Exact WKB analysis of non-adiabatic transition probabilities for three levels

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Abstract

The Schrödinger equation $id\psi/dt = \eta H\psi$ with a large parameter η and an appropriate 3×3 matrix H is studied by the exact WKB method, i.e., WKB analysis based on the Borel resummation. Transition probabilities of solutions of the equation are explicitly calculated with the help of the connection formula for WKB solutions. Since a 3×3 system is considered, addition of new Stokes curves is necessary to obtain the correct connection formula (Berk-Nevins-Roberts' observation), and we present a practically useful procedure for finding required new Stokes curves.

1 Introduction

In this paper we discuss a Landau-Zener type problem for three levels (cf. [CH], [BE], [J2] and references cited there) from the viewpoint of exact WKB analysis, i.e., WKB analysis based on the Borel resummation. (Cf. [V], [P], [DDP], [AKT1], [AKT2], [T2] and references cited there.) To be more specific, we consider the following equation

$$i\frac{d}{dt}\psi = \eta H(t,\eta)\psi, \tag{1.1}$$

where ψ is a 3-vector and $H(t,\eta)$ is a 3×3 matrix with polynomial entries that depends on a large parameter η in the manner specified below.

$$H(t,\eta) = H_0(t) + \eta^{-1/2}H_{1/2}, \tag{1.2}$$

where

$$H_0(t) = \begin{pmatrix} \rho_1(t) & & 0 \\ & \rho_2(t) & \\ 0 & & \rho_3(t) \end{pmatrix} \tag{1.3}$$

with $\rho_j(t)$ $(j = 1, 2, 3)$ being a real polynomial and

$$H_{1/2} = \begin{pmatrix} 0 & c_{12} & c_{13} \\ \overline{c_{12}} & 0 & c_{23} \\ \overline{c_{13}} & \overline{c_{23}} & 0 \end{pmatrix} \tag{1.4}$$

with c_{jk} $(1 \le j, k \le 3)$ being a complex constant. Throughout this paper we further assume

$$(1.5) \qquad (\rho_1 - \rho_2)(\rho_1 - \rho_3)(\rho_2 - \rho_3) = 0 \quad \text{has only real and simple zeros.}$$

Our task is then to relate the behavior of $\psi(t)$ for $t \to -\infty$ and that for $t \to +\infty$, that is, the transition probabilities. To formulate the problem mathematically, we follow the idea of Brundobler-Elser ([BE]) that one should compare the asymptotic behavior of $\psi(t)$ near $t = -\infty$ and that near $t = +\infty$. In our approach, we consider WKB solutions of (1.1) that can be readily expanded asymptotically near $t = -\infty$ or $t = +\infty$ and we then apply the connection formula to relate the behavior of WKB solutions near $t = -\infty$ with that near $t = +\infty$. Although this may sound to be a traditional and standard approach, there exist substantial troubles in putting this program into practice, due to the fact that (1.1) is a 3×3, not 2×2, system:

The first trouble is that WKB analysis for systems is not well-developed, at least compared with that for single equations. The second problem is that Stokes curves for an $n \times n$ system $(n \ge 3)$ may cross and that we have to add new Stokes curves to obtain a correct and consistent connection formula for WKB solutions, as was first observed by Berk-Nevins-Roberts ([BNR]).

The first issue has recently been essentially ameliorated by one of us ([T2]) through the establishment of an exact WKB theoretic result that enables us to reduce a system to a canonical one near a (double) turning point. (For the convenience of the reader, we give in Appendix a summary of the core part of [T2] that is relevant to our analysis, omitting the detailed estimation of the coefficients of η^{-j} of the transformation.)

The second issue is discussed in Section 3 with an emphasis on showing a practically efficient rule to detect the virtual turning point (called a new turning point in [AKT1]) from which a required new Stokes curve emanates. We show in Section 2 (a simple model example) and in Section 4 (the general case) how effectively these mathematical results are used to calculate the transition probabilities of solutions of the equation (1.1). We note that most of the results given in Section 3 and Section 4 can be generalized to equations for n-levels with $n \ge 4$, although, for the sake of simplicity, we confine our consideration to the 3-level problem.

In ending this Introduction, we remark that the particular η-dependence of H given in (1.2) neatly explains, as we show in this paper, the non-adiabatic character of the Landau-Zener problem, as was first observed by

Hagedorn ([H]) in the 2-level case. (See also [J1].) It may be worth mentioning the title of [Z] clearly indicates the non-adiabatic character of the problem.

2 Landau-Zener model for three levels

In this section we study the following straightforward generalization to three levels of the original Landau-Zener model for two levels:

(2.1)

$$i\frac{d}{dt}\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\end{pmatrix} = \eta\left[\begin{pmatrix} b_1t+a & 0 & 0\\ 0 & b_2t & 0\\ 0 & 0 & b_3t\end{pmatrix} + \eta^{-1/2}\begin{pmatrix} 0 & c_{12} & c_{13}\\ \overline{c_{12}} & 0 & c_{23}\\ \overline{c_{13}} & \overline{c_{23}} & 0\end{pmatrix}\right]\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\end{pmatrix},$$

where b_j's are mutually distinct real constants and a is a real constant. That is, we study (1.1) with $\rho_1(t) = b_1t + a$, $\rho_2(t) = b_2t$ and $\rho_3(t) = b_3t$. Note that every three level problem with $\rho_j(t)$ being a real polynomial of degree one can be reduced to the above form by using the translation $t \mapsto t - t_0$ and the gauge transformation $\psi = {}^t(\psi_1, \psi_2, \psi_3) \mapsto e^{i\theta t}\psi$ where t_0 and θ are real constants. In order to fix the situation, we suppose

$$0 < b_1 < b_2 < b_3 \quad \text{and} \quad 0 < a. \tag{2.2}$$

Letting t_{jk} denote the solution of the equation $\rho_j(t) = \rho_k(t)$, we then find

$$0 = t_{23} < t_{13} < t_{12}. \tag{2.3}$$

The three level problem (2.1) has a WKB solution $\psi^{(j)}$ ($j = 1, 2, 3$) of the following form:

(2.4)

$$\psi^{(j)} = \eta^{-1/2}\exp\left(\frac{\eta}{i}\int_0^t \rho_j(t)dt\right)(\rho_k-\rho_j)^{-\kappa_{kj}}(\rho_l-\rho_j)^{-\kappa_{lj}}\left(e^{(j)} + O\left(\eta^{-1/2}\right)\right),$$

where $e^{(j)} = {}^t(e_1^{(j)}, e_2^{(j)}, e_3^{(j)})$ is a unit vector satisfying

$$e_\beta^{(\alpha)} = \delta_{\alpha\beta} \quad (\alpha, \beta = 1, 2, 3), \tag{2.5}$$

$\kappa_{\alpha\beta}$ ($\alpha, \beta = 1, 2, 3$) denotes a Landau-Zener parameter

$$\kappa_{\alpha\beta} = \frac{i|c_{\alpha\beta}|^2}{b_\beta - b_\alpha} \tag{2.6}$$

(we define $c_{\alpha\beta} = \overline{c_{\beta\alpha}}$ when $\alpha > \beta$ for the notational convenience), and $\{j,k,l\}$ is a permutation of $\{1,2,3\}$, i.e., $\{j,k,l\} = \{1,2,3\}$ holds as sets. (Here and in what follows we add an extra factor $\eta^{-1/2}$ to WKB solutions so that their Borel transform and Borel sum may be readily defined.) We further assume that the branch of multivalued analytic functions $(\rho_\alpha - \rho_\beta)^{-\kappa_{\alpha\beta}}$ is determined as follows:

$$\text{(2.7)} \qquad \text{As } t \to -\infty \qquad \begin{aligned} &\arg(\rho_\alpha - \rho_\beta) = 0 \quad \text{for } \alpha < \beta, \\ &\arg(\rho_\alpha - \rho_\beta) = \pi \quad \text{for } \alpha > \beta. \end{aligned}$$

$$\text{(2.8)} \qquad \text{As } t \to +\infty \qquad \begin{aligned} &\arg(\rho_\alpha - \rho_\beta) = -\pi \quad \text{for } \alpha < \beta, \\ &\arg(\rho_\alpha - \rho_\beta) = 0 \quad \text{for } \alpha > \beta. \end{aligned}$$

See Appendix for the construction of a WKB solution . Note that the solution (2.4) is normalized in such a way that the endpoint of the frequency $\int_0^t \rho_j(t)dt$ is taken to be the origin etc.

If we introduce new fundamental systems $\psi^{\pm,(j)}$ of solutions of (2.1) defined by

$$\psi^{\pm,(j)} = N^{\pm,(j)} \psi^{(j)} \tag{2.9}$$

with

$$\left\{ \begin{array}{lcl} N^{-,(1)} &=& e^{-i\pi(\kappa_{12}+\kappa_{13})} + O\left(\eta^{-1/2}\right), \\ N^{-,(2)} &=& e^{-i\pi\kappa_{23}} + O\left(\eta^{-1/2}\right), \\ N^{-,(3)} &=& 1 + O\left(\eta^{-1/2}\right), \end{array} \right. \tag{2.10}$$

$$\left\{ \begin{array}{lcl} N^{+,(1)} &=& 1 + O\left(\eta^{-1/2}\right), \\ N^{+,(2)} &=& e^{-i\pi\kappa_{12}} + O\left(\eta^{-1/2}\right), \\ N^{+,(3)} &=& e^{-i\pi(\kappa_{23}+\kappa_{13})} + O\left(\eta^{-1/2}\right), \end{array} \right. \tag{2.11}$$

then $\psi^{\pm,(j)}$'s respectively show the following asymptotic behavior near $t = \pm\infty$:

$$\lim_{t \to \pm\infty} \left| \psi_k^{\pm,(j)}(t) \right| = \delta_{jk} \quad (j,k = 1,2,3). \tag{2.12}$$

Hence, letting $\widetilde{S}$ denote the connection matrix for the WKB solution $\psi^{(j)}$ from $t = -\infty$ to $+\infty$, we find that the matrix

$$\begin{pmatrix} N^{+,(1)} & 0 & 0 \\ 0 & N^{+,(2)} & 0 \\ 0 & 0 & N^{+,(3)} \end{pmatrix}^{-1} \widetilde{S} \begin{pmatrix} N^{-,(1)} & 0 & 0 \\ 0 & N^{-,(2)} & 0 \\ 0 & 0 & N^{-,(3)} \end{pmatrix} \tag{2.13}$$

and the square of the modulus of each entry of (2.13) respectively describe the S-matrix and the transition probabilities for the equation (2.1). In what follows we try to compute the connection matrix $\widetilde{S}$.

A turning point of (2.1) is a crossing point of two energy levels, that is, a point t_{jk} satisfying $\rho_j(t_{jk}) = \rho_k(t_{jk})$ $(j, k = 1, 2, 3)$. A Stokes curve of (2.1) is, by definition, a solution curve of the direction field

$$\mathrm{Im}\left(\frac{1}{i}\left(\rho_j(t) - \rho_k(t)\right)dt\right) = 0 \tag{2.14}$$

emanating from a turning point t_{jk}. A new Stokes curve is defined in a similar manner by replacing a turning point with a virtual turning point (cf. [AKT1]; see Section 3 also). In what follows we use the terminology "a (new) Stokes curve of type (j, k)" to emphasize the index of $\rho(t)$ appearing in the definition (2.14) of the corresponding direction field. Another terminology "a (new) Stokes curve of type $(j > k)$" is also used to specify the dominance relation between WKB solutions on the curve (for example, "type $(j > k)$" indicates that the WKB solution $\psi^{(j)}$ is dominant over the WKB solution $\psi^{(k)}$ along the portion of the curve). The Stokes geometry, i.e., the configuration of turning points and (new) Stokes curves of (2.1) can be illustrated as follows:

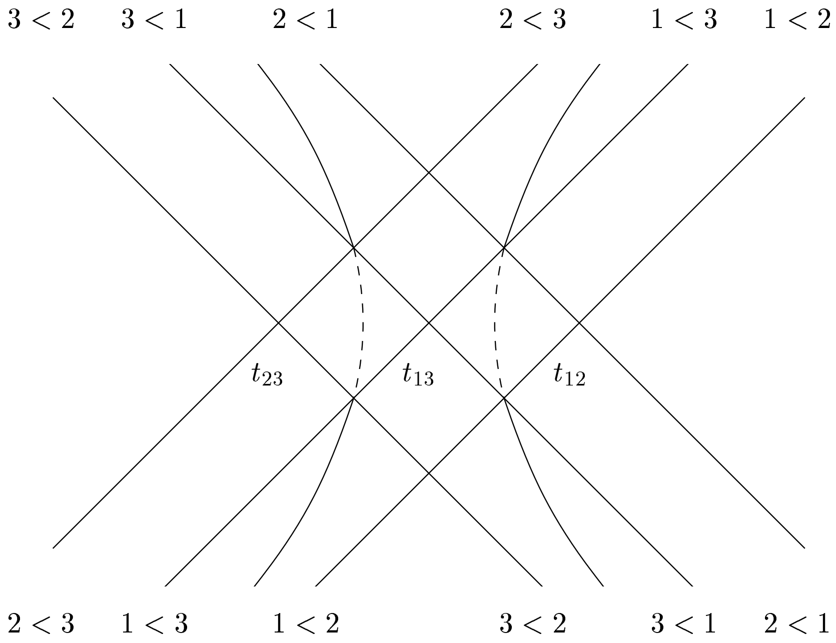


Figure 2.1 : Stokes geometry of (2.1).

In Figure 2.1 a broken segment indicates that the portion of a (new) Stokes curve is irrelevant to the Stokes phenomena. (See [AKT1, p. 77].) Each Borel resummed WKB solution $\psi^{(j)}$ of (2.1) thus becomes well-defined except on solid segments of (new) Stokes curves shown in Figure 2.1.

Remark 2.1 For the equation (2.1) we can analytically determine the location of all possible virtual turning points. Hence, as far as we restrict our consideration to a compact set in the complex t-plane, we can draw all possible (new) Stokes curves numerically. After doing that, we determine whether each segment of (new) Stokes curves is solid (i.e., a Stokes phenomenon occurs on the segment) or broken (i.e., no Stokes phenomena occur on the segment) by applying the following three rules:

(2.15a)
a segment with a turning point as endpoint should be solid,

(2.15b)
a segment containing a virtual turning point should be broken,

(2.15c)
at a crossing point t_0 of three new or ordinary Stokes curves Γ_1, Γ_2, and Γ_3 respectively of type $(j > k)$, $(k > l)$ and $(j > l)$, the following should hold for the six segments $\Gamma_m^{\pm}$ of Γ_m $(m = 1, 2, 3)$ having t_0 as common endpoint:

(i) for $m = 1, 2$ (i.e., for Stokes curves of "adjacent type") both Γ_m^+ and Γ_m^- are solid, or both are broken,

(ii) if the four segments $\Gamma_m^{\pm}$ $(m = 1, 2)$ are all solid, one of $\Gamma_3^{\pm}$'s is solid (i.e., both of $\Gamma_3^{\pm}$'s are solid, or one is solid and the other is broken). Otherwise, both of $\Gamma_3^{\pm}$'s are solid, or both are broken.

