

Adiabatic transition probability for a tangential crossing

Takuya WATANABE

(Received May 8, 2006)

(Revised June 15, 2006)

ABSTRACT. We consider a time-dependent Schrödinger equation whose Hamiltonian is a 2×2 real symmetric matrix. We study, using an exact WKB method, the adiabatic limit of the transition probability in the case where several complex eigenvalue crossing points accumulate to one real point.

1. Introduction

We consider the time-dependent Schrödinger equation:

$$ih \frac{d}{dt} \psi(t) = \mathcal{H}(t, \varepsilon) \psi(t), \quad \mathcal{H}(t, \varepsilon) = \begin{pmatrix} V(t) & \varepsilon \\ \varepsilon & -V(t) \end{pmatrix} \quad (1)$$

on \mathbf{R} , where ε and h are small positive parameters and $V(t)$ is a real-valued function. $\psi(t)$ is a vector-valued function with complex components. This equation (1) describes the adiabatic time evolution associated to the Hamiltonian $\mathcal{H}(\varepsilon, h)$. This 2×2 real symmetric and trace-free matrix $\mathcal{H}(\varepsilon, h)$ has two real eigenvalues $E_{\pm}(t, \varepsilon) = \pm \sqrt{V(t)^2 + \varepsilon^2}$. The difference of these eigenvalues

$$E_+ - E_- = 2\sqrt{V(t)^2 + \varepsilon^2}$$

is strictly positive for all $t \in \mathbf{R}$ and has its minimum 2ε at the zeros of $V(t)$.

From the physical point of view, the two different unperturbed energy levels $V(t)$ and $-V(t)$ cross each other at the zeros of $V(t)$ and ε is the interaction at the intersection. Because of this interaction, $E_+(t, \varepsilon)$ and $E_-(t, \varepsilon)$ do not cross (*avoided crossing*), but the transition occurs by the quantum effect. The parameter h is the adiabatic parameter and the quantum effect becomes small in the adiabatic limit. On the other hand, ε is the gap at the avoided crossing. One expects, then, that the transition probability $P(\varepsilon, h)$ is small when h is small while it is large when ε is small. It is an interesting problem to study its asymptotic behavior as both ε and h go to 0.

Mathematics Subject Classification. 34E20, 34E25, 81Q20.

Key words and phrases. Adiabatic limit. Transition probability. Singular perturbation. Exact WKB method.

The study of the transition probability P has its origin at the works by L. D. Landau [L] and C. Zener [Z]. In 1932, they studied the case $V(t) = at$, where a is a positive constant, and derived the following explicit formula:

$$P = \exp\left[-\frac{\pi\varepsilon^2}{ah}\right]$$

for all positive ε and h . This is the so-called *Landau-Zener formula*.

There have been many studies about the transition probability in the adiabatic limit $h \rightarrow 0$ (see the summaries [BT], [HJ], [T]). Among those, we refer to a series of studies by A. Joye, H. Kunz and C.-E. Pfister ([J1], [JKP], [JP1], [JP2]). They studied the real symmetric matrix-valued Hamiltonian:

$$\mathcal{H}(t) = \begin{pmatrix} V(t) & W(t) \\ W(t) & -V(t) \end{pmatrix},$$

where the difference of the eigenvalues $2\sqrt{V(t)^2 + W(t)^2}$ does not vanish for $t \in \mathbf{R}$. They express the adiabatic limit of the transition probability in terms of actions between complex eigenvalue crossing points:

$$\{t \in \mathbf{C}; V(t)^2 + W(t)^2 = 0\},$$

which we call *turning points* in this paper.

In this paper we consider $V(t)$ which vanishes at one point of order n , and compute the asymptotic behavior of $P(\varepsilon, h)$ as $(\varepsilon, h) \rightarrow (0, 0)$ under the condition $h/\varepsilon^{(n+1)/n} \rightarrow 0$. In case $n = 1$, this problem is studied in more general settings by [CLP] and [Ro].

Recently new approaches of an exact WKB method have been studied. These approaches give the rigorous argument to the divergent power series solution on the singular perturbation h . [AKT] studied the Hamiltonian, which is a 3×3 real symmetric matrix with polynomial elements, by the exact WKB method based on the Borel resummation. In this paper we apply the exact WKB method developed by C. Gérard and A. Grigis [GG], and S. Fujiié, C. Lasser and L. Nedelec [FLN] to this adiabatic transition problem. This method enables us to express the Wronskian of two exact WKB solutions as a convergent series defined inductively by integrations along a path. Careful observations of the phase function on the path give us the asymptotic behavior of the Wronskian as $(\varepsilon, h) \rightarrow (0, 0)$ with $h/\varepsilon^{(n+1)/n} \rightarrow 0$.

Finally we remark that this is similar to the scattering problem for Schrödinger operator over the maximum of the potential. See [Ra], [FR] for a non-degenerate maximum case and [BM] for a degenerate maximum case.

This paper is organized as follows: In §2 we define the transition probability and state the results. In §3 we review the exact WKB method for a family of 2×2 systems used in [FLN] and express the Jost solutions as exact

WKB solutions. In §4 we calculate the scattering matrix using the Wronskian of the exact WKB solutions and finally in §5, we compute the asymptotic expansion of the action with respect to ε .

2. Definitions and results

We first define the scattering matrix and the transition probability for the equation (1) under the following assumptions on $V(t)$:

(A) $V(t)$ is real-valued on \mathbf{R} and there exist two real numbers $0 < \theta_0 < \pi/2$ and $\rho > 0$ such that $V(t)$ is analytic in the complex domain:

$$\mathcal{S} = \{t \in \mathbf{C}; |\operatorname{Im} t| < |\operatorname{Re} t| \tan \theta_0\} \cup \{|\operatorname{Im} t| < \rho\}.$$

(B) There exist two real non-zero constants E_r, E_l and $\sigma > 1$ such that

$$V(t) = \begin{cases} E_r + O(|t|^{-\sigma}) & \text{as } \operatorname{Re} t \rightarrow +\infty \text{ in } \mathcal{S}, \\ E_l + O(|t|^{-\sigma}) & \text{as } \operatorname{Re} t \rightarrow -\infty \text{ in } \mathcal{S}. \end{cases}$$

Under the conditions (A) and (B), there exist four solutions $\psi_+^r, \psi_-^r, \psi_+^l,$ and ψ_-^l to (1) uniquely defined by the following asymptotic conditions:

$$\begin{aligned} \psi_+^r(t) &\sim \exp\left[+\frac{i}{h}\sqrt{E_r^2 + \varepsilon^2 t}\right] \begin{pmatrix} -\sin \theta_r \\ \cos \theta_r \end{pmatrix}, & \text{as } \operatorname{Re} t \rightarrow +\infty \text{ in } \mathcal{S}, \\ \psi_-^r(t) &\sim \exp\left[-\frac{i}{h}\sqrt{E_r^2 + \varepsilon^2 t}\right] \begin{pmatrix} \cos \theta_r \\ \sin \theta_r \end{pmatrix}, & \text{as } \operatorname{Re} t \rightarrow +\infty \text{ in } \mathcal{S}, \\ \psi_+^l(t) &\sim \exp\left[+\frac{i}{h}\sqrt{E_l^2 + \varepsilon^2 t}\right] \begin{pmatrix} -\sin \theta_l \\ \cos \theta_l \end{pmatrix}, & \text{as } \operatorname{Re} t \rightarrow -\infty \text{ in } \mathcal{S}, \\ \psi_-^l(t) &\sim \exp\left[-\frac{i}{h}\sqrt{E_l^2 + \varepsilon^2 t}\right] \begin{pmatrix} \cos \theta_l \\ \sin \theta_l \end{pmatrix}, & \text{as } \operatorname{Re} t \rightarrow -\infty \text{ in } \mathcal{S}, \end{aligned}$$

where $\tan 2\theta_r = \varepsilon/E_r$ and $\tan 2\theta_l = \varepsilon/E_l$ ($0 < \theta_r, \theta_l < \pi/2$). These solutions are called *Jost solutions* to (1). We notice that the principal term of each Jost solution, for example $\exp[+\frac{i}{h}\sqrt{E_r^2 + \varepsilon^2 t}](-\sin \theta_r \cos \theta_r)$, is a solution to the constant coefficient system:

$$ih \frac{d}{dt} \psi(t) = \begin{pmatrix} E_r & \varepsilon \\ \varepsilon & -E_r \end{pmatrix} \psi(t).$$

The pairs of Jost solutions (ψ_+^r, ψ_-^r) and (ψ_+^l, ψ_-^l) are orthonormal bases on \mathbf{C}^2 for any fixed t . Moreover they have the following relations:

$$\psi_{\pm}^r(t) = \mp \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \overline{\psi_{\mp}^r(t)}, \quad \psi_{\pm}^l(t) = \mp \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \overline{\psi_{\mp}^l(t)}. \tag{2}$$

The scattering matrix S is defined as the change of bases of Jost solutions:

$$(\psi_+^l \quad \psi_-^l) = (\psi_+^r \quad \psi_-^r)S(\varepsilon, h), \quad S(\varepsilon, h) = \begin{pmatrix} s_{11}(\varepsilon, h) & s_{12}(\varepsilon, h) \\ s_{21}(\varepsilon, h) & s_{22}(\varepsilon, h) \end{pmatrix}.$$

S is an unitary matrix independent of t and moreover, by (2),

$$s_{11}(\varepsilon, h) = \overline{s_{22}(\varepsilon, h)}, \quad s_{12}(\varepsilon, h) = -\overline{s_{21}(\varepsilon, h)}.$$

The transition probability $P(\varepsilon, h)$ is defined by

$$P(\varepsilon, h) = |s_{21}(\varepsilon, h)|^2.$$

Let us assume

(C) $V(t) = 0$ if and only if $t = 0$.

Then the eigenvalues have the so-called *avoided crossing* at the origin. We call *turning point* a complex zero of $V(t)^2 + \varepsilon^2$, and in particular, *simple turning point* if it is a simple zero.

