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Adiabatic Transition Probability for a Small Eigenvalue Gap at Two Points

By

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Abstract

Let us consider a 2-level adiabatic transition problem. We study by using an exact WKB method the asymptotic behavior of the transition probability as the eigenvalue gap parameter, as well as the adiabatic parameter, tends to 0.

§ 1. Introduction

In these notes we consider the 2×2 system of first order differential equations:

$$ih\frac{d}{dt}\psi(t) = H(t,\varepsilon)\psi(t), \quad H(t,\varepsilon) = \begin{pmatrix} V(t) & \varepsilon \\ \varepsilon & -V(t) \end{pmatrix}, \tag{1.1}$$

where h and ε are small positive parameters. h is called an adiabatic parameter. $V(t)$ satisfies the following assumptions:

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

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

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

$$V(t) = \begin{cases} 5E_r + O(|t|^{-\sigma}) & \text{as } \mathrm{Re}\, t \to +\infty \quad \text{in } \mathcal{S}, \\ E_l + O(|t|^{-\sigma}) & \text{as } \mathrm{Re}\, t \to -\infty \quad \text{in } \mathcal{S}. \end{cases}$$

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The 2×2 matrix $H(t,\varepsilon)$ is trace-free real-symmetric matrix. $H(t,\varepsilon)$ has positive and negative eigenvalues $E_\pm(t,\varepsilon) = \pm\sqrt{V(t)^2+\varepsilon^2}$.

Under the conditions **(A)** and **(B)**, there exist four solutions ψ_+^r, ψ_-^r, ψ_+^l, and ψ_-^l to (1.1) uniquely defined by the following asymptotic conditions:

$$
\begin{aligned}
&\psi_+^r(t) \sim \exp\Big[+\frac{i}{h}\sqrt{E_r^2+\varepsilon^2}\,t\Big]\begin{pmatrix}-\sin\theta_r\\ \cos\theta_r\end{pmatrix}, \quad \text{as} \quad \operatorname{Re} t \to +\infty \quad \text{in} \quad \mathcal{S},\\
&\psi_-^r(t) \sim \exp\Big[-\frac{i}{h}\sqrt{E_r^2+\varepsilon^2}\,t\Big]\begin{pmatrix}\cos\theta_r\\ \sin\theta_r\end{pmatrix}, \quad \text{as} \quad \operatorname{Re} t \to +\infty \quad \text{in} \quad \mathcal{S},\\
&\psi_+^l(t) \sim \exp\Big[+\frac{i}{h}\sqrt{E_l^2+\varepsilon^2}\,t\Big]\begin{pmatrix}-\sin\theta_l\\ \cos\theta_l\end{pmatrix}, \quad \text{as} \quad \operatorname{Re} t \to -\infty \quad \text{in} \quad \mathcal{S},\\
&\psi_-^l(t) \sim \exp\Big[-\frac{i}{h}\sqrt{E_l^2+\varepsilon^2}\,t\Big]\begin{pmatrix}\cos\theta_l\\ \sin\theta_l\end{pmatrix}, \quad \text{as} \quad \operatorname{Re} t \to -\infty \quad \text{in} \quad \mathcal{S},
\end{aligned}
\tag{1.2}
$$

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 the *Jost solutions* to (1.1). 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.

Definition 1.1. The *scattering matrix* $S(\varepsilon,h) = \big(s_{kl}(\varepsilon,h)\big)_{1\le k,l\le 2}$ is defined as the change of bases of Jost solutions:

$$(\psi_+^l \ \psi_-^l) = (\psi_+^r \ \psi_-^r)S(\varepsilon,h).$$

Note that the scattering matrix $S(\varepsilon,h)$ is unitary. The *transition probability* $P(\varepsilon,h)$ is defined by

$$P(\varepsilon,h) = |s_{21}(\varepsilon,h)|^2 = |s_{12}(\varepsilon,h)|^2.$$

In this paper we assume that

(C) $V(t)$ vanishes at two points $t = x$, y $(x > y)$ on $\mathbb{R}$.

Then the difference of eigenvalues (eigenvalue gap) attains the minimum 2ε at $t = x$, y. It is expected that the transition probability is governed by the zeros of $V(t)$.

In the special case where $V(t) = at$ $(a > 0)$ called Landau-Zener model, it was shown by Landau and Zener in 1932 ([L], [Z]) that the transition probability is given by the so-called Landau-Zener formula:

$$P(\varepsilon,h) = \exp\Big[-\frac{\pi\varepsilon^2}{ah}\Big] \tag{1.3}$$

for any $\varepsilon > 0$, $h > 0$. Note that small parameters ε and h play opposite roles for $P(\varepsilon,h)$ from (1.3). Our problem is studying what makes a contribution to the asymptotic behavior of $P(\varepsilon,h)$ as the adiabatic parameter h and the eigenvalue gap ε tend to 0.

