valid for $a < x < b$.

The representation (14), however, is sufficient for the connection only in main, zero order in λ^{-1} ($k = 0$ in (7) and (3a)). The connection in higher orders in λ^{-1} requires some generalization of the integral representation (14); one has to take into account the nonlinear terms of eq. (13), neglected in eq. (14).

1.3. We will construct such a generalization in the form

$$\psi(x, \lambda) = \int_C \exp\{\lambda[L(p) + p(x-a)]\}\,\kappa(p, \lambda)dp \ , \tag{17}$$

where

$$\kappa(p, \lambda) = \sum_{n=0}^{\infty} \kappa_n(p)\lambda^{-n+1/2} \ . \tag{18}$$

1.4. In Sec.2 we explain the construction of the function $L(p)$ and the localization of the saddle points of the exponential in eq. (17).

In Sec.3 we explain the construction of the functions $\kappa_n(p)$ (18).

In our considerations we substantially use the multiple differentiation of the composite function formula

$$\left(\frac{d}{dz}\right)^n F(\phi(z)) = n! \sum_{\substack{k_1, k_2, \ldots, k_n \\ \sum_{i=1}^{n} ik_i = n \\ k \equiv \sum_{i=1}^{n} k_i}} F^{(k)}(\phi(z)) \prod_{i=1}^{n} \left(\left(\frac{\phi^{(i)}(z)}{i!}\right)^{k_i} \frac{1}{k_i!}\right) \tag{19}$$

(the summation runs over all nonnegetive integer values of $k_1, k_2, \ldots, k_n$ restricted by the condition $\sum_{i=1}^{n} ik_i = n$).
This formula can be easily verified by induction.

1.5. Unfortunately, I am not able to determine the localization of the contour C in eq. (17) sufficiently accurately. One can only suppose that the integral (17), if $\lambda|x-a| \to \infty$, is determined by the saddle points, described in sec.2.

2. THE FUNCTION L(p)

Here we determine the function L(p).

Let us require the function (17) to have asymptotics (3), (7), (10) as $x < a$, $\lambda \to +\infty$.

Suppose the integral (17) at $x<a$ to be determined by the only saddle point $p = p(x)$; then one has

$$-S(x) = p(x)(x-a) + L(p(x)) \tag{20}$$

and

$$x - a + L'(p(x)) = 0; \tag{21}$$

the function x(p), inverse to p(x), satisfies the equation

$$x(p) - a + L'(p) = 0. \tag{22}$$

Differentiating eq. (20) with respect to x gives (with account of eq. (21))

$$S'(x) + p(x) = 0 \tag{23}$$

or

$$S'(x(p)) + p = 0. \tag{24}$$

Note that eq. (21) may have several roots p(x), but eq. (23) has only one root (for $x < a$).

2.1. Equations (10) and (13) imply

$$S(x) = \sum_{n=0}^{\infty} S_n (a-x)^{n+3/2}. \tag{25}$$

It follows from eqs. (23), (25) that

$$p(x) = \sum_{n=0}^{\infty} S_n (n+3/2)(a-x)^{n+1/2} \tag{26}$$

whence

$$a - x(p) = \sum_{n=0}^{\infty} \alpha_n p^{2n+2}. \tag{27}$$

The latter equation with eqs. (22) and (20) gives

$$L(p) = \sum_{n=0}^{\infty} \frac{\alpha_n}{2n+3} p^{2n+3}. \tag{28}$$

2.2. One has

$$Y \equiv \frac{d^2}{dp^2}[p(x-a) + L(p)]|_{p=p(x)} = L''(p(x)) = -\frac{dx(p)}{dp} =$$

$$= -\frac{1}{dp(x)/dx} = \frac{1}{S''(x)} = -\left(\frac{d\sqrt{f(x)}}{dx}\right)^{-1} > 0 \tag{29}$$

in some interval

$$a-\delta < x < a, \quad \delta > 0. \tag{30}$$

This result implies the point $p = p(x)$ to be a minimum of the exponential in the integral (17) for real p (if $a-\delta<x<a$), so that the contour C has to be parallel to the imaginary axis at the point $p = p(x)$.

