

An exact WKB approach to the 2-level adiabatic transition problems

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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 \mathbb{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 $t \in \mathbb{R}$ 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.

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]). The adiabatic limit of the transition probability is expressed in terms of actions between complex eigenvalue crossing points:

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

which we call *turning points*.

In this proceeding we consider more general $V(t)$ which vanishes at one point to 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 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 gives us their 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.

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 \mathbb{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:

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

(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 $\psi_+^r, \psi_-^r, \psi_+^l, \psi_-^l$ to (1) uniquely defined by the following asymptotic conditions:

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

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 \mathbb{C}^2 for any fixed t . Moreover they have the following relations:

$$\psi_{\pm}^r(t) = \mp \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \overline{\psi_{\mp}^r(t)}, \quad \psi_{\pm}^l(t) = \mp \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \overline{\psi_{\mp}^l(t)}. \quad (3)$$

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

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

S is an unitary matrix independent of t and moreover, by (3),

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

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 $n \in \mathbb{N} = \{1, 2, \dots\}$ 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*

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

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

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

In case $n = 1$ we notice that this theorem implies the result in [J2]. In case $n \geq 2$ we 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

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

Put $V(z) = \frac{V^{(n)}(0)}{n!} z^n v(z)$ then $v(0) = 1$. We can compute the asymptotic expansions of the action integral.

Lemma 2.1. $A_j(\varepsilon)$ is an analytic function of $\varepsilon^{1/n}$ at $t = 0$ and has the following Maclaurin expansion:

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

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

We can refer to [W] for this proof. From this lemma, we have the following proposition:

Proposition 2.1.

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

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

and

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

2) If there exists $m \in \mathbb{N}$ 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

$$\text{Im}(A_1(\varepsilon) - A_n(\varepsilon)) = 2C_{2m} \left(\sin \frac{m}{n} \pi \right) \varepsilon^{\frac{n+2m}{n}} + O \left(\varepsilon^{\frac{n+2m+2}{n}} \right), \quad (4)$$

where

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

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

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

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

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

$$P_0(\varepsilon, h) = \exp \left[-\frac{2\text{Im} A_1(\varepsilon)}{h} \right] \left(1 + O \left(\exp \left[\left(2C_{2m} \left(\sin \frac{m}{n} \pi \right) + \delta \right) \frac{\varepsilon^{\frac{n+2m}{n}}}{h} \right] \right) \right) \quad (5)$$

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

$$P_0(\varepsilon, h) = \exp \left[-\frac{2\text{Im} A_n(\varepsilon)}{h} \right] \left(1 + O \left(\exp \left[- \left(2C_{2m} \left(\sin \frac{m}{n} \pi \right) - \delta \right) \frac{\varepsilon^{\frac{n+2m}{n}}}{h} \right] \right) \right) \quad (6)$$

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

3 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 Shorödinger equations.

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

$$\frac{h}{i} \frac{d}{dt} \phi(t) = \begin{pmatrix} 0 & \alpha(t) \\ -\beta(t) & 0 \end{pmatrix} \phi(t). \quad (7)$$

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

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

$$z(t) - z(t_0) = \frac{2i}{3} (\alpha(t)\beta(t))' \Big|_{t=t_0} (t - t_0)^{\frac{3}{2}} (1 + g(t - t_0)), \quad (8)$$

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

We put $\phi(t) = e^{\pm z/h} \varphi_{\pm}(z)$ and reduce (7) to the next equation in the variable z :

$$\frac{h}{i} \frac{d}{dz} \varphi_{\pm}(z) = \begin{pmatrix} \pm i & H^{-2}(z) \\ -H^2(z) & \pm i \end{pmatrix} \varphi_{\pm}(z), \quad (9)$$

where $H(z(t)) = (\beta(t)/\alpha(t))^{1/4}$. 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 $w_{\pm}(z)$:

$$\frac{d}{dz} w_{\pm}(z) = \begin{pmatrix} 0 & \frac{H'(z)}{H(z)} \\ \frac{H'(z)}{H(z)} & \mp \frac{2}{h} \end{pmatrix} w_{\pm}(z), \quad (10)$$

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:

$$\left\{ \begin{array}{l} w_{\pm,-1}(z) = 0, \quad w_{\pm,0}(z) = 1, \\ \frac{d}{dz} w_{\pm,2k}(z) = \frac{H'(z)}{H(z)} w_{\pm,2k-1}(z) \quad (k \geq 0), \\ \left(\frac{d}{dz} \pm \frac{2}{h} \right) w_{\pm,2k+1}(z) = \frac{H'(z)}{H(z)} w_{\pm,2k}(z) \quad (k \geq 0). \end{array} \right. \quad (11)$$

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 (10) formally.