Let $n \in \mathbf{N} = \{1, 2, \dots\}$ be the number such that $V^{(k)}(0) = 0$ for $0 \leq k < n$ and $V^{(n)}(0) \neq 0$. We can assume $V^{(n)}(0) > 0$ without loss of generality. Then there are $2n$ simple turning points $T_j(\varepsilon)$ and $\overline{T_j(\varepsilon)}$ ($j = 1, \dots, n$) with $0 < \arg T_1 < \dots < \arg T_n < \pi$ which converge at the origin as ε tends to 0. We define the action integral $A_j(\varepsilon)$ by,

$$A_j(\varepsilon) = 2 \int_0^{T_j(\varepsilon)} \sqrt{V(t)^2 + \varepsilon^2} dt,$$

where the integration path is the complex segment from 0 to $T_j(\varepsilon)$ and the branch of the square root is ε at $t = 0$. Our main result is the following asymptotic formula of $P(\varepsilon, h)$ when ε and h are both small.

THEOREM 2.1. *Assume (A), (B), and (C). If $n = 1$ there exists $\varepsilon_0 > 0$ such that we have*

$$P(\varepsilon, h) = \exp\left[-\frac{2 \operatorname{Im} A_1(\varepsilon)}{h}\right] (1 + O(h)) \quad \text{as } h \rightarrow 0$$

uniformly for $\varepsilon \in (0, \varepsilon_0)$. If $n \geq 2$ there exists $\varepsilon_0 > 0$ such that, for all $\varepsilon \in (0, \varepsilon_0)$, we have

$$P(\varepsilon, h) = \left| \exp\left[\frac{i}{h} A_1(\varepsilon)\right] + (-1)^{n+1} \exp\left[\frac{i}{h} A_n(\varepsilon)\right] \right|^2 \left(1 + O\left(\frac{h}{\varepsilon^{(n+1)/n}}\right)\right)$$

as $\frac{h}{\varepsilon^{(n+1)/n}} \rightarrow 0$.

Remark that $h/\varepsilon^{(n+1)/n}$ appears in an obvious way in the case $V(t) = t^n$. By a simple rescaling $t = \varepsilon^{1/n}\tau$, (1) is reduced to

$$i \frac{h}{\varepsilon^{(n+1)/n}} \frac{d}{d\tau} \phi(\tau) = \begin{pmatrix} \tau^n & 1 \\ 1 & -\tau^n \end{pmatrix} \phi(\tau),$$

where $\psi(\varepsilon^{1/n}\tau) = \phi(\tau)$.

Let us study the asymptotic behavior of

$$P_0(\varepsilon, h) = \left| \exp \left[\frac{i}{h} A_1(\varepsilon) \right] + (-1)^{n+1} \exp \left[\frac{i}{h} A_n(\varepsilon) \right] \right|^2$$

in case $n \geq 2$ when both ε and h go to 0. We rewrite it as

$$\begin{aligned} P_0(\varepsilon, h) = & \exp \left[-\frac{\operatorname{Im}(A_1(\varepsilon) + A_n(\varepsilon))}{h} \right] \left(\exp \left[\frac{\operatorname{Im}(A_1(\varepsilon) - A_n(\varepsilon))}{h} \right] \right. \\ & \left. + \exp \left[\frac{\operatorname{Im}(A_n(\varepsilon) - A_1(\varepsilon))}{h} \right] + (-1)^{n+1} 2 \cos \left[\frac{\operatorname{Re}(A_1(\varepsilon) - A_n(\varepsilon))}{h} \right] \right). \end{aligned}$$

Then by computing the asymptotic expansions of the action integrals $A_1(\varepsilon)$ and $A_n(\varepsilon)$ (see §5) we have the following proposition:

PROPOSITION 2.1.

1) If $V^{(n+2l-1)}(0) = 0$ for all $l \in \mathbf{N}$, then

$$\operatorname{Im} A_1(\varepsilon) = \operatorname{Im} A_n(\varepsilon)$$

and

$$P_0(\varepsilon, h) = 2 \exp \left[-\frac{2 \operatorname{Im} A_1(\varepsilon)}{h} \right] \left(1 + (-1)^{n+1} \cos \left[\frac{\operatorname{Re}(A_1(\varepsilon) - A_n(\varepsilon))}{h} \right] \right).$$

2) If there exists $m \in \mathbf{N}$ such that $V^{(n+2l-1)}(0) = 0$ ($l = 0, \dots, m-1$) and $V^{(n+2m-1)}(0) \neq 0$, then for sufficiently small ε

$$\operatorname{Im}(A_1(\varepsilon) - A_n(\varepsilon)) = 2C_{2m} \left(\sin \frac{m}{n} \pi \right) \varepsilon^{(n+2m)/n} + O(\varepsilon^{(n+2m+2)/n}), \quad (3)$$

where

$$C_{2m} = -\frac{2m\sqrt{\pi}\Gamma\left(\frac{m}{n}\right)V^{(n+2m-1)}(0)}{n\Gamma(n+2m+1)\Gamma\left(\frac{n+2m}{2n}\right)} \left(\frac{n!}{V^{(n)}(0)} \right)^{(n+2m)/n},$$

and the asymptotic behavior of $P_0(\varepsilon, h)$ as $(\varepsilon, h) \rightarrow (0, 0)$ is given by the following formulae:

(i) When $\varepsilon^{(n+2m)/n}/h \rightarrow 0$,

$$P_0(\varepsilon, h) = 2 \exp \left[-\frac{\operatorname{Im}(A_1(\varepsilon) + A_n(\varepsilon))}{h} \right] \\ \times \left(1 + (-1)^{n+1} \cos \left[\frac{\operatorname{Re}(A_1(\varepsilon) - A_n(\varepsilon))}{h} \right] + O \left(\frac{\varepsilon^{(2(n+2m))/n}}{h^2} \right) \right).$$

(ii) When $h/\varepsilon^{(n+2m)/n} \rightarrow 0$,

$$P_0(\varepsilon, h) \\ = \exp \left[-\frac{2 \operatorname{Im} A_1(\varepsilon)}{h} \right] \left(1 + O \left(\exp \left[\left(2C_{2m} \left(\sin \frac{m}{n} \pi \right) + \delta \right) \frac{\varepsilon^{(n+2m)/n}}{h} \right] \right) \right) \quad (4)$$

for any positive constant δ if $m/n \notin \mathbf{N}$ and $V^{(n+2m-1)}(0) \sin \frac{m}{n} \pi > 0$ (i.e. $C_{2m} \sin \frac{m}{n} \pi < 0$) and

$$P_0(\varepsilon, h) \\ = \exp \left[-\frac{2 \operatorname{Im} A_n(\varepsilon)}{h} \right] \left(1 + O \left(\exp \left[-\left(2C_{2m} \left(\sin \frac{m}{n} \pi \right) - \delta \right) \frac{\varepsilon^{(n+2m)/n}}{h} \right] \right) \right) \quad (5)$$

for any positive constant δ if $m/n \notin \mathbf{N}$ and $V^{(n+2m-1)}(0) \sin \frac{m}{n} \pi < 0$ (i.e. $C_{2m} \sin \frac{m}{n} \pi > 0$).

3. Preliminary

3.1 Review of the exact WKB method

We use as a basic tool the *exact WKB method* for 2×2 systems introduced in [FLN], which is a natural extension of the method in [GG] for Schrödinger equations. We first review it.

Let us consider the following 2×2 system of first order differential equations:

$$\frac{h}{i} \frac{d}{dt} \phi(t) = \begin{pmatrix} 0 & \alpha(t) \\ -\beta(t) & 0 \end{pmatrix} \phi(t). \quad (6)$$

The functions $\alpha(t)$ and $\beta(t)$ are assumed to be holomorphic in a simply connected domain $\Omega \subset \mathbf{C}$.

First of all we make the change of variables $t \mapsto z$

$$z(t; t_0) = \int_{t_0}^t \sqrt{\alpha(\tau)\beta(\tau)} d\tau,$$

where t_0 is a fixed base point of Ω . If Ω_1 is a simply connected open subset of Ω in which $\alpha(t)\beta(t)$ does not vanish, the mapping z is bijective from Ω_1

to $z(\Omega_1)$ for a given determination of $(\alpha(t)\beta(t))^{1/2}$. Zeros of $\alpha(t)$ and $\beta(t)$ are called *turning points*. If t_0 is a simple turning point, we get

$$z(t) - z(t_0) = \frac{2i}{3} (\alpha(t)\beta(t))'|_{t=t_0} (t - t_0)^{3/2} (1 + g(t - t_0)), \quad (7)$$

where $g(t)$ is holomorphic and $g(0) = 0$.