In the case of the equation (2.1) these rules determine the attribute of being "solid or broken" for all the segments of (new) Stokes curves and consequently we obtain Figure 2.1 where all crossing points of Stokes curves are non-ordered. (For the definition of a non-ordered crossing point, see the begining of Section 3.) Taking account of the Riemann sheet structure of singular points of Borel transformed WKB solutions, we find that the three rules listed above are natural requirements or ansatz to be expected (cf. [AKT1]).

Since we deal with the connection problem along the real axis, the two new Stokes curves appearing in Figure 2.1 are irrelevant to our problem. (They are broken curves near the real axis.) It suffices to discuss the connection formula on ordinary Stokes curves emanating from turning points. As is shown in Appendix, at each turning point t_{jk} the equation (2.1) can be reduced to a Landau-Zener model for two levels

(2.16)
$$i\frac{d}{dz}\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} = \eta\left[\begin{pmatrix} -z & 0 \\ 0 & z \end{pmatrix} + \sum_{m=0}^{\infty} \eta^{-(m+1)/2}\begin{pmatrix} 0 & \mu_{m/2} \\ \nu_{m/2} & 0 \end{pmatrix}\right]\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}$$

with two "invariants" $\mu = \mu_0 + \eta^{-1/2}\mu_{1/2} + \cdots$ and $\nu = \nu_0 + \eta^{-1/2}\nu_{1/2} + \cdots$. Furthermore, on a Stokes curve $\{z \in \mathbb{C}\,;\ \arg z = \pi/4\}$, for example, of (2.16) (to be more precise, when one crosses $\{\arg z = \pi/4\}$ anticlockwise), we have the connection formula

(2.17)
$$\varphi^{(+)} \longmapsto \varphi^{(+)}, \quad \varphi^{(-)} \longmapsto \varphi^{(-)} - 2^{i\mu\nu/2}\eta^{i\mu\nu/2}\mu\frac{\sqrt{\pi}}{\Gamma(i\mu\nu/2+1)}e^{\pi(i+\mu\nu)/4}\varphi^{(+)}$$

for the following fundamental system of solutions of (2.16):

$$
\begin{aligned}
\varphi^{(+)} &= \eta^{-1/2}\left\{\begin{pmatrix} 1 \\ \frac{-\eta^{-1/2}\nu_0}{2z} \end{pmatrix}+\cdots\right\}e^{i\eta z^2/2}z^{i\mu_0\nu_0/2}(1+\cdots), \\
\varphi^{(-)} &= \eta^{-1/2}\left\{\begin{pmatrix} \frac{\eta^{-1/2}\mu_0}{2z} \\ 1 \end{pmatrix}+\cdots\right\}e^{-i\eta z^2/2}z^{-i\mu_0\nu_0/2}(1+\cdots).
\end{aligned}
\tag{2.18}
$$

(See [T1] or [T2].) We can thus expect that the same connection formula with (2.17) holds also for the equation (2.1) on a Stokes curve emanating from a turning point when we adopt solutions which correspond to (2.18) through the reduction as (part of) fundamental system of solutions.

For example, let us consider the turning point t_{12}. The explicit scheme for constructing the reduction to (2.16) near t_{12} described in Appendix tells us that (the top order part of) the invariants μ and ν at t_{12} are respectively given by

$$
\mu_0 = \sqrt{\frac{2}{b_2-b_1}}c_{12}, \quad \nu_0 = \sqrt{\frac{2}{b_2-b_1}}\overline{c_{12}}
\tag{2.19}
$$

(cf. (A.54) in Appendix). In particular,

$$
\frac{i\mu_0\nu_0}{2} = \frac{i|c_{12}|^2}{b_2-b_1}
\tag{2.20}
$$

coincides with the Landau-Zener parameter κ_{12}. Further, if we introduce local WKB solutions $\psi_0^{(1)}$ and $\psi_0^{(2)}$ near $t = t_{12}$ by

$$
\begin{aligned}
\psi_0^{(1)} &= \eta^{-1/2}\exp\left(\frac{\eta}{i}\int_{t_{12}}^{t}\rho_1(t)dt\right)\left(\sqrt{\frac{b_2-b_1}{2}}(t-t_{12})\right)^{\kappa_{12}} \\
&\quad\times\left(\frac{\rho_3-\rho_1}{(\rho_3-\rho_1)(t_{12})}\right)^{\kappa_{13}}\left(e^{(1)}+O\left(\eta^{-1/2}\right)\right), \\
\psi_0^{(2)} &= \eta^{-1/2}\exp\left(\frac{\eta}{i}\int_{t_{12}}^{t}\rho_2(t)dt\right)\left(\sqrt{\frac{b_2-b_1}{2}}(t-t_{12})\right)^{-\kappa_{12}} \\
&\quad\times\left(\frac{\rho_3-\rho_2}{(\rho_3-\rho_2)(t_{12})}\right)^{\kappa_{23}}\left(e^{(2)}+O\left(\eta^{-1/2}\right)\right)
\end{aligned}
\tag{2.21}
$$

(where $e^{(j)}$ is a unit vector satisfying (2.5)), we find that $\psi_0^{(j)}$ ($j = 1, 2$) corresponds to $\varphi^{(\pm)}$ through the reduction to (2.16) near t_{12} (cf. (A.62) in

Appendix). Hence it can be expected that the same connection formula with (2.17) holds for $\psi_0^{(j)}$ $(j=1,2)$ on a Stokes curve emanating from t_{12}. As $\psi_0^{(j)}$ and $\psi^{(j)}$ are related by

$$
\begin{aligned}
\psi_0^{(1)} &= (2(b_2-b_1))^{-\kappa_{12}/2}\left(\frac{b_3-b_2}{b_2-b_1}a\right)^{-\kappa_{13}} \\
&\qquad \times e^{i\eta(a/(b_2-b_1))^2(b_2-b_1/2)}\left(1+O(\eta^{-1/2})\right)\psi^{(1)}, \\
\psi_0^{(2)} &= e^{-i\pi\kappa_{12}}(2(b_2-b_1))^{\kappa_{12}/2}\left(\frac{b_3-b_2}{b_2-b_1}a\right)^{-\kappa_{23}} \\
&\qquad \times e^{i\eta(a/(b_2-b_1))^2(b_2/2)}\left(1+O(\eta^{-1/2})\right)\psi^{(2)},
\end{aligned}
\tag{2.22}
$$

we conclude that $\psi^{(j)}$ $(j=1,2)$ should satisfy the following connection formula when they are analytically continued from the left to the right across the two Stokes curves emanating from t_{12} in the upper half-plane:

$$
\begin{cases}
\psi^{(1)} \longmapsto (1+\alpha_{12}^{-}\alpha_{12}^{+})\psi^{(1)}-\alpha_{12}^{-}\psi^{(2)} \\
\psi^{(2)} \longmapsto \psi^{(2)}-\alpha_{12}^{+}\psi^{(1)},
\end{cases}
\tag{2.23}
$$

where

$$
\begin{aligned}
\alpha_{12}^{\pm} &= c_{12}^{\pm}\frac{i\sqrt{2\pi}}{\Gamma(1\pm\kappa_{12})}\left(e^{\pm i\pi/2}(b_2-b_1)\right)^{-1/2}(2\eta)^{\pm\kappa_{12}}e^{(1/2\mp1)i\pi\kappa_{12}}\beta_{12}^{\pm1}, \\
\beta_{12} &= e^{i\pi\kappa_{12}}(2(b_2-b_1))^{-\kappa_{12}}\left(\frac{b_3-b_2}{b_2-b_1}a\right)^{\kappa_{23}-\kappa_{13}}e^{i\eta a^2/(2(b_2-b_1))}, \\
& c_{12}^{+}=c_{12}, \quad c_{12}^{-}=\overline{c_{12}}.
\end{aligned}
\tag{2.24}
$$

(In (2.24) we have omitted the symbol $(1+O(\eta^{-1/2}))$ for the sake of simplicity. We use the same abbreviation in what follows if there is no fear of confusions.) In other words, if we let M_{12} denote

$$
\begin{pmatrix}
1+\alpha_{12}^{-}\alpha_{12}^{+} & -\alpha_{12}^{+} & 0 \\
-\alpha_{12}^{-} & 1 & 0 \\
0 & 0 & 1
\end{pmatrix},
\tag{2.25}
$$

$\psi^{(j)}$'s enjoy the following connection formula when they are analytically continued from the left to the right near t_{12}:

$$
\left(\psi^{(1)},\psi^{(2)},\psi^{(3)}\right)\longmapsto\left(\psi^{(1)},\psi^{(2)},\psi^{(3)}\right)M_{12}.
\tag{2.26}
$$

In a similar manner, we can show that the invariants at $t_{23}=0$ satisfy

$$\mu_0=\sqrt{\frac{2}{b_3-b_2}}c_{23},\quad \nu_0=\sqrt{\frac{2}{b_3-b_2}}\overline{c_{23}},\quad \frac{i\mu_0\nu_0}{2}=\frac{i|c_{23}|^2}{b_3-b_2}=\kappa_{23}, \tag{2.27}$$

and the following connection formula holds when $\psi^{(j)}$ $(j=2,3)$ are analytically continued from the left to the right across the two Stokes curves emanating from $t_{23}=0$ in the upper half-plane:

$$\begin{cases} \psi^{(2)} & \longmapsto & (1+\alpha_{23}^{-}\alpha_{23}^{+})\psi^{(2)}-\alpha_{23}^{-}\psi^{(3)} \\ \psi^{(3)} & \longmapsto & \psi^{(3)}-\alpha_{23}^{+}\psi^{(2)}, \end{cases} \tag{2.28}$$

where

$$\begin{gathered} \alpha_{23}^{\pm}=c_{23}^{\pm}\frac{i\sqrt{2\pi}}{\Gamma(1\pm\kappa_{23})}\left(e^{\pm i\pi/2}(b_3-b_2)\right)^{-1/2}(2\eta)^{\pm\kappa_{23}}e^{(1/2\mp1)i\pi\kappa_{23}}\beta_{23}^{\pm1}, \\ \beta_{23}=e^{i\pi\kappa_{23}}(2(b_3-b_2))^{-\kappa_{23}}a^{\kappa_{12}-\kappa_{13}}, \\ c_{23}^{+}=c_{23},\quad c_{23}^{-}=\overline{c_{23}}. \end{gathered} \tag{2.29}$$

That is,

$$\left(\psi^{(1)},\psi^{(2)},\psi^{(3)}\right)\longmapsto\left(\psi^{(1)},\psi^{(2)},\psi^{(3)}\right)M_{23}, \tag{2.30}$$

where

$$M_{23}=\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1+\alpha_{23}^{-}\alpha_{23}^{+} & -\alpha_{23}^{+} \\ 0 & -\alpha_{23}^{-} & 1 \end{pmatrix}. \tag{2.31}$$

Furthermore, at t_{13} we have

$$\mu_0=\sqrt{\frac{2}{b_3-b_1}}c_{13},\quad \nu_0=\sqrt{\frac{2}{b_3-b_1}}\overline{c_{13}},\quad \frac{i\mu_0\nu_0}{2}=\frac{i|c_{13}|^2}{b_3-b_1}=\kappa_{13}, \tag{2.32}$$

and

$$\begin{cases} \psi^{(1)} & \longmapsto & (1+\alpha_{13}^{-}\alpha_{13}^{+})\psi^{(1)}-\alpha_{13}^{-}\psi^{(3)} \\ \psi^{(3)} & \longmapsto & \psi^{(3)}-\alpha_{13}^{+}\psi^{(1)}, \end{cases} \tag{2.33}$$

where
(2.34)
$$\alpha_{13}^{\pm} = c_{13}^{\pm}\frac{i\sqrt{2\pi}}{\Gamma(1 \pm \kappa_{13})}\left(e^{\pm i\pi/2}(b_3 - b_1)\right)^{-1/2}(2\eta)^{\pm\kappa_{13}}e^{(1/2\mp 1)i\pi\kappa_{13}}\beta_{13}^{\pm 1},$$
$$\beta_{13} = e^{i\pi(-\kappa_{12}+\kappa_{23}+\kappa_{13})}(2(b_3 - b_1))^{-\kappa_{13}}\left(\frac{b_3 - b_2}{b_3 - b_1}a\right)^{-\kappa_{12}-\kappa_{23}}e^{i\eta a^2/(2(b_3-b_1))},$$
$$c_{13}^{+} = c_{13}, \quad c_{13}^{-} = \overline{c_{13}}.$$
That is,
$$\left(\psi^{(1)}, \psi^{(2)}, \psi^{(3)}\right) \longmapsto \left(\psi^{(1)}, \psi^{(2)}, \psi^{(3)}\right) M_{13}, \tag{2.35}$$
where
$$M_{13} = \begin{pmatrix} 1 + \alpha_{13}^{-}\alpha_{13}^{+} & 0 & -\alpha_{13}^{+} \\ 0 & 1 & 0 \\ -\alpha_{13}^{-} & 0 & 1 \end{pmatrix}. \tag{2.36}$$

The connection matrix $\widetilde{S}$ for the WKB solution $\psi^{(j)}$ from $t = -\infty$ to $+\infty$ is then computed as the product $M_{12}M_{13}M_{23}$. The result is as follows:
$$\begin{pmatrix} e^{2i\pi(\kappa_{12}+\kappa_{13})} & \alpha_{23}^{-}\alpha_{13}^{+}e^{2i\pi\kappa_{12}} - \alpha_{12}^{+}e^{2i\pi\kappa_{23}} & -\alpha_{13}^{+}e^{2i\pi\kappa_{12}} + \alpha_{12}^{+}\alpha_{23}^{+} \\ -\alpha_{12}^{-}e^{2i\pi\kappa_{13}} & -\alpha_{12}^{-}\alpha_{23}^{-}\alpha_{13}^{+} + e^{2i\pi\kappa_{23}} & \alpha_{12}^{-}\alpha_{13}^{+} - \alpha_{23}^{+} \\ -\alpha_{13}^{-} & -\alpha_{23}^{-} & 1 \end{pmatrix}. \tag{2.37}$$
Finally, it follows from (2.13) and (2.37) that (the top order part of) the S-matrix for the equation (2.1) becomes
(2.38)
$$\begin{pmatrix} e^{i\pi(\kappa_{12}+\kappa_{13})} & \alpha_{23}^{-}\alpha_{13}^{+}e^{i\pi(2\kappa_{12}-\kappa_{23})} - \alpha_{12}^{+}e^{i\pi\kappa_{23}} & -\alpha_{13}^{+}e^{2i\pi\kappa_{12}} + \alpha_{12}^{+}\alpha_{23}^{+} \\ -\alpha_{12}^{-}e^{i\pi\kappa_{13}} & -\alpha_{12}^{-}\alpha_{23}^{-}\alpha_{13}^{+}e^{i\pi(\kappa_{12}-\kappa_{23})} + e^{i\pi(\kappa_{12}+\kappa_{23})} & (\alpha_{12}^{-}\alpha_{13}^{+} - \alpha_{23}^{+})e^{i\pi\kappa_{12}} \\ -\alpha_{13}^{-}e^{i\pi(-\kappa_{12}+\kappa_{23})} & -\alpha_{23}^{-}e^{i\pi\kappa_{13}} & e^{i\pi(\kappa_{23}+\kappa_{13})} \end{pmatrix}.$$

Thus we have been able to compute the S-matrix for the Landau-Zener model (2.1) for three levels by using the exact WKB analysis. It is based on the reduction to a Landau-Zener model for two levels at a turning point, i.e., a crossing point of energy levels. The Landau-Zener parameters appear in the computation as (the top order part of) the invariants at turning points.