§ 2. Results

We first introduce so-called *turning points* which play an important role in the exact WKB method. They are by definition the zeros of $V(t)^2+\varepsilon^2$. Let n (resp. m) be the order of the zero $t=x$ (resp. y) and suppose $V(x)=V'(x)=\cdots=V^{(n-1)}(x)=0$ and $V^{(n)}(x)\neq 0$ (resp. $V(y)=V'(y)=\cdots=V^{(m-1)}(y)=0$ and $V^{(m)}(y)\neq 0$). We can assume $V^{(n)}(x)>0$ without loss of generality. Then there are $2n$ simple turning points around $t=x$, which are denoted by $x_j(\varepsilon)$ and $\overline{x}_j(\varepsilon)$ $(j=1,\dots,n)$, and they behave like

$$x_j(\varepsilon)\sim x+\left(\frac{n!}{|V^{(n)}(x)|}\right)^{1/n}\exp\left[\frac{(2j-1)\pi i}{2n}\right]\varepsilon^{1/n}\qquad \text{as}\quad \varepsilon\to 0.$$

There are also $2m$ simple turning points around $t=y$, which are denoted by $y_j(\varepsilon)$ and $\overline{y}_j(\varepsilon)$ $(j=1,\dots,m)$, and they have similar asymptotic behaviors.

We define the action integrals $A_j(\varepsilon)$ and $B_j(\varepsilon)$ by

$$A_j(\varepsilon)=2\int_x^{x_j(\varepsilon)}\sqrt{V(t)^2+\varepsilon^2}\,dt,\quad B_j(\varepsilon)=2\int_y^{y_j(\varepsilon)}\sqrt{V(t)^2+\varepsilon^2}\,dt, \tag{2.1}$$

where the integration path of $A_j(\varepsilon)$ (resp. $B_j(\varepsilon)$) is the complex segment from x to $x_j(\varepsilon)$ (resp. from y to $y_j(\varepsilon)$) and the branch of the square root is ε at $t=x$. Moreover we introduce the real-valued action integral:

$$R(\varepsilon)=2\int_y^x\sqrt{V(t)^2+\varepsilon^2}\,dt.$$

We shall observe the asymptotic behaviors of the action integrals for sufficiently small ε in § 3.2.

§ 2.1. Related Results

There exist many preceding studies on adiabatic transition problems (see [HJ], [T]). We here refer to the results by Joye-Mileti-Pfister and Joye in the case where the eigenvalue gap is fixed. They indicated in [JMP], [J1] that the asymptotic behavior of the transition probability as $h\to 0$ is determined by the geometrical structure generated by the Stokes lines closest to the real axis among those passing through turning points (see § 4.1).

On the other hand when the eigenvalue gap, in particular the off-diagonal part ε in our Hamiltonian $H(t,\varepsilon)$, tends to 0, the number of real zeros of $V(t)$ and their vanishing order are relevant. Here is a result in the case where $V(t)$ vanishes only at one point $t=x$.

Theorem 2.1 ([W]). *Assume $V(t)$ vanishes only at one point $t=x$.*

(i) *If* $n=1$, *then there exists* $\varepsilon_0>0$ *such that*

$$P(\varepsilon,h)=\exp\Big[-\frac{2}{h}\operatorname{Im}A_1(\varepsilon)\Big](1+O(h)) \qquad as \quad h\to 0, \tag{2.2}$$

uniformly for any $\varepsilon\in(0,\varepsilon_0)$.

(ii) *If* $n\geq 2$, *then there exists* $\varepsilon_0>0$ *such that for any* $\varepsilon\in(0,\varepsilon_0)$

$$P(\varepsilon,h)=\Big|\exp\Big[\frac{i}{h}A_1(\varepsilon)\Big]+(-1)^{n+1}\exp\Big[\frac{i}{h}A_n(\varepsilon)\Big]\Big|^2\Big(1+O\Big(\frac{h}{\varepsilon^{(n+1)/n}}\Big)\Big) \tag{2.3}$$

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

Remark. The asymptotic formula (2.2) is a natural extension of the Landau-Zener formula (1.3) (see [H], [J2]). In the case where $n\geq 2$, the asymptotic behavior of $P(\varepsilon,h)$ is not determined only by the geometrical structures of Stokes lines but by the relations between ε and h in addition to the asymptotic condition: $h/\varepsilon^{(n+1)/n}\to 0$ (see [W, Proposition 2.1]).

§ 2.2. Main Results

We state our results according to the vanishing order n, m.

Theorem 2.2. *If* $n=m=1$, *there exists* $\varepsilon_0>0$ *such that we have for any* $\varepsilon\in(0,\varepsilon_0)$

$$P(\varepsilon,h)=\Big|\exp\Big[\frac{i}{h}\big(A_1(\varepsilon)+R(\varepsilon)\big)\Big]-\exp\Big[\frac{i}{h}B_1(\varepsilon)\Big]\Big|^2\Big(1+O\Big(\frac{h}{\varepsilon^2}\Big)\Big) \tag{2.4}$$

as $h/\varepsilon^2\to 0$.

Theorem 2.3. *If* $n=1$ *and* $m\geq 2$, *there exists* $\varepsilon_0>0$ *such that we have for any* $\varepsilon\in(0,\varepsilon_0)$

$$P(\varepsilon,h)=\exp\Big[-\frac{2}{h}\operatorname{Im}A_1(\varepsilon)\Big]\Big(1+O\Big(\frac{h}{\varepsilon^{(m+1)/m}}\Big)\Big) \quad \text{as} \quad \frac{h}{\varepsilon^{(m+1)/m}}\to 0. \tag{2.5}$$