2.3. Let us now consider the case $x>a$. Equation (26) gives for $x>a$ two values of $p(x)$:

$$p(x) = \pm i \sum_{n=0}^{\infty} S_n (n+3/2)(x-a)^{n+1/2} (-)^n. \tag{31}$$

The value of integral (17) for $x>a$ is defined by two saddle points (31).

2.4. Thus we have constructed the function $L(p)$ and have defined the localization of the eq. (17) integrand saddle points.

3. THE FUNCTION $\kappa(p,\lambda)$

The function $\psi(x,\lambda)$ has to satisfy the equation

$$T \equiv \left[-\frac{d^2}{dx^2} + \lambda^2 \sum_{m=1}^{\infty} C_m (x-a)^m\right]\psi(x,\lambda) = 0 =$$

$$= \lambda^2 \int_C dp\, e^{\lambda p(x-a)} \left[-p^2 + \sum_{m=1}^{\infty} C_m \left(-\frac{1}{\lambda}\frac{d}{dp}\right)^m\right] e^{\lambda L(p)} \kappa(p,\lambda) = \tag{32}$$

$$= \lambda^2 \int dp\, e^{\lambda p(x-a)} \Big[-p^2 e^{\lambda L(p)} \kappa(p,\lambda) + \sum_{m=1}^{\infty}\sum_{n=0}^{m} C_m \frac{m!(-1/\lambda)^m}{n!(m-n)!} \times$$

$$\times \left[\left(\frac{d}{dp}\right)^n e^{\lambda L(p)}\right]\left[\left(\frac{d}{dp}\right)^{m-n} \kappa(p,\lambda)\right]\Big] =$$

$$= \lambda^2 \int dp \exp\{\lambda[p(x-a) + L(p)]\}\{p^2 \kappa(p,\lambda) + \sum_{m=1}^{\infty} \sum_{n=0}^{m} C_m \frac{m!(-)^m}{(m-n)!} \times$$

$$\times \sum_{\substack{k_1, k_2, \ldots, k_n \\ \sum_{i=1}^{n} ik_i = n}} \lambda^{\sum_1^n k_i - m} \prod_{i=1}^{n} \left(\frac{1}{k_i!}\left(\frac{L^{(i)}(p)}{i!}\right)^{k_i}\right) \left(\frac{d}{dp}\right)^{m-n} \kappa(p,\lambda)\};$$

we have used eq. (19).

Continuing the equality, introducing notation $k_0 = m - n$, $q = k_0 + 2k_2 + 3k_3 + \ldots nk_n$ and using eq. (13) we obtain

$$0 = T \equiv \lambda^2 \int dp \exp\{\lambda[p(x-a) + L(p)]\}\{-p^2 \kappa(p,\lambda) + \sum_{m=1}^{\infty} \sum_{k_0=0}^{m} \frac{\kappa^{(k_0)}(p,\lambda)}{k_0!} \times$$

$$\times \sum_{\substack{q, k_2, k_3, \ldots, k_q \\ q = k_0 + 2k_2 + \ldots qk_q \leq m}} \frac{m!\, L'(p)^{m-q} C_m (-)^m}{(m-q)!\, \lambda^{k_0 + k_2 + 2k_3 + \ldots (q-1)k_q}} \prod_{i=2}^{q} \left(\frac{1}{k_i!}\left(\frac{L^{(i)}(p)}{i!}\right)^{k_i}\right)\} = \tag{33}$$

$$= \lambda^2 \int dp \exp\{\lambda[p(x-a) + L(p)]\}\{-p^2 \kappa(p,\lambda) + \sum_{q=0}^{\infty} (-)^q f^{(q)}(a - L'(p)) \times$$

$$\times \sum_{\substack{k_0, k_2, \ldots k_q \\ k_0 + \sum_2^q ik_i = q \\ k \equiv \sum_2^q k_i}} \frac{\kappa^{(k_0)}(p,\lambda)}{k_0!\, \lambda^{q-k}} \prod_{i=2}^{q} \left(\frac{1}{k_i!}\left(\frac{L^{(i)}(p)}{i!}\right)^{k_i}\right)\},$$