We put $\phi(t) = e^{\pm z/h} \varphi_{\pm}(z)$ and reduce (6) to the next equation in the variable z :

$$\frac{h}{i} \frac{d}{dz} \varphi_{\pm}(z) = \begin{pmatrix} \pm i & H^{-2}(z) \\ -H^2(z) & \pm i \end{pmatrix} \varphi_{\pm}(z), \quad (8)$$

where $H(z(t)) = (\beta(t)/\alpha(t))^{1/4}$. Moreover we change unknown function $\varphi_{\pm}(z) = M_{\pm}(z)w_{\pm}(z)$, where $M_{\pm}(z)$ is given by

$$M_{\pm}(z) = \begin{pmatrix} H^{-1}(z) & H^{-1}(z) \\ \mp iH(z) & \pm iH(z) \end{pmatrix}.$$

Consequently, we obtain the first order differential equation of $w_{\pm}(z)$:

$$\frac{d}{dz} w_{\pm}(z) = \begin{pmatrix} 0 & \frac{H'(z)}{H(z)} \\ \frac{H'(z)}{H(z)} & \mp \frac{2}{h} \end{pmatrix} w_{\pm}(z), \quad (9)$$

where $H'(z)$ stands for $\frac{d}{dz}H(z)$. We notice that $M_{\pm}(z(t))$ and $w_{\pm}(z(t))$ are independent of t_0 . We define the sequences of functions $\{w_{\pm,n}(z; z_1)\}_{n=0}^{\infty}$ by the following differential recurrent relations:

$$\begin{cases} w_{\pm,-1}(z) = 0, & w_{\pm,0}(z) = 1, \\ \frac{d}{dz} w_{\pm,2k}(z) = \frac{H'(z)}{H(z)} w_{\pm,2k-1}(z) & (k \geq 0), \\ \left(\frac{d}{dz} \pm \frac{2}{h}\right) w_{\pm,2k+1}(z) = \frac{H'(z)}{H(z)} w_{\pm,2k}(z) & (k \geq 0). \end{cases} \quad (10)$$

The vector-valued functions $w_{\pm}(z(t)) = \begin{pmatrix} w_{\pm}^e(z(t)) \\ w_{\pm}^o(z(t)) \end{pmatrix}$ with

$$w_{\pm}^e(z(t)) = \sum_{k \geq 0} w_{\pm,2k}(z(t)), \quad w_{\pm}^o(z(t)) = \sum_{k \geq 0} w_{\pm,2k-1}(z(t)),$$

satisfy (9) formally.

$H'(z)/H(z)$ is, in terms of t ,

$$\frac{\frac{d}{dz}H(z(t))}{H(z(t))} = \frac{\alpha(t)\beta'(t) - \alpha'(t)\beta(t)}{4i(\alpha(t)\beta(t))^{3/2}}. \tag{11}$$

From (7) and (11), we see that $H'(z)/H(z)$ has a simple pole at $z = z(t_0)$.

We fix a point $z_1 = z(t_1)$ with $t_1 \in \Omega_1$ and take the initial conditions to $w_{\pm,n}(z_1) = 0$ for every $n \in \mathbf{N}$. Then the differential recurrent equations (10) are transformed to the integral recurrent equations:

$$\begin{cases} w_{\pm,0}(z; z_1) = 1, \\ w_{\pm,2k+1}(z; z_1) = \int_{z_1}^z e^{\pm(2/h)(\zeta-z)} \frac{H'(\zeta)}{H(\zeta)} w_{\pm,2k}(\zeta; z_1) d\zeta \quad (k \geq 0), \\ w_{\pm,2k}(z; z_1) = \int_{z_1}^z \frac{H'(\zeta)}{H(\zeta)} w_{\pm,2k-1}(\zeta; z_1) d\zeta \quad (k \geq 1). \end{cases}$$

From these integral representations, we obtain the following proposition on the convergence of these formal series.

PROPOSITION 3.1. *The elements of the function $w_{\pm}(z; z_1)$:*

$$w_{\pm}^e(z; z_1) = \sum_{k \geq 0} w_{\pm,2k}(z; z_1), \quad w_{\pm}^o(z; z_1) = \sum_{k \geq 0} w_{\pm,2k-1}(z; z_1) \tag{12}$$

converge absolutely and uniformly in a neighborhood of $z = z_1$.

Hence $w_{\pm}(z; z_1)$ are exact solutions to the equation (9) and

$$\phi_{\pm}(t, h; t_0, t_1) = e^{\pm z(t; t_0)/h} M_{\pm}(z(t)) w_{\pm}(z(t), h; z(t_1)). \tag{13}$$

define exact solutions to (6). We call $\phi_{\pm}(t, h; t_0, t_1)$ *exact WKB solutions*. (13) are holomorphic in a neighborhood of $t = t_1$, and extended to Ω analytically because (13) satisfy (6) with the holomorphic coefficients in Ω . We call t_0 the base point of the phase and t_1 the base point of the symbol.

The series (12) are also asymptotic expansions as $h \rightarrow 0$ in certain domains.

PROPOSITION 3.2. *There exist a positive integer N and a positive constant h_0 such that, for all $h \in (0, h_0)$, we have*

$$w_{\pm}^e(z(t), h; z(t_1)) - \sum_{k=0}^{N-1} w_{\pm,2k}(z(t), h; z(t_1)) = O(h^N),$$

$$w_{\pm}^o(z(t), h; z(t_1)) - \sum_{k=0}^{N-1} w_{\pm,2k-1}(z(t), h; z(t_1)) = O(h^N),$$

uniformly in Ω_{\pm} , where $\Omega_{\pm} = \{t \in \Omega_1; \text{ there exists a curve from } t_1 \text{ to } t \text{ along which } \pm \text{Re } z(t) \text{ increases strictly}\}$.

Moreover the Wronskian between two exact WKB solutions $\mathcal{W}[\phi(t), \tilde{\phi}(t)] = \det(\phi(t) \tilde{\phi}(t))$ is given by w_+^e :

PROPOSITION 3.3. *Linearly independent exact WKB solutions $\phi_+(t, h; t_0, t_1)$ and $\phi_-(t, h; t_0, t_2)$ satisfy the following Wronskian formula:*

$$\mathcal{W}[\phi_+(t, h; t_0, t_1), \phi_-(t, h; t_0, t_2)] = 2iw_+^e(z(t_2); z(t_1)).$$

In particular, if there exists a curve from t_1 to t_2 along which $\text{Re } z(t)$ increases strictly,

$$\mathcal{W}[\phi_+(t, h; t_0, t_1), \phi_-(t, h; t_0, t_2)] = 2i(1 + O(h)).$$

We notice that the Wronskian is independent of the variable t because the matrix of right-hand side of (6) is trace-free. The latter claim is evident from Proposition 3.2.

Finally, we introduce the so-called *Stokes line*.

DEFINITION 3.1 (Stokes line). *The Stokes lines passing by $t = t_0$ in Ω are defined as the set:*

$$\left\{ t \in \Omega; \text{Re} \int_{t_0}^t \sqrt{\alpha(\tau)\beta(\tau)} d\tau = 0 \right\}.$$

A Stokes line is a level set of the real part of the WKB phase function $z(t; t_0)$. The turning points are the branch points of $z(t; t_0)$.

If $\text{Re } z(t)$ increases along an oriented curve, then this curve is transversal to Stokes lines. Such a curve is called *canonical curve*.

3.2 WKB expression of the Jost solutions

In this subsection, we express the Jost solutions as exact WKB solutions to

(1). By the change of the unknown function $\psi(t) = Q\phi(t)$, $Q = \frac{1}{2} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$, (1) is reduced to an equation of the form (6):

$$\frac{\hbar}{i} \frac{d}{dt} \phi(t) = \begin{pmatrix} 0 & -iV(t) - \varepsilon \\ iV(t) - \varepsilon & 0 \end{pmatrix} \phi(t). \tag{14}$$

In this case, the phase function $z(t; t_0)$

$$z(t; t_0) = i \int_{t_0}^t \sqrt{V(\tau)^2 + \varepsilon^2} d\tau \quad (t_0 \in \mathcal{S}).$$

If ρ and θ_0 are small enough, there exists no turning point in \mathcal{S} . Therefore $z(t; t_0)$ is a single-valued function in such a Riemann surface. Recalling that we take the branch of $\sqrt{V(t)^2 + \varepsilon^2}$ which is ε at $t=0$, we see that $\operatorname{Re} z(t)$ increases as $\operatorname{Im} t$ decreases, and $\operatorname{Im} z(t)$ increases as $\operatorname{Re} t$ increases. Similarly

$$H(z(t)) = \sqrt[4]{\frac{-iV(t) + \varepsilon}{-iV(t) - \varepsilon}}$$

has neither zero nor pole in \mathcal{S} and the branch of $H(z(t))$ is $e^{\pi/4}$ at $t=0$.

We construct the exact WKB solutions which have the same behavior as Jost solutions as $|t| \rightarrow \infty$ as in [Ra]. First, we define unbounded simply connected domains \mathcal{S}_R^r and \mathcal{S}_R^l by

$$\begin{aligned}\mathcal{S}_R^r &= \mathcal{S} \cap \{t \in \mathbf{C}; \operatorname{Re} t > R\}, \\ \mathcal{S}_R^l &= \mathcal{S} \cap \{t \in \mathbf{C}; \operatorname{Re} t < -R\},\end{aligned}$$

where R is a positive constant. For $t \in \mathcal{S}_R^{r,l}$, we define the phase functions $z^{r,l}(t)$ with base points at infinity by

$$\begin{aligned}z^r(t) &= i \int_{\infty}^t (\sqrt{V(\tau)^2 + \varepsilon^2} - \lambda_r) d\tau + i\lambda_r t, \\ z^l(t) &= i \int_{-\infty}^t (\sqrt{V(\tau)^2 + \varepsilon^2} - \lambda_l) d\tau + i\lambda_l t,\end{aligned}$$

where $\lambda_{r,l} = \sqrt{E_{r,l}^2 + \varepsilon^2}$. Note that these integrals are convergent thanks to the assumption **(B)**. These are also primitives of $i\sqrt{V(t)^2 + \varepsilon^2}$ and satisfy for any $t_0 \in \mathcal{S}_R^{r,l}$

$$z^{r,l}(t) = z^{r,l}(t_0) + z(t; t_0).$$

Next we construct the symbol functions with base points at infinity. One sees that for all $t \in \mathcal{S}_R^l$, there exist infinite paths ending at t , $\gamma_{\pm}^l(t)$, which are asymptotic to the line $\operatorname{Im} \tau = \mp \delta \operatorname{Re} \tau$ ($\delta > 0$) as $\operatorname{Re} \tau \rightarrow -\infty$ and meet the Stokes line transversally (Stokes lines are asymptotic to horizontal lines. See §4.1 and Figure 1). For $t \in \mathcal{S}_R^r$ one similarly defines the paths $\gamma_{\pm}^r(t)$ which are asymptotic to the lines $\operatorname{Im} \tau = \pm \delta \operatorname{Re} \tau$ as $\operatorname{Re} \tau \rightarrow +\infty$.