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

$$\frac{\frac{d}{dz}H(z(t))}{H(z(t))} = \frac{\alpha(t)\beta'(t) - \alpha'(t)\beta(t)}{4i(\alpha(t)\beta(t))^{3/2}}. \quad (12)$$

From (8) and (12), 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 $n \in \mathbb{N}$. Then the differential recurrent equations (11) are transformed to the integral recurrent equations:

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

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

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

$$w_{\pm}^e(z; z_1) = \sum_{k \geq 0} w_{\pm,2k}(z; z_1) \quad w_{\pm}^o(z; z_1) = \sum_{k \geq 0} w_{\pm,2k-1}(z; z_1) \quad (13)$$

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

Hence $w_{\pm}(z; z_1)$ are exact solutions to the equation (10) and

$$\phi_{\pm}(t, h; t_0, t_1) = e^{\pm z(t; t_0)/h} M_{\pm}(z(t)) w_{\pm}(z(t), h; z(t_1)). \quad (14)$$

define exact solutions to (7). We call $\phi_{\pm}(t, h; t_0, t_1)$ *exact WKB solutions*. (14) are holomorphic in a neighborhood of $t = t_1$, and extended to Ω analytically because (14) satisfy (7) 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 (13) 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*

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

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_{\pm}^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:*

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

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

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

Notice that the Wronskian is independent of the variable t because the matrix of right-hand side of (7) is trace-free. The latter claim is evident from Proposition 3.2.

4 Stokes geometry

We introduce the so-called *Stokes line*, which plays an important role in our problem.

Definition 4.1 (Stokes line). *The Stokes lines passing by $t = t_0$ in \mathcal{S} are defined as the set:*

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

A Stokes line is a level set of the real part of the WKB phase function $z(t; t_0)$ referring to (16). 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*.

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 $r \in \mathbb{N}$, 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 $t = t_0$.

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 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 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 2.1, we see that the principal terms of the action integrals for ε small enough have the relation:

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

under the determination of $\sqrt{V(t)^2 + \varepsilon^2}$ the same as the action integral. Therefore, for sufficiently small ε , the Stokes geometry in S is as in Figure 1. Even if the number of turning points increases, the geometrical structures of the Stokes lines in S is essentially invariant.

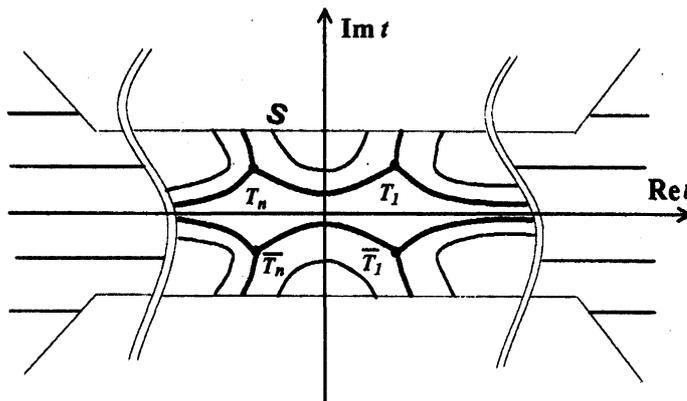


Figure 1: Stokes geometry

5 Proof

We can express the elements of the scattering matrix by the Wronskians between Jost solutions. To calculate these Wronskians, we shall take two steps. The first step is that we construct the exact WKB solutions satisfying the asymptotic condition (2) at infinity. The second step is that we connect those solutions around the turning points near the real axis. In this proceeding, we summarize the result of the first step as Proposition 5.1 and state the second step.

