Collision Problem in Atomic Physics and Resurgent Analysis

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Abstract

In this paper we consider the adiabatic approximation of the atomic collision problem. We show that the computation of transmission probabilities in this approximation can be done by means of the resurgent analysis method. We present a computational algorythm for transmission probabilities and give the mathematical verification of this algorythm. All considerations are carried out on the simple but representative example of two-level Zener model. The preliminary knowledge of the atomic physics and the resurgent analysis is not supposed.

Introduction

The role of motion invariants of dinamic systems in classical mechanics seems quite evident. It is well-known that for conservative systems, that is, for the systems whose Hamiltonians do not depend on the time explicitely, one of such invatiants is the Cartan

integral invariant

$$I = \oint p\,dx. \tag{1}$$

At the same time, for nonconservative systems the question of motion invariants is significantly more complicated. An important step in the solution of this problem was done in remarkable papers [1], [2] by Paul Ehrenfest who introduced there the notion of an adiabatic invariant – one of the fundamental notions of mechanics.

To illustrate the above mentioned notion we consider an one-dimensional time-dependent Schrödinger equation with the Hamiltonian of the form

$$H = \frac{mv^2}{2} + V(x, \alpha t),$$

α being a small parameter. In the latter equation the potential V can depend on the time t only via the variable $\tau = \alpha t$ which can be called a *slow time*.

Then, as it was shown by Ehrenfest, integral 1 is preserved in the adiabatic approximation, that is the relation

$$\oint p\,dx = \text{const} + O(\alpha)$$

takes place.

For multidimensional problems the similar result is easily obtained from the one-dimensional one provided that the variables can be divided in the corresponding Schrödinger equation, since in this case the multidimensional problem can be reduced to several one-dimensional ones. However, it can be shown that for general multidimensional problems the similar result fails (this can be demonstrated by the well-known Fermi example).

The next result in this direction was obtained by A. N. Vasilliev in early eightees. He has shown that the expression for adiabatic invariants can be improved by adding lower-order terms in h:

$$I = \oint p\,dx + hI_1 + h^2 I_2 + \dots$$

such that the quantity I will be preserved in the evolution. Thus, the notion of adiabatic invariants was introduced in the most general situation.

Further, the adiabatic invariants were a predmet of investigation in a lot of physical and mathematical papers. We mention here the papers [3], [4], [5], [6], [7].

So, there arises a problem of investigation of Schrödinger equations in the adiabatic approximation. This means that one has to investigate the asymptotic behavior of

solutions to the time-dependent Schrödinger equation

$$ih\frac{\partial\psi}{\partial t} = \left[-\frac{h^2}{2m}\Delta + V(x, \alpha t)\right]\psi \tag{2}$$

as $\alpha \to 0$. The first result in this direction was obtained by M. Born and V. Fock [4]. They have proved that the quantum states are preserved in the main term of the adiabatic aproximation, that is, that if the solution to (2) satisfies the 'initial conditions' of the form

$$\lim_{t\to-\infty} \psi = \psi_n$$

for some eigenfunction ψ_n of the Hamiltonian

$$-\frac{h^2}{2m}\Delta + V(x, -\infty),$$

then

$$\lim_{\alpha\to 0} \psi = \psi_n(x, R) \exp\left[\frac{i}{h}\int E_n(R)\, dR\right]$$

where $\psi_n(x, R)$ is an eigenfunction of the instanteneous Hamiltonian

$$-\frac{h^2}{2m}\Delta + V(x, \tau)$$

corresponding to the eigenvalues $E_n(R)$ (these are called *adiabatic potential curves*), and τ is the above mentioned slow time.

We remark also that, due to the well-known Wigner theorem adiabatic potential curves do not intersect one another.

The further investigation of the problem was done for different models. We mention here the *Zener model* (see [8]) for which the Hamiltonian is a two-dimensional operator with the matrix

$$\begin{pmatrix} \alpha a_1 t & b \\ b & \alpha a_2 t \end{pmatrix}.$$

The Schrödinger equation for this model can be solved explicitely and then the asymptotics as $\alpha \to 0$ can be computed from the explicit expression for the solution. It occurs that the transitions between the two states involved in this problems are of exponential order $O\left(e^{-\Delta/\alpha}\right)$, where Δ (the so-called Massey parameter) has the sense of the shortest distance between the two adiabatic potential curves in question.

The next model which is worth mentioning is the so-called *Rosen-Zener-Demkov model* [9], [10]. This is also a two-level model admitting the explicit solutions, and the corresponding Hamiltonian is given by the matrix

$$\begin{pmatrix} 0 & e^{-a\tau} \\ e^{-a\tau} & \Delta \end{pmatrix},$$

where a and Δ are some positive parameters. The asymptotic analysis of the exact solution gives us the following value of the transition probability

$$P = \sum_{n=1}^{\infty} e^{-\frac{n\Delta}{a}}.$$

The next step in the investigation of the finite-level models was done in the paper [11] by E. C. G. Stueckelberg. In this paper the two-level model

$$i\alpha \frac{d}{d\tau} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} a(\tau) & b(\tau) \\ b(\tau) & c(\tau) \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}$$

was considered. The asymptotic expansion involving exponentially decreasing terms (such as the transition probabilities are) was obtained in this paper with the help of continuation of the solution to the complex plane and using the technique of model equations in a neighbourhood of the (complex) turning point.

Finally, let us turn our attention to the general problem of atomic collisions. To be short, we shall consider here the problem which involves one electron and two nuclei. The time-dependent Schrödinger equation for such a problem is

$$i\frac{\partial \psi}{\partial t} = -\Delta\psi + \left(\frac{Z_1}{\left|\vec{r} - \vec{R}_1\right|} + \frac{Z_2}{\left|\vec{r} - \vec{R}_2\right|} \right) \psi,$$

where $\vec{r} = (x, y, z)$ is the electron radius-vector, $\vec{R}_1$ and $\vec{R}_2$ are radius-vectors of the nuclei with charges Z_1 and Z_2, and Δ is the Laplace operator with respect to the electrone variables (x, y, z) (see Figure 1). It is supposed that the two nuclei in question are moving with respect to each other with the relative velocity v which is exactly the small parameter of the adiabatic approximation. Such problems were considered from physical point of view by E. Solov'ev (see [12]). The analysis of this problem can be divided into two parts: the computation of the corresponding adiabatic potential curves $E_j(\tau)$ ($\tau = vt$, as above), and the construction of the adiabatic asymptotics in the problem with known E_j.