3 A recipé for finding a complete Stokes geometry

As Berk-Nevins-Roberts ([BNR]) first discovered, addition of a new Stokes curve is necessary for obtaining a correct and consistent connection formula for WKB solutions near an ordered crossing point of Stokes curves. (For the reference of the reader, let us note that a crossing point of two Stokes curves respectively of type $(j > k)$ and of type $(l > m)$ $(j, k, l, m \in \{1, 2, 3\})$ is said to be ordered if $k = l$ or $j = m$. If a crossing point is not ordered, we say it is unordered, or non-ordered.) Later [AKT1] detected a point from which a new Stokes curve emanates, by studying the singularity structure of Borel transforms of WKB solutions. The point is called "a new turning point" in [AKT1], but we now coin the name "a virtual turning point". (The background of this naming is that such a point is intrinsically determined by the operator, independent of arg η on which a new Stokes curve depends, and that the new Stokes curve is irrelevant to the Stokes phenomena of WKB solutions in a neighborhood of the virtual turning point. Actually a new Stokes curve is designated by a broken line near a virtual turning point, indicating that no Stokes phenomenon is observed there, as discussed in Section 2. (Cf. [AKT1]).) The argument in [AKT1] is based on a mathematical result for a linear partial differential operator with simple characteristics, which appears as the Borel transform of the ordinary differential operator in question. In contrast to the operators discussed in [AKT1] operators discussed in this paper are with double turning points as a consequence of (1.5), and hence their Borel transforms are not with simple characteristics but rather with multiple characteristics. Singularities of solutions of such operators propagate along the so-called bicharacteristic chain, that is, they bifurcate along two mutually tangent bicharacteristic curves at a point where the simple characteristic condition is violated, that is, at a double turning point ([KKO], [P], [T2]).

An explicit and analytic form of a bicharacteristic chain $b(\kappa, T; \alpha, c)$ is given by (3.1) below, where κ is a multi-index $(k_1, k_2, \ldots, k_n)$ with $k_l \in \{1, 2, 3\}$ $(l = 1, 2, \ldots, n)$ such that $k_l \neq k_{l+1}$ $(l = 1, 2, \ldots, n-1)$, $T = (t^{(1)}, \ldots, t^{(n-1)})$ is a set of turning points such that $\rho_{k_l}(t^{(l)}) = \rho_{k_{l+1}}(t^{(l)})$ $(l = 1, 2, \ldots, n-1)$, and α and c are some constants.

(3.1)

$$
\begin{aligned}
&b(\kappa, T; \alpha, c) = \{(y,t) \in \mathbb{C}^2; y = i\int_\alpha^t \rho_{k_1} dt + c\} \\
&\cup \{(y,t) \in \mathbb{C}^2; y = i\int_{t^{(1)}}^t \rho_{k_2} dt + i\int_\alpha^{t^{(1)}} \rho_{k_1} dt + c\} \\
&\cup \cdots \cup \{(y,t) \in \mathbb{C}^2; y = i\int_{t^{(n-1)}}^t \rho_{k_n} dt + i\sum_{l=1}^{n-2}\int_{t^{(l)}}^{t^{(l+1)}} \rho_{k_{l+1}} dt + i\int_\alpha^{t^{(1)}} \rho_{k_1} dt + c\}.
\end{aligned}
$$

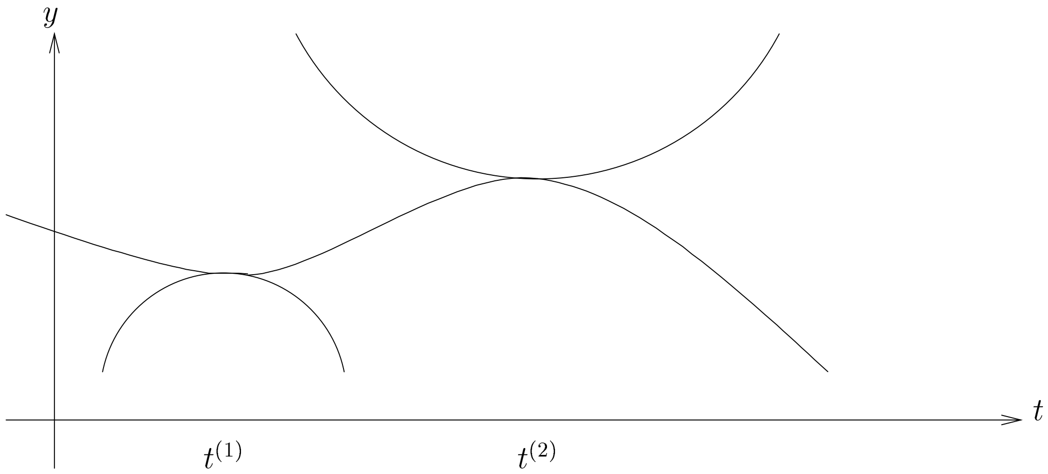


Figure 3.1: An example of a bicharacteristic chain.

Therefore, by replacing "a bicharacteristic curve" with "a bicharacteristic chain" in the reasoning of [AKT1], we conclude that a virtual turning point for (1.1) is the t-component of a self-intersection point of a bicharacteristic chain $b(\kappa, T; \alpha, c)$ with α being a turning point t_{jk_1}, i.e., $\rho_j(t_{jk_1}) = \rho_{k_1}(t_{jk_1})$ ($j \neq k_1, k_n$). As it is clear that c is irrelevant to the value of the t-component of a self-intersection point, we choose c to be 0 in what follows. If we let $k_0 = k_{n+1}$ and $t^{(0)}$ respectively denote j and t_{jk}, we find that the defining equation of a virtual turning point is determined by a multi-index $K = (k_0, k_1, \ldots, k_n)$ that satisfies $k_l \neq k_{l+1}$ for $l = 0, 1, \ldots, n$ [recall that

$k_{n+1} = k_0$ by the definition] and a K-dependent set T of turning points; the concrete form of the equation is given by $(3.3)_{K,T}$ below. Here and in what follows we always assume the condition (3.2) below to avoid the degeneracy that a bicharacteristic chain contains a closed loop:

(3.2) For any point α such that $\rho_{k_0}(\alpha) = \rho_{k_n}(\alpha)$,

$$-\int_{t^{(0)}}^{\alpha} \rho_{k_0} dt + \int_{t^{(n-1)}}^{\alpha} \rho_{k_n} dt + \sum_{l=1}^{n-1} \int_{t^{(l-1)}}^{t^{(l)}} \rho_{k_l} dt \neq 0.$$

$$(3.3)_{K,T} \qquad \int_{t^{(0)}}^{t} \rho_{k_0} dt = \int_{t^{(n-1)}}^{t} \rho_{k_n} dt + \sum_{l=1}^{n-1} \int_{t^{(l-1)}}^{t^{(l)}} \rho_{k_l} dt.$$

This equation enjoys the following important property:

Reflecting the double turning point character of the equation (1.1), the equation $(3.3)_{K,T}$ is quite complicated in its appearance. However, since $\rho_j(t)$ $(j = 1, 2, 3)$ is a polynomial, $(3.3)_{K,T}$ is an algebraic equation, and hence it admits only finitely many solutions. This presents a clear contrast to the situation for operators with simple discriminants ([AKT1]), where the defining equation of a virtual turning point is highly transcendental, and finding out its solutions is a difficult job in spite of the fact that there seems to exist infinitely many solutions (cf. [AKT1, pp.82-83]).

Making use of this significant property of $(3.3)_{K,T}$, we now present a recipé for adding new Stokes curves to resolve ordered crossings. Here "to resolve ordered crossings" means "to add an appropriate Stokes curve passing through an ordered crossing point so that a consistent connection formula for WKB solutions may be found" (cf. [AKT1, pp.83-84]). To describe the procedure concretely, let us introduce the following diagram which schematically describes the equation $(3.3)_{K,T}$; we call it a bicharacteristic diagram. The diagram is determined by (K, T), just as in the case of the equation $(3.3)_{K,T}$. Here K is a multi-index $(k_0, k_1, \ldots, k_n)$ with $k_l \in \{1, 2, 3\}$ $(l = 0, 1, \ldots, n)$ such that $k_l \neq k_{l+1}$ $(l = 0, 1, \ldots, n-1)$ and $k_0 \neq k_n$, and T is a set of turning points $\{t^{(0)}, t^{(1)}, \ldots, t^{(n-1)}\}$ such that

$$\rho_{k_l}(t^{(l)}) = \rho_{k_{l+1}}(t^{(l)}) \ (l = 0, 1, \ldots, n-1).$$

To such data (K, T) we assign a diagram $D(K, T)$ in the following manner: Diagram $D(K, T)$ consists of $(n-1)$ line segments labeled by k_l $(l = 1, \ldots, n-1)$, two half lines respectively labeled by k_0 and k_n, and n points labeled by

$t^{(l)}$ $(l = 0, 1, \ldots, n-1)$, so that the line k_l and the line k_{l+1} are hinged by the point $t^{(l)}$ $(l = 0, 1, \ldots, n-1)$. As a convention we let the half lines cross, and line segments are located in a linear order. To maintain the flavor of a bicharacteristic chain (cf. Figure 3.1), we draw line segments as curvilinear ones, but this is just a matter of taste. (See Figure 3.2 below.)

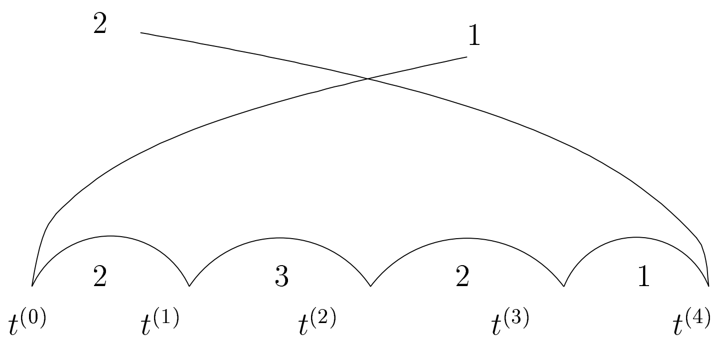
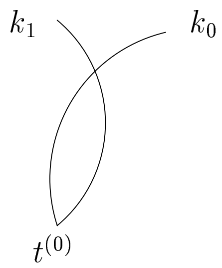


Figure 3.2: A bicharacteristic diagram with $K = (1, 2, 3, 2, 1, 2)$.

Remark 3.1 As a convention we consider $D(K_0, T_0)$ with $K_0 = (k_0, k_1)$ and $T_0 = (t^{(0)})$ as a bicharacteristic diagram, that is,



is, by definition, regarded as a bicharacteristic diagram. As simple zeros of $(3.3)_{K_0,T_0}$ are irrelevant to the Stokes phenomena, we concentratre our attention to double zeros in this case. But, then, the assumption (3.2) ensures that the only double zero of $(3.3)_{K_0,T_0}$ is $t = t^{(0)}$, that is, not a virtual turning point but an ordinary turning point is designated by the diagram $D(K_0, T_0)$.

For the practical application of bicharacteristic diagrams, the notions of their contractions and junctions are important. The contraction of a bicharacteristic diagram is the following procedure: if the points $t^{(l)}$ and $t^{(l+1)}$ are the same we replace the triplet of lines (k_l, k_{l+1}, k_{l+2}) by one line k_l. Note that $t^{(l)} = t^{(l+1)}$ entails $k_l = k_{l+2}$, as we are considering double turning points for three levels. For example, if $t^{(3)} = t^{(4)}$ in the diagram in Figure 3.2, its contraction becomes the diagram shown in Figure 3.3 below.

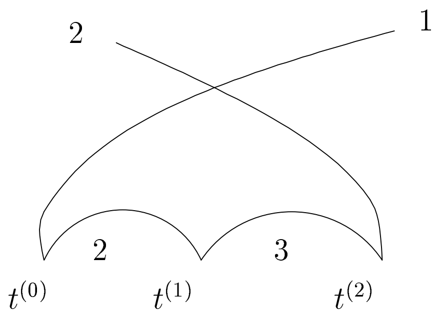


Figure 3.3: Contraction of the diagram in Figure 3.2.

Note that the contraction procedure is a counterpart of the vanishing of the integral

$$\int_{t^{(l)}}^{t^{(l+1)}} \rho_{k_{l+1}} dt$$

in $(3.3)_{K,T}$.

Junction of two bicharacteristic diagrams $D(K,T)$ and $D(K',T')$ is defined if $K = (k_0, \ldots, k_n)$ and $K' = (k'_0, \ldots, k'_m)$ satisfy the following condition:

(3.4) $\qquad \{k_0, k_n, k'_0, k'_m\}$ coincides with $\{1, 2, 3\}$ as sets.

Note that $k_0 \neq k_n$ and $k'_0 \neq k'_m$ by the assumption. Hence it suffices to define the "junction" $D(K,T)\#D(K',T')$ of $D(K,T)$ and $D(K',T')$ when

(3.4′) $\qquad k_0 = 1,\ k_n = 3,\ k'_0 = 3$ and $k'_m = 2.$

To define the junction let k_{n+l} and $t^{(n+l)}$ respectively denote k'_l and $t'^{(l)}$ for $l = 0, 1, \ldots, m-1$. This re-numbering is well-defined by the assumption (3.4′). The $D(K,T)\#D(K',T')$ is then obtained by joining $t^{(n-1)}$ and $t^{(n)}$ by k_n $(= 3)$.

