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Non-trivial prefactors in adiabatic transition probabilities induced by high-order complex degeneracies

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Abstract. The adiabatic limit of the transition probability for two-level systems driven by real symmetric time-dependent Hamiltonians is considered. When the Hamiltonian depends analytically on time, the transition probability is governed, in simple cases, by a complex eigenvalue crossing point which is, generically, a square root branching point for the eigenvalues. In such a case, the transition probability is given by the Dykhne formula, the recently discovered geometric prefactor being equal to one. In this paper we deal with the general situation where the relevant eigenvalue crossing point is a branching point of order $n/2$, $n \geq 1$, for the eigenvalues and a zero of order $m \geq 0$ for the Hamiltonian itself. The analysis shows that the Dykhne formula must be completed by a novel prefactor which depends on both n and m . In particular, this prefactor can take the value zero, in contrast to the geometrical prefactor. We also consider the case where the transition probability is governed by N complex eigenvalue crossing points of different orders n_j and m_j , $j = 1, \dots, N$. The end result displays an interference phenomenon between the individual prefactors similar to the case of generic eigenvalue crossing points $n_j = 1$ and $m_j = 0$ considered earlier.

1. Introduction

The adiabatic limit of the time-dependent Schrödinger equation

$$i\varepsilon \frac{\partial}{\partial t} \psi(t) = H(t) \psi(t) \quad \varepsilon \rightarrow 0 \quad (1.1)$$

has been the object of renewed interest for several years now. The origin of this renewal of interest is the seminal paper by Berry [1] in which he showed that the adiabatic theorem of quantum mechanics could generate a phase factor of non-trivial geometric meaning. After the abstract formulation of the geometric content of this result by Simon [2], several theoretical as well as experimental works were devoted to this geometric phase and its generalizations [3]. Another important aspect of the adiabatic theorem of quantum mechanics has also been recently reconsidered, namely the rigorous estimation of the (vanishing) transition probabilities between spectrally isolated subspaces. This aspect specialized to two-level systems is the main concern of this paper. Consider a two-level system driven by an analytic time-dependent Hamiltonian $H(t)$ whose eigenvalues $e_1(t)$ and $e_2(t)$ are separated by a gap for any time t . It is known since the pioneering works of Landau [4], Zener [5] and Dykhne [6], that the transition probability $\mathcal{P}(\varepsilon)$ between the eigenvectors of the system over infinite time is exponentially small in the adiabaticity parameter ε , as ε tends to zero. However, the asymptotic formula proposed in [4] and [6] for real symmetric Hamiltonians, known as the Dykhne formula, was rigorized much later

by Davis and Pechukas [7] and by Hwang and Pechukas [8]. This formula shows that in simple cases the transition probability is governed by one of the complex crossing points of the analytic continuations of the eigenvalues, i.e. points z_j such that $e_1(z_j) = e_2(z_j)$. Generically, the complex eigenvalue crossing points are square root branching points for the difference of the eigenvalues:

$$e_1(z) - e_2(z) \simeq (z - z_j)^{1/2}. \quad (1.2)$$

If z_1 is the relevant eigenvalue crossing, which is assumed to be generic, then the Dykhne formula reads

$$\mathcal{P}(\varepsilon) \simeq \exp \left\{ -\frac{2}{\varepsilon} \left| \operatorname{Im} \int_0^{z_1} e_1(z) - e_2(z) dz \right| \right\} \quad \text{as } \varepsilon \rightarrow 0. \quad (1.3)$$

It was pointed out recently by Berry [9] and Joye *et al* [10] independently that the Dykhne formula (1.3) must be completed by a prefactor of the form $\exp\{2 \operatorname{Im} \theta\}$ when applied to generic complex Hermitian two-level Hamiltonians. This prefactor is geometric in nature and is given by the analytic continuation of the geometric phase mentioned above around the relevant complex eigenvalue crossing point. For real symmetric Hamiltonians, this prefactor reduces to 1, yielding back the familiar Dykhne formula for the transition probability. The geometric prefactor was measured successfully by Zwanziger *et al* [11] in a spin experiment.

More general expressions for $\mathcal{P}(\varepsilon)$ can be found in [12–15], whereas a phenomenon of interferences is studied in [16] when several eigenvalue crossing points govern the transition probability. Similar problems were also considered for more general systems [17, 18] and the reduction of general problems to the study of two-level systems was legitimated in [19]. In particular, the so called Landau–Zener formula was rigorized in [20] and [21]. See also [22].

The main purpose of this paper is to study the asymptotic of the transition probability for two-level systems driven by real symmetric Hamiltonians displaying complex eigenvalue crossing points of higher orders. This means that we consider the general behaviour (see hypothesis (iv))

$$e_1(z) - e_2(z) \simeq (z - z_1)^{n/2} \quad n \geq 1 \quad (1.4)$$

close to the relevant crossing point z_1 , instead of the generic square root behaviour (1.2). Let us give a heuristic description of the physically expected behaviour of the transition probability $\mathcal{P}(\varepsilon)$ in this situation. Assume for the discussion that z_1 is close to the real axis. Thus the two levels $e_1(t)$ and $e_2(t)$ for real t become close to each other in a neighbourhood of z_1 . Now if n takes a larger value than 1, the levels will be close to one another on a larger region of the real axis. As a consequence, the transition between the levels should be enhanced and the transition probability should be increased. On the other hand, the Hamiltonian $H(z)$ itself may possess a zero of high order at the degeneracy point z_1 (1.4) of the levels:

$$H(z) \simeq (z - z_1)^m. \quad (1.5)$$

(Then, necessarily $2m \leq n$, see lemma 3.1.) This means that, although the levels are close to each other in that region, the coupling between them is very weak. As a consequence, the transition probability should be decreased. The asymptotic formula for $\mathcal{P}(\varepsilon)$ in the adiabatic limit $\varepsilon \rightarrow 0$ must thus reflect the competition between these two conflicting effects.

Our study of this problem in the simple case described above of one relevant eigenvalue crossing point z_1 characterized by the integers n and m , leads to the appearance of a non-trivial prefactor in the asymptotic formula for the transition probability (see corollary 2.1):

$$\mathcal{P}(\varepsilon) \simeq 4 \sin^2 \left(\frac{\pi(n - 2m)}{2(n + 2)} \right) \exp \left\{ - \frac{2}{\varepsilon} \left| \operatorname{Im} \int_0^{z_1} e_1(z) - e_2(z) dz \right| \right\} \quad \text{as } \varepsilon \rightarrow 0. \quad (1.6)$$

The novel prefactor $4 \sin^2(\pi(n - 2m)/2(n + 2))$ is induced by the high-order complex degeneracy z_1 and is not of geometrical origin. This prefactor reduces to 1 if z_1 is a generic complex eigenvalue crossing ($n = 1, m = 0$). For a given order n of the degeneracy, it can take $n/2 + 1$ (respectively $(n + 1)/2$) different values depending on m , if n is even (respectively odd). Moreover, it describes correctly the competition described above: if we set $m = 0$, i.e. $H(z_1) \neq 0$, we see that the exponential function is multiplied by a factor greater or equal to 1, which can get close to 4 if n is large. This is the behaviour expected for close levels and large coupling. In contrast, if we take for m the largest admissible value $m = (n - 1)/2$, assuming n to be odd, the prefactor is less or equal to 1 and can get close to 0 if n is large. This describes the effect of the weak coupling between the levels if the Hamiltonian is highly degenerate at the high-order complex degeneracy of the levels. Moreover, if n is even, the value $m = n/2$ yields a prefactor exactly equal to zero, and this for any value of n . This means that when the eigenvalue crossing is the consequence of a degeneracy of the Hamiltonian, the coupling between the levels becomes ineffective (to the leading order). For other intermediate values of m , the balance between the two extreme situations is described by the sine in the prefactor. Note that the prefactor is equal to 1 if $m = \frac{1}{2}n - 1 \in \mathbb{N}$. Naturally, the exponential decay rate in (1.6) also depends on n . An explicit example displaying a non-trivial prefactor is studied in section 4.

This result can be extended to the cases where the transition probability between the two levels is governed by several eigenvalue crossings $z_j, j = 1, 2, \dots, N$, each one being characterized by the integers n_j and $m_j, (2m_j \leq n_j)$ defined as above (see conditions (iv) to (vi)). The end result for $\mathcal{P}(\varepsilon)$ is given by the sum of the contributions of each individual eigenvalue crossing point (see theorem 2.1):

$$\mathcal{P}(\varepsilon) \simeq \left| \sum_{j=1}^N 2\sigma_j \sin \left(\frac{\pi(n_j - 2m_j)}{2(n_j + 2)} \right) \exp \left\{ - \frac{i}{\varepsilon} \int_0^{z_j} e_1(z) - e_2(z) dz \right\} \right|^2 \quad \text{as } \varepsilon \rightarrow 0 \quad (1.7)$$

where $\sigma_j = \pm 1$ is determined explicitly. In such a case we have

$$\begin{aligned} \operatorname{Im} \int_0^{z_j} e_1(z) - e_2(z) dz &= \operatorname{Im} \int_0^{z_1} e_1(z) - e_2(z) dz \\ &= - \left| \operatorname{Im} \int_0^{z_1} e_1(z) - e_2(z) dz \right| < 0 \quad j = 1, 2, \dots, N. \end{aligned} \quad (1.8)$$

This formula generalizes (1.6) in the same way as the result of [16] generalizes the case of generic eigenvalue crossings considered in [10]. As in the corresponding result of [16], the main feature of (1.7) is that it takes into account the phases of the individual transition amplitudes which induce interferences in the asymptotic expression of $\mathcal{P}(\varepsilon)$, as $\varepsilon \rightarrow 0$. For a more detailed discussion of this phenomenon and numerical illustrations of it, we refer the reader to [16].