Theorem 2.4. *If* $m\geq n\geq 2$, *there exists* $\varepsilon_0>0$ *such that we have for any* $\varepsilon\in(0,\varepsilon_0)$

$$P(\varepsilon,h)=\Big|\exp\Big[\frac{i}{h}\big(A_1(\varepsilon)+R(\varepsilon)\big)\Big]+(-1)^{n+1}\exp\Big[\frac{i}{h}\big(A_n(\varepsilon)+R(\varepsilon)\big)\Big]$$
$$+(-1)^n\exp\Big[\frac{i}{h}B_1(\varepsilon)\Big]+(-1)^{n+m+1}\exp\Big[\frac{i}{h}B_m(\varepsilon)\Big]\Big|^2\Big(1+O\Big(\frac{h}{\varepsilon^{(n+1)/n}}\Big)\Big)$$

as $h/\varepsilon^{(n+1)/n} \to 0$. *In particular, if* $m > n$ *we have*

$$P(\varepsilon,h) = \left|\exp\left[\frac{i}{h}A_1(\varepsilon)\right] + (-1)^{n+1}\exp\left[\frac{i}{h}A_n(\varepsilon)\right]\right|^2 \left(1 + O\left(\frac{h}{\varepsilon^{(n+1)/n}}\right)\right) \tag{2.6}$$

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

Remark. The principal terms of the asymptotic formulae (2.4) and (2.3) are the same in the sense that the action integrals which appear in each principal term are defined by the two turning points closest to the real axis. In fact they have essentially the same Stokes geometry. Similarly the principal term of (2.5) is the same as that of (2.2) and the asymptotic formula (2.6) is exactly the same as (2.3). From above considerations, it is expected that turning points around the lowest order zero make a major contribution to the asymptotic behavior of $P(\varepsilon, h)$.

If $V(t)$ vanishes at more than two points, we can express the scattering matrix by means of the product of the transfer matrices (see § 4).

§ 3. Preliminary

§ 3.1. Exact WKB Method for 2×2 System

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

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

$$\frac{h}{i}\frac{d}{dt}\phi(t) = \begin{pmatrix} 0 & \alpha(t) \\ -\beta(t) & 0 \end{pmatrix} \phi(t). \tag{3.1}$$

The functions $\alpha(t)$ and $\beta(t)$ are assumed to be holomorphic in a simply connected domain $\Omega \subset \mathbb{C}$ and they do not vanish in a domain $\Omega_1 \subset \Omega$. These zeros of $\alpha(t)\beta(t)$ are called *turning points* and coincide with those mentioned in §2. Note that the equation (1.1) can be reduced to this anti-diagonal system (3.1) by $\psi(t) \mapsto \frac{1}{2}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \phi(t)$.

The exact WKB solutions to (3.1) are the following form:

$$\phi_\pm(t,h;t_0,t_1) = e^{\pm z(t;t_0)/h}\, M_\pm(z(t))\boldsymbol{w}_\pm(z(t),h;z(t_1)) \tag{3.2}$$

for two base points $t_0 \in \Omega$, $t_1 \in \Omega_1$, where

$$z(t;t_0) = \int_{t_0}^{t} \sqrt{\alpha(\tau)\beta(\tau)}\, d\tau, \tag{3.3}$$

$$M_{\pm}(z(t)) = \begin{pmatrix} K(z(t))^{-1} & K(z(t))^{-1} \\ \mp iK(z(t)) & \pm iK(z(t)) \end{pmatrix}, \quad K(z(t)) = \sqrt[4]{\frac{\beta(t)}{\alpha(t)}}, \tag{3.4}$$

$$\boldsymbol{w}_{\pm}(z(t),h;z(t_1)) = \begin{pmatrix} w_{\pm}^{e}(z(t),h;z(t_1)) \\ w_{\pm}^{o}(z(t),h;z(t_1)) \end{pmatrix} = \sum_{k\geq 0} \begin{pmatrix} w_{\pm,2k}(z(t),h;z(t_1)) \\ w_{\pm,2k-1}(z(t),h;z(t_1)) \end{pmatrix}. \tag{3.5}$$

Here the sequences of functions $\{w_{\pm,n}(z;z_1)\}_{n=0}^{\infty}$, where $z_1 = z(t_1)$ are defined by the integral recurrent relations:

$$\begin{cases} w_{\pm,0}(z;z_1) = 1, \qquad w_{\pm,-1}(z;z_1) = 0 \\ w_{\pm,2k+1}(z;z_1) = \displaystyle\int_{z_1}^{z} e^{\pm\frac{2}{h}(\zeta - z)} \frac{K'(\zeta)}{K(\zeta)}\, w_{\pm,2k}(\zeta,\zeta_1)\, d\zeta, \\ w_{\pm,2k}(z;z_1) = \displaystyle\int_{z_1}^{z} \frac{K'(\zeta)}{K(\zeta)}\, w_{\pm,2k-1}(\zeta;\zeta_1)\, d\zeta. \end{cases} \tag{3.6}$$

The phase function (3.3) is a solution to an eikonal equation and has singularities of turning points at branch points of the integrand. On the other hand, the symbol function (3.5) are determined by the integral recurrent relations. Hence we see that the elements of the function $\boldsymbol{w}_{\pm}(z;z_1)$ converge absolutely and uniformly in a neighborhood of $z = z_1$ (see [FLN], [W]). Such solutions (3.2) constructed by the way above are exact solutions to (3.1).

The exact WKB solutions (3.2) are holomorphic in a neighborhood of $t = t_1$, and extended analytically to Ω because (3.2) satisfy the equation (3.1) with holomorphic coefficients in Ω. We call t_0 the base point of the phase and t_1 the base point of the symbol. We remark that the pair of exact WKB solutions $\phi_+(t,h;t_0,t_1)$, $\phi_-(t,h;t_0,t_1)$ are linearly independent.