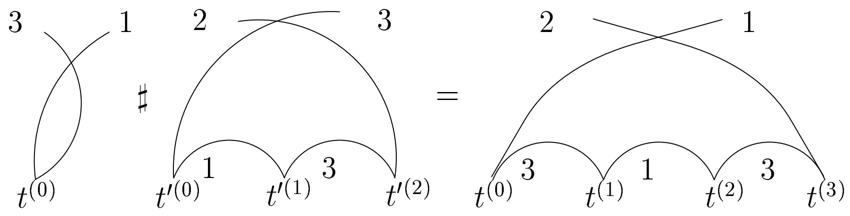
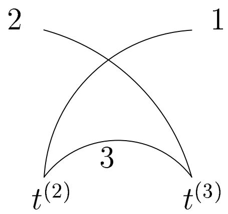


Figure 3.4: Junction of bicharacteristic diagrams.

Note that contraction may often be applied to the resulting diagram. For example, if $t^{(0)} = t'^{(0)}$ in the example in Figure 3.4, the resulting diagram may be contracted to the following:



The importance of the notion "junction" lies in the following fact (3.5):

(3.5) Suppose two (ordinary or new) Stokes curves σ_1 and σ_2 cross at a point a. Suppose further that σ_j $(j = 1, 2)$ emanates from a (virtual or ordinary) turning point designated by the bicharacteristic diagram $D(K_j, T_j)$ $(j = 1, 2,$ respectively). As condition (3.4) is satisfied in this case, we may assume (3.4′). If we consider the union σ of Stokes curves of type $(1, 2)$ that emanate from solutions of $(3.3)_{K,T}$ that corresponds to the bicharacteristic diagram $D(K, T) = D(K_1, T_1)\#D(K_2, T_2)$, then the crossing point a is contained in σ.

To validate the fact (3.5), we let $R_j(t)$ denote $\int_0^t \rho_j dt$ $(j = 1, 2, 3)$. (The lower endpoint 0 is chosen just for a uniform normalization.) By the assumptions, the Stokes curve σ_1 is given by

$$\text{(3.6)} \qquad \mathrm{Im}\,(i(R_1(t) - R_3(t))) = \mathrm{Im}\,(i(R_1(t_*) - R_3(t_*))),$$

where t_* is a solution of $(3.3)_{K_1,T_1}$. As $\rho_j(t)$ is a real polynomial by the assumption, (3.6) can be rewritten as

$$\mathrm{Re}\,(R_1(t) - R_3(t)) = \mathrm{Re}\,(R_1(t_*) - R_3(t_*)). \tag{3.7}$$

Similarly, σ_2 is given by

$$\mathrm{Re}\,(R_3(t) - R_2(t)) = \mathrm{Re}\,(R_3(t_{**}) - R_2(t_{**})), \tag{3.8}$$

where t_{**} is a solution of $(3.3)_{K_2,T_2}$. To write down the equations for t_* and t_{**}, let K_1 and K_2 be given respectively by $(k_0\ (=1), k_1, \ldots, k_n\ (=3))$ and $(k_n\ (=3), k_{n+1}, \ldots, k_{n+m}\ (=2))$, and let T_1 and T_2 be given respectively by $(t^{(0)}, \ldots, t^{(n-1)})$ and $(t^{(n)}, \ldots, t^{(n+m-1)})$. Then we find

$$\begin{aligned} &R_1(t_*) - R_1(t^{(0)}) \\ &\quad = R_3(t_*) - R_3(t^{(n-1)}) + \sum_{l=1}^{n-1}(R_{k_l}(t^{(l)}) - R_{k_l}(t^{(l-1)})), \end{aligned} \tag{3.9}$$

$$\begin{aligned} &R_3(t_{**}) - R_3(t^{(n)}) \\ &\quad = R_2(t_{**}) - R_2(t^{(n+m-1)}) + \sum_{l=1}^{m-1}(R_{k_{l+n}}(t^{(l+n)}) - R_{k_{l+n}}(t^{(l+n-1)})). \end{aligned} \tag{3.10}$$

On the other hand, σ is given by

$$\mathrm{Re}\,(R_1(t) - R_2(t)) = \mathrm{Re}\,(R_1(\tilde{t_*}) - R_2(\tilde{t_*})), \tag{3.11}$$

where $\tilde{t}_*$ satisfies

$$\begin{aligned} &R_1(\tilde{t}_*) - R_1(t^{(0)}) \\ &\quad = R_2(\tilde{t}_*) - R_2(t^{(n+m-1)}) + \sum_{l=1}^{n-1} R_{k_l}(t^{(l)}) - R_{k_l}(t^{(l-1)}) \\ &\qquad + R_3(t^{(n)}) - R_3(t^{(n-1)}) + \sum_{l=1}^{m-1} R_{k_{l+n}}(t^{(l+n)}) - R_{k_{l+n}}(t^{(l+n-1)}). \end{aligned} \tag{3.12}$$

Since a lies both on σ_1 and on σ_2, we find from (3.7) and (3.8)

$$\mathrm{Re}\,(R_1(a) - R_2(a)) = \mathrm{Re}\,(R_1(t_*) - R_3(t_*) + R_3(t_{**}) - R_2(t_{**})). \tag{3.13}$$

Furthermore it follows from (3.9) and (3.10) that

$$
\begin{aligned}
(3.14)\quad & R_1(t_*) - R_3(t_*) + R_3(t_{**}) - R_2(t_{**}) \\
&= R_1(t^{(0)}) - R_3(t^{(n-1)}) + \sum_{l=1}^{n-1} \big(R_{k_l}(t^{(l)}) - R_{k_l}(t^{(l-1)})\big) \\
&+ R_3(t^{(n)}) - R_2(t^{(n+m-1)}) + \sum_{l=1}^{m-1} \big(R_{k_{l+n}}(t^{(l+n)}) - R_{k_{l+n}}(t^{(l+n-1)})\big).
\end{aligned}
$$

It then follows from (3.12) that this coincides with $(R_1(\widetilde{t_*}) - R_2(\widetilde{t_*}))$. Therefore a lies on the Stokes curve σ, i.e.,

$$
\operatorname{Re}(R_1(a) - R_2(a)) = \operatorname{Re}(R_1(\widetilde{t_*}) - R_2(\widetilde{t_*})). \tag{3.15}
$$

This confirms the fact (3.5).

Remark 3.2 It is worth mentioning that the crossing point a in (3.5) may be either ordered or non-ordered, although we use the fact (3.5) to resolve an ordered crossing.

Let us now show how to use the fact (3.5) in obtaining a complete Stokes geometry, i.e., a Stokes geometry without ordered crossing points. We discuss Example 3.1 below in a somewhat detailed manner; it gives us several interesting lessons. Some other examples are included at the end of this section without any discussions.

Example 3.1 Let $\rho_1 = 1$, $\rho_2 = t/2$ and $\rho_3 = t^2$. Then the configuration of ordinary Stokes curves is given by Figure 3.5 below.

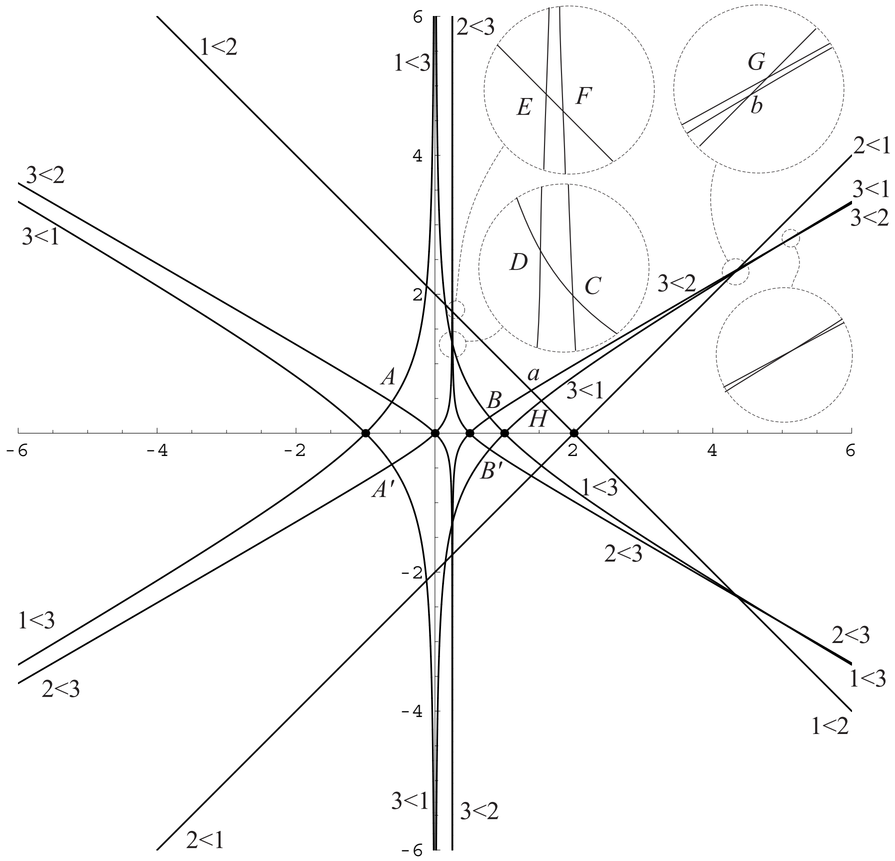
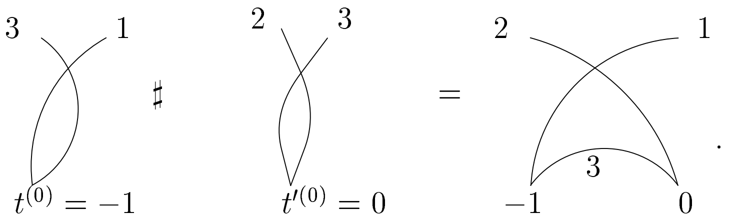


Figure 3.5: Ordinary Stokes curves of Example 3.1.

Because of the reality of ρ_j the geometry is symmetric with respect to the real axis. Hence we mainly study the geometry in the first and the second quadrants. There is one ordered crossing point A in the second quadrant. Together with its mirror image A' in the third quadrant, this ordered crossing should be resolved by a new Stokes curve emanating from a virtual turning point satisfying $(3.3)_{K,T}$ with

(3.16) $D(K,T) =$



The explicit form of $(3.3)_{K,T}$ is as follows in this case:

$$t + 1 = \frac{t^{\,2}}{4} + \frac{1}{3}\,. \tag{3.17}$$

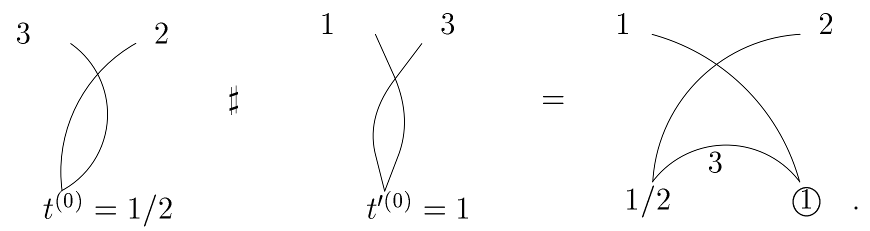
We then find a new Stokes curve of type $(1, 2)$ emanating from $t = 2 - \sqrt{20/3}$ resolves ordered crossing points A and A' simultaneously.

Let us now examine the configuration of (ordinary) Stokes curves in the region

$$\{t \in \mathbb{C}; 0 < \mathrm{Re}\ t < 1, \mathrm{Im}\ t > 0\}.$$

In this region we observe three ordered crossing points, labeled respectively by B, E and F in Figure 3.5. We first concentrate our attention to the point B; points E and F shall be discussed after we finish the study of the effect of resolving the ordered crossing point B. The point B is a crossing point of a Stokes curve emanating from $t = 1/2$ and that emanating from $t = 1$. Hence it should be resolved, again together with its mirror image B', by a new Stokes curve emanating from a virtual turning point determined by $(3.3)_{K,T}$, where $D(K,T)$ is given by (3.18) below:

(3.18)



Here and in what follows, a circled integer like ① indicates a turning point, not an index.) The explicit form of $(3.3)_{K,T}$ in this case is as follows:

$$\frac{t^2}{4} - \frac{1}{16} = t - 1 + \frac{1}{3} - \frac{1}{24} \ . \tag{3.19}$$

We then see that a new Stokes curve of type $(1, 2)$ passing through the virtual turnning point $t = 2 - \sqrt{17/12}$ resolves the ordered crossings simultaneously.

Let us now trace this new Stokes curve in $\{t \in \mathbb{C}; \operatorname{Im} t > 0\}$. There it is of type $(2 > 1)$ and its concrete form is shown in Figure 3.6 below.

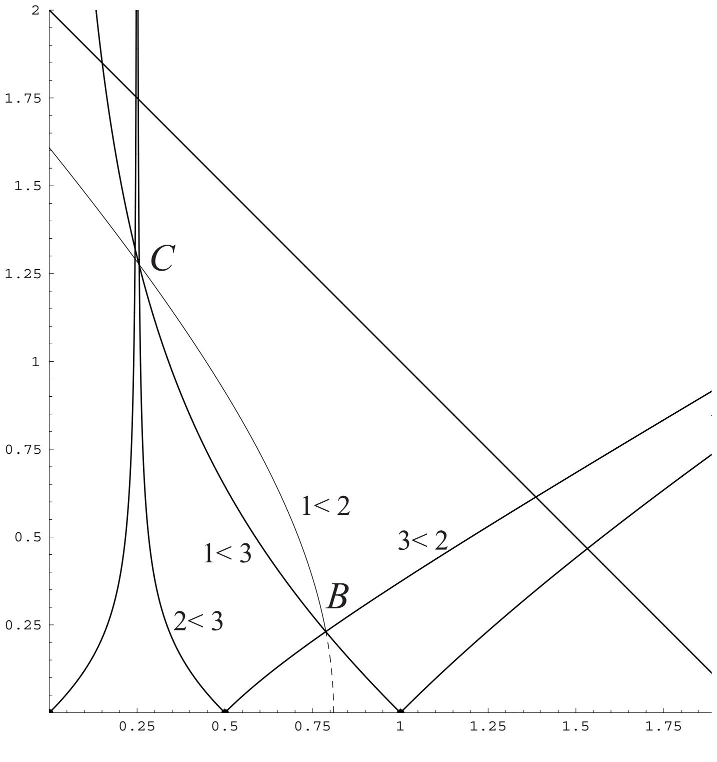
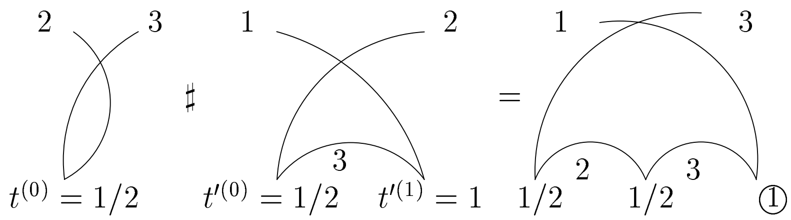


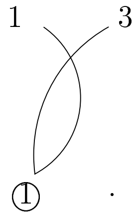
Figure 3.6: New Stokes curve resolving the ordered crossing point B.