First of all, 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 (7):

$$\frac{h}{i} \frac{d}{dt} \phi(t) = \begin{pmatrix} 0 & -iV(t) - \varepsilon \\ iV(t) - \varepsilon & 0 \end{pmatrix} \phi(t). \quad (15)$$

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

$$z(t; t_0) = i \int_{t_0}^t \sqrt{V(\tau)^2 + \varepsilon^2} d\tau \quad (t_0 \in \mathcal{S}). \quad (16)$$

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 around the real axis. Similarly the branch of

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

is $e^{\pi/4}$ at $t = 0$. 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

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

because the Wronskian calculation is independent of t . Then we sum the first step as follows:

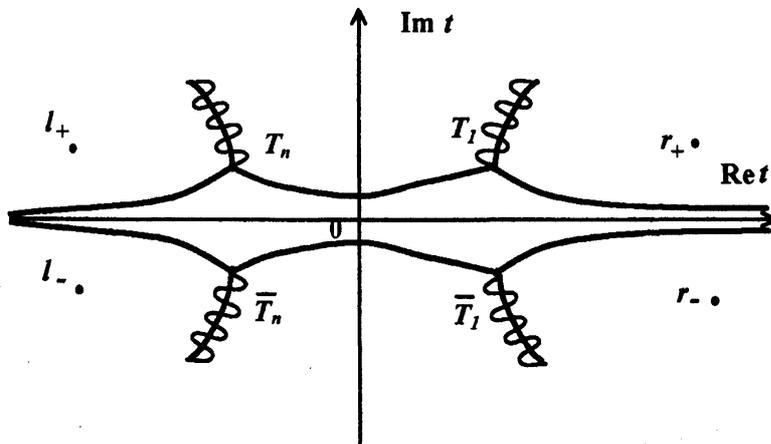


Figure 2: symbol base points

Proposition 5.1. *We obtain the following relations between the Jost solutions and the exact WKB solutions:*

$$\begin{aligned}\psi_+^r(t) &= -Q \exp \left[\frac{i}{2\hbar} \left(-A_\infty(\varepsilon) + A_1(\varepsilon) \right) \right] \phi_+^{(1)}(r_+) (1 + O(\hbar)), \\ \psi_-^r(t) &= -iQ \exp \left[\frac{i}{2\hbar} \left(A_\infty(\varepsilon) - \overline{A_1(\varepsilon)} \right) \right] \phi_-^{(1)}(r_-) (1 + O(\hbar)), \\ \psi_+^l(t) &= -Q \exp \left[\frac{i}{2\hbar} \left(-A_{-\infty}(\varepsilon) + A_n(\varepsilon) \right) \right] \phi_+^{(n)}(l_+) (1 + O(\hbar)), \\ \psi_-^l(t) &= -iQ \exp \left[\frac{i}{2\hbar} \left(A_{-\infty}(\varepsilon) - \overline{A_n(\varepsilon)} \right) \right] \phi_-^{(\bar{n})}(l_-) (1 + O(\hbar)),\end{aligned}$$

where

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

and $O(\hbar)$ is uniform for small ε .

We can refer to [W] for the proof of this proposition. Now we explain the second step of connecting the exact WKB solutions around the avoided crossing.

5.1 Transition at the avoided crossing

The elements of the scattering matrix can be expressed by Wronskians.

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

From Proposition 5.1, we obtain the diagonal and off-diagonal elements:

$$\begin{aligned}\frac{\mathcal{W}[\psi_+^r, \psi_+^l]}{\mathcal{W}[\psi_+^r, \psi_-^r]} &= -i \exp \left[\frac{i}{2\hbar} \left(-A_{-\infty}(\varepsilon) - A_\infty(\varepsilon) + \overline{A_1(\varepsilon)} + A_n(\varepsilon) \right) \right] \\ &\quad \times \frac{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_+^{(n)}(l_+)]}{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(1)}(r_-)]} (1 + O(\hbar)),\end{aligned}\quad (17)$$

$$\begin{aligned}\frac{\mathcal{W}[\psi_+^r, \psi_-^l]}{\mathcal{W}[\psi_+^r, \psi_-^r]} &= \exp \left[\frac{i}{2\hbar} \left(A_{-\infty}(\varepsilon) - A_\infty(\varepsilon) + \overline{A_1(\varepsilon)} - \overline{A_n(\varepsilon)} \right) \right] \\ &\quad \times \frac{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(\bar{n})}(l_-)]}{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(1)}(r_-)]} (1 + O(\hbar)).\end{aligned}\quad (18)$$

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.