We also denote by $\Gamma_{\pm}^r(z)$ (resp. $\Gamma_{\pm}^l(z)$) the infinite oriented paths $z^r(\gamma_{\pm}^r(t))$ (resp. $z^l(\gamma_{\pm}^l(t))$) ending at $z^r(t)$ (resp. $z^l(t)$). We remark that $\Gamma_{-}^r(z)$ (resp. $\Gamma_{+}^l(z)$) is asymptotic to the line $\operatorname{Im} \zeta = \frac{1}{\delta} \operatorname{Re} \zeta$ as $\operatorname{Re} \zeta \rightarrow +\infty$ (resp.

$\operatorname{Re} \zeta \rightarrow -\infty$), and similarly that $\Gamma_+^r(z)$ (resp. $\Gamma_-^l(z)$) is asymptotic to the line $\operatorname{Im} \zeta = -\frac{1}{\delta} \operatorname{Re} \zeta$ as $\operatorname{Re} \zeta \rightarrow -\infty$ (resp. $\operatorname{Re} \zeta \rightarrow +\infty$).

Let $\Gamma_{\pm}^{r,l}(z)$ be the paths defined above. The system of recurrence equations

$$\begin{cases} w_{\pm,0}^{r,l}(z) = 1, \\ w_{\pm,2k+1}^{r,l}(z) = \int_{\Gamma_{\pm}^{r,l}(z)} e^{\pm(2/h)(\zeta-z)} \frac{H'(\zeta)}{H(\zeta)} w_{\pm,2k}^{r,l}(\zeta) d\zeta & (k \geq 0), \\ w_{\pm,2k}^{r,l}(z) = \int_{\Gamma_{\pm}^{r,l}(z)} \frac{H'(\zeta)}{H(\zeta)} w_{\pm,2k-1}^{r,l}(\zeta) d\zeta & (k \geq 1), \end{cases}$$

define the sequences of functions $\{w_{\pm,n}^{r,l}(z)\}_{n=0}^{\infty}$. We define

$$w_{\pm;even}^{r,l}(z) = \sum_{k \geq 0} w_{\pm,2k}^{r,l}(z), \quad w_{\pm;odd}^{r,l}(z) = \sum_{k \geq 0} w_{\pm,2k-1}^{r,l}(z),$$

$$w_{\pm}^{r,l}(z) = \begin{pmatrix} \sum_{k \geq 0} w_{\pm,2k}^{r,l}(z) \\ \sum_{k \geq 0} w_{\pm,2k-1}^{r,l}(z) \end{pmatrix}.$$

The convergence of $\sum_{k \geq 0} w_{\pm,2k}^{r,l}(z(t))$ and $\sum_{k \geq 0} w_{\pm,2k-1}^{r,l}(z(t))$ follows from the fact that

$$\frac{d}{dz} \frac{H(z(t))}{H(z(t))} = -\frac{\varepsilon V'(t)}{2(V(t)^2 + \varepsilon^2)^{3/2}}$$

belongs to $L^2(\Gamma_{\pm}^{r,l}(z))$ thanks to the assumptions **(A)** and **(B)**. Moreover we see that

$$\lim_{t \rightarrow +\infty} w_{\pm,n}^r(t) = 0 \quad \lim_{t \rightarrow -\infty} w_{\pm,n}^l(t) = 0 \quad \forall n \in \mathbf{N}. \quad (15)$$

The corresponding WKB solutions $\phi_{\pm}^r(t)$ and $\phi_{\pm}^l(t)$ written by

$$\phi_{\pm}^r(t) = \exp\left[\pm \frac{z^r(t)}{h}\right] M_{\pm}(z(t)) w_{\pm}^r(z(t)),$$

$$\phi_{\pm}^l(t) = \exp\left[\pm \frac{z^l(t)}{h}\right] M_{\pm}(z(t)) w_{\pm}^l(z(t)),$$

have the following relations with the Jost solutions.

PROPOSITION 3.4. *For any fixed $h > 0$, the exact WKB solutions $\phi_{\pm}^r(t)$ and $\phi_{\pm}^l(t)$ have the following asymptotic behaviors as t goes to $\pm\infty$.*

$$\begin{aligned}\phi_{\pm}^r(t) &= \exp\left[\pm\frac{i}{h}(\lambda_r t + o(1))\right] \begin{pmatrix} ie^{-i\theta_r} \\ \mp e^{i\theta_r} \end{pmatrix} & \text{as } t \rightarrow +\infty, \\ \phi_{\pm}^l(t) &= \exp\left[\pm\frac{i}{h}(\lambda_l t + o(1))\right] \begin{pmatrix} ie^{-i\theta_l} \\ \mp e^{i\theta_l} \end{pmatrix} & \text{as } t \rightarrow -\infty.\end{aligned}$$

Consequently, we obtain the following relations between the Jost solutions and the exact WKB solutions:

$$\begin{aligned}\psi_+^r(t) &= -Q\phi_+^r(t), & \psi_-^r(t) &= -iQ\phi_-^r(t), \\ \psi_+^l(t) &= -Q\phi_+^l(t), & \psi_-^l(t) &= -iQ\phi_-^l(t).\end{aligned}$$

PROOF. The asymptotic behavior of the phase function $z^r(t)$ (resp. $z^l(t)$) is evident from the definition. That of the symbol functions is also obvious from (15) so that we have

$$\lim_{t \rightarrow +\infty} w_{\pm}^r(t) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \lim_{t \rightarrow -\infty} w_{\pm}^l(t) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

We consider the asymptotic behaviors of $M_{\pm}(z(t))$. When $E_l > 0$, we get

$$\begin{aligned}\lim_{t \rightarrow +\infty} (-iV(t) - \varepsilon) &= \lambda_r \exp\left[i\left(\frac{3}{2}\pi - 2\theta_r\right)\right], \\ \lim_{t \rightarrow +\infty} (-iV(t) + \varepsilon) &= \lambda_r \exp\left[i\left(-\frac{\pi}{2} + 2\theta_r\right)\right], \\ \lim_{t \rightarrow -\infty} (-iV(t) - \varepsilon) &= \lambda_l \exp\left[i\left(\frac{3}{2}\pi - 2\theta_l\right)\right], \\ \lim_{t \rightarrow -\infty} (-iV(t) + \varepsilon) &= \lambda_l \exp\left[i\left(-\frac{\pi}{2} + 2\theta_l\right)\right].\end{aligned}$$

Notice that in case $E_l < 0$ these asymptotic behaviors as $t \rightarrow -\infty$ are the same as in case $E_l > 0$, so we calculate

$$\lim_{t \rightarrow +\infty} H(z(t)) = -ie^{i\theta_r}, \quad \lim_{t \rightarrow -\infty} H(z(t)) = -ie^{i\theta_l}.$$

Therefore we obtain

$$\lim_{t \rightarrow +\infty} M_{\pm}(z(t)) = \begin{pmatrix} ie^{-i\theta_r} & ie^{-i\theta_r} \\ \mp e^{i\theta_r} & \pm e^{i\theta_r} \end{pmatrix}, \quad \lim_{t \rightarrow -\infty} M_{\pm}(z(t)) = \begin{pmatrix} ie^{-i\theta_l} & ie^{-i\theta_l} \\ \mp e^{i\theta_l} & \pm e^{i\theta_l} \end{pmatrix}.$$

Hence we calculate the asymptotic behaviors of $\phi_{\pm}^r(t)$ and $\phi_{\pm}^l(t)$ from above consideration. In addition, we return $\phi_{\pm}^r(t)$ and $\phi_{\pm}^l(t)$ to the solutions to (1).

$$\begin{aligned}
 Q\phi_+^r(t) &\sim \exp\left[+\frac{i}{\hbar}\lambda_r t\right] \begin{pmatrix} \sin \theta_r \\ -\cos \theta_r \end{pmatrix}, \\
 Q\phi_-^r(t) &\sim i \exp\left[-\frac{i}{\hbar}\lambda_r t\right] \begin{pmatrix} \cos \theta_r \\ \sin \theta_r \end{pmatrix} \quad \text{as } t \rightarrow +\infty, \\
 Q\phi_+^l(t) &\sim \exp\left[+\frac{i}{\hbar}\lambda_l t\right] \begin{pmatrix} \sin \theta_l \\ -\cos \theta_l \end{pmatrix}, \\
 Q\phi_-^l(t) &\sim i \exp\left[-\frac{i}{\hbar}\lambda_l t\right] \begin{pmatrix} \cos \theta_l \\ \sin \theta_l \end{pmatrix} \quad \text{as } t \rightarrow -\infty. \quad \square
 \end{aligned}$$

4. Connection of the exact WKB solutions

The elements of the scattering matrix can be expressed by Wronskians of Jost solutions:

$$S = \frac{1}{\mathcal{W}[\phi_+^r, \phi_-^r]} \begin{pmatrix} \mathcal{W}[\phi_+^l, \phi_-^r] & i\mathcal{W}[\phi_-^l, \phi_-^r] \\ -i\mathcal{W}[\phi_+^r, \phi_+^l] & \mathcal{W}[\phi_+^r, \phi_-^l] \end{pmatrix}.$$

In order to know the asymptotic property of the Wronskian of two exact WKB solutions there should be a canonical curve between their symbol base points (see Proposition 3.3). If it is not the case, it is necessary to define some intermediate exact WKB solutions. First we investigate the geometrical structure of Stokes lines.