Then the new Stokes curve in question crosses at C another (ordinary)Stokes curve of type $(3 > 2)$, which might appear to be a newly created ordered crossing point. The candidate for resolving this possible ordered crossing point is given by $(3.3)_{K,T}$ with $D(K,T)$ being given by (3.20) below.

(3.20)


,

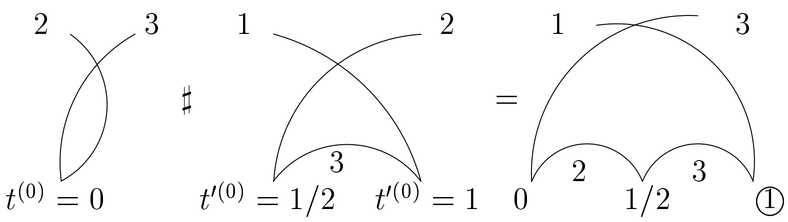
which is contracted to (3.21) below:

(3.21)


.

Thus the "new Stokes curve" to be added to resolve the "ordered crossing point" C is actually an ordinary Stokes curve. As a matter of fact one can readily confirm analytically (i.e., without the aid of a computer) that the point C is a non-ordered crossing point of ordinary Stokes curves respectively of type $(3 > 1)$ and of type $(3 > 2)$. Otherwise stated, three Stokes curves meet at the point C. As Rule (2.15c) in Section 2 tells us, the (new) Stokes curve of type $(2 > 1)$, i.e., of "adjacent type" thus remains to be a solid line after passing through the crossing point C, and it further crosses another ordinary Stokes curve of type $(3 > 2)$ emanating from $t = 0$. The crossing point D is ordered, and a new Stokes curve that resolves this ordered crossing point emanates from a virtual turning point defined by $(3.3)_{K,T}$ with $D(K,T)$ being given by (3.22) below.

(3.22)



Hence the explicit form of $(3.3)_{K,T}$ reads as follows:

(3.23)
$$\frac{t^3}{3} = t - 1 + \frac{1}{16} + \frac{1}{3} - \frac{1}{24}.$$

As shown in Figure 3.7 below, we can then confirm that a new Stokes curve emanating from $t = 1 - \delta \quad (\delta > 0)$ that satisfies (3.23) passes through the point D, resolving the ordered crossing point.

Although this new Stokes curve of type $(3 > 1)$ does not cross any more Stokes curves, the new Stokes curve of type $(2 > 1)$ further cross (in the second quadrant) another Stokes curve of type $(3 > 1)$ that emanates from $t = -1$. But, the crossing point is non-ordered. Thus, as far as these new Stokes curves are concerned, no problems remain.

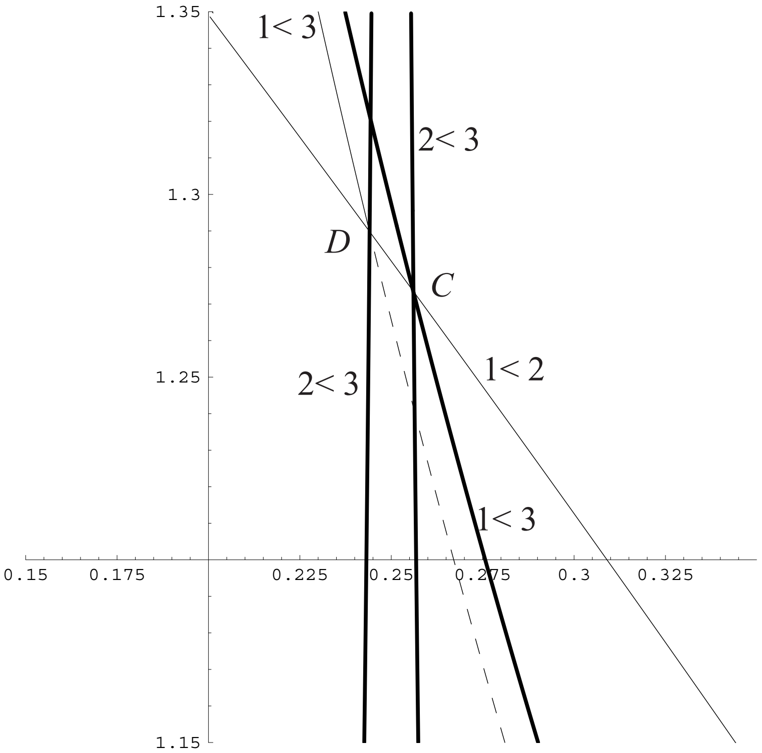
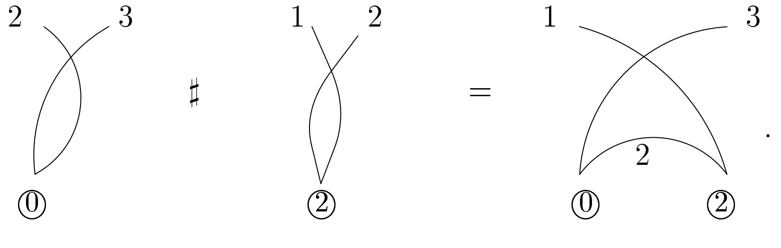


Figure 3.7: New Stokes curve resolving the ordered crossing point D.

Now let us come back to the study of points E and F. The ordered crossing point E is an intersection point of the Stokes curve emanating from 0 with type $(3 > 2)$ and that emanating from 2 with type $(2 > 1)$; hence it should be resolved by a new Stokes curve emanating from a virtual turning point defined by $(3.3)_{K,T}$ with $D(K,T)$ being given by (3.24) below.

(3.24)



The concrete form of the equation is:

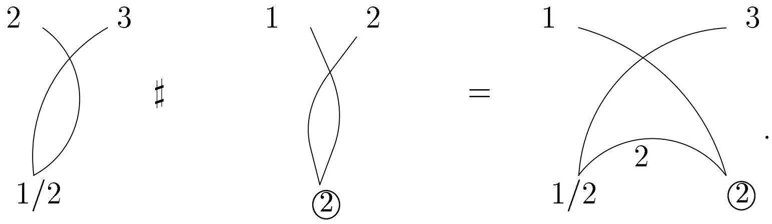
$$\frac{t^3}{3} = t - 2 + 1. \tag{3.25}$$

We can easily check that this equation has one solution t_* in the first quadrant (near $1.1 + 0.7\sqrt{-1}$), and the Stokes curve of type $(3 > 1)$ that emanates from t_* passes through the point E, resolving the ordered crossing. A similar discussion shows that we are to seek for a solution t_{**} of the equation

$$\frac{t^3}{3} - \frac{1}{24} = t - 2 + 1 - \frac{1}{16}, \tag{3.26}$$

which is read off from the following diagram (3.27):

(3.27) $D_F \underset{\text{det}}{=}$



Extending this new Stokes curve beyond t_{**}, we are naturally led to the study of the configuration of ordinary Stokes curves in the region $\{t \in \mathbb{C}; \mathrm{Re}\ t > 1, \mathrm{Im}\ t > 0\}$. As we see in Figure 3.5 there exist two ordered crossing points G and H in the region. Interestingly enough, the defining equation for a virtual turning point needed to resolve G is the same as (3.26), because the associated bicharacteristic diagram is the same as D_F. It may be worth noting that the new Stokes curve in question also passes through the non-ordered crossing point a. See Figure 3.8 below. Note that this new Stokes curve changes its type at t_{**}; thus both F and G are simultaneously resolved by one new Stokes curve.

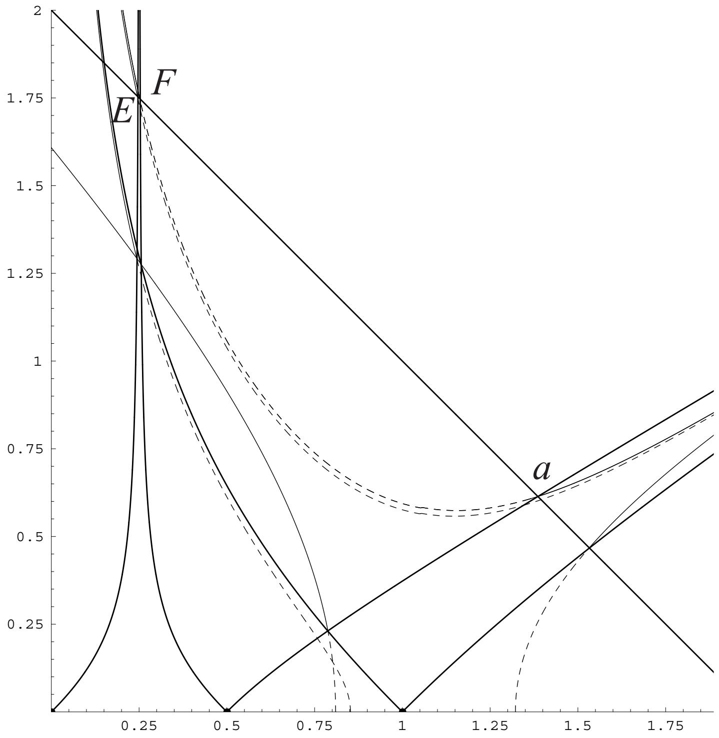
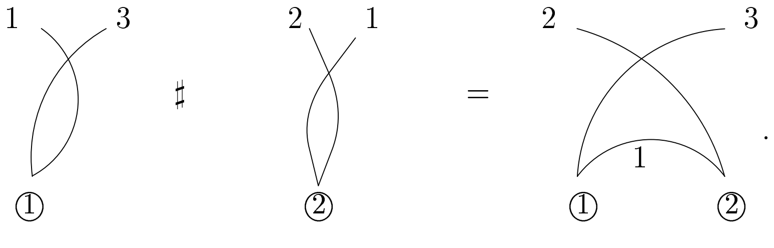


Figure 3.8: New Stokes curve resolving two ordered crossing points F and G simultaneously.

Finally let us study the ordered crossing point H in Figure 3.5. Since it is a crossing point of the Stokes curve emanating from 1 with type $(1 > 3)$ and that emanating from 2 with type $(2 > 1)$, the associated bicharacteristic diagram is given by (3.28) below:

(3.28)

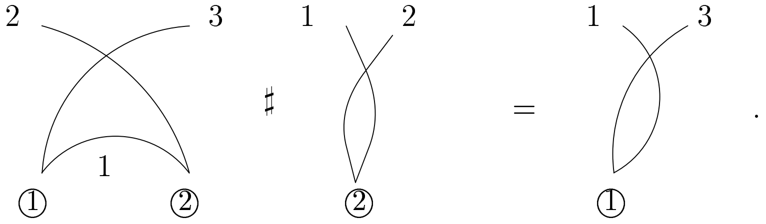


Hence the defining equation of the required virtual turning point is

$$\frac{t^3}{3} - \frac{1}{3} = \frac{t^2}{4} - 1 + (2 - 1). \tag{3.29}$$

As this equation has one real solution t_0 ($\fallingdotseq 1.3$), a new Stokes curve emanating from t_0 resolves H, together with its mirror image H' simultaneously. Extending this new Stokes curve beyond H, we find that it intersects with an ordinary Stokes curve emanating from 2 and that emanating from 1. Fortunately these three Stokes curves meet at one and the same point b. (Cf. Figure 3.9 below.) This fact can be immediately understood if we use bicharacteristic diagrams; for example, at the potential ordered crossing point, say δ, of the Stokes curve of type $(1 > 2)$ and the new Stokes curve emanating from t_0 with type $(2 > 3)$ near δ should be resolved by a new Stokes curve that emanates from a virtual turning point whose defining equation is $(3.3)_{K,T}$ with $D(K, T)$ being given by (3.30) below:

(3.30)



This means that the new Stokes curve is actually an ordinary Stokes curve emanating from 1. Therefore δ coincides with b, the non-ordered crossing point of an ordinary Stokes curve of type $(1 > 2)$ and that of type $(1 > 3)$.

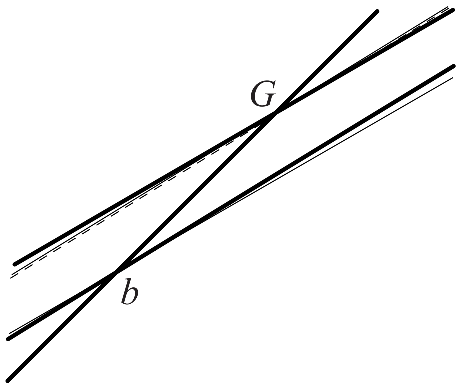


Figure 3.9: Three Stokes curves meeting at the point b.

Thus we have resolved all the ordered crossing points of ordinary Stokes curves together with all the newly created ones by the addition of new Stokes curves. The resulting Stokes geometry is as follows.

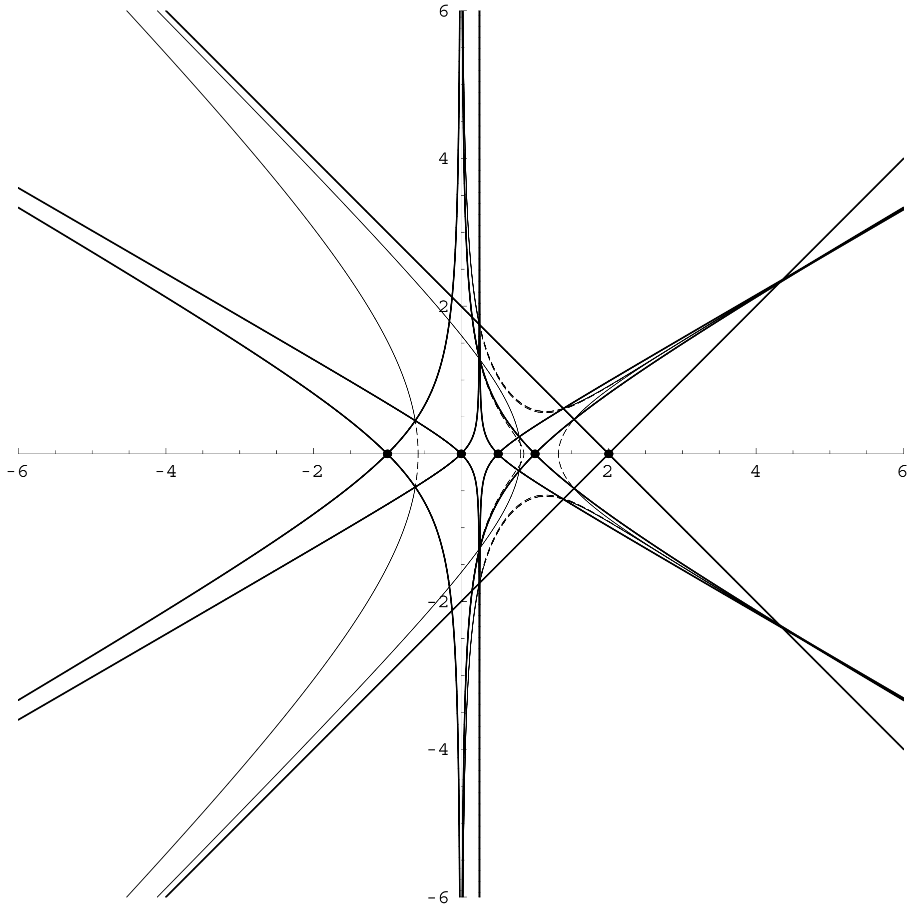


Figure 3.10: Complete Stokes geometry of Example 3.1.