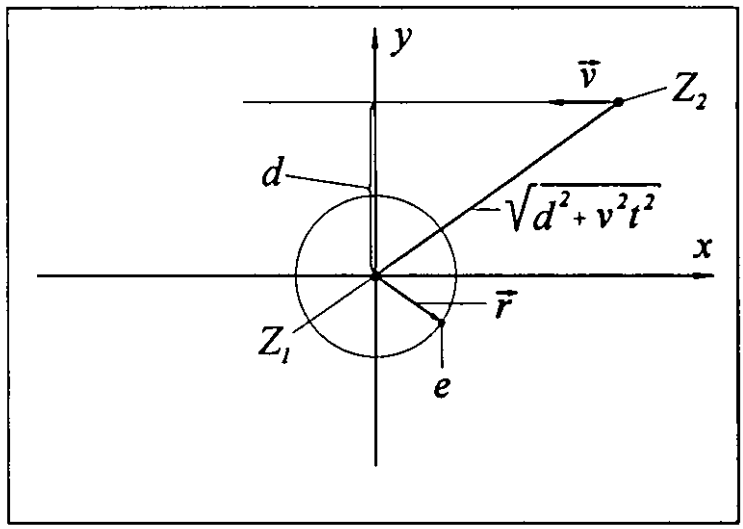

Figure 1: The simplest atomic collision.

The present paper is aimed at the investigation of the second of the two problems listed above by means of the resurgent analysis.

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1 Statement of the problem

To begin with, we recall shortly the general statement of the problem.

Consider a proton and some atom (hydrogen, for example) moving with respect to each other with the relative velocity v. Then, in the adiabatic approximation one can treat the motion of the heavy particles as a classical one, and the motion of the electron as a quantum one. Thus, the transitions between electronic states in this system are described with the help of the following Schrödinger equation:

$$i\frac{\partial\psi(x,t)}{\partial t} = \widehat{H}(R)\psi(x,t). \tag{3}$$

Here $\widehat{H}(R)$ is the electronic Hamiltonian of the diatomic quasimolecule (the exact form of the Hamiltonian $\widehat{H}(R)$ is not of importance for us), $x = (x^1, x^2, x^3)$ are electronic coordinates, and R is the internuclear distance, which can be written down in the form

$$R = \sqrt{d^2 + v^2 t^2},$$

d being an impact parameter[1] (see Figure 1; we neglect the curvature of the classical trajectories of the heavy particles).

We recall that the *adiabatic approximation* is exactly the asymptotic expansion of the unknown function $\psi(x,t)$ with respect to the small parameter v.

Further, we are mostly interested in the computation of probabilities of transitions between different electronic states occurring as a result of the described collision. From this viewpoint it seems natural to pass to the *population of the atomic states*[2] representation, that is, to expand the electron wave function $\psi(x,t)$ over the basis $\{\psi_j(x,R)\}$ consisting of the eigenfunctions of the instantaneous electronic Hamiltonian $\widehat{H}(R)$:

$$\psi(x,t) = \sum_j c_j(t)\psi_j(x, R(t)), \tag{4}$$

where

$$\widehat{H}(R)\psi_j(x,R) = E_j(R)\,\psi_j(x,R).$$

The eigenvalues $E_j(R)$ playing the role of effective potential are called *adiabatic potential curves* in the adiabatic approximation. The functions $c_j(t)$ on the right in (4) describe the evolution of the population of the j-th electronic state during the collision; clearly, these functions depend on the parameter v.

The naturality of representation (4) is confirmed by the Born-Fock theorem [4] which claims that the population numbers $|c_j(t)|$ do not change during a collision in the limit $v \to 0$, that is,

$$\lim_{v\to 0} |c_j(t)| = \text{const}.$$

The above stated problem prescribes also the 'initial conditions' for the functions $c_j(t)$ in question. Namely, if we investigate probabilities of the transitions from the state j_0 to all other states, it is natural to put

$$\lim_{t\to-\infty} c_j(t) = \begin{cases} 1, & j = j_0, \\ 0, & j \neq j_0. \end{cases}$$

[1] Here and below we use atomic units for which $h = 1$, $m = 1$.

[2] In physics the probability for an electron to be in the given atomic space is called a population of this state.

Then the probabilities of the transition from the state j_0 to the state j are given by

$$p_{j_0 j} = \left| \lim_{t \to +\infty} c_j(t) \right|^2 .$$

Substituting expression (4) into equation (3) and expanding the result of the substitution over the basis $\{\psi_j(x, R)\}$, we obtain the following (infinite) system of differential equations for the functions $c_j(t)$:

$$i \frac{\partial c_j(t)}{\partial t} = \sum_k H_{jk}(t)\, c_k(t), \tag{5}$$

where the (infinite) matrix $\|H_{jk}(t)\|$ is the expression of the Hamiltonian $\widehat{H}(t)$ in the considered representation. To separate the small parameter v explicitely, we introduce the new variable $\tau = vt$ ('slow' time), thus rewriting (5) in the form

$$iv \frac{\partial c_j(\tau, v)}{\partial \tau} = \sum_k H_{jk}(\tau)\, c_k(\tau, v), \tag{6}$$

where the functions $H_{jk}(\tau)$ depend on the variable τ in a regular way.

Now we shall introduce the finite-level approximation, which is based on the following facts. First of all, as it was already mentioned (Born-Fock theorem), the principal term of the adiabatic approximation corresponds to the absence of the transitions between different electronic states. Moreover, as it was already mentioned in the Introduction, the probabilities of the transitions $p_{j_0 j}$ and, hence, the subsequent terms of the asymptotics of the functions $c_j(t)$ in the adiabatic approximation decrease exponentially as $v \to 0$ with the exponential factor $e^{-\Delta/v}$, where Δ is the shortest distance between the corresponding adiabatic potential curves (see Figure 2; one can see that the transitions between different states can occur in the region in which the distance between the curves is minimal – the so-called region of quasiintersection). This means that, if we are intended to investigate the asymptotic behavior of $c_j(t)$ in the variable v modulo exponential terms with some fixed type, we can include into consideration only a finite number of components $c_k(t)$ corresponding to energy levels $E_k(R)$ closest to the given potential curve $E_{j_0}(R)$. Therefore we arrive at the *finite-dimensional model* which coincides in form with (6) but with a *finite* matrix $\|H_{jk}(\tau)\|$.