4.1 Stokes geometry

Let us consider the geometrical properties of Stokes lines. In our case the Stokes line passing by $t = t_0$ is the set

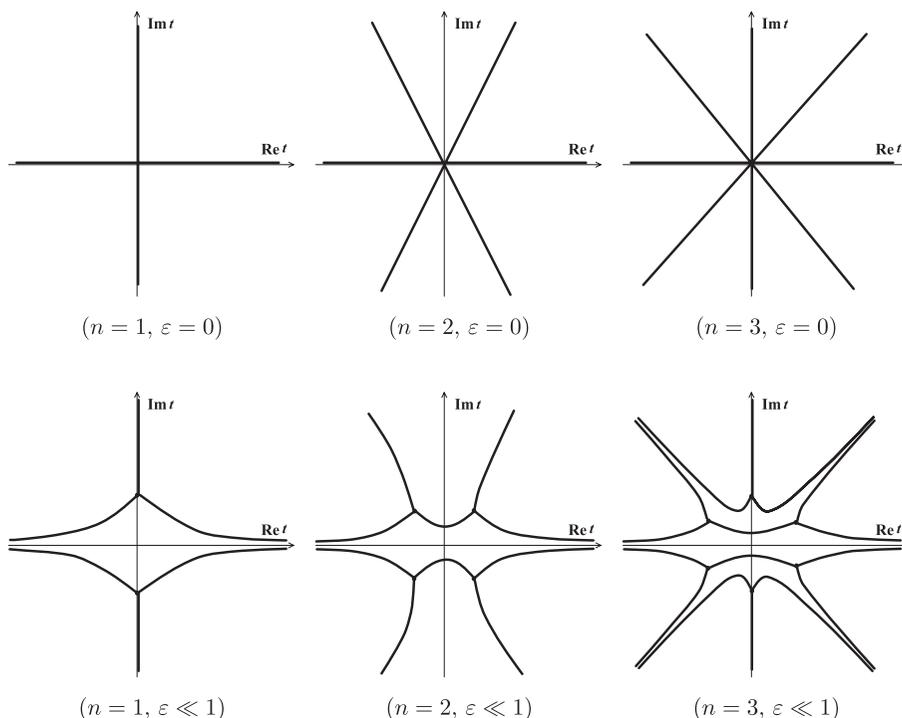
$$\left\{ t \in \mathcal{S}; \operatorname{Im} \int_{t_0}^t \sqrt{V(\tau)^2 + \varepsilon^2} d\tau = 0 \right\},$$

that is the level set of $z(t; t_0)$.

We first state the local properties of Stokes lines near a fixed point $t_0 \in \mathcal{S}$.

- (i) If t_0 is not a turning point, then $z(t; t_0)$ is conformal near $t = t_0$.
- (ii) If t_0 is a turning point of order $r \in \mathbf{N}$, that is $V(t)^2 + \varepsilon^2 = (t - t_0)^r \tilde{V}(t)$ with $\tilde{V}(0) \neq 0$, then there exist $r + 2$ Stokes lines emanating from $t = t_0$ and every angle between two closest Stokes lines is $2\pi/(r + 2)$ at $t = t_0$.

We illustrate the Stokes lines passing by the turning points in case $V(t) = t^n$ for $\varepsilon = 0$ and for ε positive and small.



From the assumptions **(A)** and **(B)**, Stokes lines are symmetric with respect to the real axis and the real axis itself is a Stokes line. At infinity in \mathcal{S} the Stokes lines are asymptotic to horizontal lines $\text{Im } t = \text{const.}$

If ε is sufficiently small, there exist $2n$ turning points $T_j(\varepsilon)$ and $\bar{T}_j(\varepsilon)$ ($j = 1, \dots, n$) in a neighborhood of each root of $(V^{(n)}(0)/n!)^2 t^{2n} + \varepsilon^2 = 0$. It is possible to take $\rho = \rho(\varepsilon)$ and θ_0 properly small, so that \mathcal{S} includes only four turning points $T_1, T_n, \bar{T}_1,$ and \bar{T}_n . Moreover the Stokes lines emanating from these turning points are not connected with those from the other $2n - 4$ turning points. Indeed, by Lemma 5.1, we see that the principal terms of the action integrals for ε small enough have the relation:

$$\max\{\text{Im } A_1(\varepsilon), \text{Im } A_n(\varepsilon)\} < \min\{\text{Im } A_2(\varepsilon), \dots, \text{Im } A_{n-1}(\varepsilon)\}.$$

For sufficiently small ε , the Stokes geometry in \mathcal{S} is as in Figure 1.

The larger the number n is, the more complicated the Stokes geometry becomes. However, if we restrict ourselves to a properly restricted domain \mathcal{S} , it has always the same structure. Hence we calculate Wronskians between $\phi_{\pm}^r(t)$ and $\phi_{\pm}^l(t)$ defined in \mathcal{S}_R^r and \mathcal{S}_R^l with the exact WKB solutions defined in a neighborhood of the turning points near the real axis as in Figure 1.

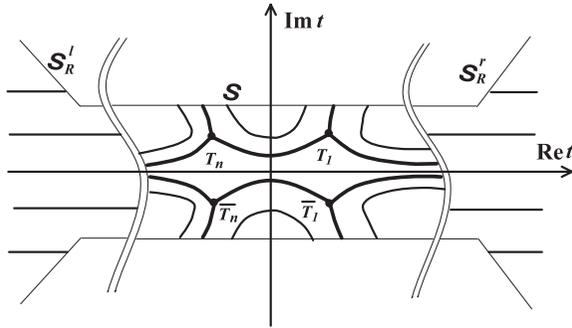


Fig. 1. Stokes geometry

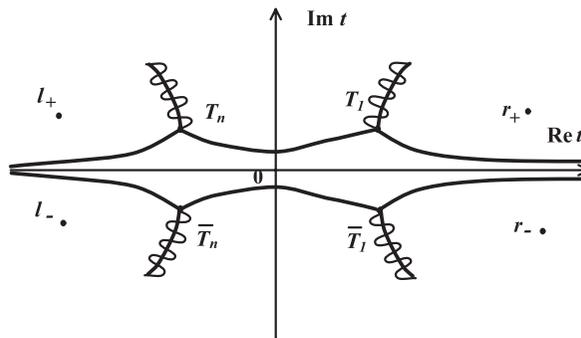


Fig. 2. Symbol base points

4.2 Transition at the avoided crossing

We first reduce our problem to a local connection problem near the avoided crossing. We introduce four symbol base points r_+ , r_- , l_+ , l_- and make the branch cuts as in Figure 2. We write, for short, the exact WKB solutions by

$$\phi_{\pm}(t, h; T_j, t_1) = \phi_{\pm}^{(j)}(t_1), \quad \phi_{\pm}(t, h; \bar{T}_j, t_1) = \phi_{\pm}^{(\bar{j})}(t_1).$$

We have the following relations between these and $\phi_{\pm}^{r,l}(t)$:

$$\begin{aligned} \phi_+^r(t) &= \exp\left[+\frac{z^r(T_1)}{h}\right] \phi_+^{(1)}(r_+)(1 + O(h)), \\ \phi_-^r(t) &= \exp\left[-\frac{z^r(\bar{T}_1)}{h}\right] \phi_-^{(\bar{1})}(r_-)(1 + O(h)), \end{aligned}$$

$$\begin{aligned}\phi_+^l(t) &= \exp\left[+\frac{z^l(T_n)}{h}\right]\phi_+^{(n)}(l_+)(1+O(h)), \\ \phi_-^l(t) &= \exp\left[-\frac{z^l(\bar{T}_n)}{h}\right]\phi_-^{(\bar{n})}(l_-)(1+O(h)),\end{aligned}$$

where $O(h)$ is uniform for small ε . From the above relations, we obtain

LEMMA 4.1.

$$\begin{aligned}\frac{\mathcal{W}[\phi_+^r, \phi_-^l]}{\mathcal{W}[\phi_+^r, \phi_-^r]} &= \exp\left[\frac{i}{2h}(A_{-\infty}(\varepsilon) - A_\infty(\varepsilon) + \overline{A_1(\varepsilon)} - \overline{A_n(\varepsilon)})\right] \\ &\quad \times \frac{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(\bar{n})}(l_-)]}{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(\bar{1})}(r_-)]}(1+O(h)), \\ \frac{\mathcal{W}[\phi_+^r, \phi_+^l]}{\mathcal{W}[\phi_+^r, \phi_-^r]} &= \exp\left[\frac{i}{2h}(-A_{-\infty}(\varepsilon) - A_\infty(\varepsilon) + \overline{A_1(\varepsilon)} + A_n(\varepsilon))\right] \\ &\quad \times \frac{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_+^{(n)}(l_+)]}{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(\bar{1})}(r_-)]}(1+O(h)),\end{aligned}$$

where

$$A_\infty(\varepsilon) = 2 \int_0^\infty (\sqrt{V(t)^2 + \varepsilon^2} - \lambda_r) dt, \quad A_{-\infty}(\varepsilon) = 2 \int_0^{-\infty} (\sqrt{V(t)^2 + \varepsilon^2} - \lambda_l) dt$$

and $O(h)$ is uniform for small ε .

Two Wronskians $\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(\bar{1})}(r_-)]$ and $\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(\bar{n})}(l_-)]$ can be calculated directly by Proposition 3.3 as follows.

$$\begin{aligned}\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(\bar{1})}(r_-)] &= \exp\left[-\frac{i}{2h}(A_1(\varepsilon) - \overline{A_1(\varepsilon)})\right]\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(1)}(r_-)], \\ &= 2i \exp\left[-\frac{i}{2h}(A_1(\varepsilon) - \overline{A_1(\varepsilon)})\right]w_+^e(z(r_-); z(r_+)), \\ \mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(\bar{n})}(l_-)] &= \exp\left[-\frac{i}{2h}(A_1(\varepsilon) - \overline{A_n(\varepsilon)})\right]\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(1)}(l_-)], \\ &= 2i \exp\left[-\frac{i}{2h}(A_1(\varepsilon) - \overline{A_n(\varepsilon)})\right]w_+^e(z(l_-); z(r_+)).\end{aligned}$$

Therefore we have

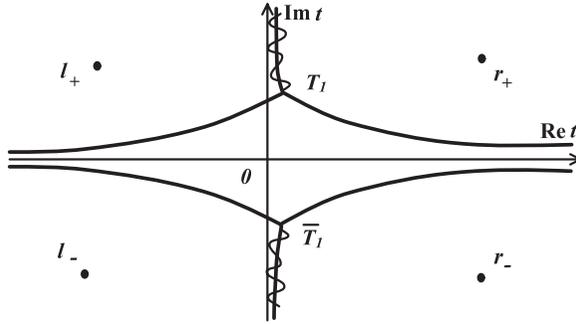


Fig. 3. Stokes geometry $n = 1$

$$\frac{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(\bar{n})}(L_-)]}{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(\bar{1})}(r_-)]} = \exp\left[\frac{i}{2h}(\overline{A_n(\varepsilon)} - \overline{A_1(\varepsilon)})\right] \frac{w_+^e(z(L_-); z(r_+))}{w_+^e(z(r_-); z(r_+))}. \quad (16)$$

By Proposition 3.2, we can obtain the asymptotic expansions of these Wronskians as $\hbar \rightarrow 0$ for the reason why there exist canonical curves from r_+ to either r_- or L_- (see §4.3).