For the reference of the reader, we present two examples of completed Stokes geometry. We omit the explanations how to obtain them. They are actually simpler to analyze than Example 3.1, as points like D, i.e., newly created ordered crossing points do not appear in Examples 3.2 and 3.3.

Example 3.2 *($\rho_1 = 0, \rho_2 = t$ and $\rho_3 = t^2 - 2$.)*

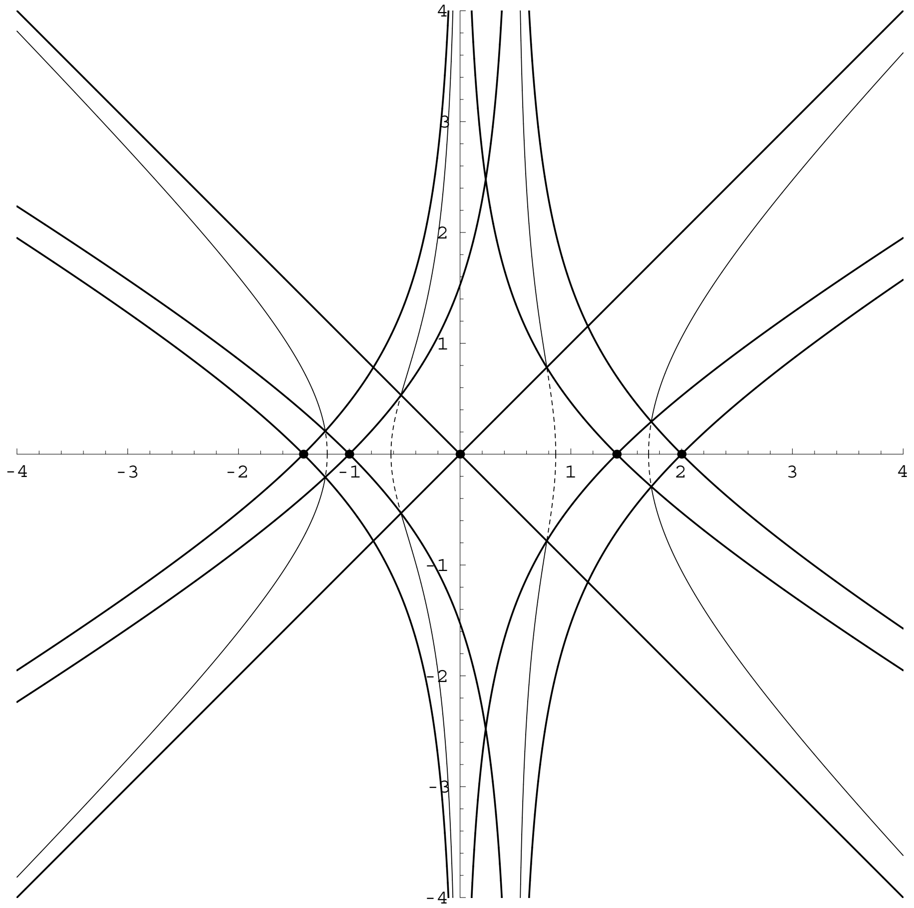


Figure 3.11: Complete Stokes geometry of Example 3.2.

Example 3.3 *($\rho_1 = 1 - 5t^2 + t^4, \rho_2 = -\frac{3}{2}t^2$ and $\rho_3 = -2.$)*

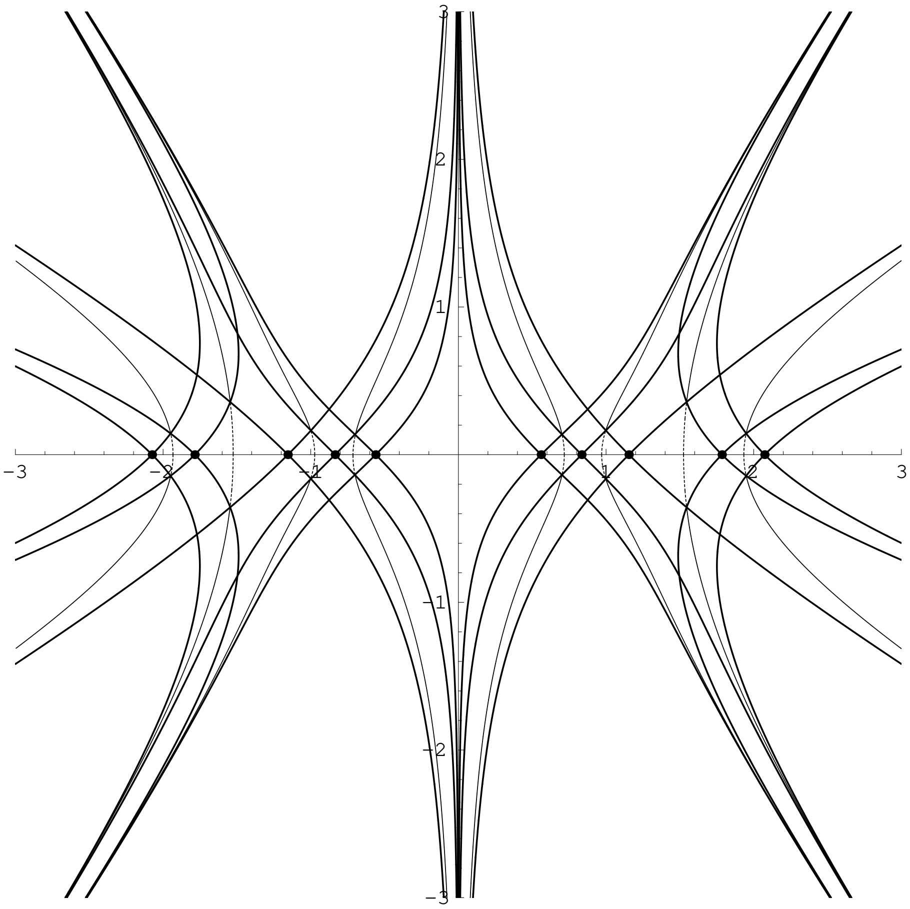


Figure 3.12: Complete Stokes geometry of Example 3.3.

4 Computation of the transition probabilities: General case

In this section we present a general recipé for computing the transition probabilities from $t = -\infty$ to $t = +\infty$ of solutions of (1.1). An important observation for obtaining such a general result is that, thanks to the reality assumption (1.5), a new Stokes curve emanating from a non-real virtual turning point never crosses the real axis. To confirm this, let us consider a non-real virtual turning point t_* determined by $(3.3)_{K,T}$ with appropriate K and T. That is, t_* is a solution of

$$(4.1)\qquad \int_0^{t_*} (\rho_{k_0} - \rho_{k_n})\, dt = \int_0^{t^{(0)}} \rho_{k_0} dt - \int_0^{t^{(n-1)}} \rho_{k_n} dt + \sum_{l=1}^{n-1} \int_{t^{(l-1)}}^{t^{(l)}} \rho_{k_l} dt.$$

Since (1.5) entails the right-hand side of (4.1) is real, the mirror image $\overline{t}_*$ of t_* (with respect to the real axis) is also a virtual turning point. (In fact, $\overline{t}_*$ also satisfies (4.1).) Furthermore the same reasoning shows that the mirror image $\overline{\sigma}$ of the new Stokes curve σ emanating from t_* is a new Stokes curve emanating from $\overline{t}_*$. If σ meets with the real axis and if the union $\sigma \cup \overline{\sigma}$ is non-singular as t ranges from t_* to $\overline{t}_*$ along it, we find

$$(4.2)\qquad \operatorname{Im} \int_{t_*}^{t} (\rho_{k_0} - \rho_{k_n}) dt \text{ is monotonically increasing or decreasing.}$$

But, as both t_* and $\overline{t}_*$ are solutions of the same equation (4.1) and hence $\displaystyle\int_{t_*}^{\overline{t}_*} (\rho_{k_0} - \rho_{k_n}) dt = 0$ holds, this means $t_* = \overline{t}_*$, contradicting the assumption that t_* is non-real. Hence there exists a singular point, say α, of the curve $\sigma \cup \overline{\sigma}$. By virtue of the Cauchy-Riemann equation for the integral $\displaystyle\int_{t_*}^{t} (\rho_{k_0} - \rho_{k_n}) dt$, we find

$$(4.3)\qquad \rho_{k_0}(\alpha) = \rho_{k_n}(\alpha).$$

Therefore α is a turning point. Hence it lies on the real axis by the assumption (1.5). In particular, $\displaystyle\int_{t_*}^{\alpha} (\rho_{k_0} - \rho_{k_n}) dt$ is real, while it is purely imaginary as α is on the new Stokes curve $\sigma \cup \overline{\sigma}$. Hence the integral $\displaystyle\int_{t_*}^{\alpha} (\rho_{k_0} - \rho_{k_n}) dt$ must be zero and, by the same reasoning as above, α should coincide with t_*, again leading to a contradiction. Thus we have confirmed that a new Stokes curve emanating from a non-real virtual turning point never meets with the real axis.

On the other hand, a new Stokes curve emanating from a virtual turning point on the real axis is a broken line near the real axis, that is, it is irrelevant to the Stokes phenomena of WKB solutions. To be very strict, we have to pay some special attention to the case where a virtual turning point and an ordinary turning point happen to coincide. This degenerate case is, however, eliminated by the assumption (3.2). Thus it suffices to take into account the effect of ordinary Stokes curves in a complete Stokes geometry (i.e., a collection of Stokes curves whose crossing points are all non-ordered), as far as we are concerned with the connection problems near the real axis.

Hence we can compute the transition probabilities for a general three level problem (1.1) in the following manner: First, as a fundamental system of solutions, we consider the following WKB solutions $\psi^{(j)}$ $(j = 1, 2, 3)$:

(4.4)
$$\psi^{(j)} = \eta^{-1/2} \exp\left(\frac{\eta}{i}\int_{t_0}^{t} \rho_j(t)dt + \frac{1}{i}\int_{t_0}^{t}\left(\frac{|c_{jk}|^2}{\rho_j - \rho_k} + \frac{|c_{jl}|^2}{\rho_j - \rho_l}\right)dt\right)\left(e^{(j)} + O\left(\eta^{-1/2}\right)\right),$$

where t_0 is a base point which is arbitrarily fixed (as far as it does not coincide with a turning point), $e^{(j)}$ is a unit vector satisfying (2.5), and $\{j, k, l\}$ is a permutation of $\{1, 2, 3\}$. We choose normalization constants $N^{\pm,(j)}$ so that $\psi^{\pm,(j)} = N^{\pm,(j)}\psi^{(j)}$ may satisfy (2.12). Note that, in view of the asymptotic behavior of WKB solutions near $t = \pm\infty$, we can choose $N^{\pm,(j)} = 1$ except when $\rho_j - \rho_k$ is a polynomial of degree one for some k. Next, we list up all the (real) turning points $\{t_{jk}\}$ and arrange them in an increasing order like $\{t_{jk}^{[n]}\}_{n=1,\dots,N}$, that is, we number $\{t_{jk}\}$ by counting them from the left (i.e., from $t = -\infty$). Then, our WKB solutions $\psi^{(j)}$ $(j = 1, 2, 3)$ should satisfy the following connection formula when they are analytically continued from the left to the right across the two Stokes curves emanating from $t_{jk}^{[n]}$ in the upper half-plane:

$$(4.5)\qquad \begin{cases} \psi^{(j)} & \longmapsto \quad (1 + \alpha_{jk}^{[n],-}\alpha_{jk}^{[n],+})\psi^{(j)} - \alpha_{jk}^{[n],-}\psi^{(k)} \\ \psi^{(k)} & \longmapsto \quad \psi^{(k)} - \alpha_{jk}^{[n],+}\psi^{(j)}. \end{cases}$$

Here we are assuming that

$$(4.6)\qquad \lambda_{jk}^{[n]} \overset{\text{def}}{=} \frac{d}{dt}(\rho_k - \rho_j)\Big|_{t=t_{jk}^{[n]}} > 0$$

holds (by exchanging the indices j and k we may assume (4.6) without loss of generality) and (the top order part of) $\alpha_{jk}^{[n],\pm}$ is given as follows:

$$(4.7)\quad \alpha_{jk}^{[n],\pm} = c_{jk}^{\pm}\frac{i\sqrt{2\pi}}{\Gamma(1 \pm \kappa_{jk}^{[n]})}\left(e^{\pm i\pi/2}\lambda_{jk}^{[n]}\right)^{-1/2}(2\eta)^{\pm\kappa_{jk}^{[n]}}e^{(1/2\mp 1)i\pi\kappa_{jk}^{[n]}}(\beta_{jk}^{[n]})^{\pm 1},$$

where

$$c_{jk}^{+} = c_{jk}, \quad c_{jk}^{-} = \overline{c_{jk}}, \quad \kappa_{jk}^{[n]} = \frac{i|c_{jk}|^2}{\lambda_{jk}^{[n]}}, \tag{4.8}$$

and $\beta_{jk}^{[n]}$ can be computed by comparing the WKB solutions (4.4) with the following:

(4.9)

$$\begin{aligned} \psi_0^{(j)} &= \eta^{-1/2} \exp\left(\frac{\eta}{i}\int_{t_{jk}^{[n]}}^{t} \rho_j(t)dt + \frac{1}{i}\int_{t_{jk}^{[n]}}^{t} \left(|c_{jk}|^2\left(\frac{1}{\rho_j-\rho_k} + \frac{1}{\lambda_{jk}^{[n]}(t-t_{jk}^{[n]})}\right)\right.\right. \\ &\quad \left.\left. + \frac{|c_{jl}|^2}{\rho_j-\rho_l}\right)dt\right)\left(\frac{\lambda_{jk}^{[n]}(t-t_{jk}^{[n]})^2}{2}\right)^{\kappa_{jk}^{[n]}/2} \left(e^{(j)} + O\left(\eta^{-1/2}\right)\right), \\ \psi_0^{(k)} &= \eta^{-1/2} \exp\left(\frac{\eta}{i}\int_{t_{jk}^{[n]}}^{t} \rho_k(t)dt + \frac{1}{i}\int_{t_{jk}^{[n]}}^{t} \left(-|c_{jk}|^2\left(\frac{1}{\rho_j-\rho_k} + \frac{1}{\lambda_{jk}^{[n]}(t-t_{jk}^{[n]})}\right)\right.\right. \\ &\quad \left.\left. + \frac{|c_{kl}|^2}{\rho_k-\rho_l}\right)dt\right)\left(\frac{\lambda_{jk}^{[n]}(t-t_{jk}^{[n]})^2}{2}\right)^{-\kappa_{jk}^{[n]}/2} \left(e^{(k)} + O\left(\eta^{-1/2}\right)\right), \end{aligned}$$

that is, $\beta_{jk}^{[n]}$ is determined by

$$\beta_{jk}^{[n]} = \frac{\gamma_j^{[n]}}{\gamma_k^{[n]}} \tag{4.10}$$

where

$$\psi_0^{(j)} = \gamma_j^{[n]}\psi^{(j)}, \quad \psi_0^{(k)} = \gamma_k^{[n]}\psi^{(k)}. \tag{4.11}$$

Note that the WKB solutions (4.9) correspond to the solutions (2.18) of the Landau-Zener model (2.16) for two levels through the reduction to (2.16) near $t_{jk}^{[n]}$. As is done in Section 2, the connection formula (4.5) can also be expressed with some 3×3 matrix $M^{[n]}$ in the following manner:

$$\left(\psi^{(1)}, \psi^{(2)}, \psi^{(3)}\right) \longmapsto \left(\psi^{(1)}, \psi^{(2)}, \psi^{(3)}\right) M^{[n]}. \tag{4.12}$$

Since a Stokes curve emanating from an ordinary turning point never meets again with the real axis (which can be verified by the same reasoning as that

used to confirm that a new Stokes curve emanating from a non-real virtual turning point does not cross the real axis), we thus conclude that
(4.13)

$$\begin{pmatrix} N^{+,(1)} & 0 & 0 \\ 0 & N^{+,(2)} & 0 \\ 0 & 0 & N^{+,(3)} \end{pmatrix}^{-1} M^{[N]} \cdots M^{[1]} \begin{pmatrix} N^{-,(1)} & 0 & 0 \\ 0 & N^{-,(2)} & 0 \\ 0 & 0 & N^{-,(3)} \end{pmatrix}$$

describes the S-matrix for the equation (1.1).

Appendix Reduction to a Landau-Zener model for two levels at a turning point

In this Appendix we construct a formal reduction of our three level problem (1.1) with the Hamiltonian given by (1.2) to a Landau-Zener model for two levels at a turning point. Similar reductions have already been discussed for systems of the form (1.1) with $H(t,\eta) = H_0(t) + \eta^{-1}H_1(t) + \eta^{-2}H_2(t) + \cdots$, that is, when $H(t,\eta)$ is a formal power series in η^{-1} with holomorphic coefficients, at a simple turning point in [W] and at a double turning point in [T2]. The argument employed in this Appendix is a slight modification of that used in [T2].

Before discussing the reduction at a turning point, we first review briefly the construction of WKB solutions of (1.1) as a preliminary. To construct WKB solutions, we use the following formal diagonalization of (1.1) (cf. [W], [T2]): Since the top order part of (1.1) (with respect to η) is already diagonal by the assumption (1.3), we start with the diagonalization of the order 1/2 part. For this purpose we consider a change of unknown functions of the form

$$\psi = \left(1 + \eta^{-1/2}P_{1/2}(t)\right)\varphi. \tag{A.1}$$

Then φ should satisfy

$$\begin{aligned} i\frac{d}{dt}\varphi &= \eta\left((1+\eta^{-1/2}P_{1/2})^{-1}(H_0+\eta^{-1/2}H_{1/2})(1+\eta^{-1/2}P_{1/2}) \right. \\ &\qquad \left. - i\eta^{-3/2}(1+\eta^{-1/2}P_{1/2})^{-1}\frac{dP_{1/2}}{dt}\right)\varphi \\ &= \eta\left(H_0 + \eta^{-1/2}\left(H_{1/2} + [H_0, P_{1/2}]\right) + \cdots\right)\varphi, \end{aligned} \tag{A.2}$$

where [,] denotes the commutator of two matrices. Hence, if we define each off-diagonal entry $(P_{1/2})_{jk}$ $(j \neq k)$ of $P_{1/2}(t)$ by

$$(P_{1/2})_{jk} = -\frac{c_{jk}}{\rho_j(t) - \rho_k(t)} \tag{A.3}$$

(here we are assuming $c_{jk} = \overline{c_{kj}}$ for $j > k$), the order 1/2 part of (A.2) vanishes as all the diagonal components of $H_{1/2}(t)$ are zero by the assumption (1.4). This procedure can be continued up to arbitrarily higher orders, that is, for an arbitrary integer n we can diagonalize (1.1) up to order $n/2$ by introducing a change of unknown functions $\psi = (1 + \eta^{-n/2} P_{n/2}(t))\varphi$ in a recursive way. Hence we find a formal transformation

$$\psi = R(t,\eta)\varphi, \quad R(t,\eta) = 1 + \eta^{-1/2} R_{1/2}(t) + \cdots = (1 + \eta^{-1/2} P_{1/2})(1 + \eta^{-1} P_1) \cdots \tag{A.4}$$

which transforms the equation (1.1) into

$$i\frac{d}{dt}\varphi = \eta \left[H_0(t) + \eta^{-1} \tilde{H}_1(t) + \eta^{-3/2} \tilde{H}_{3/2}(t) + \cdots \right] \varphi \tag{A.5}$$

where every matrix $\tilde{H}_{n/2}(t)$ is diagonal. Since the diagonalized system (A.5) can be readily solved, we thus obtain a formal solution of (1.1) of the form

$$\psi^{(j)} = \exp\left(\frac{\eta}{i} \int^t \rho_j(t) dt \right) \sum_{m=0}^{\infty} \psi^{(j)}_{m/2}(t) \eta^{-(m+1)/2} \tag{A.6}$$

(where each $\psi^{(j)}_{m/2}(t)$ is an n-vector) by substituting a solution of (A.5) whose k-th components are all zero except for $k = j$ into the right-hand side of the transformation (A.4).

For example, in the case of the equation (2.1), i.e., a generalization of the Landau-Zener model to three levels, the first few terms of the transformation (A.4) and those of the diagonalized system (A.5) are given as follows:

$$R_{1/2} = \begin{pmatrix} 0 & \frac{c_{12}}{\rho_2 - \rho_1} & \frac{c_{13}}{\rho_3 - \rho_1} \\ \frac{\overline{c_{12}}}{\rho_1 - \rho_2} & 0 & \frac{c_{23}}{\rho_3 - \rho_2} \\ \frac{\overline{c_{13}}}{\rho_1 - \rho_3} & \frac{\overline{c_{23}}}{\rho_2 - \rho_3} & 0 \end{pmatrix}, \tag{A.7}$$

$$R_1 = \begin{pmatrix} 0 & \frac{\overline{c_{23}} c_{13}}{(\rho_2 - \rho_1)(\rho_2 - \rho_3)} & \frac{c_{12} c_{23}}{(\rho_3 - \rho_1)(\rho_3 - \rho_2)} \\ \frac{c_{23} \overline{c_{13}}}{(\rho_1 - \rho_2)(\rho_1 - \rho_3)} & 0 & \frac{\overline{c_{12}} c_{13}}{(\rho_3 - \rho_1)(\rho_3 - \rho_2)} \\ \frac{\overline{c_{12}}\, \overline{c_{23}}}{(\rho_1 - \rho_2)(\rho_1 - \rho_3)} & \frac{c_{12} \overline{c_{13}}}{(\rho_2 - \rho_1)(\rho_2 - \rho_3)} & 0 \end{pmatrix}, \tag{A.8}$$

$$\text{(A.9)} \qquad H_0 = \begin{pmatrix} \rho_1 & 0 & 0 \\ 0 & \rho_2 & 0 \\ 0 & 0 & \rho_3 \end{pmatrix},$$

$$\text{(A.10)} \qquad \tilde{H}_1 = \begin{pmatrix} \frac{|c_{12}|^2}{\rho_1-\rho_2} + \frac{|c_{13}|^2}{\rho_1-\rho_3} & 0 & 0 \\ 0 & \frac{|c_{12}|^2}{\rho_2-\rho_1} + \frac{|c_{23}|^2}{\rho_2-\rho_3} & 0 \\ 0 & 0 & \frac{|c_{13}|^2}{\rho_3-\rho_1} + \frac{|c_{23}|^2}{\rho_3-\rho_2} \end{pmatrix},$$

$$\text{(A.11)} \qquad \tilde{H}_{3/2} = (c_{12}c_{23}\overline{c_{13}} + \overline{c_{12}}\ \overline{c_{23}}c_{13}) \begin{pmatrix} \frac{1}{(\rho_1-\rho_2)(\rho_1-\rho_3)} & 0 & 0 \\ 0 & \frac{1}{(\rho_2-\rho_1)(\rho_2-\rho_3)} & 0 \\ 0 & 0 & \frac{1}{(\rho_3-\rho_1)(\rho_3-\rho_2)} \end{pmatrix},$$

where $\rho_1(t) = b_1 t + a$, $\rho_2(t) = b_2 t$ and $\rho_3(t) = b_3 t$. Hence, letting $e^{(j)}$ denote a unit vector satisfying $e^{(j)}_k = \delta_{jk}$, we find that (2.1) has the following WKB solutions:

(A.12)

$$\begin{aligned} \psi^{(j)} &= \eta^{-1/2} \exp\left(\frac{\eta}{i}\int^t \left(\rho_j(t) + \eta^{-1}\left(\frac{|c_{kj}|^2}{\rho_j-\rho_k} + \frac{|c_{lj}|^2}{\rho_j-\rho_l}\right) + O(\eta^{-3/2})\right) dt\right) \\ &\qquad \times \left(e^{(j)} + O(\eta^{-1/2})\right) \\ &= \eta^{-1/2} \exp\left(\frac{\eta}{i}\int^t \rho_j(t)dt\right) (\rho_k-\rho_j)^{-\kappa_{kj}} (\rho_l-\rho_j)^{-\kappa_{lj}} \left(e^{(j)} + O\left(\eta^{-1/2}\right)\right). \end{aligned}$$

Here $\kappa_{\alpha\beta}$ denotes a Landau-Zener parameter (2.6) and $\{j,k,l\}$ is a permutation of $\{1,2,3\}$.

In order to seek for the explicit form of the connection formula for Borel sums of these WKB solutions, we now discuss the reduction at a turning point. Since we assume that only two of the $\rho_j(t)$'s merge at a turning point (cf. (1.5)), we can decompose the system (1.1) into the direct sum of two smaller systems, one of which is of size 2×2 and the other of which is of size 1×1, by the following transformation near the turning point in question:

$$\text{(A.13)} \qquad \psi = S(t,\eta)\varphi, \quad S(t,\eta) = 1 + \eta^{-1/2}S_{1/2}(t) + \eta^{-1}S_1(t) + \cdots$$

where each entry of $S_{j/2}(t)$ is holomorphic near the turning point ("block diagonalization"; cf. [W], [T2]). Thus it suffices to consider the reduction of a 2×2 system. Furthermore, as every turning point is a double turning point by virtue of (1.5), by employing a gauge transformation

$$\psi = \exp\left(\frac{\eta}{2i}\int_{t_{jk}}^{t} \operatorname{trace} H_0(t)dt\right)\varphi \tag{A.14}$$

and a change of variables defined by

$$z\frac{dz}{dt} = \sqrt{\Delta(t)}, \quad \text{i.e.,} \quad z = \left(2\int_{t_{jk}}^{t} \sqrt{\Delta(t)}dt\right)^{1/2}, \tag{A.15}$$

where t_{jk} is the turning point in question and $\Delta(t)$ denotes the discriminant of the characteristic equation of $H_0(t)$, we can convert the top order part H_0 into the following form:

$$H_0 = \begin{pmatrix} -z & 0 \\ 0 & z \end{pmatrix}. \tag{A.16}$$

Hence, in what follows, we discuss the reduction of the following 2×2 system to a Landau-Zener model (2.16) for two levels at a turning point $z=0$:

$$i\frac{d}{dz}\psi = \eta\left[H_0(z) + \eta^{-1/2}H_{1/2}(z) + \cdots\right]\psi, \tag{A.17}$$

where

$$\begin{aligned} &H_0(z) = \begin{pmatrix} -z & 0 \\ 0 & z \end{pmatrix}, \quad H_{1/2}(z) = \begin{pmatrix} 0 & b_{1/2}(z) \\ c_{1/2}(z) & 0 \end{pmatrix}, \quad \text{and} \\ &H_{j/2}(z) = \begin{pmatrix} a_{j/2}(z) & b_{j/2}(z) \\ c_{j/2}(z) & d_{j/2}(z) \end{pmatrix} \quad (j \geq 2). \end{aligned} \tag{A.18}$$

First, we consider the following transformation

$$\psi = (P_0 + \eta^{-1/2}Q_{1/2})\varphi \tag{A.19}$$

with

$$P_0 = \begin{pmatrix} p(z) & 0 \\ 0 & q(z) \end{pmatrix} \ (p(0)q(0) \neq 0), \ Q_{1/2} = \begin{pmatrix} 0 & r(z) \\ s(z) & 0 \end{pmatrix}. \tag{A.20}$$

By (A.19) the equation (A.17) is transformed into

$$i\frac{d}{dz}\varphi = \eta\left[H_0(z) + \eta^{-1/2}\tilde{H}_{1/2}(z) + \eta^{-1}\tilde{H}_1(z) + \cdots\right]\varphi \tag{A.21}$$

where

$$\tilde{H}_{1/2}(z) = \begin{pmatrix} 0 & \frac{q}{p}b_{1/2} - 2\frac{r}{p}z \\ \frac{p}{q}c_{1/2} + 2\frac{s}{q}z & 0 \end{pmatrix} \tag{A.22}$$

and

(A.23)

$$\tilde{H}_1(z) = \begin{pmatrix} a_1 + \frac{s}{p}b_{1/2} - \frac{r}{q}c_{1/2} - 2\frac{rs}{pq}z - i\frac{p'}{p} & \frac{q}{p}b_1 \\ \frac{p}{q}c_1 & d_1 - \frac{s}{p}b_{1/2} + \frac{r}{q}c_{1/2} + 2\frac{rs}{pq}z - i\frac{q'}{q} \end{pmatrix}.$$

Hence, if we require

$$\frac{q}{p}b_{1/2} - 2\frac{r}{p}z = b_{1/2}(0), \tag{A.24}$$

$$\frac{p}{q}c_{1/2} + 2\frac{s}{q}z = c_{1/2}(0), \tag{A.25}$$

$$a_1 + \frac{s}{p}b_{1/2} - \frac{r}{q}c_{1/2} - 2\frac{rs}{pq}z - i\frac{p'}{p} = 0, \tag{A.26}$$

$$d_1 - \frac{s}{p}b_{1/2} + \frac{r}{q}c_{1/2} + 2\frac{rs}{pq}z - i\frac{q'}{q} = 0, \tag{A.27}$$

we can let the off-diagonal entries of $\tilde{H}_{1/2}$ be independent of z and let the diagonal components of $\tilde{H}_1$ vanish. The requirements (A.24), ..., (A.27) are attained by defining p and q by

$$pq = \exp\left(\frac{1}{i}\int_0^z (a_1 + d_1)dz\right), \tag{A.28}$$

$$b_{1/2}c_{1/2} - b_{1/2}(0)c_{1/2}(0) - z\left[(a_1 - d_1) - i\frac{d}{dz}\left(\log\frac{p}{q}\right)\right] = 0, \tag{A.29}$$

$$p(0) = q(0) = 1 \tag{A.30}$$

and choosing r and s so that they satisfy (A.24) (A.25) respectively. (Note that the sum of (A.26) and (A.27) is an immediate consequence of (A.28) and that their difference follows from (A.24), (A.25) and (A.29).)