Now we can formulate the corresponding mathematical problem.
Consider the system

$$iv \frac{\partial c_j(\tau, v)}{\partial \tau} = \sum_k H_{jk}(\tau)\, c_k(\tau, v), \; j = 1, 2, \ldots, n \tag{7}$$

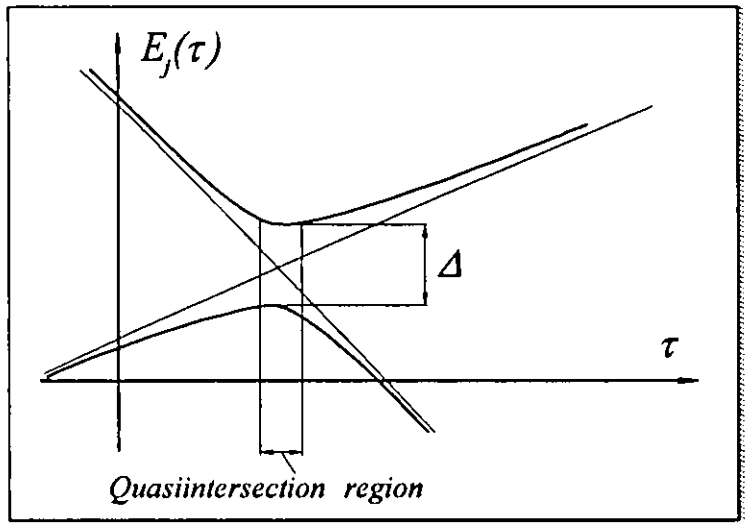

Figure 2: Quasiintersection.

of ordinary differential equations with the 'initial data'

$$\lim_{\tau \to -\infty} c_j(\tau, v) = \begin{cases} 1, & j = j_0, \\ 0, & j \neq j_0. \end{cases} \tag{8}$$

with respect to the n unknowns

$$\{c_j(\tau, v),\ j = 1, 2, \ldots, n\}.$$

The problem is to investigate the asymptotic behavior of solution to this system as $v \to 0$ with exponential accuracy of arbitrary exponential type.

The above formulated problem will be solved in this paper with the help of the resurgent analysis (see, for example [13]). To be short and clear, we shall present all the calculations for the simplest Zener model, though all the computational procedure can be applied to general problem of the type (7), (8). We recall that for Zener model the matrix $\widehat{H}(\tau) = \|H_{jk}(\tau)\|$ has the form

$$\widehat{H}(\tau) = \begin{pmatrix} a_1\tau & b_1 & b_2 & \ldots \\ b_1 & a_2\tau & 0 & \ldots \\ b_2 & 0 & a_3\tau & \ldots \\ \ldots & \ldots & \ldots & \ldots \end{pmatrix},$$

so that for the corresponding two-level model the matrix $\widehat{H}(\tau)$ is given by

$$\widehat{H}(\tau) = \begin{pmatrix} a_1\tau & b \\ b & a_2\tau \end{pmatrix}$$

with some real values of the constants a, b, λ. To be definite, we shall choose $a_1 = -2$, $b = -1$, $a_2 = 0$, thus considering the following system of two ordinary differential equations:

$$\begin{cases} -iv\dfrac{dc_1}{d\tau} = 2\tau c_1 + c_2, \\ -iv\dfrac{dc_2}{d\tau} = c_1. \end{cases} \tag{9}$$

In accordance with the resurgent analysis method, we search for solutions to system (9) in the form

$$\begin{aligned} c_1(\tau, v) &= \mathcal{L}[C_1(\tau, s)], \\ c_2(\tau, v) &= \mathcal{L}[C_2(\tau, s)], \end{aligned} \tag{10}$$

where $C_j(\tau, s)$, $j = 1, 2$ are endlessly-continuable[3] analytic functions in the variable s and $\mathcal{L}[C_j]$ is the Laplace transform[4] of the function $C_j(\tau, s)$ in the variable s, taken at some of its ramification point $s = S(\tau)$:

$$c_j(\tau, v) = \mathcal{L}[C_j(\tau, s)] = \int_{\Gamma(\tau)} e^{\frac{i}{v}s} C_j(\tau, s)\, ds. \tag{11}$$

In the latter formula $\Gamma(\tau)$ is a standard contour encircling the singularity point $s = S(\tau)$ of the function $C_j(\tau, s)$ (see Figure 3). Clearly, as it is usual in the resurgent analysis, we have to investigate the asymptotic behavior of the functions in question not only for real but for complex values of τ. In general, to do this one have to require that the coefficients of the considered system of ordinary differential equation has entire coefficient; in our model example this requirement is obviously fulfilled. Now, substituting expressions (11) for the components $c_j(\tau, v)$ of the solution into the system (9) we obtain the following system for the unknowns $C_j(\tau, s)$:

$$\begin{cases} \dfrac{\partial C_1}{\partial \tau} = -2\tau\dfrac{\partial C_1}{\partial s} - \dfrac{\partial C_2}{\partial s}, \\ \dfrac{\partial C_2}{\partial \tau} = -\dfrac{\partial C_1}{\partial s}. \end{cases} \tag{12}$$

Later on, as we shall see below, one can suppose that the solution $\{C_j(\tau, s)\}$ of the latter system has *simple singularities*, that is, the singularities of the form

$$C_j(\tau, s) = \frac{a_0(\tau)}{s - S(\tau)} + \ln(s - S(\tau)) \sum_{j=0}^{\infty} \frac{(s - S(\tau))^j}{j!} a_{j+1}(\tau) \tag{13}$$

[3] An *endlessly-continuable* function is, roughly speaking, an analytic function having a discrete set of singularities on its Riemannian surface (for exact definitions see, for example, [14], [13]).

[4] In the sequel we shall see that the functons c_j will be represented as a sum of Laplace transforms of the functions C_j taken in different points of ramification of these functions (see formula (21) below). At present this fact is not of importance for us.