We state some properties of the exact WKB solutions. The Wronskian between two exact WKB solutions $[\phi(t),\widetilde{\phi}(t)] = \det\big(\phi(t)\ \widetilde{\phi}(t)\big)$ is given by w_{+}^{e}:

Proposition 3.1. *Any exact WKB solutions $\phi_+(t;t_0,t_1)$ and $\phi_-(t;t_0,t_2)$ with the same base point t_0 of the phase satisfy the Wronskian formula:*

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

We note that the Wronskian is independent of the variable t because the matrix of right side of (3.1) is trace-free.

The convergent series (3.5) of the function $\boldsymbol{w}_{\pm}(z(t),h;z(t_1))$ constructed by (3.6) are also asymptotic expansions on h in the domains $\Omega_{\pm} \subset \Omega_1$ in which there exists a curve from t_1 to t along which $\pm \operatorname{Re} z(t)$ increases strictly.

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*

$$w_{\pm}^{e}(z(t), h; z(t_1)) - \sum_{k=0}^{N-1} w_{\pm,2k}(z(t), h; z(t_1)) = O(h^N), \tag{3.7}$$

$$w_{\pm}^{o}(z(t), h; z(t_1)) - \sum_{k=0}^{N-1} w_{\pm,2k-1}(z(t), h; z(t_1)) = O(h^N), \tag{3.8}$$

uniformly in $\Omega_{\pm}$.

We introduce the so-called *Stokes line*, which characterizes the asymptotic behavior of the exact WKB solution as h tends to 0.

Definition 3.3. The Stokes lines emanating from $t = t_0$ in Ω are defined as the set:

$$\Big\{ t \in \Omega;\ \mathrm{Re} \int_{t_0}^{t} \sqrt{\alpha(\tau)\beta(\tau)}\, d\tau = 0 \Big\}.$$

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

If $\mathrm{Re}\, z(t)$ strictly increases along an oriented curve, such a curve is called a *canonical curve*. In fact a canonical curve is transversal to Stokes lines. We can characterize the asymptotic behavior of the Wronskian between the linearly independent exact WKB solutions in terms of canonical curve.

Proposition 3.4. *If there exists a canonical curve from t_1 to t_2,*

$$[\phi_+(t, h; t_0, t_1), \phi_-(t, h; t_0, t_2)] = 2i\,(1 + O(h)) \qquad \text{as} \quad h \to 0.$$

§ 3.2. Action Integral

In this subsection we give the asymptotic behaviors of the action integrals (2.1). These are important to study the decay rate of $P(\varepsilon, h)$ and the geometrical structures of the Stokes lines.

We see that there exist the relations between the action integral defined in §2 and the phase function (3.3): $A_j(\varepsilon) = iz(x_j(\varepsilon); x)/2$, $B_j(\varepsilon) = iz(y_j(\varepsilon); y)/2$. Put $V(t) = \dfrac{V^{(n)}(x)}{n!}(t-x)^n v_x(t-x)$, where $v_x(t)$ are holomorphic near $t = 0$ and $v_x(0) = 1$ (resp. $V(t) = \dfrac{V^{(m)}(y)}{m!}(t-y)^m v_y(t-y)$) respectively.

Lemma 3.5. *$A_j(\varepsilon)$ is an analytic function of $\varepsilon^{1/n}$ at $t = x$ and has the following expansion:*

$$A_j(\varepsilon) = \sum_{q=1}^{\infty} X_q \exp\Big[\frac{(2j-1)q\pi i}{2n}\Big] \varepsilon^{(n+q)/n} \qquad (j = 1, \dots, n), \tag{3.9}$$

where $X_q = \dfrac{\sqrt{\pi}\,\Gamma(q/(2n))}{(n+q)\,\Gamma(q)\,\Gamma((n+q)/(2n))}\left(\dfrac{n!}{|V^{(n)}(x)|}\right)^{q/n}\left[\dfrac{d^{q-1}}{dz^{q-1}}(v_x(z)^{-q/n})\right]_{z=0}$.

Remark. $B_j(\varepsilon)$ is also an analytic function of $\varepsilon^{1/m}$ at $t = y$ and has a similar expansion.

To consider the scattering matrix, we define the action integrals $R_\infty(\varepsilon)$ and $R_{-\infty}(\varepsilon)$, which have $\pm\infty$ as the end points of the integration paths, by

$$R_\infty(\varepsilon) = 2\int_x^\infty (\sqrt{V(t)^2+\varepsilon^2} - \lambda_r)\,dt,$$
$$R_{-\infty}(\varepsilon) = 2\int_y^{-\infty} (\sqrt{V(t)^2+\varepsilon^2} - \lambda_l)\,dt,$$

where $\lambda_r = \sqrt{E_r^2+\varepsilon^2}$ and $\lambda_l = \sqrt{E_l^2+\varepsilon^2}$. Note that $R_\infty(\varepsilon)$ and $R_{-\infty}(\varepsilon)$ are real-valued as well as $R(\varepsilon)$.

§ 4. Outline of Proofs

The proof of each theorem is reduced to studying the asymptotic expansions of the elements of the scattering matrix as $h \to 0$ by means of the exact WKB method in § 3.1. In short the scattering matrix can be expressed by the products of the change of bases (*transfer matrix*) between the exact WKB solutions which has a valid asymptotic expansion on h in a complex domain separated by Stokes lines near the real axis. We first study the geometrical structures of Stokes lines in some cases and define such exact WKB solutions. In § 4.2 we give the expression of the scattering matrix with the transfer matrix near each zero of $V(t)$.