In a similar manner we inductively use the transformation

$$\psi = (1 + \eta^{-(n-1)/2}P_{(n-1)/2} + \eta^{-n/2}Q_{n/2})\varphi \tag{A.31}$$

$(n \geq 2)$ with

(A.32)
$$P_{(n-1)/2} = \begin{pmatrix} p_{(n-1)/2}(z) & 0 \\ 0 & q_{(n-1)/2}(z) \end{pmatrix}, \quad Q_{n/2} = \begin{pmatrix} 0 & r_{n/2}(z) \\ s_{n/2}(z) & 0 \end{pmatrix}$$

to make the off-diagonal entries of the order $n/2$ part be independent of z and the diagonal components of the order $(n+1)/2$ part vanish. As a matter of fact, under the induction hypothesis that $H_{j/2}(z)$ has been already converted to a canonical form (2.16) for $j \leq n-1$ and the diagonal components of $H_{n/2}(z)$ vanish, (A.31) transforms the equation (A.17) into

(A.33)
$$i\frac{d}{dz}\varphi = \eta \left[H_0 + \cdots + \eta^{-(n-1)/2} H_{(n-1)/2} + \eta^{-n/2}\tilde{H}_{n/2} + \eta^{-(n+1)/2}\tilde{H}_{(n+1)/2} + \cdots\right]\varphi,$$

where the diagonal components of $\tilde{H}_{n/2}(z)$ are both equal to 0, its off-diagonal entries are given by

$$b_{n/2} - (p_{(n-1)/2} - q_{(n-1)/2})\mu_{1/2} - 2r_{n/2}z, \tag{A.34}$$
$$c_{n/2} + (p_{(n-1)/2} - q_{(n-1)/2})\nu_{1/2} + 2s_{n/2}z, \tag{A.35}$$

and the diagonal components of $\tilde{H}_{(n+1)/2}$ are of the following form:

$$a_{(n+1)/2} + s_{n/2}\mu_{1/2} - r_{n/2}\nu_{1/2} - ip'_{(n-1)/2}, \tag{A.36}$$
$$d_{(n+1)/2} - s_{n/2}\mu_{1/2} + r_{n/2}\nu_{1/2} - iq'_{(n-1)/2}. \tag{A.37}$$

Hence, if we define $p_{(n-1)/2}$ and $q_{(n-1)/2}$ by

$$p_{(n-1)/2} + q_{(n-1)/2} = \frac{1}{i}\int_0^z (a_{(n+1)/2} + d_{(n+1)/2})dz, \tag{A.38}$$
$$\begin{aligned}&(b_{n/2} - b_{n/2}(0))\nu_{1/2} + (c_{n/2} - c_{n/2}(0))\mu_{1/2} \\ &\quad - z\left[(a_{(n+1)/2} - d_{(n+1)/2}) - i\frac{d}{dz}(p_{(n-1)/2} - q_{(n-1)/2})\right] = 0,\end{aligned} \tag{A.39}$$
$$p_{(n-1)/2}(0) = q_{(n-1)/2}(0) = 0 \tag{A.40}$$

and determine $r_{n/2}$ and $s_{n/2}$ so that they satisfy

$$b_{n/2} - (p_{(n-1)/2} - q_{(n-1)/2})\mu_{1/2} - 2r_{n/2}z = b_{n/2}(0), \tag{A.41}$$
$$c_{n/2} + (p_{(n-1)/2} - q_{(n-1)/2})\nu_{1/2} + 2s_{n/2}z = c_{n/2}(0), \tag{A.42}$$

then the equation (A.33) turns out to be of the desired form. We have thus constructed a transformation

$$\psi = T(z,\eta)\varphi, \tag{A.43}$$

where

$$\begin{aligned} T(z,\eta) &= T_0(z) + \eta^{-1/2}T_{1/2}(z) + \eta^{-1}T_1(z) + \cdots \\ &= (P_0 + \eta^{-1/2}Q_{1/2})(1 + \eta^{-1/2}P_{1/2} + \eta^{-1}Q_1)\cdots, \end{aligned} \tag{A.44}$$

which reduces the equation (A.17) to a Landau-Zener model (2.16) for two levels at a turning point $z = 0$.

In the case of our Landau-Zener model (2.1) for three levels, the system can be block-diagonalized near a turning point, say, $t_{12} = a/(b_2 - b_1)$ by the following:

$$S_{1/2} = \begin{pmatrix} 0 & 0 & \frac{c_{13}}{\rho_3-\rho_1} \\ 0 & 0 & \frac{c_{23}}{\rho_3-\rho_2} \\ -\frac{\overline{c_{13}}}{\rho_3-\rho_1} & -\frac{\overline{c_{23}}}{\rho_3-\rho_2} & 0 \end{pmatrix}, \tag{A.45}$$

$$S_1 = \begin{pmatrix} 0 & 0 & \frac{c_{12}c_{23}}{(\rho_3-\rho_1)(\rho_3-\rho_2)} \\ 0 & 0 & \frac{\overline{c_{12}}c_{13}}{(\rho_3-\rho_1)(\rho_3-\rho_2)} \\ -\frac{\overline{c_{12}}\,\overline{c_{23}}}{(\rho_3-\rho_1)(\rho_3-\rho_2)} & -\frac{c_{12}\overline{c_{13}}}{(\rho_3-\rho_1)(\rho_3-\rho_2)} & 0 \end{pmatrix}. \tag{A.46}$$

This block-diagonalizer together with a gauge transformation

$$\psi = \exp\left(\frac{\eta}{2i}\int_{t_{12}}^{t}(\rho_1+\rho_2)dt\right)\varphi \tag{A.47}$$

and a change of variables

$$z = z(t) = \sqrt{\frac{b_2-b_1}{2}}(t - t_{12}) \tag{A.48}$$

reduces the 3×3 system (2.1) to the following 2×2 system:

$$i\frac{d}{dz}\psi = \eta\left[H_0(z) + \eta^{-1/2}H_{1/2}(z) + \cdots\right]\psi, \tag{A.49}$$

where

$$H_0 = \begin{pmatrix} -z & 0 \\ 0 & z \end{pmatrix}, \tag{A.50}$$

$$H_{1/2} = \sqrt{\frac{2}{b_2 - b_1}} \begin{pmatrix} 0 & c_{12} \\ \overline{c_{12}} & 0 \end{pmatrix}, \tag{A.51}$$

$$H_1 = -\sqrt{\frac{2}{b_2 - b_1}} \begin{pmatrix} \frac{|c_{13}|^2}{\rho_3 - \rho_1} & \frac{\overline{c_{23}} c_{13}}{\rho_3 - \rho_2} \\ \frac{c_{23}\overline{c_{13}}}{\rho_3 - \rho_1} & \frac{|c_{23}|^2}{\rho_3 - \rho_2} \end{pmatrix}, \tag{A.52}$$

$$H_{3/2} = -\sqrt{\frac{2}{b_2 - b_1}} \begin{pmatrix} \frac{\overline{c_{12}}\ \overline{c_{23}} c_{13}}{(\rho_3 - \rho_1)(\rho_3 - \rho_2)} & \frac{c_{12}|c_{13}|^2}{(\rho_3 - \rho_1)^2} \\ \frac{\overline{c_{12}}|c_{23}|^2}{(\rho_3 - \rho_2)^2} & \frac{c_{12}c_{23}\overline{c_{13}}}{(\rho_3 - \rho_1)(\rho_3 - \rho_2)} \end{pmatrix}. \tag{A.53}$$

(Here each ρ_j is regarded as a function of the new variable z.) The system (A.47) can be transformed into a Landau-Zener model (2.16) for two levels with the invariants

$$\mu_0 = \sqrt{\frac{2}{b_2 - b_1}} c_{12}, \quad \nu_0 = \sqrt{\frac{2}{b_2 - b_1}} \overline{c_{12}}, \tag{A.54}$$

$$\mu_{1/2} = -\frac{\sqrt{2(b_2 - b_1)}}{a(b_3 - b_2)} \overline{c_{23}} c_{13}, \quad \nu_{1/2} = -\frac{\sqrt{2(b_2 - b_1)}}{a(b_3 - b_2)} c_{23}\overline{c_{13}} \tag{A.55}$$

by the transformation (A.43) with

(A.56)

$$T_0 = \begin{pmatrix} \rho_{13}^{\kappa_{13}} & 0 \\ 0 & \rho_{23}^{\kappa_{23}} \end{pmatrix},$$

(A.57)

$$T_{1/2} =$$
$$\begin{pmatrix} \frac{i(c_{12}c_{23}\overline{c_{13}} + \overline{c_{12}}\ \overline{c_{23}} c_{13})}{a(b_3 - b_2)} \rho_{13}^{\kappa_{13}} \log \rho_{13} & -\frac{c_{12}}{\sqrt{2(b_2 - b_1)}} \frac{1}{z} (\rho_{13}^{\kappa_{13}} - \rho_{23}^{\kappa_{23}}) \\ -\frac{\overline{c_{12}}}{\sqrt{2(b_2 - b_1)}} \frac{1}{z} (\rho_{13}^{\kappa_{13}} - \rho_{23}^{\kappa_{23}}) & -\frac{i(c_{12}c_{23}\overline{c_{13}} + \overline{c_{12}}\ \overline{c_{23}} c_{13})}{a(b_3 - b_2)} \rho_{23}^{\kappa_{23}} \log \rho_{23} \end{pmatrix},$$

and the upper off-diagonal entry and the lower one of T_1 being respectively given by

$$\begin{aligned} &\frac{\overline{c_{23}} c_{13} \sqrt{b_2 - b_1}}{\sqrt{2} a(b_3 - b_2)} \frac{1}{z} (\rho_{13}^{\kappa_{13}} - \rho_{23}^{\kappa_{23} - 1}) \\ &\quad - \frac{i c_{12}(c_{12}c_{23}\overline{c_{13}} + \overline{c_{12}}\ \overline{c_{23}} c_{13})}{a\sqrt{2(b_2 - b_1)}(b_3 - b_2)} \frac{1}{z} (\rho_{13}^{\kappa_{13}} \log \rho_{13} - \rho_{23}^{\kappa_{23}} \log \rho_{23}), \end{aligned} \tag{A.58}$$

$$\text{(A.59)}\qquad \frac{c_{23}\overline{c_{13}}\sqrt{b_2-b_1}}{\sqrt{2}a(b_3-b_2)}\frac{1}{z}(\rho_{13}^{\kappa_{13}-1}-\rho_{23}^{\kappa_{23}}) - \frac{i\overline{c_{12}}(c_{12}c_{23}\overline{c_{13}}+\overline{c_{12}}\ \overline{c_{23}}c_{13})}{a\sqrt{2(b_2-b_1)}(b_3-b_2)}\frac{1}{z}(\rho_{13}^{\kappa_{13}}\log\rho_{13}-\rho_{23}^{\kappa_{23}}\log\rho_{23}),$$

where ρ_{13} and ρ_{23} respectively denote the following:

$$\text{(A.60)}\qquad \rho_{13} = \frac{\rho_3-\rho_1}{(\rho_3-\rho_1)\big|_{z=0}} = \frac{\sqrt{2(b_2-b_1)}}{a}\frac{b_3-b_1}{b_3-b_2}z+1,$$

$$\text{(A.61)}\qquad \rho_{23} = \frac{\rho_3-\rho_2}{(\rho_3-\rho_2)\big|_{z=0}} = \frac{\sqrt{2(b_2-b_1)}}{a}z+1.$$

We finally remark that the reduction constructed in this Appendix transforms a WKB solution of (1.1) into a WKB solution of the Landau-Zener model for two levels. In the case of a turning point t_{12} of the system (2.1), letting $\psi_0^{(j)}$ $(j=1,2)$ denote a WKB solution (2.21) of (2.1), we can verify by straightforward computations that the following relations hold between $\psi_0^{(j)}$ and the WKB solutions $\varphi^{(\pm)}$ of the Landau-Zener model for two levels described by (2.18):

(A.62)

$$\begin{cases} \psi_0^{(1)} = S(t,\eta)\exp\left(\dfrac{\eta}{2i}\displaystyle\int_{t_{12}}^{t}(\rho_1+\rho_2)dt\right)\begin{pmatrix} T(z,\eta)\varphi^{(+)} \\ 0 \end{pmatrix}\Bigg|_{z=z(t)}\left(1+O\left(\eta^{-1}\right)\right), \\ \psi_0^{(2)} = S(t,\eta)\exp\left(\dfrac{\eta}{2i}\displaystyle\int_{t_{12}}^{t}(\rho_1+\rho_2)dt\right)\begin{pmatrix} T(z,\eta)\varphi^{(-)} \\ 0 \end{pmatrix}\Bigg|_{z=z(t)}\left(1+O\left(\eta^{-1}\right)\right). \end{cases}$$

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