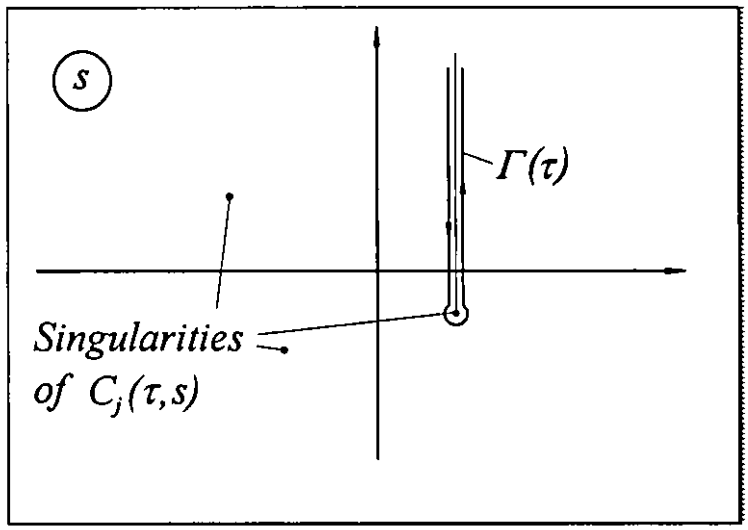

Figure 3: The standard integration contour.

near each its singular point $s = S(\tau)$ (see [13]). In this case expression (11) can be considered as a result of resummation of the corresponding WKB-series

$$e^{\frac{i}{v}S(\tau)} \sum_{j=0}^{\infty} v^j a_j(\tau). \tag{14}$$

However, as it is known, the asymptotics of the solution can involve different number of WKB-terms for different points x (the so-called Stokes phenomenon). So, to investigate the solution with the help of the resurgent analysis, one has to:

– investigate the *resurgent structure* of the solution, that is, to determine the values of actions for all WKB-terms which can be possibly involved in the asymptotic expansion;

– investigate the *Stokes phenomenon*, that is to determine which singularities of the type (13) will contribute to the asymptotic expansion for different values of x.

This program will be realized in the subsequent Sections.

2 Resurgent structure of solutions

Our first goal is the computation of the resurgent structure of the functions $c_j(\tau, v)$, that is, of the structure of set of singularities of the functions $C_j(\tau, s)$. As follows from formulas (13), (14) above, the resurgent structure of a solution plays an important role in investigation of its WKB-expansion. Namely, if $s = S(\tau)$ is an equation of the

set of singularities of the solution and $\{S_j(\tau)\}$ are different branches of (ramifying, in general) function $S(\tau)$, then $S_j(\tau)$ play the role of actions in WKB-terms of the asymptotic expansion of the solution.

Clearly, the question whether there exists a resurgent solution to a system of the form (7) is not a simple one. In our book [13] we prove the existence of the full system of resurgent solutions to an ordinary differential equation of arbitrary order with polynomial coefficients. The results obtained there can be generalized to the systems of ordinary differential equations, and we can prove the existence of an endlessly-continuable solution with simple singularities to problem (7), (8) (in the case of system of equations with polynomial coefficients) with singularities at points

$$s = S_j(\tau),$$

where $S_j(\tau)$ are different branches of (ramifying, in general) solution of the corresponding Hamilton-Jacobi equation. For system (12) the Hamilton-Jacobi equation reads

$$\begin{vmatrix} 2\tau - S'(\tau) & 1 \\ 1 & -S'(\tau) \end{vmatrix} = [S'(\tau)]^2 - 2\tau S'(\tau) - 1 = 0. \tag{15}$$

We remark that for the particular system (9) the existence of resurgent solutions with simple singularities can be proved directly. To do this, we shall search for the solution to this system in the form of a Laplace integral

$$\begin{cases} c_1(\tau, v) = \int\limits_\gamma \exp\left[\frac{i}{v} p\tau\right] A_1(p, v)\, dp, \\ c_2(\tau, v) = \int\limits_\gamma \exp\left[\frac{i}{v} p\tau\right] A_2(p, v)\, dp, \end{cases}$$

where the functions $A_1(p, v)$ and $A_2(p, v)$, as well as the integration contour γ, are unknowns. Substituting the latter relations to the system (9), we obtain for $A_1(p, v)$, $A_2(p, v)$ the following system of equations:

$$\begin{cases} pA_1 = 2iv\frac{dA_1}{dp} + A_2, \\ pA_2 = A_1. \end{cases}$$

The solution to the obtained system is given by

$$A_1(p, v) = \exp\left\{\frac{i}{v}\left[-\frac{p^2}{4} + \frac{1}{2}\ln p\right]\right\},$$
$$A_2(p, v) = p^{-1}\exp\left\{\frac{i}{v}\left[-\frac{p^2}{4} + \frac{1}{2}\ln p\right]\right\},$$

so that the corresponding solution (c_1, c_2) to (9) has the form

$$\begin{cases} c_1(\tau, v) = \int\limits_\gamma \exp\left\{\frac{i}{v}\left[p\tau - \frac{p^2}{4} + \frac{1}{2}\ln p\right]\right\} dp, \\ c_2(\tau, v) = \int\limits_\gamma \exp\left\{\frac{i}{v}\left[p\tau - \frac{p^2}{4} + \frac{1}{2}\ln p\right]\right\} p^{-1}\, dp. \end{cases} \tag{16}$$

In the latter integrals one have to choose the integration contour γ in such a way that these integrals converge. The example of such a contour is drawn on Figure 4; one can choose any contour coming to

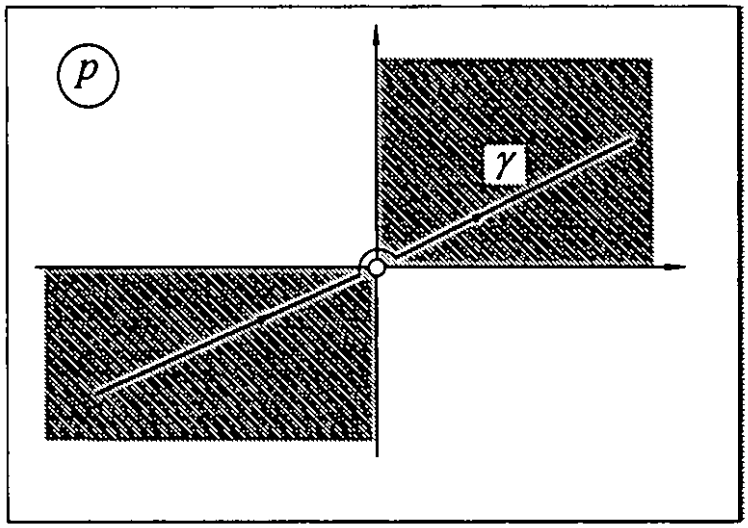

Figure 4: The choice of the contour γ.

infinity in regions of exponential decrease of the integrang (marked on the Figure) and avoiding the polar singularity $p = 0$ of the integrand.