The presence of a non-trivial prefactor in formula (1.6) was noticed by Solov'ev in [23, 24]. However, the case $m = 0$ only is dealt with, so that the conflicting effects described above are not taken into account. Moreover, no estimates on the error terms are given in these works, as explicitly stated by the author. Finally, the same result can be obtained by using the concept of superadiabatic evolution [12, 18, 19] and by following the ideas presented in [12]. This approach was developed independently for the case $m = 0$ by Berry and Lim [25].

A similar phenomenon, although less general, takes place in the study of the semiclassical limit of the stationary one-dimensional Schrödinger equation

$$-\hbar^2 \frac{d^2}{dx^2} \varphi(x) + V(x)\varphi(x) = E\varphi(x) \quad \text{as } \hbar \rightarrow 0 \quad (1.9)$$

when $E > \sup_{x \in \mathbb{R}} V(x)$. Indeed, the mathematical structure of the computation of the above barrier reflection coefficient $R(\hbar)$ and of the transition probability $\mathcal{P}(\varepsilon)$ are quite similar, as noted in [4, 6–8]. Assuming that V is analytic, the role of the complex eigenvalue crossing points is played here by the complex turning points z_j such that $V(z_j) = E$. They are generically simple zeros of $E - V(z)$. If z_1 is the relevant generic turning point, the reflection coefficient is given by a decreasing exponential in $1/\hbar$ with decay rate $-4|\operatorname{Im} \int_0^{z_1} \sqrt{E - V(z)} dz|$ [7, 8]. When applied to this semiclassical context and assuming that z_1 is a zero of order $n \geq 1$ of $E - V(z)$, our analysis yields (see theorem 5.1)

$$R(\hbar) \simeq 4 \sin^2 \left(\frac{\pi n}{2(n+2)} \right) \exp \left\{ -\frac{4}{\hbar} \left| \operatorname{Im} \int_0^{z_1} \sqrt{E - V(z)} dz \right| \right\} \quad \text{as } \hbar \rightarrow 0. \quad (1.10)$$

The appearance of a prefactor for non-generic turning points was already recognized by Pokrovskii and Khalatnikov in 1961 [26]. Then this problem was reconsidered and generalized in [27–31]. In particular, in [28] Berry used an original method in which $R(\hbar)$ is represented by a convergent multiple reflections series. However, no rigorous derivation of equation (1.10) can be found in the literature. Note that the prefactor here is entirely characterized by the order n of the zero of $E - V(z)$ and is always greater than 1. This property reflects the fact that the semiclassical problem depends on one function only, $E - V(z)$, whereas the adiabatic problem is determined by two independent functions $B_1(z)$ and $B_3(z)$ (see below). Although formula (1.10) is not new in this context, we transpose our rigorous analysis of the adiabatic problem to the semiclassical problem in section 5 to provide explicit error bounds which are lacking in the treatments quoted above. Again, the result can be generalized to cases where the reflection coefficient is determined by several turning points of arbitrary orders (see theorem 5.1).

The plan of the paper is as follows. We give in section 2 a precise formulation of our main result in the adiabatic context. Section 3 contains the proof of the theorem and we deal with an explicit example in section 4. The application of our analysis to the semiclassical computation of the above barrier reflection coefficient is briefly exposed in section 5.

2. Main result

We consider the singular limit $\varepsilon \rightarrow 0$ of the equation

$$i\varepsilon \frac{\partial}{\partial t} \psi(t) = H(t)\psi(t) \quad t \in \mathbb{R} \quad (2.1)$$

where the Hamiltonian $H(t)$ is a 2×2 real symmetric matrix

$$H(t) = \begin{pmatrix} B_3(t) & B_1(t) \\ B_1(t) & -B_3(t) \end{pmatrix}. \quad (2.2)$$

We assume the following regularity conditions.

- (i) The Hamiltonian $H(t)$ is analytic in a strip $S_a = \{z = t + is \in \mathbb{C} \mid |s| \leq a\}$.
- (ii) There exist two non-zero real symmetric matrices $H(\pm\infty)$ such that

$$\lim_{t \rightarrow \pm\infty} \sup_{|s| \leq a} \|H(t) - H(\pm\infty)\| |t|^{1+\alpha} = 0 \tag{2.3}$$

for some $\alpha > 0$.

Moreover, we suppose that the eigenvalues of $H(t)$, $e_1(t)$ and $e_2(t)$, are separated by a gap during the whole evolution:

(iii)

$$e_2(t) - e_1(t) \geq g > 0 \quad \forall t \in \mathbb{R}. \tag{2.4}$$

The eigenvalues are given on the real axis by the expressions

$$e_j(t) = (-1)^j \sqrt{\rho(t)} \tag{2.5}$$

where

$$\rho(t) = B_1^2(t) + B_3^2(t) \tag{2.6}$$

is strictly positive. The function $\rho(t)$ is analytic in S_a whereas the analytic continuations $e_j(z)$ of the eigenvalues $e_j(t)$ are generally multivalued in S_a . The complex eigenvalue crossings give rise to branching points for $e_j(z)$ which coincide with the zeros of $\rho(z)$, the analytic continuation of $\rho(t)$. We select on the real axis a set of normalized instantaneous eigenvectors $\varphi_j(t)$

$$H(t)\varphi_j(t) = e_j(t)\varphi_j(t) \quad t \in \mathbb{R}, \quad j = 1, 2 \tag{2.7}$$

by requiring that

$$\langle \varphi_j(t) | \frac{d}{dt} \varphi_j(t) \rangle \equiv 0 \quad j = 1, 2 \tag{2.8}$$

($\langle \cdot | \cdot \rangle$ being the usual scalar product in \mathbb{C}^2). It is a standard result that these vectors are unique up to an overall phase factor (see [32]). Moreover, their analytic continuations, $\varphi_j(z)$, are multivalued in S_a , with singularities at the eigenvalue crossings, as shown explicitly in [10] and [16]. Our condition (ii) insures the existence of the limits $\varphi_j(\pm\infty)$, $j = 1, 2$.

We expand the solution $\psi(t)$ of (2.1) on the eigenvectors just defined as

$$\psi(t) = \sum_{j=1}^2 c_j(t) \exp \left\{ -\frac{i}{\varepsilon} \int_0^t e_j(s) ds \right\} \varphi_j(t) \quad t \in \mathbb{R}. \tag{2.9}$$

The unknown coefficients $c_j(t)$ satisfy then the equation

$$\frac{d}{dt} c_k(t) = \sum_{j=1}^2 a_{kj}(t) \exp \left\{ (-1)^j \frac{i}{\varepsilon} \Delta(t) \right\} c_j(t) \quad j \neq k \in \{1, 2\} \tag{2.10}$$

where

$$\Delta(t) = \int_0^t (e_1(s) - e_2(s)) ds = -2 \int_0^t \sqrt{\rho(s)} ds \tag{2.11}$$

$$a_{kj}(t) = -\left\langle \varphi_k(t) \left| \frac{d}{dt} \varphi_j(t) \right. \right\rangle \quad t \in \mathbb{R}. \tag{2.12}$$

By condition (ii) again, the limits $c_j(\pm\infty)$, $j = 1, 2$, exist. We consider a solution $\psi(t)$ which, as $t \rightarrow -\infty$, is asymptotically an eigenstate of $H(-\infty)$ associated with $e_1(-\infty)$, i.e. we choose

$$c_1(-\infty) = 1 \quad c_2(-\infty) = 0. \tag{2.13}$$

We want to compute the probability to find the system at $t = +\infty$ in the eigenstate associated with $e_2(+\infty)$, i.e. the transition probability

$$\mathcal{P}(\varepsilon) = |c_2(+\infty)|^2. \tag{2.14}$$

As noted in the introduction, the transition probability is governed the complex eigenvalue crossings of the Hamiltonian. In this paper we consider the general situation characterized by

(iv) The set X of zeros of $\rho(z)$ in S_a consists of $2n$ interior points $z_1, \bar{z}_1, z_2, \bar{z}_2, \dots, z_n, \bar{z}_n$, where z_k and \bar{z}_k are zeros of order $n_k \geq 1$, $k = 1, \dots, n$ ($\text{Im } z_k > 0$ by convention).

Moreover, the number of vanishing derivatives of the Hamiltonian at the eigenvalue crossing z_k is of importance. Hence we further introduce:

(v) Let $m_k \geq 0$ be the order of z_k considered as a zero of $H(z)$. We have $2m_k \leq n_k$.

The inequality $2m_k \leq n_k$ is always satisfied, as shown in lemma 3.1.