However we must be careful in calculating the Wronskian $\mathcal{W}[\phi_+^{(1)}(r_+), \phi_+^{(n)}(l_+)]$, because there exist remarkable differences on the geometrical structures of the Stokes lines whether $n = 1$ or $n \geq 2$. Therefore we will separately discuss the cases where $V(t)$ has a simple zero or a zero of higher order.

4.2.1 Transition at a simple zero

In the case where $n = 1$, there are two simple turning points $T_1(\varepsilon)$ and $\overline{T_1(\varepsilon)}$. The calculation of $\mathcal{W}[\phi_+^{(1)}(r_+), \phi_+^{(1)}(l_+)]$ is the connection problem at the turning point of order 1 over the branch cut as in Figure 3. Let \hat{l}_+ be the same point as l_+ but continued from r_+ passing by the branch cut from T_1 .

PROPOSITION 4.1. *If $n = 1$, we obtain*

$$\mathcal{W}[\phi_+^{(1)}(r_+), \phi_+^{(1)}(l_+)] = -2w_+^e(z(\hat{l}_+); z(r_+)).$$

PROOF OF PROPOSITION 4.1. We can not apply Proposition 3.3 to this calculation directly. Therefore we consider the following lemma, which gives the relation between exact WKB solutions on the different Riemann surfaces.

LEMMA 4.2. *Let T be a simple turning point and $t_1 \neq T$ sufficiently close to T . Then*

$$\phi_{\pm}(t; T, T + (\hat{t}_1 - T)e^{-2\pi i}) = \begin{cases} i\phi_{\mp}(t; T, \hat{t}_1) & (T \text{ is a zero of } V(t) - i\varepsilon), \\ -i\phi_{\mp}(t; T, \hat{t}_1) & (T \text{ is a zero of } V(t) + i\varepsilon). \end{cases}$$

T_1 is a simple zero of $V(t) - i\varepsilon$. Since l_+ is obtained from \hat{l}_+ after turning clockwise around T_1 , one has from Lemma 4.2 $\phi_+^{(1)}(l_+) = i\phi_-^{(1)}(\hat{l}_+)$. Hence

$$\mathcal{W}[\phi_+^{(1)}(r_+), \phi_+^{(1)}(l_+)] = i\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(1)}(\hat{l}_+)].$$

We apply Proposition 3.3 to this Wronskian then Proposition 4.1 is obtained. □

Hence the Wronskian of the exact WKB solutions in Lemma 4.1 is given by

$$\frac{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_+^{(1)}(l_+)]}{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(1)}(r_-)]} = i \exp\left[\frac{i}{h} \operatorname{Im} A_1(\varepsilon)\right] \frac{w_+^e(z(\hat{l}_+); z(r_+))}{w_+^e(z(r_-); z(r_+))}. \tag{17}$$

For the symbol base \hat{l}_+ on another Riemann surface, there exists a canonical curve from r_+ to \hat{l}_+ passing through the branch cut.

4.2.2 Transition at a zero of higher order

In case $n \geq 2$, the geometrical structures of the Stokes lines emanating from four turning points T_1, T_n, \bar{T}_1 and \bar{T}_n are classified into three cases $\operatorname{Re} z(T_1) > \operatorname{Re} z(T_n)$, $\operatorname{Re} z(T_1) = \operatorname{Re} z(T_n)$ and $\operatorname{Re} z(T_1) < \operatorname{Re} z(T_n)$ (Figure 4, 5, 6).

We introduce the two symbol base points δ and $\bar{\delta}$ on the imaginary axis such that

$$\max\{\operatorname{Re} z(T_2), \operatorname{Re} z(T_{n-1})\} < \operatorname{Re} z(\delta) < \min\{\operatorname{Re} z(T_1), \operatorname{Re} z(T_n)\}$$

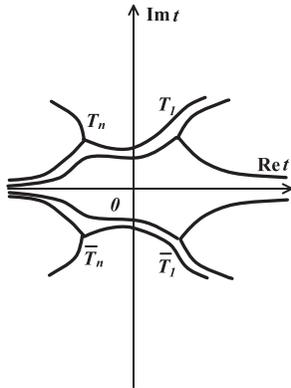


Fig. 4. $\operatorname{Re} z(T_n; T_1) < 0$

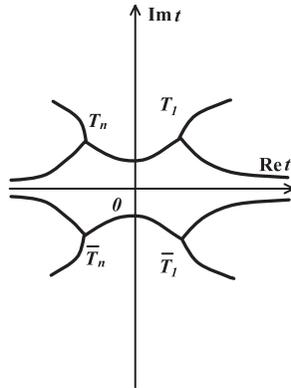


Fig. 5. $\operatorname{Re} z(T_n; T_1) = 0$

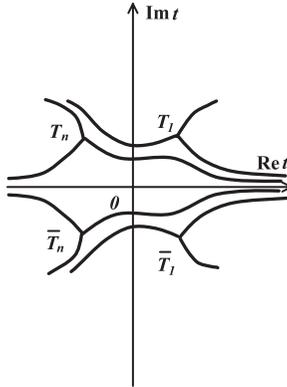


Fig. 6. $\text{Re } z(T_n; T_1) > 0$

and consider linearly independent intermediate exact WKB solutions $(\phi_+(t; T_1, \delta), \phi_-(t; T_1, \bar{\delta}))$ and $(\phi_+(t; T_n, \delta), \phi_-(t; T_n, \bar{\delta}))$. Let \hat{l}_+, \hat{r}_+ be the same point as l_+, r_+ but continued from δ passing through the branch cuts as in Figure 2. Then one sees that $l_+ = T_n + (\hat{l}_+ - T_n)e^{-2\pi i}$ and $r_+ = T_1 + (\hat{r}_+ - T_1)e^{2\pi i}$.

PROPOSITION 4.2. *If $n \geq 2$, we obtain*

$$\begin{aligned} \mathcal{W}[\phi_+^{(1)}(r_+), \phi_+^{(n)}(l_+)] &= -2 \left((-1)^{n+1} \frac{w_+^e(z(\bar{\delta}); z(r_+))w_+^e(z(\hat{l}_+); z(\delta))}{w_+^e(z(\bar{\delta}); z(\delta))} \exp\left[\frac{z(T_n; T_1)}{h}\right] \right. \\ &\quad \left. + \frac{w_+^e(z(\bar{\delta}); z(l_+))w_+^e(z(\hat{r}_+); z(\delta))}{w_+^e(z(\bar{\delta}); z(\delta))} \exp\left[\frac{z(T_1; T_n)}{h}\right] \right). \end{aligned}$$

PROOF. The exact WKB solutions $\phi_+(t; T_1, \delta), \phi_-(t; T_1, \bar{\delta}), \phi_+(t; T_n, \delta)$ and $\phi_-(t; T_n, \bar{\delta})$ have the well-defined semiclassical asymptotic expansions in the direction from the symbol base points to the phase base points. Now the pairs of $(\phi_+(t; T_1, \delta), \phi_-(t; T_1, \bar{\delta}))$ and $(\phi_+(t; T_n, \delta), \phi_-(t; T_n, \bar{\delta}))$ are fundamental bases of the space of solutions each other. So $\phi_+(t; T_1, r_+)$ and $\phi_+(t; T_n, l_+)$ are written by the linear combinations:

$$\begin{aligned} \phi_+^{(1)}(r_+) &= \frac{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(1)}(\bar{\delta})]}{\mathcal{W}[\phi_+^{(1)}(\delta), \phi_-^{(1)}(\bar{\delta})]} \phi_+^{(1)}(\delta) + \frac{\mathcal{W}[\phi_+^{(1)}(\delta), \phi_+^{(1)}(r_+)]}{\mathcal{W}[\phi_+^{(1)}(\delta), \phi_-^{(1)}(\bar{\delta})]} \phi_-^{(1)}(\bar{\delta}), \\ \phi_+^{(n)}(l_+) &= \frac{\mathcal{W}[\phi_+^{(n)}(l_+), \phi_-^{(n)}(\bar{\delta})]}{\mathcal{W}[\phi_+^{(n)}(\delta), \phi_-^{(n)}(\bar{\delta})]} \phi_+^{(n)}(\delta) + \frac{\mathcal{W}[\phi_+^{(n)}(\delta), \phi_+^{(n)}(l_+)]}{\mathcal{W}[\phi_+^{(n)}(\delta), \phi_-^{(n)}(\bar{\delta})]} \phi_-^{(n)}(\bar{\delta}). \end{aligned}$$