Let us now rewrite the obtained expressions for solutions in the form of resurgent functions. To do this, we perform the variable change

$$s = p\tau - \frac{p^2}{4} + \frac{1}{2}\ln p \tag{17}$$

in (16), thus reducing the expression for the solutions to the form

$$\begin{cases} c_1(\tau, v) = \int\limits_\gamma \exp\left[\frac{i}{v}s\right] \frac{dp}{ds}(\tau, s)\, dp, \\ c_2(\tau, v) = \int\limits_\gamma \exp\left[\frac{i}{v}s\right]\, p^{-1}(\tau, s) \frac{dp}{ds}(\tau, s)\, dp, \end{cases}$$

where $p(\tau, s)$ is a solution to equation (17) with respect to p.

Now it is evident that the singularities of the functions

$$\begin{cases} C_1(\tau, s) = \frac{dp}{ds}(\tau, s), \\ C_2(\tau, s) = p^{-1}(\tau, s) \frac{dp}{ds}(\tau, s), \end{cases}$$

are posited at those points where the variable change given by (17) degenerates. These points can be found from (17) together with

$$\frac{\partial}{\partial p}\left\{p\tau - \frac{p^2}{4} + \frac{1}{2}\ln p\right\} = \tau - \frac{p}{2} + \frac{1}{2p} = 0$$

and are given by

$$s = S(\tau) = -\frac{1}{4} + \frac{\tau^2}{2} + \frac{1}{2}\tau\sqrt{\tau^2+1} + \frac{1}{2}\ln\left(\tau + \sqrt{\tau^2+1}\right). \tag{18}$$

One can immediately verify that the function $S(\tau)$ determined by the latter relation is a solution to the Hamilton-Jacobi equation (15).

The constructed solution is not a solution with simple singularities in the above sense. However, it is easy to construct a solution with simple singularities applying the operator $(\partial/\partial s)^{-1/2}$ to both of the functions $C_1(\tau, s)$ and $C_2(\tau, s)$ (the definition of this operator one can find in [15], [16], [13]).

Let us continue the investigation of the resurgent structure of a solution to (12). Deriving $S'(\tau)$ from the Hamilton-Jacobi equation (15) we obtain the expression for the corresponding adiabatic potential curves

$$E(\tau) = S'(\tau) = \tau + \sqrt{\tau^2 + 1} \tag{19}$$

(the two different determinations of the square root correspond to the two adiabatic potential curves in question). Now, integrating the obtained result along paths in the complex τ-plane from the origin to the arbitrary point τ, we obtain the equation of the singularity set of the solution $(C_1(\tau, s), C_2(\tau, s))$ to system (12) in the form[5]

$$s = S(\tau) = \frac{\tau^2}{2} + \frac{1}{2}\tau\sqrt{\tau^2 + 1} + \frac{1}{2}\ln\left(\tau + \sqrt{\tau^2 + 1}\right). \tag{20}$$

The obtained set of singularities is drawn on Figure 5 a) — c) for three different values of the variable τ. Namely, Figure 5 a) corresponds to some real negative value of τ, Figure 5 b) corresponds to $\tau = 0$, and Figure 5 c) corresponds to some positive real value of τ.

One can see that for any τ the singularity set of the solution consists of two different lattices with step $i\pi$. For any real value of τ the first from these two lattices, corresponding to the positive determination of the square root in expression (20), contains one real point, and the other contains no real point at all. When the variable τ changes from $-\infty$ to 0, these two lattices are moving one to another in the direction of the real axis. Then (at the value $\tau = 0$) they go through each other and continue their motion as τ varies from 0 to $+\infty$ such that the distance between them infinitely increases.

Let us denote by S_+ (correspondingly, S_-) the real value of the function given by (20) for positive determination of $\sqrt{\tau^2 + 1}$ (correspondingly, the value of the function $S(\tau)$ having the imaginary part equal to $i\pi/2$ for negative determination of $\sqrt{\tau^2 + 1}$). It is clear that the solution $(c_1(\tau, v), c_2(\tau, v))$ to system (9) which is given by expression (11) with the integration contour $\Gamma(\tau)$ encircling the point $S_+(\tau)$ (or any other point of the first lattice) corresponds to the adiabatic potential curve $E_+(\tau)$ (with the positive value of $\sqrt{\tau^2 + 1}$) whereas the same expression with $\Gamma(\tau)$ encircling the point $S_-(\tau)$ (or

[5]This expression differ from the expression (18) obtained above up to an additive constant $-1/4$. Since the choice of the arbitrary constant in the action function is inessential, we use below the most simple normalization.

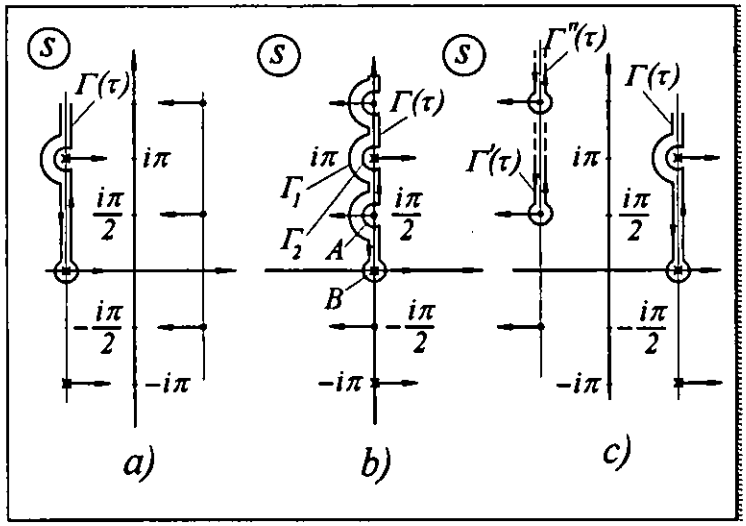

Figure 5: Resurgent structure of the solution.

any other point of the second lattice) gives us a solution corresponding to the adiabatic potential curve $E_-(\tau)$ (with the negative value of $\sqrt{\tau^2+1}$). Thus, to satisfy the 'initial conditions' of the considered problem one has to choose for $\tau < 0$ the solution given by (11) with the integration contour $\Gamma(\tau)$ drawn on Figure 5 a).