As usual in this type of analysis, the Stokes lines of the problem play an important role. They are defined through the analytic continuations of the function (2.11),

$$\Delta(z) = -2 \int_0^z \sqrt{\rho(s)} ds \tag{2.15}$$

where the path of integration from 0 to z belongs to $S_a \setminus X$. This function has branching points at the points of X and is defined by continuity if $z \in X$. The Stokes lines of the problem are defined by the set of level lines

$$\text{Im } \Delta(z) = \text{Im } \Delta(z_k) \quad \forall z \in S_a, \quad k = 1, \dots, n. \tag{2.16}$$

(Confusion should be avoided here between our definition (2.16) of Stokes lines and the other convention consisting in calling the level lines $\text{Re } \Delta(z) = \text{Re } \Delta(z_k)$ Stokes lines.) There are $n_k + 2$ branches of Stokes lines emanating from a zero z_k of $\rho(z)$ of order n_k , as verified by a local argument (see e.g. [33]). We now state our last hypothesis which concerns the global behaviour of the Stokes lines:

(vi) There exist N eigenvalue crossings z_1, \dots, z_N and a Stokes line $t \mapsto \gamma(t)$, $t \in \mathbb{R}$, in S_a which passes through z_1, \dots, z_N and satisfies

$$\lim_{t \rightarrow \pm\infty} \text{Re } \gamma(t) = \pm\infty \quad \sup_{t \in \mathbb{R}} |\text{Im } \gamma(t)| < a. \tag{2.17}$$

This assumption may look merely technical at first sight, however it allows the N eigenvalue crossings governing the transition probability to be determined, which is obviously an essential issue. For a detailed investigation of this important aspect and a geometric interpretation of it, we refer the reader to [10].

Theorem 2.1. Let $H(t)$ be a real symmetric 2×2 (traceless) matrix satisfying conditions (i) to (vi) and let $\psi(t)$ be a solution of the Schrödinger equation (2.1). Then, there exist constants $\varepsilon^* > 0$ and $p > 0$ such that the transition probability $\mathcal{P}(\varepsilon)$ defined by (2.13) and (2.14) is given for any $\varepsilon < \varepsilon^*$ by

$$\mathcal{P}(\varepsilon) = \left| \sum_{j=1}^N 2\sigma_j \sin \left(\frac{\pi(n_j - 2m_j)}{2(n_j + 2)} \right) \exp \left\{ -\frac{i}{\varepsilon} \Delta(z_j) \right\} \right|^2 + \mathcal{O} \left(\varepsilon^p \exp \left\{ -\frac{2}{\varepsilon} |\operatorname{Im} \Delta(z_1)| \right\} \right) \tag{2.18}$$

where $\Delta(z_j) = \int_0^{z_j} e_1(z) - e_2(z) dz$, $\sigma_j = \pm 1$ and $2m_j \leq n_j$.

Remarks.

- The value of σ_j is determined by the phase of $(d^{m_j}/dz^{m_j})B_1(z_j)$, see lemma 3.1.
- An explicit value for the power p is given in lemma 3.3. However, as noticed in [16], this power is not the optimal one and the error term is probably much smaller than the estimate obtained here.
- Since the relevant eigenvalue crossings are located on the same Stokes line γ , we immediately have, for all $j = 1, \dots, N$,

$$\operatorname{Im} \Delta(z_j) = \operatorname{Im} \Delta(z_1) = -|\operatorname{Im} \Delta(z_1)| < 0. \tag{2.19}$$

- The assumption (ii) can be weakened a little, see the example and [15].
- If the boundary conditions (2.13) are reversed, the transition probability $\mathcal{P}(\varepsilon) = |c_1(\infty)|^2$ is given by the same formula, as noted in [16].

Setting $N = 1$ we have the immediate:

Corollary 2.1. Under the same hypotheses as in theorem 2.1, and with the notation $n_1 \equiv n$, $m_1 \equiv m$, there exist constants $\varepsilon^* > 0$ and $p > 0$ such that

$$\mathcal{P}(\varepsilon) = \left(4 \sin^2 \left(\frac{\pi(n - 2m)}{2(n + 2)} \right) + \mathcal{O}(\varepsilon^p) \right) \exp \left\{ -\frac{2}{\varepsilon} |\operatorname{Im} \Delta(z_1)| \right\} \tag{2.20}$$

for any $\varepsilon < \varepsilon^*$.

This yields the prefactor discussed in the introduction.

3. Proof of the result

We show theorem 2.1 by following a direct generalization of the method used in [16]. Let us briefly recall the strategy. Using the analyticity of the problem, we consider the differential equation (2.10) for the coefficients along the Stokes line γ of condition (vi), rather than on the real axis, except in the neighbourhood of the singular points. The singularities of this equation are precisely the eigenvalue crossing points which are located on γ . Around these singularities we solve exactly a comparison equation which captures the dominant features of the equation. Then, we asymptotically match this approximation with the solution of (2.10) obtained along the Stokes line, which we control by using an integration by parts.

Let us recall some general facts which are proven in [10] and [16], under conditions (i) to (vi):

- The simply connected domain Ω defined by its border $\partial\Omega = \gamma \cup \bar{\gamma}$ contains no point of X in its interior.
- The functions $\Delta(t)$ and $a_{kj}(t)$ defined in (2.11) and (2.12) possess single-valued analytic continuations $\Delta(z)$ and $a_{kj}(z)$, $\forall z \in \Omega \setminus X$.
- The expression of the couplings $a_{kj}(z)$ in terms of the functions $B_k(z)$ reads in our case

$$a_{kj}(z) = -\frac{(-1)^j}{\rho(z)} \left(\frac{B_3(z)\rho'(z)}{4B_1(z)} - \frac{B'_3(z)\rho(z)}{2B_1(z)} \right) \tag{3.1}$$

provided $\rho(z)B_1(z) \neq 0$ and with the notation $' = d/dz$ (lemma 3.1 of [16]). Moreover, we can exchange the indices of the functions $B_k(z)$ in this formula.

- The coefficients $c_j(t)$ thus admit single-valued analytic extensions $c_j(z)$ in $\Omega \setminus X$ such that

$$\lim_{t \rightarrow \pm\infty} |c_j(t + is) - c_j(\pm\infty)| \quad t + is \in \Omega. \tag{3.2}$$

These properties allow us to consider the analytic continuation of the system (2.10) along $\gamma(t)$ in particular, with boundary conditions

$$c_1(\gamma(-\infty)) = 1 \quad c_2(\gamma(-\infty)) = 0 \tag{3.3}$$

to compute

$$\mathcal{P}(\varepsilon) = |c_2(\gamma(+\infty))|^2. \tag{3.4}$$

3.1. Study of the singularities

Let z_0 denote any one of the points of X belonging to γ , characterized by the integers $n \geq 1$ and $m \geq 0$ such that

$$\rho(z) = r(z_0)(z - z_0)^n + \mathcal{O}((z - z_0)^{n+1}) \quad r(z_0) \neq 0 \tag{3.5}$$

$$H(z) = h(z_0)(z - z_0)^m + \mathcal{O}((z - z_0)^{m+1}) \quad h(z_0) \neq 0. \tag{3.6}$$

Lemma 3.1.

- (a) The integers n and m are such that $2m \leq n$.
- (b) Using the notation $f^{(m)}(z) \equiv (d^m/dz^m)f(z)$, we have the behaviours
 - (i) if $2m < n$

$$a_{kj}(z) = (-1)^j i \sigma_0 \frac{(n - 2m)}{4(z - z_0)} + \mathcal{O}(1) \tag{3.7}$$

where σ_0 is defined by $B_3^{(m)}(z_0) = i\sigma_0 B_1^{(m)}(z_0) \neq 0$;

- (ii) if $2m = n$

$$a_{kj}(z) = \mathcal{O}(1) \tag{3.8}$$

for z in a neighbourhood of z_0 .

Remarks.

- The factor $n - 2m$ describes quantitatively the conflicting effects discussed in the introduction on the strength of the couplings a_{kj} between the levels.

- If $n - 2m = 0$, the couplings are analytic at z_0 which allows us to use a simple method to estimate the transition probability in this case.

Proof. It follows from (3.6) that one of the functions $B_j(z)$ at least has a zero of order m at z_0 . Hence we can assume that

$$B_1(z) = \frac{B_1^{(m)}(z_0)}{m!} (z - z_0)^m + \mathcal{O}((z - z_0)^{m+1}) \tag{3.9}$$

with $B_1^{(m)}(z_0) \neq 0$, so that

$$B_1^2(z) = \left(\frac{B_1^{(m)}(z_0)}{m!} \right)^2 (z - z_0)^{2m} + \mathcal{O}((z - z_0)^{2m+1}). \tag{3.10}$$

Similar expressions hold for $B_3(z)$ and $B_3^2(z)$ with $|B_3^{(m)}(z_0)| \geq 0$, hence $2m \leq n$ is a consequence of (3.5).

Assume that $2m < n$. Then we have

$$(B_1^2(z) + B_3^2(z))^{(2m)}|_{z=z_0} = 0 \tag{3.11}$$

so that

$$(B_3^2)^{(2m)}(z_0) = -(B_1^2)^{(2m)}(z_0) \neq 0. \tag{3.12}$$

Thus we can write

$$B_3(z) = \frac{B_3^{(m)}(z_0)}{m!} (z - z_0)^m + \mathcal{O}((z - z_0)^{m+1}) \tag{3.13}$$

with

$$B_3^{(m)}(z_0) = \frac{m!}{\sqrt{(2m)!}} \sqrt{(B_3^2)^{(2m)}(z_0)} \equiv i\sigma_0 B_1^{(m)}(z_0). \tag{3.14}$$

It remains to insert these expressions in (3.1) to obtain assertion (i).