Two Wronskians $\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(\bar{1})}(r_-)]$, $\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(\bar{n})}(l_-)]$ in (18) can be calculated directly by Proposition 3.3 as follows.

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

Therefore we have

$$\frac{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(\bar{n})}(l_-)]}{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(\bar{1})}(r_-)]} = \exp\left[\frac{i}{2h}\left(\overline{A_n(\varepsilon)} - \overline{A_1(\varepsilon)}\right)\right] \frac{w_+^e(z(l_-); z(r_+))}{w_+^e(z(r_-); z(r_+))}. \quad (19)$$

By Proposition 3.2, we can obtain the asymptotic expansions of these Wronskians as $h \rightarrow 0$ for the reason why there exist canonical curves from r_+ to either r_- or l_- (see §5.2).

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.

5.1.1 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 .

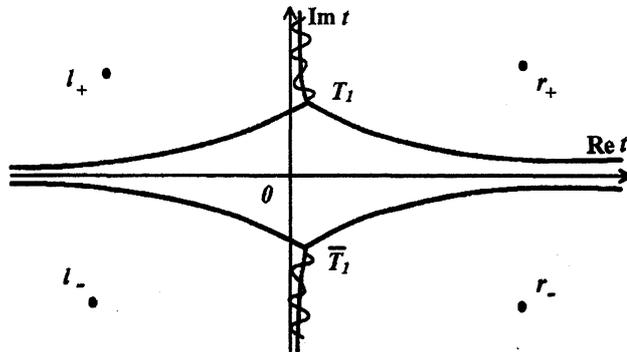
Proposition 5.2. *If $n = 1$, we obtain*

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

Proof of Proposition 5.2. We can not apply Proposition 3.3 to this calculation directly. Therefore we consider the following lemma, which give the relation between exact WKB solutions on the different Riemann surfaces.

Lemma 5.1. *Let T be a simple turning point and $t_1 \neq T$ sufficiently close to T . Then*

$$\phi_{\pm}(t; T, T + (t_1 - T)e^{-2\pi i}) = \begin{cases} i\phi_{\mp}(t; T_k, \hat{t}_1) & (T \text{ is a zero of } V(t) - i\varepsilon), \\ -i\phi_{\mp}(t; T_k, \hat{t}_1) & (T \text{ is a zero of } V(t) + i\varepsilon). \end{cases}$$

Figure 3: Stokes geometry $n = 1$

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 5.1. $\phi_+^{(1)}(l_+) = i\phi_-^{(1)}(\hat{l}_+)$. 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 5.2 is obtained. \square

Hence the Wronskian of the exact WKB solutions in (17) is given by

$$\frac{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_+^{(1)}(l_+)]}{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(1)}(r_-)]} = i \exp \left[\frac{i}{\hbar} \text{Im} A_1(\varepsilon) \right] \frac{w_+^e(z(\hat{l}_+); z(r_+))}{w_+^e(z(r_-); z(r_+))}. \quad (20)$$

For the symbol base \hat{l}_+ on the another Riemann surface, there exists a canonical curve from r_+ to \hat{l}_+ passing through the branch cut (see §5.2).

5.1.2 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 $\text{Re } z(T_1) > \text{Re } z(T_n)$, $\text{Re } z(T_1) = \text{Re } z(T_n)$ and $\text{Re } z(T_1) < \text{Re } z(T_n)$ (see Figure 4, 5, 6).

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

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

Then we can 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 see that $l_+ = T_n + (\hat{l}_+ - T_n)e^{-2\pi i}$ and $r_+ = T_1 + (\hat{r}_+ - T_1)e^{2\pi i}$.