or

$$0 = T \equiv \lambda^2 \int_C dp \exp[\lambda[p(x-a) + L(p)] \times$$

$$\times \{[-p^2 + f(a - L'(p))]\kappa(p,\lambda) - f'(a - L'(p))\kappa'(p,\lambda) + \tag{34}$$

$$+ f''(a - L'(p))\left[\frac{\kappa''(p,\lambda)}{2!\lambda^2} + \frac{L''(p)}{2!} \frac{\kappa(p,\lambda)}{0!\lambda}\right] -$$

$$- f'''(a - L'(p))\left[\frac{\kappa'''(p,\lambda)}{3!\lambda^3} + \frac{\kappa'(p,\lambda)}{1!} \frac{L''(p)}{2!\lambda^2} + \frac{\kappa(p,\lambda)}{0!} \frac{L'''(p)}{3!\lambda^2}\right] +$$

$$+ O(\lambda^{-3})\}$$

Equating the expression in braces to zero allows one to determine the function $\kappa(p, \lambda)$. With account of eqs. (22), (23) one can transform the first term in braces according to

$$[-p^2 + f(a - L'(p))]\kappa(p,\lambda) =$$
$$= [-S'(x(p))^2 + f(x(p))]\,\kappa(p,\lambda)\ ; \tag{35}$$

eq. (5), as taken for complex x, $x = x(p)$, $p \in C$, implies the latter expression to disappear.

3.1. Substituting the expansion (18) into eq. (34) gives the equations defining the functions $\kappa_n(p), n=0,1,2,...$

$$-f'(a - L'(p))\kappa_0'(p) + f''(a - L'(p))\,L''(p)\kappa_0(p)/2 = 0\,; \tag{36}$$

$$-f'(a - L'(p))\kappa_1'(p) + f''(a - L'(p))L''(p)\kappa_1(p)/2 +$$
$$+ f''(a - L'(p))\kappa_0''(p)/2 - \tag{37}$$
$$- f'''(a - L'(p))\,[\kappa_0'(p)\,L''(p)/2 + \kappa_0(p)L'''(p)/6\,] = 0\,,$$

whence

$$\kappa_0(p) = A_0\,[-f'(a - L'(p))]^{1/2}\,, \tag{38}$$

$$\kappa_1(p) = \kappa_0(p)\{\int_0^p [\,\frac{f''(a - L'(s))}{2f'(a - L'(s))}\kappa_0''(s) - \frac{f'''(a - L'(s))}{f'(a - L'(s))}...]\frac{ds}{\kappa_0(s)} + A\ ),$$

3.2. So, we have constructed the function $\kappa(p, \lambda)$.

4. CONCLUDING REMARKS

Expanding the function (17) by the saddle point method for $x<a$ and $x>a$ allows one to get connected representations $\psi(x, \lambda)$ of the form (3), (7) and (3a). So we have got the solution of the problem, stated in the item 1.2.2.

The integral representation we have got enables one, e.g., to calculate quasiclassical energy levels in any desired order in λ^{-1}. Note, however, that the first five terms of this expansion have been constructed /2-4/ without the knowledge of our integral representation.

4.1. Let us show for illustration that eq. (17) gives formula (11). The main saddle point term of eq. (17) at $x < a$ is

$$\psi(x,\lambda) \sim e^{-\lambda S(x)} \kappa_0(p(x))(L''(p(x)))^{-1/2}$$

here $\kappa_0(p(x)) = [-f'(x)]^{-1/2}$ according to eqs. (38) and (22) and $L''(p) = -2[f(x)]^{1/2}/f'(x)$ according to eq. (29), so, we arrive to eq. (11).

4.2. Note in conclusion that the integral representation we have got allows rather a simple generalization to the case of multidimensional quasiclassics; one has only to know the function $S(x)$, satisfying the multidimensional eq. (5), and the part of the dividing surface, which is a generalization of the turning point to the case of multidimensional quasiclassics.

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