§ 4.1. Stokes Geometry

In this paper we call *Stokes geometry* the geometrical structures of the Stokes lines emanating from turning points. We remark that the Stokes geometry near the real axis differs according to the orders of zeros of $V(t)$. See Figures 1, 2, and 3 for different Stokes geometries.

Let r, $\bar{r}$, l, and $\bar{l}$ be four base points of the symbol as in each figure. We make the branch cuts dashed lines as in each figure. Recalling that we take the branch of $\sqrt{V(t)^2+\varepsilon^2}$ which is ε at $t = x$, we see that around the real axis $\mathrm{Re}\,z(t)$ is increases as $\mathrm{Im}\,t$ decreases and $\mathrm{Im}\,z(t)$ increases as $\mathrm{Re}\,t$ increases.

For any n, $m \in \mathbb{N}$ we consider four exact WKB solutions:

$$
(4.1)\quad
\begin{aligned}
\phi_+(t;x_1,r) &= \exp\Big[+\frac{z(t;x_1)}{h}\Big] M_+(z(t))\boldsymbol{w}_+(z(t);z(r)),\\
\phi_-(t;\overline{x}_1,\overline{r}) &= \exp\Big[-\frac{z(t;\overline{x}_1)}{h}\Big] M_-(z(t))\boldsymbol{w}_-(z(t);z(\overline{r})),\\
\phi_+(t;y_m,l) &= \exp\Big[+\frac{z(t;y_m)}{h}\Big] M_+(z(t))\boldsymbol{w}_+(z(t);z(l)),\\
\phi_-(t;\overline{y}_m,\overline{l}) &= \exp\Big[-\frac{z(t;\overline{y}_m)}{h}\Big] M_-(z(t))\boldsymbol{w}_-(z(t);z(\overline{l})).
\end{aligned}
$$

Note that each exact WKB solution has a valid asymptotic expansion on h in the direction toward its phase base point from its symbol base point.

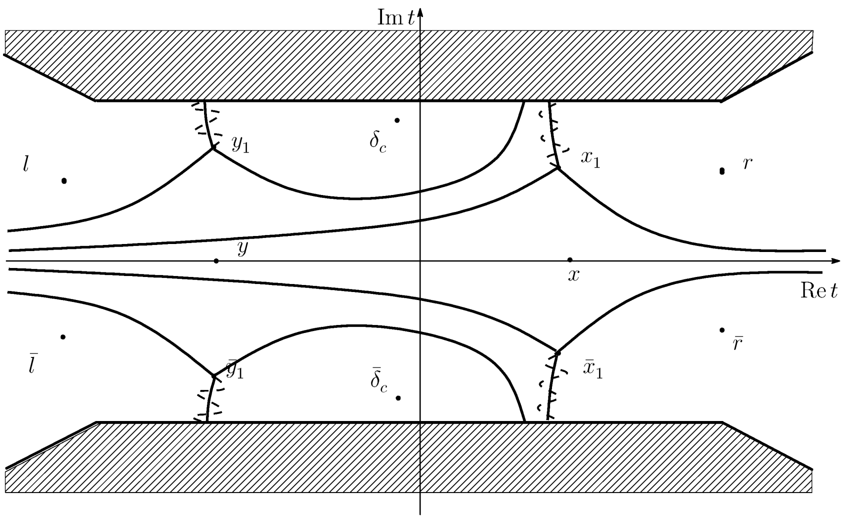

Figure 1. $n = m = 1$, $\operatorname{Im} A_1(\varepsilon) < \operatorname{Im} B_1(\varepsilon)$

Let δ_c and $\overline{\delta}_c$ as in Figures 1, 2 and 3 be the intermediate symbol base points in $\mathcal{S}$ satisfying

$$
(4.2)\qquad \max\{|\operatorname{Re} z(x_n)|,\, |\operatorname{Re} z(y_1)|\} < |\operatorname{Re} z(\delta_c)| < \min\{|\operatorname{Re} z(x_{n-1})|,\, |\operatorname{Re} z(y_2)|\}
$$

for sufficiently small ε. In fact we note, from Lemma 3.5, that the inequality $\operatorname{Re} z(x_n) > \operatorname{Re} z(y_1)$ holds for sufficiently small ε if $n > m$. Then we consider the intermediate exact WKB solutions:

$$
\begin{aligned}
\phi_+(t;x_n,\delta_c) &= \exp\Big[+\frac{z(t;x_n)}{h}\Big] M_+(z(t))\boldsymbol{w}_+(z(t);z(\delta_c)),\\
\phi_-(t;\overline{x}_n,\overline{\delta}_c) &= \exp\Big[-\frac{z(t;\overline{x}_n)}{h}\Big] M_-(z(t))\boldsymbol{w}_-(z(t);z(\overline{\delta}_c)),\\
\phi_+(t;y_1,\delta_c) &= \exp\Big[+\frac{z(t;y_1)}{h}\Big] M_+(z(t))\boldsymbol{w}_+(z(t);z(\delta_c)),
\end{aligned}
$$

$$\phi_-(t;\overline{y}_1,\overline{\delta}_c)=\exp\Big[-\frac{z(t;\overline{y}_1)}{h}\Big]M_-(z(t))\boldsymbol{w}_-(z(t);z(\overline{\delta}_c)),$$

whose asymptotic expansions in h are valid in the direction toward four turning points from the symbol base points δ_c, $\overline{\delta}_c$.