If $2m = n$, then $|B_3^{(n/2)}(z_0)| \geq 0$ and (3.1) again yields the result. □

Let us segment the Stokes line γ in several parts containing no eigenvalue crossing points in the following way. We introduce $z_j^\pm \in \gamma$ such that z_j^\pm are in the neighbourhood of $z_j \in X$ and z_j^- is first met when we follow γ from $-\infty$ to $+\infty$, see figure 1. Let us also define the points $\zeta_j^\pm \in \gamma$ which are a finite distance away from z_j and such that ζ_j^+ is between z_j^+ and z_{j+1}^- , and $\zeta_j^+ = \zeta_{j+1}^-$, as in figure 1. We set $\zeta_1^- = -\infty$ and $\zeta_N^+ = +\infty$. The

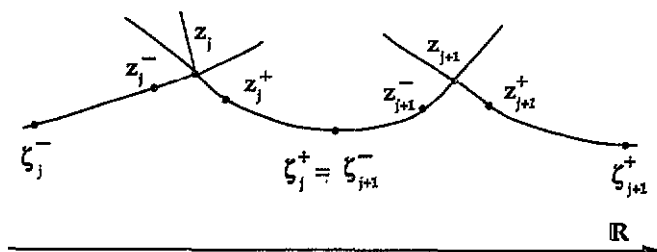


Figure 1. Definition of the points z_j^\pm and ζ_j^\pm .

segment of Stokes line γ delimited by ζ_j^- and ζ_j^+ is denoted by γ_j , whereas the segment delimited by ζ_j^\pm and z_j^\pm is denoted by γ_j^\pm .

We consider the system (2.10) along the portion of Stokes line γ_0^- delimited by ζ_0^- and z_0^- , (the index 0 still denoting any index). Let us estimate $c_j(z_0^-)$ as functions of $c_j(\zeta_0^-)$. In order to do so we work with the more appropriate variables

$$\widehat{c}_1(z) = c_1(z) \quad \widehat{c}_2(z) = \exp\left\{\frac{i}{\varepsilon}\Delta(z_0)\right\} c_2(z) \quad (3.15)$$

satisfying the equations

$$\begin{aligned} \widehat{c}_1(z) &= \widehat{c}_1(\zeta) + \int_{\zeta}^z a_{12}(z') \exp\left\{\frac{i}{\varepsilon}(\Delta(z') - \Delta(z_0))\right\} \widehat{c}_2(z') dz' \\ \widehat{c}_2(z) &= \widehat{c}_2(\zeta) + \int_{\zeta}^z a_{21}(z') \exp\left\{-\frac{i}{\varepsilon}(\Delta(z') - \Delta(z_0))\right\} \widehat{c}_1(z') dz' \end{aligned} \quad (3.16)$$

for any ζ and z in Ω . Performing an integration by parts we have

$$\begin{aligned} \widehat{c}_1(z) &= \widehat{c}_1(\zeta) + \frac{\varepsilon}{i} \frac{a_{12}}{\Delta'}(z') \exp\left\{\frac{i}{\varepsilon}(\Delta(z') - \Delta(z_0))\right\} \widehat{c}_2(z') \Big|_{\zeta}^z \\ &\quad - \frac{\varepsilon}{i} \int_{\zeta}^z \left(\frac{a_{12}}{\Delta'}\right)'(z') \exp\left\{\frac{i}{\varepsilon}(\Delta(z') - \Delta(z_0))\right\} \widehat{c}_2(z') dz' \\ &\quad - \frac{\varepsilon}{i} \int_{\zeta}^z \frac{a_{12}a_{21}}{\Delta'}(z') \widehat{c}_1(z') dz' \\ \widehat{c}_2(z) &= \widehat{c}_2(\zeta) - \frac{\varepsilon}{i} \frac{a_{21}}{\Delta'}(z') \exp\left\{-\frac{i}{\varepsilon}(\Delta(z') - \Delta(z_0))\right\} \widehat{c}_1(z') \Big|_{\zeta}^z \\ &\quad + \frac{\varepsilon}{i} \int_{\zeta}^z \left(\frac{a_{21}}{\Delta'}\right)'(z') \exp\left\{-\frac{i}{\varepsilon}(\Delta(z') - \Delta(z_0))\right\} \widehat{c}_1(z') dz' \\ &\quad + \frac{\varepsilon}{i} \int_{\zeta}^z \frac{a_{12}a_{21}}{\Delta'}(z') \widehat{c}_2(z') dz'. \end{aligned} \quad (3.17)$$

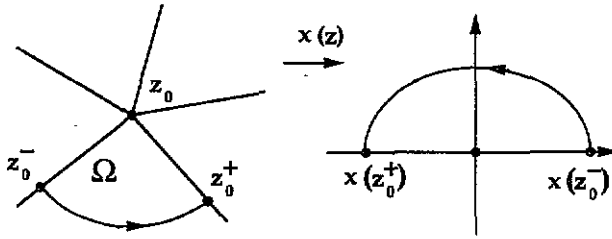


Figure 2. The analytic continuation of $x(z)$ inside Ω .

3.2. Case $2m < n$

From now on we assume that $2m < n$. The case $2m = n$ is treated below. Using lemma 3.1 and (3.5), if z is close to z_0^- we can find constants independent of j and z (which we denote generically by κ) such that

$$\begin{aligned} \left| \frac{a_{kj'}}{\Delta'}(z) \right| &\leq \frac{\kappa}{|z - z_0|^{(n+2)/2}} \\ \left| \left(\frac{a_{kj}}{\Delta'} \right)'(z) \right| &\leq \frac{\kappa}{|z - z_0|^{(n+4)/2}} \\ \left| \frac{a_{12}a_{21}}{\Delta'}(z) \right| &\leq \frac{\kappa}{|z - z_0|^{(n+4)/2}}. \end{aligned} \tag{3.18}$$

As $z \in \gamma_0^-$, we can assume that the above estimates hold for any such z . We set $\|\widehat{c}_k\| = \sup_{z \in \gamma_0^-} |\widehat{c}_k(z)|$ and $\delta = |z_0^- - z_0|$ so that using the property

$$\text{Im } \Delta(z) = \text{Im } \Delta(z_0) \quad \forall z \in \gamma_0^- \tag{3.19}$$

we obtain for all $z \in \gamma_0^-$

$$\begin{aligned} |\widehat{c}_1(z)| &\leq |\widehat{c}_1(z_0^-)| + \kappa \frac{\varepsilon}{\delta^{(n+2)/2}} (\|\widehat{c}_1\| + \|\widehat{c}_2\|) \\ |\widehat{c}_2(z)| &\leq |\widehat{c}_2(z_0^-)| + \kappa \frac{\varepsilon}{\delta^{(n+2)/2}} (\|\widehat{c}_1\| + \|\widehat{c}_2\|). \end{aligned} \tag{3.20}$$

Hence, taking the supremum over $z \in \gamma_0^-$ and summing the resulting inequalities, we get

$$\|\widehat{c}_1\| + \|\widehat{c}_2\| \leq |\widehat{c}_1(z_0^-)| + |\widehat{c}_2(z_0^-)| + 2\kappa \frac{\varepsilon}{\delta^{(n+2)/2}} (\|\widehat{c}_1\| + \|\widehat{c}_2\|), \tag{3.21}$$

Then, choosing ε small enough so that $2\kappa\varepsilon/\delta^{(n+2)/2} < 1/2$,

$$\|\widehat{c}_1\| + \|\widehat{c}_2\| \leq \kappa (|\widehat{c}_1(z_0^-)| + |\widehat{c}_2(z_0^-)|) \tag{3.22}$$

for another constant κ . Coming back to (3.17), we obtain under these conditions and for all $z \in \gamma_0^-$

$$|\widehat{c}_k(z) - \widehat{c}_k(z_0^-)| \leq \kappa \frac{\varepsilon}{\delta^{(n+2)/2}} (|\widehat{c}_1(z_0^-)| + |\widehat{c}_2(z_0^-)|). \tag{3.23}$$

We can perform the same type of analysis on the segment γ_0^+ delimited by z_0^+ and z_0^+ . Setting $\delta = |z_0^+ - z_0|$ we obtain similarly

$$|\widehat{c}_k(z) - \widehat{c}_k(z_0^+)| \leq \kappa \frac{\varepsilon}{\delta^{(n+2)/2}} (|\widehat{c}_1(z_0^+)| + |\widehat{c}_2(z_0^+)|) \tag{3.24}$$

for all $z \in \gamma_0^+$.

3.3. Comparison equation

We now turn to the determination of the comparison equation valid in the neighbourhood of the singularity z_0 . Its exact solution will allow us to express the coefficients $\widehat{c}_k(z_0^+)$ as functions of $\widehat{c}_k(z_0^-)$, up to errors which we master below. These coefficients satisfy

$$\begin{aligned}\widehat{c}_1'(z) &= a_{12}(z) \exp\left\{\frac{i}{\varepsilon}(\Delta(z) - \Delta(z_0))\right\} \widehat{c}_2(z) \\ \widehat{c}_2'(z) &= a_{21}(z) \exp\left\{-\frac{i}{\varepsilon}(\Delta(z) - \Delta(z_0))\right\} \widehat{c}_1(z).\end{aligned}\tag{3.25}$$