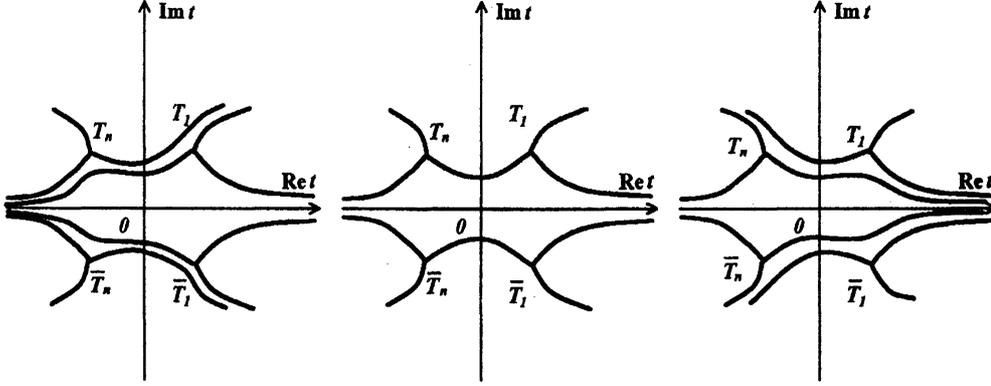


Figure 4: $\operatorname{Re} z(T_n, T_1) < 0$ Figure 5: $\operatorname{Re} z(T_n, T_1) = 0$ Figure 6: $\operatorname{Re} z(T_n, T_1) > 0$

Proposition 5.3. *If $n \geq 2$, we obtain*

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

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. 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 same as the connection at the turning point of order 1. Notice that 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 5.1, 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,

$$\phi_+^{(1)}(r_+) = \frac{w_+^e(z(\bar{\delta}); z(r_+))}{w_+^e(z(\bar{\delta}); z(\delta))} \phi_+^{(1)}(\delta) - i \frac{w_+^e(z(\hat{r}_+); z(\delta))}{w_+^e(z(\bar{\delta}); z(\delta))} \phi_-^{(1)}(\bar{\delta}),$$

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

From these relations, we have Proposition 5.3. □

Applying Proposition 5.3, we have

$$\begin{aligned}
\frac{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_+^{(n)}(l_+)]}{\mathcal{W}[\phi_+^{(1)}(r_+), \phi_-^{(1)}(r_-)]} &= i \exp \left[-\frac{i}{2h} \left(\overline{A_1(\varepsilon)} + A_n(\varepsilon) \right) \right] \frac{1}{w_+^e(z(r_-); z(r_+))} \\
&\quad \times \left((-1)^{n+1} \frac{w_+^e(z(\bar{\delta}); z(r_+)) w_+^e(z(\hat{l}_+); z(\delta))}{w_+^e(z(\bar{\delta}); z(\delta))} \exp \left[\frac{i}{h} A_n(\varepsilon) \right] \right. \\
&\quad \left. + \frac{w_+^e(z(\bar{\delta}); z(l_+)) w_+^e(z(\hat{r}_+); z(\delta))}{w_+^e(z(\bar{\delta}); z(\delta))} \exp \left[\frac{i}{h} A_1(\varepsilon) \right] \right) \quad (21)
\end{aligned}$$

Note that there exists a canonical curve for each Wronskian calculation (see §5.2).

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

About the calculations of the asymptotic expansions of the Wronskian (19), (20), (21) 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 figures of the canonical curve on the complex z -plane, where the phase base point is equal to 0.

For the Wronskian in (19), 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

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

By Lemma 2.1, we have

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

In case $n = 1$, for the Wronskian in (20), 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 $n = 1$,

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

WKB solutions as follows:

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

$$w_+^e(z(\hat{r}_+); z(l_+)) = 1 + O\left(\frac{h}{\operatorname{Re} z(T_1) - \operatorname{Re} z(T_n)}\right) \quad \text{as } h \rightarrow 0.$$

By Lemma 2.1, we have

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

The asymptotic expansions (6), (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).

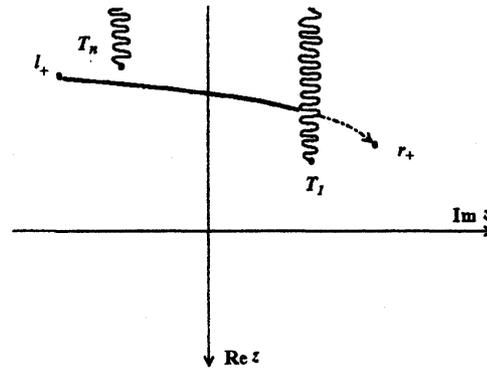


Figure 9: $n \geq 2$, $\operatorname{Re} z(T_n) < \operatorname{Re} z(T_1)$

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