These Wronskian calculations are the same as the connection at the turning point of order 1. Notice that the turning point $T_n(\varepsilon)$ is a zero of $V(t) - i\varepsilon$ when n is odd and that of $V(t) + i\varepsilon$ when n is even. By Lemma 4.2, we have $\phi_+^{(1)}(r_+) = -i\phi_-^{(1)}(\hat{r}_+)$, $\phi_+^{(n)}(l_+) = (-1)^{n+1}i\phi_-^{(n)}(\hat{l}_+)$ and then, by Proposition 3.3,

$$\begin{aligned} \phi_+^{(1)}(r_+) &= \frac{w_+^e(z(\bar{\delta}); z(r_+))}{w_+^e(z(\bar{\delta}); z(\delta))} \phi_+^{(1)}(\delta) - i \frac{w_+^e(z(\hat{r}_+); z(\delta))}{w_+^e(z(\bar{\delta}); z(\delta))} \phi_-^{(1)}(\bar{\delta}) \\ \phi_+^{(n)}(l_+) &= \frac{w_+^e(z(\bar{\delta}); z(l_+))}{w_+^e(z(\bar{\delta}); z(\delta))} \phi_+^{(n)}(\delta) + (-1)^{n+1}i \frac{w_+^e(z(\hat{l}_+); z(\delta))}{w_+^e(z(\bar{\delta}); z(\delta))} \phi_-^{(n)}(\bar{\delta}) \\ &= \frac{w_+^e(z(\bar{\delta}); z(l_+))}{w_+^e(z(\bar{\delta}); z(\delta))} e^{z(T_1; T_n)/h} \phi_+^{(1)}(\delta) \\ &\quad + (-1)^{n+1}i \frac{w_+^e(z(\hat{l}_+); z(\delta))}{w_+^e(z(\bar{\delta}); z(\delta))} e^{z(T_n; T_1)/h} \phi_-^{(1)}(\bar{\delta}). \end{aligned}$$

From these relations, we have Proposition 4.2. □

Applying Proposition 4.2, we have

$$\begin{aligned} \frac{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_+^{(n)}(l_+)]}{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(1)}(r_-)]} &= i \exp \left[-\frac{i}{2h} (\overline{A_1(\varepsilon)} + A_n(\varepsilon)) \right] \frac{1}{w_+^e(z(r_-); z(r_+))} \\ &\quad \left((-1)^{n+1} \frac{w_+^e(z(\bar{\delta}); z(r_+))w_+^e(z(\hat{l}_+); z(\delta))}{w_+^e(z(\bar{\delta}); z(\delta))} \exp \left[\frac{i}{h} A_n(\varepsilon) \right] \right. \\ &\quad \left. + \frac{w_+^e(z(\bar{\delta}); z(l_+))w_+^e(z(\hat{r}_+); z(\delta))}{w_+^e(z(\bar{\delta}); z(\delta))} \exp \left[\frac{i}{h} A_1(\varepsilon) \right] \right). \end{aligned} \tag{18}$$

Note that there exists a canonical curve for each Wronskian calculation.

4.3 Asymptotics of the Wronskians as $h \rightarrow 0$

About the calculations of the asymptotic expansions of the Wronskian (16), (17), (18) as $h \rightarrow 0$, we must pay attention to the distance between the canonical curve and the turning points on the complex z -plane because $z = z(T_j)$ are simple poles of $H'(z)/H(z)$. We give the figure of the canonical curve on the complex z -plane, where the phase base point is equal to 0.

For the Wronskian in (16), the canonical curve from $z(r_+)$ to $z(l_-)$ passes between $z(T_1)$ and $z(\bar{T}_1)$ as in Figure 7. Therefore we get

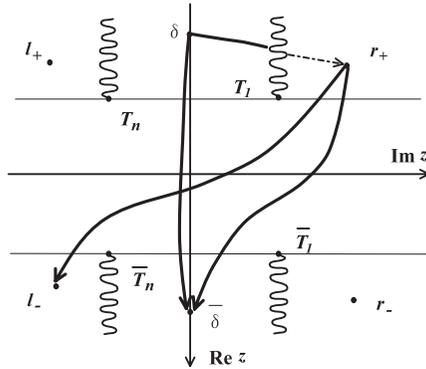


Fig. 7. $n \geq 2$, $\text{Re } z(T_n) = \text{Re } z(T_1)$

$$w_+^e(z(l_-); z(r_+)) = 1 + O\left(\frac{h}{\text{Re } z(\bar{T}_1) - \text{Re } z(T_1)}\right) \quad \text{as } h \rightarrow 0.$$

By Lemma 5.1, we have

$$\text{Re } z(\bar{T}_1) - \text{Re } z(T_1) = O(\varepsilon^{(n+1)/n}) \quad \text{as } \varepsilon \rightarrow 0.$$

In case $n = 1$, for the Wronskian in (17), the canonical curve from $z(r_+)$ to $z(\hat{l}_+)$ through the branch cut passes over $z(T_1)$ as in Figure 8.

$$w_+^e(z(\hat{l}_+); z(r_+)) = 1 + O(h) \quad \text{as } h \rightarrow 0.$$

Therefore we obtain, in case $n = 1$,

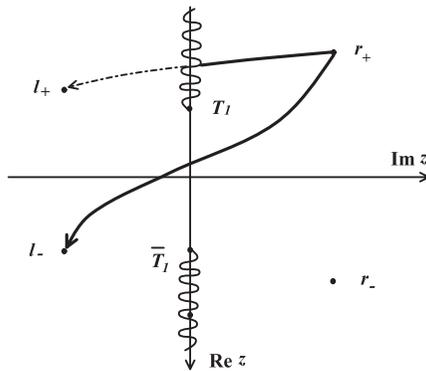


Fig. 8. $n = 1$

$$P(\varepsilon, h) = \exp\left[-\frac{2}{h} \operatorname{Im} A_1(\varepsilon)\right] (1 + O(h)) \quad \text{as } h \rightarrow 0.$$

In case $n \geq 2$ and $\operatorname{Re} z(T_n) = \operatorname{Re} z(T_1)$, for the Wronskians in (18), the canonical curve from $z(\delta)$ to $z(\bar{\delta})$ passes between $z(T_1)$ and $z(T_n)$, the canonical curve from $z(r_+)$ to $z(\bar{\delta})$ passes between $z(T_1)$ and $z(\bar{T}_1)$ and the canonical curve from $z(\delta)$ to $z(\hat{r}_+)$ through the branch cut passes between $z(T_1)$ and $z(T_2)$ as in Figure 7. Therefore we get

$$\begin{aligned} w_+^e(z(\bar{\delta}); z(\delta)) &= 1 + O\left(\frac{h}{\operatorname{Im} z(T_1) - \operatorname{Im} z(T_n)}\right) \quad \text{as } h \rightarrow 0, \\ w_+^e(z(\bar{\delta}); z(r_+)) &= 1 + O\left(\frac{h}{\operatorname{Re} z(\bar{T}_1) - \operatorname{Re} z(T_1)}\right) \quad \text{as } h \rightarrow 0, \\ w_+^e(z(\hat{r}_+); z(\delta)) &= 1 + O\left(\frac{h}{\operatorname{Re} z(T_1) - \operatorname{Re} z(T_2)}\right) \quad \text{as } h \rightarrow 0. \end{aligned}$$

By Lemma 5.1, we have

$$\begin{aligned} \operatorname{Im} z(T_1) - \operatorname{Im} z(T_n) &= O(\varepsilon^{(n+1)/n}) \quad \text{as } \varepsilon \rightarrow 0, \\ \operatorname{Re} z(\bar{T}_1) - \operatorname{Re} z(T_1) &= O(\varepsilon^{(n+1)/n}) \quad \text{as } \varepsilon \rightarrow 0, \\ \operatorname{Re} z(T_1) - \operatorname{Re} z(T_2) &= O(\varepsilon^{(n+1)/n}) \quad \text{as } \varepsilon \rightarrow 0. \end{aligned}$$

Hence we obtain Theorem 2.1 in case $n \geq 2$

$$\begin{aligned} P(\varepsilon, h) &= \left| \exp\left[\frac{i}{h} A_1(\varepsilon)\right] + (-1)^{n+1} \exp\left[\frac{i}{h} A_n(\varepsilon)\right] \right|^2 \left(1 + O\left(\frac{h}{\varepsilon^{(n+1)/n}}\right)\right) \\ &\quad \text{as } \frac{h}{\varepsilon^{(n+1)/n}} \rightarrow 0. \end{aligned}$$

We remark that there exists the canonical curve from l_+ to \hat{r}_+ in the case $\operatorname{Re} z(T_n) < \operatorname{Re} z(T_1)$ as in Figure 9. The Wronskian can be calculated without intermediate exact WKB solutions as follows:

$$\begin{aligned} \mathcal{W}[\phi_+^{(1)}(r_+), \phi_+^{(n)}(l_+)] &= \exp\left[\frac{i}{2h} (A_1(\varepsilon) - A_n(\varepsilon))\right] \mathcal{W}[\phi_+^{(1)}(r_+), \phi_+^{(1)}(l_+)] \\ &= -i \exp\left[\frac{i}{2h} (A_1(\varepsilon) - A_n(\varepsilon))\right] w_+^e(z(\hat{r}_+); z(l_+)). \\ w_+^e(z(\hat{r}_+); z(l_+)) &= 1 + O\left(\frac{h}{\operatorname{Re} z(T_1) - \operatorname{Re} z(T_n)}\right) \quad \text{as } h \rightarrow 0. \end{aligned}$$

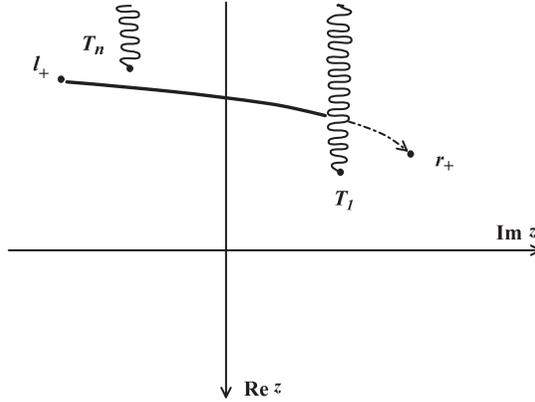


Fig. 9. $n \geq 2$, $\text{Re } z(T_n) < \text{Re } z(T_1)$

By Lemma 5.1, we have

$$\text{Re } z(T_1) - \text{Re } z(T_n) = O(\varepsilon^{(n+2m)/n}) \quad \text{as } \varepsilon \rightarrow 0.$$

The asymptotic expansions (4), (5) in Proposition 2.1 imply that $P(\varepsilon, h)$ in case $n \geq 2$ can be calculated as in case $n = 1$ when h goes to 0 faster than $\varepsilon^{(n+2m)/n}$ tends to 0 (see Figure 4).