Let us introduce a suitable new variable x by

$$\varepsilon x \equiv \Delta(z) - \Delta(z_0) = -2 \int_{z_0}^z \sqrt{\rho(z')} dz' \tag{3.26}$$

which is well defined in the neighbourhood of z_0 . Note that x depends on both ε and z_0 and that this change of variables is one to one if $z \in \Omega$. By definition, x is real if $z \in \gamma$ and since $\text{Im } \Delta(z_0) < 0$, we have

$$x(z_0^-) > 0 \quad \text{and} \quad x(z_0^+) = e^{i\pi} |x(z_0^+)| < 0 \tag{3.27}$$

when the analytic continuation of $x(z)$ from z_0^- to z_0^+ is performed along a path belonging to Ω , see figure 2. In terms of the variable x , the system (3.25) reads

$$\begin{aligned}\frac{d}{dx} \widehat{c}_1(z(x)) &= -\frac{\varepsilon}{2\sqrt{\rho(z(x))}} a_{12}(z(x)) \exp\{ix\} \widehat{c}_2(z(x)) \\ \frac{d}{dx} \widehat{c}_2(z(x)) &= -\frac{\varepsilon}{2\sqrt{\rho(z(x))}} a_{21}(z(x)) \exp\{-ix\} \widehat{c}_1(z(x))\end{aligned}\tag{3.28}$$

which we rewrite in matrix notation as

$$\frac{d}{dx} \widehat{c}(z(x)) \equiv D(x, \varepsilon) \widehat{c}(z(x)). \tag{3.29}$$

Now, using (3.5)

$$\varepsilon x = -\frac{4\sqrt{r(z_0)}}{n+2} (z - z_0)^{(n+2)/2} (1 + \mathcal{O}(z - z_0)) \tag{3.30}$$

so that

$$z - z_0 = \mathcal{O}((\varepsilon x)^{2/(n+2)}). \tag{3.31}$$

These expressions and lemma 3.1 yield

$$\begin{aligned}-\frac{\varepsilon}{2\sqrt{\rho(z)}} a_{kj}(z) &= -(-1)^j \frac{\varepsilon i \sigma_0(n-2m)}{8\sqrt{r(z_0)}(z-z_0)^{(n+2)/2}} + \varepsilon \mathcal{O}\left(\frac{1}{(z-z_0)^{n/2}}\right) \\ &= (-1)^j \frac{i \sigma_0(n-2m)}{2(n+2)} \frac{1}{x} + \frac{1}{x} \mathcal{O}((\varepsilon x)^{2/(n+2)}) + \varepsilon \mathcal{O}((\varepsilon x)^{-n/(n+2)}) \\ &= (-1)^j \frac{i \sigma_0(n-2m)}{2(n+2)} \frac{1}{x} + \mathcal{O}(\varepsilon^{2/(n+2)} x^{-n/(n+2)}).\end{aligned}\tag{3.32}$$

Keeping the leading term of this expression only, we define our comparison equation by

$$\begin{aligned} \frac{d}{dx} \tilde{c}_1(x) &= + \frac{i\sigma_0(n-2m)}{2(n+2)} \frac{e^{ix}}{x} \tilde{c}_2(x) \\ \frac{d}{dx} \tilde{c}_2(x) &= - \frac{i\sigma_0(n-2m)}{2(n+2)} \frac{e^{-ix}}{x} \tilde{c}_1(x) \end{aligned} \tag{3.33}$$

or, in matrix notation,

$$\frac{d}{dx} \tilde{c}(x) \equiv A(x) \tilde{c}(x). \tag{3.34}$$

We note for later reference that the difference between the approximate system (3.33) and (3.29) is given by the matrix $B(x, \varepsilon)$ defined by

$$D(x, \varepsilon) \equiv A(x) + B(x, \varepsilon). \tag{3.35}$$

As a consequence of the above considerations, the following estimates hold

$$\|A(x)\| \leq \frac{(n-2m)}{2(n+2)} \frac{e^{|Imx|}}{|x|} \tag{3.36}$$

$$\|B(x, \varepsilon)\| \leq \kappa \varepsilon^{2/(n+2)} \frac{e^{|Imx|}}{|x|^{n/(n+2)}} \tag{3.37}$$

where κ is some constant.

We know from (3.23) and (3.24) that we can control the solution of (3.29) along γ_0^\pm up to errors of order $\varepsilon/\delta^{(n+2)/n}$, where $\delta = |z_0^\pm - z_0| = \mathcal{O}((\varepsilon x)^{2/(n+2)})$, i.e. errors of order $1/|x|$. Hence we shall impose the matching condition $|x| \rightarrow \infty$ and $|\varepsilon x| \rightarrow 0$.

In order to compute $\tilde{c}_j(x)$, $j = 1, 2$, we convert the system (3.33) to a second-order differential equation for $\tilde{c}_1(x)$, by eliminating $\tilde{c}_2(x)$. Setting

$$d = \frac{(n-2m)}{2(n+2)} > 0 \tag{3.38}$$

we obtain the following equation for $\tilde{c}_1(x)$

$$f''(x) + \left(\frac{1}{x} - i\right) f'(x) - \frac{d^2}{x^2} f(x) = 0. \tag{3.39}$$

This equation is exactly the same as the one obtained for the value $d = 1/6$ in [16], equation (5.1). Following [16] we write the solution of (3.39) as

$$f(x) = e^{ix} x^d w(-ix) \tag{3.40}$$

where the function $w(y)$ satisfies

$$yw''(y) + (b-y)w'(y) - aw(y) = 0 \tag{3.41}$$

with $a = d + 1, b = 2d + 1$. This equation has been the object of many studies and its solutions are well known [34]. We list below the properties of interest for our problem [34] and [16].

- Two linearly independent solutions of (3.41) are given by

$$\begin{aligned} w_1(a, b, y) &= M(a, b, y) \\ w_2(a, b, y) &= y^{1-b} M(a - b + 1, 2 - b, y) \end{aligned} \tag{3.42}$$

where

$$M(a, b, y) = \frac{\Gamma(b)}{\Gamma(a)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)}{\Gamma(b+n)} \frac{y^n}{n!} \quad b \neq 0, -1, -2, \dots \tag{3.43}$$

is single valued and is called the Kummer's or confluent hypergeometric function.

- The asymptotic behaviours of w_1 and w_2 when

$$|y| \rightarrow \infty \quad -\frac{3}{2}\pi < \arg y < \frac{1}{2}\pi \tag{3.44}$$

are given by

$$\begin{aligned} w_1(a, b, y) &= e^{-ix^a} \frac{\Gamma(b)}{\Gamma(b-a)} w_1^\infty(a, b, y) + \frac{\Gamma(b)}{\Gamma(a)} w_2^\infty(a, b, y) \\ w_2(a, b, y) &= e^{-ix^{a-b+1}} \frac{\Gamma(2-b)}{\Gamma(1-a)} w_1^\infty(a, b, y) + \frac{\Gamma(2-b)}{\Gamma(a-b+1)} w_2^\infty(a, b, y) \end{aligned}$$

where

$$\begin{aligned} w_1^\infty(a, b, y) &= y^{-a} \left(1 - a(a-b+1) \frac{1}{y} + \mathcal{O}\left(\frac{1}{y^2}\right) \right) \\ w_2^\infty(a, b, y) &= y^{a-b} e^y \left(1 + (b-a)(1-a) \frac{1}{y} + \mathcal{O}\left(\frac{1}{y^2}\right) \right). \end{aligned} \tag{3.45}$$

- The derivatives of w_1 and w_2 can be expressed as

$$\begin{aligned} \frac{d}{dy} w_1(a, b, y) &= \frac{a}{b} w_1(a+1, b+1, y) \\ \frac{d}{dy} w_2(a, b, y) &= \frac{1-b}{y} w_2(a, b, y) + \frac{a-b+1}{y(2-b)} w_2(a, b-1, y). \end{aligned} \tag{3.46}$$

- Finally, we have the symmetry relations

$$\begin{aligned} w_1(a, b, e^{ix} y) &= e^{-y} w_1(b-a, b, y) \\ w_2(a, b, e^{ix} y) &= e^{ix(1-b)} e^{-y} w_2(b-a, b, y). \end{aligned} \tag{3.47}$$

Hence, making use of (3.40), the first equation (3.33) and (3.46), we can write

$$\begin{aligned} \tilde{c}_1(x) &= e^{ix} (px^d w_1(d+1, 2d+1, -ix) + qx^d w_2(d+1, 2d+1, -ix)) \\ \tilde{c}_2(x) &= -\frac{i}{\sigma_0 d} \left(p \left\{ ix^{d+1} w_1(d+1, 2d+1, -ix) + dx^d w_1(d+1, 2d+1, -ix) \right. \right. \\ &\quad \left. \left. - i \frac{d+1}{2d+1} x^{d+1} w_1(d+2, 2d+2, -ix) \right\} \right. \\ &\quad \left. + q \left\{ ix^{d+1} w_2(d+1, 2d+1, -ix) - dx^d w_2(d+1, 2d+1, -ix) \right. \right. \\ &\quad \left. \left. + \frac{1-d}{1-2d} x^d w_2(d+1, 2d, -ix) \right\} \right) \end{aligned} \tag{3.48}$$

where p and q are constants. Note that the condition $2m < n$ implies that $1 - 2d \neq 0$. Let us compute the asymptotic of $\tilde{c}_j(x)$ as $|x| \rightarrow \infty$. As noted earlier, x is real and positive on γ_0^- . Hence $\arg(-ix) = -\pi/2$ on γ_0^- and we can apply the expansion (3.45) of w_j for x large and positive. After some straightforward algebra and with the identity $\Gamma(z + 1) = z\Gamma(z)$ we obtain