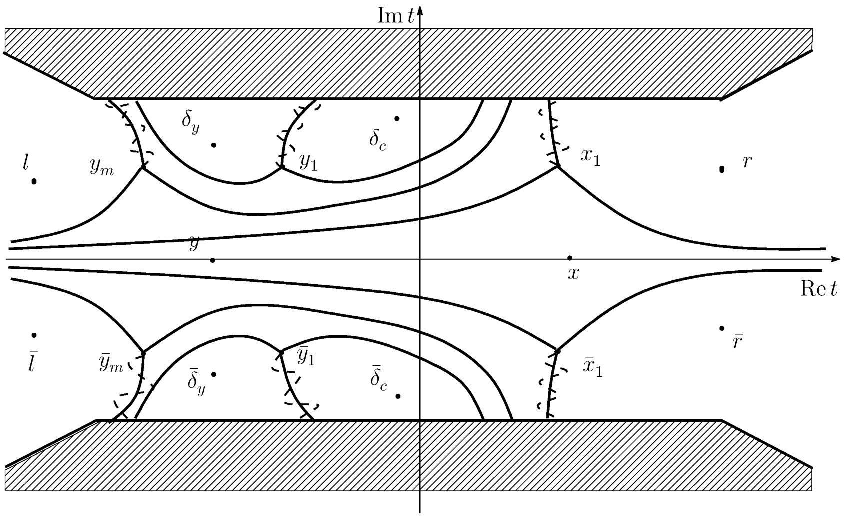

Figure 2. $n=1, m\geq 2$, $\operatorname{Im} B_1(\varepsilon)>\operatorname{Im} B_m(\varepsilon)$

§ 4.2. Scattering Matrix

We first give the relations between the Jost solutions and the exact WKB solutions (4.1) (see [Ra], [FR], [W]).

Lemma 4.1. *The following relations hold:*

$$\psi_+^r(t)=QC_1(\varepsilon,h)\exp\Big[+\frac{z^r(x_1)}{h}\Big]\phi_+(t;x_1,r),$$
$$\psi_-^r(t)=-iQC_2(\varepsilon,h)\exp\Big[-\frac{z^r(\overline{x}_1)}{h}\Big]\phi_-(t;\overline{x}_1,\overline{r}),$$
$$\psi_+^l(t)=QC_3(\varepsilon,h)\exp\Big[+\frac{z^l(y_m)}{h}\Big]\phi_+(t;y_m,l),$$
$$\psi_-^l(t)=-iQC_4(\varepsilon,h)\exp\Big[-\frac{z^l(\overline{y}_m)}{h}\Big]\phi_-(t;\overline{y}_m,\overline{l}),$$

where $Q=\frac{1}{2}\begin{pmatrix}1 & i\\ i & 1\end{pmatrix}$, *and*

$$z^r(t)=i\int_\infty^t(\sqrt{V(\tau)^2+\varepsilon^2}-\lambda_r)\,d\tau+i\lambda_r t,\qquad \Big(\lambda_r=\sqrt{E_r^2+\varepsilon^2}\,\Big)$$

$$z^l(t) = i \int_{-\infty}^{t} (\sqrt{V(\tau)^2 + \varepsilon^2} - \lambda_l)\, d\tau + i\lambda_l t, \qquad \Big(\lambda_l = \sqrt{E_l^2 + \varepsilon^2}\,\Big).$$

The coefficients $C_k(\varepsilon, h)$ are some constants depending only on ε and h, and $C_k(\varepsilon, h) = 1 + O(h)$ as h tends to 0 uniformly with respect to small ε.

We will denote such constants simply by $1 + O(h)$.

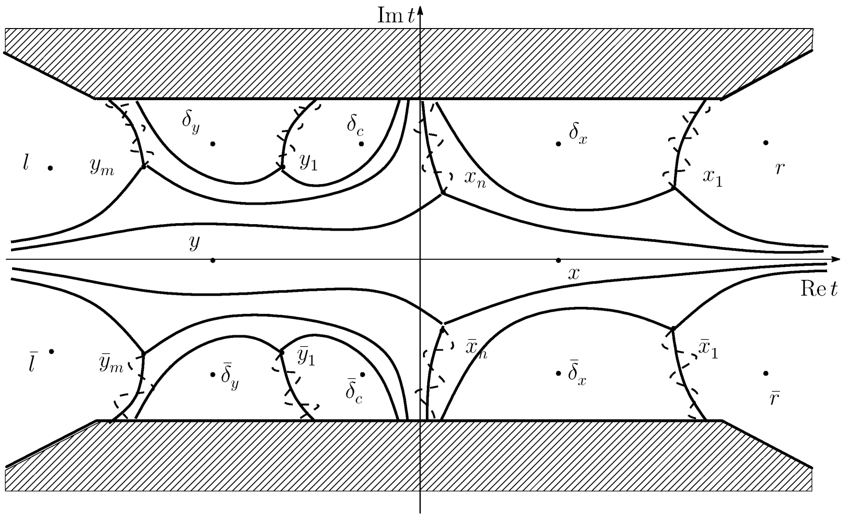

Figure 3. $m \geq n \geq 2$, $\operatorname{Im} A_1(\varepsilon) > \operatorname{Im} A_n(\varepsilon)$, $\operatorname{Im} B_1(\varepsilon) > \operatorname{Im} B_m(\varepsilon)$