Now we must continue the obtained solution to all real values of τ and calculate this solution for sufficiently large positive τ. However, as it is clear from Figure 5, when τ goes across the value $\tau = 0$, the integration contour will be intersected by infinitely many points from the second lattice of singularities. Clearly, as a result of this intersection the topology of the integration contour will be changed, since the singularity point which intersects the integration contour can extract from it one or two contours of the same type but encircling this new point of singularity. Such a phenomenon is known in the resurgent analysis as the *Stokes phenomenon* and, hence, to investigate the continuation of the solution to positive values of τ one have to include the Stokes phenomenon into consideration. This will be done in the following Section.

3 Investigation of the Stokes phenomenon

Up to the moment we have constructed a solution to equation (9) in the region $\tau < 0$. This solution is represented in a form of the integral (11) with the integration contour $\Gamma(\tau)$ drawn on Figure 5 a). However, as it was already mentioned in the end of the previous Section, the topology of the integration contour can be changed during

the continuation of the constructed solution to all real values of τ. This topological rebuilding happens at $\tau = 0$ when the integration contour is intersected by singularities of the integrand different from that encircling by the considered contour.

The mentioned topological rebuilding is due to the fact that any singular point intersecting the integration contour can extract from it some another contour of the same type. However, we do not know a priori how many contours of this kind (if any) will be extracted from the integration contour as a result of the intersection. The number of extracted contours depends on which branches of the integration contour (which is posited on the Riemannian surface of the integrand) are really intersected by the considered point of singularity. For example (see Figure 5 b)), the point A of singularity of the integrand can intersect both branches Γ_1 and Γ_2 of the integration contour (in this case two additional contours will be extracted from $\Gamma(\tau)$ as a result of the intersection). It can happen also that this point will intersect one of the branches Γ_1 and Γ_2 (in this case only one new integration contour will be originated during the intersection process). Finally, one can imagine that the point A comes along a sheet of the Riemannian surface which does not contain both Γ_1 and Γ_2 (in this case the intersection process does not lead to the appearance of new integration contours). Thus, we see that, generally speaking, the integral representation of the solution in different regions of the real axis τ will be of the form

$$c_j(\tau, v) = \sum_k \mathcal{L}_{s_k}[C_j(\tau, s)] = \sum_k \int_{\Gamma_k(\tau)} e^{\frac{i}{v}s} C_j(\tau, s)\, ds \tag{21}$$

rather than of the form (11). Here the sum is taken over some subset[6] of the set of points s_k of singularities of the integrands $C_j(\tau, s)$ and the contour $\Gamma_k(\tau)$ is a standard contours encircling the point s_k. The sum on the right in (21) can be infinite, but must contain only a finite number of points of support in any half-plane $\operatorname{Im} s < A$ for arbitrary real value of A.

From the above considerations it is clear that to compute directly the number of contours extracted it is necessary to know the global structure of the Riemannian surface of the integrand. Clearly, this task is not so simple in the general case.

Further, as we have seen above (see formulas (13) and (14)), each point s_k of singularity of the integrand in (21) corresponds to some WKB-term which *might* be included into the asymptotic expansion of the constructed solution (though can not be included in it). Actually, the WKB-term (14) is involved into the asymptotic expansion of the solution if and only if the corresponding point of singularity of the integrand

[6]This subset is called a *support* of the resurgent function in question. The notion of a support of a resurgent function is strongly connected with different physical and mathematical notions; see, for example, the paper [17] on complex rays method.

is encircled by some integration contour in the integral representation of this solution, that is, if this point corresponds to one of the terms on the right in (21). We shall refer points of singularities included into representation (21) as *active points* and all other points of singularity as *passive points* for the given value of the variable τ. As it is clear from the above considerations the property of the point to be passive or active can be changed exactly at those points τ at which one point of singularity of the integrand in (21) intersects the integration contour encircling the another point of singularity. For the considered example it can happen only for such values of τ for which the real part of the action $S_+(\tau)$ coincides with the real part of the action $S_-(\tau)$, that is, in the case, when the two lattices in question lay on one and the same vertical line in the complex plane s. The set of such points is called a *Stokes set* of the functions in question.

Later on, the Stokes set divides all the complex plane $\mathbf{C}_\tau$ into a number of regions which will be referred below as the *Stokes regions.*

Finally, there are points in the complex plane $\mathbf{C}_\tau$ which are ramification points of the adiabatic potential curves (and, consequently, the ramification points of the action function). In the resurgent analysis such points are called *focal points* of the resurgent function in question and we denote by $\mathcal{F}$ the set of focal points. As we shall see below, these points play a crucial role in the investigation of the asymptotic expansions of the solutions to the considered equations. In our example we have two focal points $\tau = \pm i$ at which two lattices of singularities of the functions $C_1(\tau, s)$ and $C_2(\tau, s)$ coincide with each other. The difference between the set of focal points and the Stokes set of the given resurgent function is that the first one has *complex* codimension 1 in the complex plane $\mathbf{C}_\tau$ whereas the second one has in this plane the *real* codimension 1. Hence, the Stokes set divides the plane $\mathbf{C}_\tau$ into Stokes regions, and the set of focal points does not divide $\mathbf{C}_\tau$ at all.

Thus, to give the full description of the Stokes phenomenon one has to determine the set of active points of singularity in each Stokes region.

One can present more exact description of the Stokes phenomenon using the notion of *microfunctions.* To come to this notion we remark that each integral on the right in (21) will not be changed if we add to the integrand some endlessly-continuable analytic function which is holomorphic in a neighbourhood of the corresponding point s_k of singularity. Thus, the value of the term in the representation (21) depends not on the functions C_1 and C_2 themselves but on the equivalence class of these functions modulo functions regular near the point s_k. Such equivalence classes are called (endlessly-continuable) *microfunctions* supported at the point s_k and are none more than singular parts of C_1 and C_2 at the point s_k. The space of microfunctions supported at the point s_k we shall denote by $\mathcal{M}_{s_k}$.

Further, as we have seen above, each term of the (exponential) WKB-expansion of the solution corresponds to exactly one term of the representation on the right in (21), that is, to exactly one

microfunction supported at some point of singularity of the integrands C_1 and C_2. Therefore, we can represent the asymptotic expansion of the functions in question as (infinite, in general) vectors

$$\begin{pmatrix} C_{1,s_1} \\ C_{1,s_2} \\ \dots \end{pmatrix}, \begin{pmatrix} C_{2,s_1} \\ C_{2,s_2} \\ \dots \end{pmatrix}, \tag{22}$$

where C_{j,s_k} are some elements of the space $\mathcal{M}_{s_k}$ for some point s_k of singularity of the function $C_j(\tau, s)$. We denote by $\mathcal{M}$ the space of vectors (22), so that the asymptotic expansion of the solution can be represented as an element from $\mathcal{M} \times \mathcal{M}$.