$$\begin{aligned} \tilde{c}_1(x) &= p \left\{ e^{id\pi/2} \frac{\Gamma(2d+1)}{\Gamma(d+1)} + \mathcal{O}\left(\frac{1}{x}\right) \right\} + q \left\{ e^{id\pi/2} \frac{\Gamma(1-2d)}{\Gamma(1-d)} + \mathcal{O}\left(\frac{1}{x}\right) \right\} \\ \tilde{c}_2(x) &= -\frac{i}{\sigma_0 d} \left(p \left\{ e^{-id\pi/2} \frac{\Gamma(2d+1)}{\Gamma(d)} + \mathcal{O}\left(\frac{1}{x}\right) \right\} \right. \\ &\quad \left. + q \left\{ e^{id3\pi/2} \frac{\Gamma(1-2d)}{\Gamma(-d)} + \mathcal{O}\left(\frac{1}{x}\right) \right\} \right) \end{aligned} \tag{3.49}$$

as $x \rightarrow +\infty$. On γ_0^+ , $x = e^{i\pi} |x|$ so that the expansions (3.45) are useless. Thus we consider the symmetry relations (3.47) to write for $x > 0$

$$\begin{aligned} \tilde{c}_1(e^{i\pi} x) &= p e^{i\pi d} x^d w_1(d, 2d+1, -ix) + q e^{-i\pi d} x^d w_2(d, 2d+1, -ix) \\ \tilde{c}_2(e^{i\pi} x) &= -\frac{i}{\sigma_0 d} e^{i\pi} \left(p e^{i\pi d} \left\{ -ix^{d+1} w_1(d, 2d+1, -ix) + dx^d w_1(d, 2d+1, -ix) \right. \right. \\ &\quad \left. \left. + i \frac{d+1}{2d+1} x^{d+1} w_1(d, 2d+2, -ix) \right\} \right. \\ &\quad \left. + q e^{-i\pi d} \left\{ -ix^{d+1} w_2(d, 2d+1, -ix) - dx^d w_2(d, 2d+1, -ix) \right. \right. \\ &\quad \left. \left. - \frac{1-d}{1-2d} x^d w_2(d-1, 2d, -ix) \right\} \right) \end{aligned} \tag{3.50}$$

and we can apply formulae (3.45) to compute the asymptotics as $x \rightarrow +\infty$. We get similarly

$$\begin{aligned} \tilde{c}_1(e^{i\pi} x) &= p \left\{ e^{id\pi/2} \frac{\Gamma(2d+1)}{\Gamma(d+1)} + \mathcal{O}\left(\frac{1}{x}\right) \right\} + q \left\{ e^{id\pi/2} \frac{\Gamma(1-2d)}{\Gamma(1-d)} + \mathcal{O}\left(\frac{1}{x}\right) \right\} \\ \tilde{c}_2(e^{i\pi} x) &= -\frac{i}{\sigma_0 d} \left(p \left\{ e^{id3\pi/2} \frac{\Gamma(2d+1)}{\Gamma(d)} + \mathcal{O}\left(\frac{1}{x}\right) \right\} \right. \\ &\quad \left. + q \left\{ e^{-id\pi/2} \frac{\Gamma(1-2d)}{\Gamma(-d)} + \mathcal{O}\left(\frac{1}{x}\right) \right\} \right) \end{aligned} \tag{3.51}$$

Thus we have:

Lemma 3.2. Let $\tilde{c}(x)$ be a vector solution of (3.34) whose asymptotics as $x \rightarrow +\infty$ is given by

$$\tilde{c}(x) = \begin{pmatrix} a \\ b \end{pmatrix} + \mathcal{O}\left(\frac{1}{x}\right). \tag{3.52}$$

Then

$$\tilde{c}(e^{i\pi} x) = Y_0 \begin{pmatrix} a \\ b \end{pmatrix} + \mathcal{O}\left(\frac{1}{x}\right) \tag{3.53}$$

where

$$Y_0 = \begin{pmatrix} 1 & 0 \\ \sigma_0^{-1} 2 \sin(\pi d) & 1 \end{pmatrix}. \tag{3.54}$$

Remarks.

- The matrix Y_0 depends explicitly on the singular point z_0 around which the analysis is performed.

- In the adiabatic context, $\sigma_0 = \pm 1$, so that $\sigma_0^{-1} = \sigma_0$. However, this is not true in the semiclassical context. This is the reason why we keep on writing σ_0^{-1} .

- Replacing d by its value $d = (n - 2m)/2(n + 2)$, we obtain the individual prefactor of corollary 2.1.

Proof. By (3.49) and (3.51) we can write

$$\tilde{c}(x) = W(x) \begin{pmatrix} p \\ q \end{pmatrix} \quad x > 0 \tag{3.55}$$

where $W(x) = W_+ + \mathcal{O}(1/x)$,

$$W_+ = e^{i d \pi / 2} \begin{pmatrix} \frac{\Gamma(2d + 1)}{\Gamma(d + 1)} & \frac{\Gamma(1 - 2d)}{\Gamma(1 - d)} \\ -\frac{i}{\sigma_0} e^{-i d \pi} \frac{\Gamma(2d + 1)}{\Gamma(d + 1)} & \frac{i}{\sigma_0} e^{i d \pi} \frac{\Gamma(1 - 2d)}{\Gamma(1 - d)} \end{pmatrix} \tag{3.56}$$

and $W(e^{i \pi} x) = W_- + \mathcal{O}(1/x)$,

$$W_- = e^{i d \pi / 2} \begin{pmatrix} \frac{\Gamma(2d + 1)}{\Gamma(d + 1)} & \frac{\Gamma(1 - 2d)}{\Gamma(1 - d)} \\ -\frac{i}{\sigma_0} e^{i d \pi} \frac{\Gamma(2d + 1)}{\Gamma(d + 1)} & \frac{i}{\sigma_0} e^{-i d \pi} \frac{\Gamma(1 - 2d)}{\Gamma(1 - d)} \end{pmatrix}. \tag{3.57}$$

Thus, by hypothesis

$$\begin{pmatrix} p \\ q \end{pmatrix} = \left(W_+^{-1} + \mathcal{O}\left(\frac{1}{x}\right) \right) \left(\begin{pmatrix} a \\ b \end{pmatrix} + \mathcal{O}\left(\frac{1}{x}\right) \right) \tag{3.58}$$

hence

$$\tilde{c}(e^{i \pi} x) = W_- W_+^{-1} \begin{pmatrix} a \\ b \end{pmatrix} + \mathcal{O}\left(\frac{1}{x}\right) \tag{3.59}$$

and we compute $W_- W_+^{-1} = Y_0$. □

3.4. Asymptotic matching

We now turn to the matching of the asymptotics obtained for $\tilde{c}(x)$ and the one given for $\hat{c}(z)$ in (3.23) and (3.24). Let us determine the error made by replacing \hat{c} by \tilde{c} in the neighbourhood of z_0 . As in [16], we denote by $U_A(x, x_0)$ and $U(x, x_0)$ the associated propagators defined by

$$\begin{aligned} U'_A(x, x_0) &= A(x)U_A(x, x_0) & U_A(x_0, x_0) &= \mathbb{I} \\ U'(x, x_0) &= (A(x) + B(x, \varepsilon))U(x, x_0) & U(x_0, x_0) &= \mathbb{I}. \end{aligned} \tag{3.60}$$

By the method of variation of the constant, we obtain the identity (see [16])

$$U(x, x_0) - U_A(x, x_0) = \int_{x_0}^x U_A(x, s) B(s, \varepsilon) U(s, x_0) ds. \tag{3.61}$$

Consider the path consisting in the following three parts in the x plane

- a rectilinear part from x_0 to 1, $x_0 > 1$,
- a semicircular part from 1 to -1 in the upper half plane,
- a rectilinear part from -1 to $-x_0$.

We want to evaluate $U(-x_0, x_0) - U_A(-x_0, x_0)$ integrated along the path just described. We decompose

$$\begin{aligned} U(-x_0, x_0) - U_A(x_0, x_0) &= (U(-x_0, -1) - U_A(-x_0, -1))U_A(-1, 1)U_A(1, x_0) \\ &\quad + U(-x_0, -1)(U(-1, 1) - U_A(-1, 1))U_A(1, x_0) \\ &\quad + U(-x_0, -1)U(-1, 1)(U(1, x_0) - U_A(1, x_0)) \end{aligned} \tag{3.62}$$

and bound each term separately. For x and y on the same branch of Stokes line, i.e. $x \cdot y > 0$, we have, b. standard estimates using (3.36) and (3.37),

$$\begin{aligned} \|U_A(x, y)\| &\leq \exp(d|\ln x/y|) \\ \|U(x, y)\| &\leq \exp(d|\ln x/y|) \exp[\kappa(|\varepsilon x|^{2/(n+2)} + |\varepsilon y|^{2/(n+2)})] \leq \kappa \exp(d|\ln x/y|) \end{aligned} \tag{3.63}$$

as $|\varepsilon x|, |\varepsilon y| \rightarrow 0$, so that by (3.61)

$$\|U(x, y) - U_A(x, y)\| \leq \kappa e^{d|\ln x/y|} (|\varepsilon x|^{2/(n+2)} + |\varepsilon y|^{2/(n+2)}). \tag{3.64}$$

Along the path $x(\theta) = e^{i\theta}$, $\theta \in [0, \pi]$, we get by similar methods

$$\|U(-1, 1) - U_A(-1, 1)\| \leq \kappa \varepsilon^{2/(n+2)}. \tag{3.65}$$

Gathering these estimates, we obtain from (3.62)

$$\|U(-x_0, x_0) - U_A(x_0, x_0)\| \leq \kappa x_0^{2d} (\varepsilon x_0)^{2/(n+2)} \tag{3.66}$$

as $\varepsilon \rightarrow 0$, $x_0 \rightarrow \infty$ and $\varepsilon x_0 \rightarrow 0$.