We next define the transfer matrices $T_r(\varepsilon, h)$ and $T_l(\varepsilon, h)$ by

$$(\psi_+^r(t)\ \psi_-^r(t)) = (\phi_+(t; x_1, r)\ \phi_-(t; \overline{x}_1, \overline{r}))T_r(\varepsilon, h),$$
$$(\psi_+^l(t)\ \psi_-^l(t)) = (\phi_+(t; y_m, l)\ \phi_-(t; \overline{y}_m, \overline{l}))T_l(\varepsilon, h),$$

and the transfer matrices $T_x(\varepsilon, h)$, $T_y(\varepsilon, h)$ around $t = x$, y and $T_c(\varepsilon, h)$:

$$(\phi_+(t; x_n, \delta_c)\ \phi_-(t; \overline{x}_n, \overline{\delta}_c)) = (\phi_+(t; x_1, \delta_r)\ \phi_-(t; \overline{x}_1, \overline{r}))T_x(\varepsilon, h),$$
$$(\phi_+(t; y_m, l)\ \phi_-(t; \overline{y}_m, \overline{l})) = (\phi_+(t; y_1, \delta_c)\ \phi_-(t; \overline{y}_1, \overline{\delta}_c))T_y(\varepsilon, h),$$
$$(\phi_+(t; y_1, \delta_c)\ \phi_-(t; \overline{y}_1, \overline{\delta}_c)) = (\phi_+(t; x_n, \delta_c)\ \phi_-(t; \overline{x}_n, \overline{\delta}_c))T_c(\varepsilon, h).$$

We see that the transfer matrices $T_r(\varepsilon, h)$, $T_l(\varepsilon, h)$, and $T_c(\varepsilon, h)$ are diagonal matrices given by

$$(4.3)\quad T_r = \begin{pmatrix} \exp\Big[\dfrac{i}{2h}(A_1 - R_\infty + 2\lambda_r x)\Big] & 0 \\ 0 & \exp\Big[\dfrac{i}{2h}(R_\infty - \overline{A}_1 - 2\lambda_r x)\Big] \end{pmatrix} (1 + O(h)),$$

$$(4.4)\quad T_l = \begin{pmatrix} \exp\Big[\frac{i}{2h}(B_m - R_{-\infty} + 2\lambda_l y)\Big] & 0 \\ 0 & \exp\Big[\frac{i}{2h}(R_{-\infty} - \overline{B}_m - 2\lambda_l y)\Big] \end{pmatrix} (1 + O(h)),$$

where $O(h)$ is uniform with respect to small ε, and

$$(4.5)\quad T_c = \begin{pmatrix} \exp\Big[\frac{i}{2h}(A_n - B_1 + R)\Big] & 0 \\ 0 & \exp\Big[-\frac{i}{2h}(\overline{A}_n - \overline{B}_1 + R)\Big] \end{pmatrix}.$$

Then the asymptotic formula of $S(\varepsilon, h)$ as h tends to 0 is given by

Proposition 4.2. *The scattering matrix $S(\varepsilon, h)$ is the product of the 2×2 matrices $T_r(\varepsilon, h)$, $T_l(\varepsilon, h)$, $T_x(\varepsilon, h)$, $T_y(\varepsilon, h)$, and $T_c(\varepsilon, h)$:*

$$(4.6)\qquad S(\varepsilon, h) = T_r^{-1}(\varepsilon, h)\, T_x(\varepsilon, h)\, T_c(\varepsilon, h)\, T_y(\varepsilon, h)\, T_l(\varepsilon, h).$$

We finally state the asymptotic formulae of the transfer matrices $T_x(\varepsilon, h)$ and $T_y(\varepsilon, h)$. Put

$$T_x(\varepsilon, h) = \begin{pmatrix} \xi_{11}(\varepsilon, h) & \xi_{12}(\varepsilon, h) \\ \xi_{21}(\varepsilon, h) & \xi_{22}(\varepsilon, h) \end{pmatrix}, \qquad T_y(\varepsilon, h) = \begin{pmatrix} \eta_{11}(\varepsilon, h) & \eta_{12}(\varepsilon, h) \\ \eta_{21}(\varepsilon, h) & \eta_{22}(\varepsilon, h) \end{pmatrix}.$$

Proposition 4.3. *$T_x(\varepsilon, h)$ satisfies the following asymptotic formulae:*
If $n = 1$, then

$$\begin{aligned}
\xi_{11}(\varepsilon, h) &= 1 + O\Big(\frac{h}{\varepsilon^2}\Big) && \text{as} \quad \frac{h}{\varepsilon^2} \to 0, \\
\xi_{12}(\varepsilon, h) &= i \exp\Big[-\frac{1}{h} \operatorname{Im} A_1(\varepsilon)\Big](1 + O(h)) && \text{as} \quad h \to 0, \\
\xi_{21}(\varepsilon, h) &= i \exp\Big[-\frac{1}{h} \operatorname{Im} A_1(\varepsilon)\Big](1 + O(h)) && \text{as} \quad h \to 0, \\
\xi_{22}(\varepsilon, h) &= 1 + O\Big(\frac{h}{\varepsilon^2}\Big) && \text{as} \quad \frac{h}{\varepsilon^2} \to 0.
\end{aligned}$$