5. Asymptotics of the action integral

To prove Proposition 2.1 we give two lemmas on the asymptotic behavior of the action integral. Put $V(z) = \frac{V^{(n)}(0)}{n!} z^n v(z)$. Then $v(0) = 1$.

LEMMA 5.1. $A_j(\varepsilon)$ is an analytic function of $\varepsilon^{1/n}$ at $t = 0$ and has the following Maclaurin expansion:

$$A_j(\varepsilon) = \sum_{k=1}^{\infty} C_k \exp\left[\frac{(2j-1)k\pi i}{2n}\right] \varepsilon^{(n+k)/n},$$

where $C_k = \frac{\sqrt{\pi} \Gamma(\frac{k}{2n})}{(n+k)(k-1)! \Gamma(\frac{n+k}{2n})} \left(\frac{n!}{V^{(n)}(0)}\right)^{k/n} \left[\frac{d^{k-1}}{dz^{k-1}} (v(z))^{-k/n}\right]_{z=0}$.

Remark that this constant C_k is equivalent to the one in Proposition 2.1.

PROOF.

$$A_j(\varepsilon) = 2 \int_0^{T_j(\varepsilon)} \sqrt{\left(\frac{V^{(n)}(0)}{n!} t^n v(t)\right)^2 + \varepsilon^2} dt.$$

By the change of variables $\varepsilon s^n = \frac{V^{(n)}(0)}{n!} t^n v(t)$, we get

$$A_j(\varepsilon) = 2\varepsilon \int_0^{\exp\{((2j-1)/2n)\pi i\}} \sqrt{s^{2n} + \varepsilon^2} \left(\frac{dt}{ds}\right) ds.$$

By the Lagrange’s formula, the Maclaurin expansion of t with respect to s is given by

$$t = \sum_{k=1}^{\infty} \frac{\varepsilon^{k/n}}{k!} \left(\frac{n!}{V^{(n)}(0)}\right)^{k/n} \left[\frac{d^{k-1}}{dz^{k-1}}(v(z)^{-k/n})\right]_{z=0} s^k,$$

and hence

$$\frac{dt}{ds} = \sum_{k=1}^{\infty} \frac{\varepsilon^{k/n}}{(k-1)!} \left(\frac{n!}{V^{(n)}(0)}\right)^{k/n} \left[\frac{d^{k-1}}{dz^{k-1}}(v(z)^{-k/n})\right]_{z=0} s^{k-1}.$$

Then the formula is obtained by term integrations and the identity

$$\int_0^{\exp\{((2j-1)/2n)\pi i\}} s^{k-1} \sqrt{s^{2n} + 1} ds = \frac{\sqrt{\pi} \Gamma(\frac{k}{2n})}{2(n+k)\Gamma(\frac{n+k}{2n})} \exp\left[\frac{(2j-1)k\pi i}{2n}\right]. \quad \square$$

To study the principal term of $\text{Im}(A_1(\varepsilon) - A_n(\varepsilon))$, we use the following lemma.

LEMMA 5.2. *Assume $v^{(2j-1)}(0) = 0$ ($j = 1, \dots, m$) for any fixed $m \in \mathbb{N}$. Then we have for any positive number σ*

$$\left[\frac{d^{2j-1}}{dz^{2j-1}}(v(z)^{-\sigma})\right]_{z=0} = 0 \quad (j = 1, \dots, m) \tag{19}$$

PROOF. We shall prove this lemma by mathematical induction with respect to m . In the case where $m = 1$, the statement (19) is evident. Assume that there exists $k \in \mathbb{N}$ such that (19) is true for all $m < k + 1$.

By the Leibniz formula, we have

$$\begin{aligned} & \left[\frac{d^{2k+1}}{dz^{2k+1}}(v(z)^{-\sigma})\right]_{z=0} \\ &= -\sigma \left[\sum_{p=0}^{2k} \binom{2k}{p} v^{(2k+1-p)}(z) \frac{d^p}{dz^p}(v(z)^{-\sigma-1})\right]_{z=0} \\ &= -\sigma v^{(2k+1)}(0) - \sigma \sum_{q=1}^k \binom{2k}{2q-1} v^{(2k-2q+2)}(0) \left[\frac{d^{2q-1}}{dz^{2q-1}}(v(z)^{-\sigma-1})\right]_{z=0}. \end{aligned}$$

The second term is zero from the assumption. If $v^{(2k+1)}(0) = 0$, (19) with $m = k + 1$ is also true. \square

From this proof, if there exists $m \in \mathbf{N}$ such that $v^{(2j-1)}(0) = 0$ ($j = 1, \dots, m-1$) and $v^{(2m-1)}(0) \neq 0$, we obtain

$$\left[\frac{d^{2m-1}}{dz^{2m-1}} (v(z)^{-\sigma}) \right]_{z=0} = -\sigma v^{(2m-1)}(0).$$

If there exists $m \in \mathbf{N}$ such that $V^{(n+2l-1)}(0) = 0$ ($l = 0, \dots, m-1$) and $V^{(n+2m-1)}(0) \neq 0$, we get the following relation between derivatives of $V(t)$ and $v(t)$:

$$v^{(2m-1)}(0) = \frac{n!}{V^{(n)}(0)} \frac{(2m-1)! V^{(n+2m-1)}(0)}{(n+2m-1)!}$$

and moreover in the case where $m \geq 2$

$$v'(0) = v^{(3)}(0) = \dots = v^{(2m-3)}(0) = 0.$$

Therefore we obtain (3).

References

- [AKT] T. Aoki, T. Kawai and Y. Takei: Exact WKB analysis of non-adiabatic transition probabilities for three levels, *J. Phys. A: Math. Gen.* **35** (2002), 2401–2430.
- [BM] H. Baklouti and M. Mnif: Asymptotique des résonances pour une barrière de potential dégénérée, *Asymptotic Analysis* **47** (2006), 19–48.
- [BT] V. Betz and S. Teufel: Landau-Zener formulae from adiabatic transition histories, preprint.
- [CLP] Y. Colin de Verdière, M. Lombardif and J. Pollët: The microlocal Landau-Zener formula, *Annales de l'I.H.P. Physique Théorique* **71**, 1 (1999), 95–127.
- [FLN] S. Fujiié, C. Lasser and L. Nedelec: Semiclassical resonances for a two-level Schrödinger operator with a conical intersection, preprint.
- [FR] S. Fujiié, and T. Ramond: Matrice de scattering et résonances associées à une orbite hétérocline, *Annales de l'I.H.P. Physique Théorique* **69**, 1 (1998), 31–82.
- [GG] C. Gérard and A. Grigis: Precise estimates of tunneling and eigenvalues near a potential barrier, *J. Diff. Equations* **42** (1988), 149–177.
- [H] G. A. Hagedorn: Proof of the Landau-Zener formula in an adiabatic limit with small eigenvalue gaps, *Commun. Math. Phys.* **136**, 4 (1991), 33–49.
- [HJ] G. A. Hagedorn and A. Joye: Recent results on non-adiabatic transitions in Quantum mechanics, *Proceedings of the 2005 UAB International Conference on Differential Equations and Mathematical Physics*, Birmingham, Alabama. March 29–April 2 (2005).
- [J1] A. Joye: Non-Trivial Prefactors in Adiabatic Transition Probabilities Induced by High-Order degeneracies, *J. Phys. A* **26** (1993), 6517–6540.
- [J2] A. Joye: Proof of the Landau-Zener formula, *Asymptotic Analysis* **9** (1994), 209–258.

- [JKP] A. Joye, H. Kunz and C.-E. Pfister: Exponential Decay and Geometric Aspect of Transition Probabilities in the Adiabatic Limit, *Ann. Phys.* **208** (1991), 299–332.
- [JP1] A. Joye and C.-E. Pfister: Superadiabatic evolution and adiabatic transition probability between two non-degenerate levels isolated in the spectrum, *J. Math. Phys.* **34** (1993), 454–479.
- [JP2] A. Joye and C.-E. Pfister: Semiclassical Asymptotics Beyond all Orders for Simple Scattering Systems, *SIAM J. Math. Anal.* **26** (1995), 944–977.
- [L] L. D. Landau: *Collected Papers of L. D. Landau*, Pergamon Press (1965).
- [M] A. Martinez: Precise exponential estimates in adiabatic theory, *J. Math. Phys.* **35** (1994), 3889–3915.
- [Ra] T. Ramond: Semiclassical study of Quantum scattering on the line, *Commun. Math. Phys.* **177** (1996), 221–254.
- [Ro] V. Rousse: Landau-Zener transitions for eigenvalue avoided crossing in the adiabatic and Born-Oppenheimer approximations, *Asymptot. Anal.* **37** (2004), no. 3–4, 293–328.
- [T] S. Teufel: *Adiabatic Perturbation Theory in Quantum Dynamics*, Springer Lecture Notes in Mathematics **1821** (2003).
- [Z] C. Zener: Non-adiabatic crossing of energy levels, *Proc. Roy. Soc. London* **137** (1932), 696–702.
- [ZN] C. Zhu and H. Nakamura: Stokes constants for a certain class of second-order ordinary differential equations, *J. Math. Phys.* **33** (1992), 2697–2717.

Takuya Watanabe

Mathematical Institute, Tohoku University

Aoba, Sendai, JAPAN, 980-8578

e-mail: sa1m31@math.tohoku.ac.jp