Now the change of the asymptotic expansion at points of the Stokes set can be treated as a homomorphism

$$\tau : \mathcal{M} \times \mathcal{M} \to \mathcal{M} \times \mathcal{M}$$

which is called a *connection homomorphism* in the resurgent analysis.

Thus, the computation of the Stokes phenomenon is exactly the computation of the Stokes homomorphism at each point on the Stokes set.

So, to compute the asymptotic expansion of the solution with the exponential accuracy, one has to solve the following two problems.

1. To compute WKB asymptotic expansions corresponding to each point of singularity.
2. To select the set of active points of singularity for each value of τ.

Then the asymptotic expansion of the solution will be simply the sum of WKB-expansions (or, more exactly, of the resums of these expansions since the corresponding asymptotic series diverge) computed at each active point for any value of τ.

We claim that both these problems can be solved with the help of complexification in the variable τ. As it was already mentioned, the solution of both problems strongly depends on the position of the ramification points of the adiabatic potential curves, or, in other words, of the focal points for the constructed solution.

Let us describe first the computation of the WKB-expansions. To do this, we first investigate the behavior of points of singularities of the functions $C_1(\tau, s)$ and $C_2(\tau, s)$ when the point τ is tracing a path l_1 in the complex plane $\mathbf{C}_\tau$ shown on Figure 6. This path having the origin at the point $\tau = 0$ goes along the imaginary axis to the point $\tau = i$, encircles this point counterclockwise and then comes back to the origin.

It is easy to verify that when τ moves along the imaginary axis from the origin to the point $\tau = i$, the singular points of the functions $C_j(\tau, s)$ will move along the trajectories shown on Figure 7 b) (on Figures 7 a) and c) the initial and the final states of this motion is shown, the points of the first lattice are shown on this Figure by crosses whereas the points of the second lattice are shown by points; in the situation

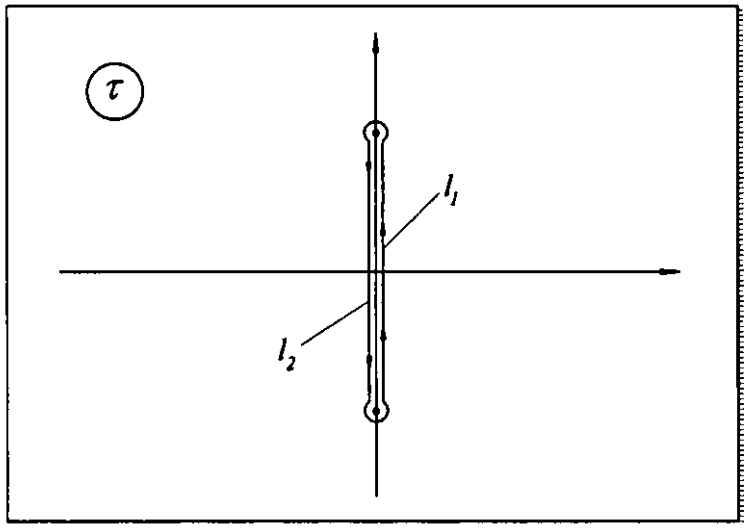

Figure 6: Paths of analytic continuation.

of Figure 7 c) these two lattices coincide with each other since $\tau = i$ is a focal point). Actually, we have

$$S_+(i\theta) = -\frac{\theta^2}{2} + i\left[\frac{\theta}{2}\sqrt{1-\theta^2} + \frac{1}{2}\mathrm{arctg}\frac{\theta}{\sqrt{1-\theta^2}}\right],$$

$$S_-(i\theta) = -\frac{\theta^2}{2} + i\left[\frac{\pi}{2} - \frac{\theta}{2}\sqrt{1-\theta^2} - \frac{1}{2}\mathrm{arctg}\frac{\theta}{\sqrt{1-\theta^2}}\right],$$

and one can easily verify that the real and imaginary parts of the two latter functions are monotonic when $0 < \theta < 1$.

Later on, when τ is at point a (see Figure 6), that is, $\theta = 1-\varepsilon$ for some small positive ε, the two points $S_+(i\theta)$ and $S_-(i\theta)$ are both close to the point $s = -1/2+i\pi/4$. When τ encircles the small loop around the focal point $\tau = i$, these two points will rotate to the angle 3π and, hence, these two points will be exchanged during this rotation. Actually, one has

$$S_\pm\left(i + \varepsilon e^{i\alpha}\right) = -\frac{1}{2} + \frac{i\pi}{4} \pm \frac{3\sqrt{2i}}{4}\varepsilon^{3/2}e^{\frac{3i\alpha}{2}} + O\left(\varepsilon^2\right).$$

The stated assertion is a direct consequence of the latter formula.

Finally, if the point τ goes back from the value $\tau = i(1-\varepsilon)$ to the origin, the two considered points will be moving back along the trajectories shown on Figure 7 b) to the initial position. Thus, as a result of tracing the path l_1 shown on Figure 6, the two

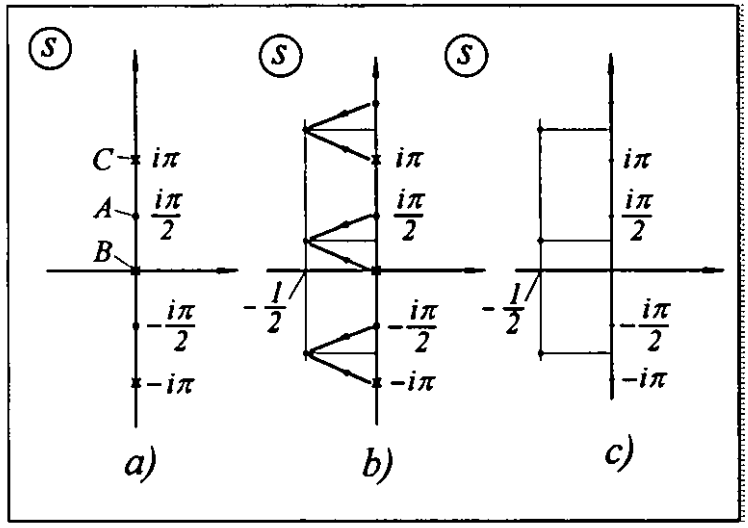

Figure 7: Dynamics of the resurgent structure along l_1.

points A and B shown on Figure 7 a) will be interchanged (as well as all other pairs of points obtained from A and B with shifting by $i\pi$).