We can now determine explicitly the scaling limit which matches these asymptotic formulae on the whole segment of Stokes line γ_0 . Let us define

$$q = \max_{j=1, \dots, N} n_j \tag{3.67}$$

and assume that

$$\hat{c}(\xi_0^-) = \begin{pmatrix} a \\ b \end{pmatrix} + \mathcal{O}(\varepsilon^{1/(q+2)}). \tag{3.68}$$

Setting

$$\varepsilon x_0 \equiv \varepsilon x(z_0^-) = \mathcal{O}((z_0^- - z_0)^{(m+2)/2}) \tag{3.69}$$

we get from (3.23)

$$\hat{c}(z_0^-) = \begin{pmatrix} a \\ b \end{pmatrix} + \mathcal{O}(\varepsilon^{1/(q+2)}) + \mathcal{O}\left(\frac{1}{x_0}\right) \quad (3.70)$$

since

$$\delta = |z_0^- - z_0| = \mathcal{O}((\varepsilon x_0)^{2/(n+2)}). \quad (3.71)$$

At that point we use U_A instead of U to compute $\hat{c}(z_0^+)$. That is we consider

$$\bar{c}(x_0) = \begin{pmatrix} a \\ b \end{pmatrix} + \mathcal{O}(\varepsilon^{1/(q+2)}) + \mathcal{O}\left(\frac{1}{x_0}\right) \quad (3.72)$$

and get from lemma 3.2

$$\bar{c}(e^{i\pi} x_0) = Y_0 \begin{pmatrix} a \\ b \end{pmatrix} + \mathcal{O}(\varepsilon^{1/(q+2)}) + \mathcal{O}\left(\frac{1}{x_0}\right). \quad (3.73)$$

We thus make an error which we estimate by (3.66)

$$\|\hat{c}(e^{i\pi} x_0) - \bar{c}(e^{i\pi} x_0)\| = \mathcal{O}(x_0^{2d} (\varepsilon x_0)^{2/(n+2)}). \quad (3.74)$$

As

$$2d + \frac{2}{n+2} = \frac{n+2-2m}{n+2} \leq 1 \quad \text{and} \quad \frac{2}{n+2} \geq \frac{2}{q+2} \quad (3.75)$$

we have

$$\hat{c}(z_0^+) = Y_0 \begin{pmatrix} a \\ b \end{pmatrix} + \mathcal{O}(\varepsilon^{1/(q+2)}) + \mathcal{O}(x_0 \varepsilon^{2/(q+2)}) + \mathcal{O}\left(\frac{1}{x_0}\right). \quad (3.76)$$

Finally, we make use of (3.24) to compute $\hat{c}(\zeta_0^+)$, assuming that $x_0 \varepsilon^{2/(q+2)} \rightarrow 0$, as $\varepsilon \rightarrow 0$. We obtain, with

$$\delta = |z_0^+ - z_0| = \mathcal{O}((\varepsilon x_0)^{2/(m+2)}) \quad (3.77)$$

$$\hat{c}(\zeta_0^+) = Y_0 \begin{pmatrix} a \\ b \end{pmatrix} + \mathcal{O}(\varepsilon^{1/(q+2)}) + \mathcal{O}(x_0 \varepsilon^{2/(q+2)}) + \mathcal{O}\left(\frac{1}{x_0}\right). \quad (3.78)$$

At that point we impose that all error terms are of the same order, i.e.

$$\varepsilon^{1/(q+2)} = x_0 \varepsilon^{2/(q+2)} = \frac{1}{x_0}. \quad (3.79)$$

We thus find

$$x_0 = \varepsilon^{-1/(q+2)} \quad (3.80)$$

which justifies our use of lemma 3.2 and yields the formula

$$\hat{c}(\zeta_0^+) = Y_0 \begin{pmatrix} a \\ b \end{pmatrix} + \mathcal{O}(\varepsilon^{1/(q+2)}). \quad (3.81)$$

We can reiterate this procedure since we are in the same conditions as we were in at the beginning of the computation.

3.5. Case $2m = n$

Consider now the case where $2m = n$, i.e. where the couplings $a_{kj}(z)$ are analytic at $z = z_0$. Between ζ_0^-, z_0^- and ζ_0^+, z_0^+ , we use (3.23) and (3.24) with $\delta^{(n+2)/2}$ replaced by $\delta^{n/2}$:

$$\begin{aligned} |\widehat{c}_k(z) - \widehat{c}_k(\zeta_0^-)| &\leq \kappa \frac{\varepsilon}{\delta^{n/2}} (|\widehat{c}_1(\zeta_0^-)| + |\widehat{c}_2(\zeta_0^-)|) \quad \forall z \in \gamma_0^- \\ |\widehat{c}_k(z) - \widehat{c}_k(z_0^+)| &\leq \kappa \frac{\varepsilon}{\delta^{n/2}} (|\widehat{c}_1(z_0^+)| + |\widehat{c}_2(z_0^+)|) \quad \forall z \in \gamma_0^+. \end{aligned} \tag{3.82}$$

Between z_0^- and z_0^+ along γ , we simply use (3.16) to obtain

$$|\widehat{c}_1(z)| \leq |\widehat{c}_1(z_0^-)| + \kappa\delta \|\widehat{c}_2\| \quad |\widehat{c}_2(z)| \leq |\widehat{c}_2(z_0^-)| + \kappa\delta \|\widehat{c}_1\| \tag{3.83}$$

where

$$\|\widehat{c}_k\| = \sup_{z \in \gamma_0 \setminus \gamma_0^+ \cup \gamma_0^-} |\widehat{c}_k(z)|. \tag{3.84}$$

Hence, provided $\kappa\delta < 1/2$ we get as above

$$|\widehat{c}_k(z) - \widehat{c}_k(z_0^-)| \leq \kappa\delta (|\widehat{c}_1(z_0^-)| + |\widehat{c}_2(z_0^-)|) \quad \forall z \in \gamma_0 \setminus \gamma_0^+ \cup \gamma_0^-. \tag{3.85}$$

Thus assuming again that

$$\widehat{c}(\zeta_0^-) = \begin{pmatrix} a \\ b \end{pmatrix} + \mathcal{O}(\varepsilon^{1/(q+2)}) \tag{3.86}$$

we get from the foregoing considerations

$$\widehat{c}(\zeta_0^+) = \begin{pmatrix} a \\ b \end{pmatrix} + \mathcal{O}(\varepsilon^{1/(q+2)}) + \mathcal{O}\left(\frac{\varepsilon}{\delta^{n/2}}\right) + \mathcal{O}(\delta). \tag{3.87}$$

Choosing $\delta = \varepsilon^{2/(n+2)}$, so that

$$\frac{\varepsilon}{\delta^{n/2}} = \delta \tag{3.88}$$

we finally obtain

$$\begin{aligned} \widehat{c}(\zeta_0^+) &= \begin{pmatrix} a \\ b \end{pmatrix} + \mathcal{O}(\varepsilon^{1/(q+2)}) + \mathcal{O}(\varepsilon^{2/(n+2)}) \\ &= Y_0 \begin{pmatrix} a \\ b \end{pmatrix} + \mathcal{O}(\varepsilon^{1/(q+2)}). \end{aligned} \tag{3.89}$$

Note that Y_0 reduces to the identity matrix when $2m = n \iff d = 0$. We can state the main lemma of this section, which is the consequence of (3.81) and (3.89):

Lemma 3.3. If

$$\widehat{c}(\zeta_0^-) = \begin{pmatrix} a \\ b \end{pmatrix} + \mathcal{O}(\varepsilon^{1/(q+2)}) \tag{3.90}$$

then

$$\widehat{c}(\zeta_0^+) = Y_0 \begin{pmatrix} a \\ b \end{pmatrix} + \mathcal{O}(\varepsilon^{1/(q+2)})$$

for all $0 \leq 2m \leq n$, where $q = \max_{j=1, \dots, N} n_j$.

Theorem 2.1 is then a direct consequence of this lemma when we go back from the coefficients $\widehat{c}(z)$ in (3.15) to the coefficients $c(z)$ and when we iterate these formulae from eigenvalue crossing point to eigenvalue crossing point. We simply have to remember that the definition of $\widehat{c}(z)$ depends on the different points z_j and that $\text{Im } \Delta(z_j) = \text{Im } \Delta(z_1)$, $j = 1, \dots, N$ (see [16]).