If $n \geq 2$, then

$$\begin{aligned}
\xi_{11}(\varepsilon, h) &= \Big(\exp\Big[\frac{i}{2h}(A_1 - A_n)\Big] + (-1)^n \exp\Big[\frac{i}{2h}(A_1 - 2\overline{A}_1 + A_n)\Big]\Big) \\
&\quad \times \Big(1 + O\Big(\frac{h}{\varepsilon^{(n+1)/n}}\Big)\Big) && \text{as} \quad \frac{h}{\varepsilon^{(n+1)/n}} \to 0, \\
\xi_{12}(\varepsilon, h) &= i\Big((-1)^{n+1} \exp\Big[\frac{i}{2h}(A_1 - \overline{A}_n)\Big] + \exp\Big[\frac{i}{2h}(A_1 - 2\overline{A}_1 + \overline{A}_n)\Big]\Big) \\
&\quad \times \Big(1 + O\Big(\frac{h}{\varepsilon^{(n+1)/n}}\Big)\Big) && \text{as} \quad \frac{h}{\varepsilon^{(n+1)/n}} \to 0,
\end{aligned}$$

$$\xi_{21}(\varepsilon,h) = i\Big((-1)^{n+1}\exp\Big[\frac{i}{2h}(A_n-\overline{A}_1)\Big]+\exp\Big[\frac{i}{2h}(2A_1-\overline{A}_1-A_n)\Big]\Big)$$
$$\times\Big(1+O\Big(\frac{h}{\varepsilon^{(n+1)/n}}\Big)\Big) \qquad \text{as} \quad \frac{h}{\varepsilon^{(n+1)/n}}\to 0,$$
$$\xi_{22}(\varepsilon,h) = \Big(\exp\Big[\frac{i}{2h}(\overline{A}_n-\overline{A}_1)\Big]+(-1)^n\exp\Big[\frac{i}{2h}(2A_1-\overline{A}_1-\overline{A}_n)\Big]\Big)$$
$$\times\Big(1+O\Big(\frac{h}{\varepsilon^{(n+1)/n}}\Big)\Big) \qquad \text{as} \quad \frac{h}{\varepsilon^{(n+1)/n}}\to 0.$$

This proposition can be proved by means of the idea in [W]. The elements of $T_x(\varepsilon,h)$ are expressed by Wronskians between the exact WKB solutions defined in § 4.1. We see that there exist a canonical curve for each Wronskian in case $n=1$. In the case where $n\geq 2$, taking account of intermediate base points of the symbol δ_x and $\overline{\delta}_x$, we also make sure of the existence of canonical curves. Therefore we obtain this proposition by Proposition 3.4. Similarly we get

Proposition 4.4. *$T_y(\varepsilon,h)$ satisfies the following asymptotic formulae:*
If $m=1$, then

$$\eta_{11}(\varepsilon,h) = 1+O\Big(\frac{h}{\varepsilon^2}\Big) \qquad \text{as} \quad \frac{h}{\varepsilon^2}\to 0,$$
$$\eta_{12}(\varepsilon,h) = (-1)^n i\,\exp\Big[-\frac{1}{h}\operatorname{Im}B_1(\varepsilon)\Big](1+O(h)) \qquad \text{as} \quad h\to 0,$$
$$\eta_{21}(\varepsilon,h) = (-1)^n i\,\exp\Big[-\frac{1}{h}\operatorname{Im}B_1(\varepsilon)\Big](1+O(h)) \qquad \text{as} \quad h\to 0,$$
$$\eta_{22}(\varepsilon,h) = 1+O\Big(\frac{h}{\varepsilon^2}\Big) \qquad \text{as} \quad \frac{h}{\varepsilon^2}\to 0.$$

If $m\geq 2$, then

$$\eta_{11}(\varepsilon,h) = \Big(\exp\Big[\frac{i}{2h}(B_1-B_m)\Big]+(-1)^m\exp\Big[\frac{i}{2h}(B_1-2\overline{B}_1+B_m)\Big]\Big)$$
$$\times\Big(1+O\Big(\frac{h}{\varepsilon^{(m+1)/m}}\Big)\Big) \qquad \text{as} \quad \frac{h}{\varepsilon^{(m+1)/m}}\to 0,$$
$$\eta_{12}(\varepsilon,h) = (-1)^n i\Big((-1)^{m+1}\exp\Big[\frac{i}{2h}(B_1-\overline{B}_m)\Big]+\exp\Big[\frac{i}{2h}(B_1-2\overline{B}_1+\overline{B}_m)\Big]\Big)$$
$$\times\Big(1+O\Big(\frac{h}{\varepsilon^{(m+1)/m}}\Big)\Big) \qquad \text{as} \quad \frac{h}{\varepsilon^{(m+1)/m}}\to 0,$$
$$\eta_{21}(\varepsilon,h) = (-1)^n i\Big((-1)^{m+1}\exp\Big[\frac{i}{2h}(B_m-\overline{B}_1)\Big]+\exp\Big[\frac{i}{2h}(2B_1-\overline{B}_1-B_m)\Big]\Big)$$
$$\times\Big(1+O\Big(\frac{h}{\varepsilon^{(m+1)/m}}\Big)\Big) \qquad \text{as} \quad \frac{h}{\varepsilon^{(m+1)/m}}\to 0,$$
$$\eta_{22}(\varepsilon,h) = \Big(\exp\Big[\frac{i}{2h}(\overline{B}_m-\overline{B}_1)\Big]+(-1)^m\exp\Big[\frac{i}{2h}(2B_1-\overline{B}_1-\overline{B}_m)\Big]\Big)$$
$$\times\Big(1+O\Big(\frac{h}{\varepsilon^{(m+1)/m}}\Big)\Big) \qquad \text{as} \quad \frac{h}{\varepsilon^{(m+1)/m}}\to 0.$$

From (4.3), (4.4), (4.5), Propositions 4.2, 4.3, and 4.4, we obtain the asymptotic expansions of the scattering matrix.

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