The loop l_1 determines an element $\bar{l}_1$ of the fundamental group $\pi_1(\mathbf{C}_\tau \backslash \mathcal{F})$ of the complement $\mathbf{C}_\tau \backslash \mathcal{F}$ of the set $\mathcal{F}$ of focal points in the plane $\mathbf{C}_\tau$. As we have shown above, the action of this element on the Riemannian surface of solutions C_1 and C_2 to system (12) interchanges the points of singularity A and B. Hence, the analytic continuation of these functions considered in a neighbourhood of the point A along the path l_1 gives the value of the same functions in a neighbourhood of the point B. Since the correspondence between expansions (13) and (14) is one-to-one, we can claim that the WKB-element corresponding to the point B is a result of the analytic continuation of the WKB-element corresponding to the point A.

The action of the element $\bar{l}_2$ of the fundamental group $\pi_1(\mathbf{C}_\tau \backslash \mathcal{F})$ corresponding to the path l_2 drawn on Figure 6 can be investigated in the similar way. However, this element interchanges the points of singularity A and C (see Figure 7 a)), not A and B.

Let us now pass to the solution of the second problem listed above. The matter is that there exists a method of computation of the Stokes phenomenon based on the so-called *resurgent equations*. This method is based on the fact that the solution $(c_1(\tau, v), c_2(\tau, v))$ to system (9) is clearly an entire function of the variable τ whereas the asymptotic series given by WKB-elements ramifies around singular points of the adiabatic potential curves. Hence, the variation of the WKB expansions originated by

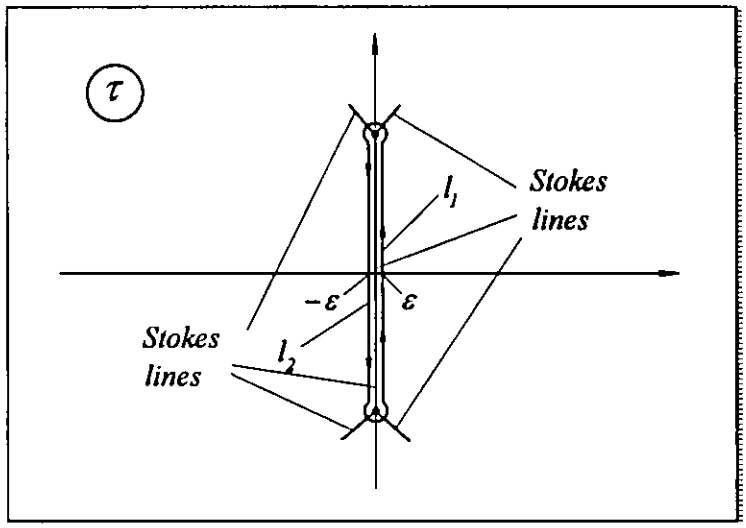

Figure 8: Computation of the Stokes phenomenon.

ramification of the action $S(\tau)$ and of the amplitude

$$a(\tau, v) = \sum_{j=0}^{\infty} v^j a_j(\tau)$$

must be cancelled out with the additional terms appearing in the asymptotics due to the Stokes phenomenon. One can write down the corresponding relations and try to obtain the information about the change of asymptotic expansions from these relations. This program can be fulfilled with the help of the so-called *alient derivative*. Unfortunately, the presentation of the theory of alient derivatives is far out of the framework of the present paper; the reader can find the detailed explanations of all this theory in [18], [14], [19], [20], [21], [13]. Here we shall mention only that the computation of changes in asymptotic expansions when intersecting Stokes lines with the help of the alient differential calculus is possible only in a neighbourhood of some focal points and only in the case when both the point defining the integration contour and the point intersecting this contour are those coinciding with one another when τ approaches this focal point. So the question arises: how can one compute the change of asymptotic expansion when one point intersect the integration contour determined by the other point if these two points are posited on some nonvanishing distance from each other? Such a situation, typical for the problems of the considered type, is shown, for example, on Figure 5 b) where the point A of singularity intersects the integration contour apart from its origin B.

The answer to this question can be obtained again with the help of the analytic continuation along paths l_1 and l_2 drawn on Figure 6 together with the corresponding Stokes lines. Namely, instead of continuation along the segment of the real axis from the point $\tau = -\varepsilon$ to the point $\tau = \varepsilon$ for some $\varepsilon > 0$ (this segment intersects one of the Stokes lines, see Figure 8) one can use the continuation along the path l_1 (drawn on the same Figure) along which the intersections with all the Stokes lines in question occurs in a neighbourhood of the focal point $\tau = i$. We have chosen the path l_1 since, as it can be seen from Figure 7 the two points A and B in question (see Figure 5 b)) are close to each other in a neighbourhood of the focal point $\tau = i$.

The result of computations of the Stokes phenomenon for the considered example is shown on Figure 5 c). Here one can see that all points of the lattice born by $S_-(\tau)$ lying above the real axis in the complex plane C_s are active for $\tau > 0$ and, hence, all these points determine nontrivial contributions to the asymptotic expansion of the solution in this region.

4 Formulation of the computational algorythm

In the previous Section we have obtained that the asymptotic expansion of the solution to (9) for $\tau > 0$ (in particular, for large real values of τ) consists of the WKB element corresponding to the adiabatic potential curve $E_+(\tau)$ and of all analytic continuations of this WKB element along paths l_1, $l_1 l_2 l_1$, $l_1 l_2 l_1 l_2 l_1$, ..., each corresponding to the adiabatic potential curve $E_-(\tau)$.

Similar one can obtain the following result valid for general problems of the form (7), (8).

The asymptotic expansion of the solution to the problem (7), (8) *for sufficiently large positive values of the variable* τ *consists of the WKB-element corresponding to the adiabatic potential curve* $E_{j_0}(\tau)$ *and of all continuations of this element along all elements of the basis of the fundamental group* $\pi_1(\mathbf{C}_\tau \backslash \mathcal{F})$ *taken with coefficients arising due to the Stokes phenomenon.*

We shall not present here the proof of the stated assertion since it goes more or less similar to the consideration of the above example. The reader can construct this proof by himself or herself.

In conclusion we remark that just the same computations lead to the asymptotic investigation of the *overbarrier reflection* phenomenon in quantum mechanics (see, for example, [22]). What is more, numerical computations in the simplest case of quadratic potential coincide exactly with the above computations for the two-level Zener model.

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