4. Example

Let us illustrate our result by the following example. We consider

$$i\varepsilon\psi'(t) = H_B(t)\psi(t) \tag{4.1}$$

where

$$H_B(t) = \frac{1}{\sqrt{t^2 + 1}} \begin{pmatrix} t & 1 \\ 1 & -t \end{pmatrix} \tag{4.2}$$

and we want to compute the transition probability $\mathcal{P}(\varepsilon)$. The Hamiltonian $H_B(t)$ can be considered as a generalization of the familiar Landau–Zener Hamiltonian which possesses no complex eigenvalue crossing points in the whole complex plane. Indeed, $H_B(t)$ has analytic continuations everywhere in the complex plane except at $z = \pm i$ where it possesses singular branching points and its eigenvalues $e_{1B}(t)$ and $e_{2B}(t)$ are identically equal to -1 and 1 . Moreover $H_B(t)$ does not tend to its limiting values $H_B(\pm\infty) = \pm I$ fast enough. Hence, the Hamiltonian $H_B(t)$ does not fit in the framework of our analysis. Nevertheless, we can convert the problem (4.1) by a simple change of variables into one to which theorem 2.1 applies. Let $s \in \mathbb{R}$ be defined by

$$s = \sinh^{-1}(t) \iff t = \sinh(s). \tag{4.3}$$

Then the vector $\varphi(s) \equiv \psi(\sinh(s))$ satisfies

$$i\varepsilon\varphi'(s) = \begin{pmatrix} \sinh(s) & 1 \\ 1 & -\sinh(s) \end{pmatrix} \varphi(s) \equiv H(s)\varphi(s). \tag{4.4}$$

The new Hamiltonian $H(s)$ is now analytic in the whole complex plane and the associated function $\rho(s)$ is given by

$$\rho(s) = 1 + \sinh^2(s) = \cosh^2(s). \tag{4.5}$$

Thus the eigenvalues

$$e_j(s) = (-1)^j \cosh(s) \quad j = 1, 2 \tag{4.6}$$

display a complex degeneracy of order 1 (i.e. characterized by $n = 2, m = 0$) at $z_1 = i(\frac{1}{2}\pi + k\pi), k = \pm 1, \pm 2, \dots$. Note, however, that $H(s)$ diverges as $s \rightarrow \pm\infty$, but this will cause no trouble, as shown below. Let us consider the degeneracy at $z_1 = i\pi/2$.

Thus

$$\Delta(z) = -2 \int_0^z \cosh(z') dz' = -2 \sinh(z) \quad \Delta(z_1) = -2i \tag{4.7}$$

so that the corresponding Stokes lines are given by the set

$$\{z \equiv x + iy \mid \sin(y) \cosh(x) = 1\} \tag{4.8}$$

described in figure 3. These lines define the border of the simply connected set Ω , which does not contain any eigenvalue crossing points in its interior. Consider now the couplings $a_{kj}(z)$ between the coefficients $c_j(z)$. We compute by means of (3.1)

$$a_{kj}(z) = \frac{(-1)^j}{2 \cosh(z)} \quad \forall z \in \Omega \setminus \{z_1\}. \tag{4.9}$$

Hence it follows that, although the Hamiltonian $H(s)$ diverges at infinity, the coefficients $c_j(s)$ possess well defined limits $c_j(\pm\infty)$ as $s \rightarrow \pm\infty$, due to the exponentially fast decay to zero of the couplings at infinity. This remark insures that $\mathcal{P}(\varepsilon)$ is well defined for this problem. Thus we can apply theorem 2.1 to get

$$\mathcal{P}(\varepsilon) = e^{-4/\varepsilon} (2 + \mathcal{O}(\varepsilon^{1/4})) \tag{4.10}$$

for ε small enough. Note that the exponential decay rate -4 is equal to $2 \operatorname{Im} \int_0^i (e_{1B}(z) - e_{2B}(z)) dz$, where i is the branching of $H_B(z)$ in the upper half plane.

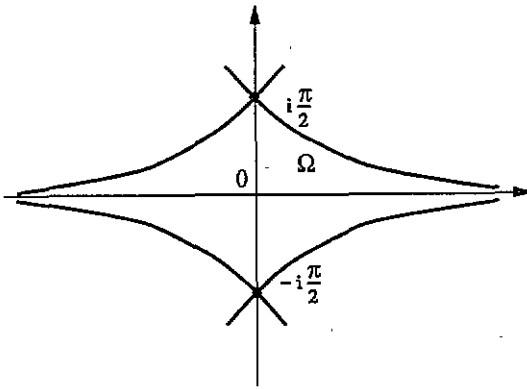


Figure 3. The Stokes lines associated with $z_1 = i\pi/2$.

5. Semiclassical context

We consider the equation

$$\hbar^2 \frac{d^2}{dx^2} \psi(x) + p^2(x) \psi(x) = 0 \tag{5.1}$$

where $p^2(x) = E - V(x)$. We assume that $V(x)$ is analytic in a strip S_a , that there exist $V(\pm\infty)$ such that

$$\lim_{x \rightarrow \pm\infty} \sup_{|y| < a} |V(x + iy) - V(\pm\infty)| |x|^{1+\alpha} = 0 \tag{5.2}$$

for some $\alpha > 0$ and that

$$\inf_{x \in \mathbb{R}} E - V(x) \geq g > 0. \tag{5.3}$$

These assumptions are equivalent to (i)–(iii) in the adiabatic context. The complex turning points are the zeros z_j of $p^2(z)$, $z \in S_a$, and the Stokes lines are the level lines

$$\text{Im } \Delta(z) = \text{Im } \Delta(z_j) \quad z \in S_a \tag{5.4}$$

where

$$\Delta(z) = -2 \int_0^z p(z') dz'. \tag{5.5}$$

We further assume that (iv) and (vi) hold. Let us write the solution of (5.1) as a combination of WKB solutions

$$\psi(x) = c_1(x) \frac{\exp[(i/\hbar) \int_0^x p(x') dx']}{\sqrt{p(x)}} + c_2(x) \frac{\exp[(-i/\hbar) \int_0^x p(x') dx']}{\sqrt{p(x)}}. \tag{5.6}$$

Then, if the coefficients satisfy the system

$$\frac{d}{dx} c(x) = \begin{pmatrix} 0 & \exp[(i/\hbar) \Delta(x)] \frac{p'(x)}{2p(x)} \\ \exp[(-i/\hbar) \Delta(x)] \frac{p'(x)}{2p(x)} & 0 \end{pmatrix} c(x) \tag{5.7}$$

then the expression (5.6) is a solution of (3.29) (see [8] for example). Consider the boundary conditions

$$c_1(-\infty) = 0 \quad c_2(-\infty) = 1 \quad (5.8)$$

which corresponds to a particule coming from $+\infty$. Then the above barrier reflection coefficient $R(\hbar)$ is defined by the ratio

$$R(\hbar) = \left| \frac{c_1(+\infty)}{c_2(+\infty)} \right|^2. \quad (5.9)$$

The conditions (5.8) are reversed with respect to the ones we have considered above. However, we can take as initial conditions

$$c_1(-\infty) = 1 \quad c_2(-\infty) = 0 \quad (5.10)$$

and use the formula

$$R(\hbar) = \frac{|c_2(+\infty)|^2}{1 + |c_2(+\infty)|^2} \quad (5.11)$$

instead of (5.9). Indeed, it is readily verified that if $(c_1(x), c_2(x))$ is a solution of (5.7) and (5.10), then $(\overline{c_2(x)}, \overline{c_1(x)})$ is another solution of (5.7) satisfying (5.8). Finally, it follows from this remark that

$$|c_1(x)|^2 - |c_2(x)|^2 = \kappa \quad \forall x \in \mathbb{R} \quad (5.12)$$

where κ is a constant determined by the initial conditions.

Consider a turning point z_0 which is a zero of order n of $E - V(z)$. Then,

$$E - V(z) = r(z_0)(z - z_0)^n(1 + \mathcal{O}(z - z_0)) \quad r(z_0) \neq 0. \quad (5.13)$$

We compute

$$\frac{p'(z)}{2p(z)} = \frac{-V'(z)}{4(E - V(z))} = \frac{n}{4(z - z_0)} + \mathcal{O}(1) \quad (5.14)$$

and

$$\Delta(z) = \Delta(z_0) - \frac{4\sqrt{r(z_0)}}{(n+2)}(z - z_0)^{(n+2)/2}(1 + \mathcal{O}(z - z_0)). \quad (5.15)$$

Note that the leading term of the couplings $p'(z)/2p(z)$ is never equal to zero in this context. We define new coefficients $\tilde{c}(x)$ as in (3.15) and the new variable x by

$$\hbar x \equiv \Delta(z) - \Delta(z_0) = -\frac{4\sqrt{r(z_0)}}{(n+2)}(z - z_0)^{(n+2)/2}(1 + \mathcal{O}(z - z_0)) \quad (5.16)$$

hence

$$z - z_0 = \mathcal{O}((\hbar x)^{2/(n+2)}). \quad (5.17)$$

We are thus led to the following comparison equation close to z_0

$$\frac{d}{dx} \tilde{c}(x) = \begin{pmatrix} 0 & \frac{n}{2(n+2)} \frac{e^{ix}}{x} \\ \frac{n}{2(n+2)} \frac{e^{-ix}}{x} & 0 \end{pmatrix} \tilde{c}(x). \quad (5.18)$$

This equation yields (3.39) again and we can use lemma 3.2 with $\sigma_0 = -i$ and $m = 0$ to compute its solution asymptotically. Finally, the error terms in the derivation of (5.18) are the same as in the adiabatic context so that the whole asymptotic analysis performed in the preceding section holds for this case as well. Hence we have the following theorem.

Theorem 5.1. Let $V(x)$ be a real analytic potential satisfying conditions (i) to (iv) and (vi) and let $\psi(x)$ be a solution of the Schrödinger equation (5.1). Then, there exist constants $\hbar^* > 0$ and $p > 0$ such that the above barrier reflection coefficient $R(\hbar)$ defined by (5.9) and (5.8) is given for any $\hbar < \hbar^*$ by

$$R(\hbar) = \left| \sum_{j=1}^N 2 \sin \left(\frac{\pi n_j}{2(n_j + 2)} \right) \exp \left\{ -\frac{i}{\hbar} \Delta(z_j) \right\} \right|^2 + \mathcal{O} \left(\varepsilon^p \exp \left\{ -\frac{2}{\varepsilon} |\operatorname{Im} \Delta(z_1)| \right\} \right) \quad (5.19)$$

where $\Delta(z_j) = -2 \int_0^{z_j} p(z) dz$.

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