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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.

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1. Introduction

In this paper we discuss a Landau–Zener type problem for three levels (cf [CH,BE,J2,CLP,JP] 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

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

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.

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

where

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

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

j

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

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

$$(\rho_1 - \rho_2)(\rho_1 - \rho_3)(\rho_2 - \rho_3) = 0$$
 has only real and simple zeros. (1.5)

Our task is then to relate the behaviour 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 behaviour 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 $+\infty$ and we then apply the connection formula to relate the behaviour of WKB solutions near $t = -\infty$ with that near $t = +\infty$. Although this may sound a traditional and standard approach, there exist substantial problems in putting this program into practice, due to the fact that (1.1) is a 3 × 3, not 2 × 2, system.

The first problem 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 necessity of additional new Stokes curves seems to be closely related to the obstacle against the construction of a dissipative domain in the approach with complex WKB method. See [JP, section 7] for illuminating discussions concerning the obstacle.)

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 the 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. See also [CLP] for a C^{∞} -counterpart of [T2]. Note, however, that results in the C^{∞} -category are not suited for the exact WKB analysis, which makes essential use of the analytic structure of the Borel transformed WKB solutions.)

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 equation (1.1). We note that most of the results given in sections 3 and 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 that the title of [Z] clearly indicates the non-adiabatic character of the problem. We also note that, as is calculated including exponentially small off-diagonal elements in [JP] (cf [J2] also), the diagonal elements of the *S*-matrix are close to 1 in the adiabatic (in the sense of [CLP]) case with no real turning points, showing a clear contrast between adiabatic type problems and Landau–Zener type problems.

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:

$$i\frac{d}{dt}\begin{pmatrix}\psi_1\\\psi_2\\\psi_3\end{pmatrix} = \eta \left[\begin{pmatrix}b_1t+a & 0 & 0\\0 & b_2t & 0\\0 & 0 & b_3t\end{pmatrix} + \eta^{-1/2} \begin{pmatrix}0 & c_{12} & c_{13}\\\frac{c_{12}}{c_{13}} & \frac{0}{c_{23}} & 0\end{pmatrix}\right] \begin{pmatrix}\psi_1\\\psi_2\\\psi_3\end{pmatrix},$$
(2.1)

where b_i 's are mutually distinct real constants and a is a real constant. That is, we study (1.1) with $\rho_1(t) = b_1 t + a$, $\rho_2(t) = b_2 t$ and $\rho_3(t) = b_3 t$. Note that every three level problem with $\rho_i(t)$ 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

$$0 < b_1 < b_2 < b_3$$
 and $0 < a$. (2.2)

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

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

$$\psi^{(j)} = \eta^{-1/2} \exp\left(\frac{\eta}{i} \int_0^t \rho_j(t) \,\mathrm{d}t\right) (\rho_k - \rho_j)^{-\kappa_{kj}} (\rho_l - \rho_j)^{-\kappa_{lj}} (e^{(j)} + \mathcal{O}(\eta^{-1/2})), \tag{2.4}$$

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

 $0 = t_{23} < t_{13} < t_{12}$

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

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

As

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

(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:

$$t \to -\infty \qquad \arg(\rho_{\alpha} - \rho_{\beta}) = 0 \qquad \text{for } \alpha < \beta, \\ \arg(\rho_{\alpha} - \rho_{\beta}) = \pi \qquad \text{for } \alpha > \beta.$$

$$(2.7)$$

As
$$t \to +\infty$$
 $\arg(\rho_{\alpha} - \rho_{\beta}) = -\pi$ for $\alpha < \beta$, (2.8)

$$\arg(\rho_{\alpha} - \rho_{\beta}) = 0 \qquad \text{for } \alpha > \beta.$$

See the appendix for the construction of a WKB solution. Note that 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

$$N^{-,(1)} = e^{-i\pi(\kappa_{12}+\kappa_{13})} + O(\eta^{-1/2}),$$

$$N^{-,(2)} = e^{-i\pi\kappa_{23}} + O(\eta^{-1/2}),$$

$$N^{-,(3)} = 1 + O(\eta^{-1/2}),$$

(2.10)

$$N^{+,(1)} = 1 + O(\eta^{-1/2}),$$

$$N^{+,(2)} = e^{-i\pi\kappa_{12}} + O(\eta^{-1/2}),$$

$$N^{+,(3)} = e^{-i\pi(\kappa_{23}+\kappa_{13})} + O(\eta^{-1/2}),$$
(2.11)

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

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

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

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

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

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

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 Stokes curve). Note that the dominance relation is uniquely determined for each Stokes curve, by which we mean, as a convention, a curvilinear half line starting from an (ordinary or virtual) turning point and going toward a point at infinity, unless any two (ordinary or virtual) turning points of the same type (j, k) are connected by a Stokes curve. The Stokes geometry, i.e. the configuration of turning points and (new) Stokes curves of (2.1) can be illustrated as in figure 1 where the small dots (resp. small rectangles) designate ordinary (resp. virtual) turning points, all of which lie on the real axis. Equation (2.1) has two relevant virtual turning points t_* and \tilde{t}_* . (We know by (3.3)_{K,T} in section 3 that they respectively satisfy

$$\int_{t_{13}}^{t_*} \rho_1 \, \mathrm{d}t = \int_{t_{23}}^{t_*} \rho_2 \, \mathrm{d}t + \int_{t_{13}}^{t_{23}} \rho_3 \, \mathrm{d}t \tag{2.15}$$

and

$$\int_{t_{12}}^{\tilde{t}_*} \rho_2 \,\mathrm{d}t = \int_{t_{13}}^{\tilde{t}_*} \rho_3 \,\mathrm{d}t + \int_{t_{12}}^{t_{13}} \rho_1 \,\mathrm{d}t. \tag{2.16}$$

Among the solutions of these equations we choose $t_* = \frac{a}{b_2 - b_1} \left(1 - \left(\frac{b_3 - b_2}{b_3 - b_1}\right)^{1/2}\right)$ and $\tilde{t}_* = a((b_2 - b_1)(b_3 - b_1))^{-1/2}$; new Stokes curves emanating from other solutions do not pass ordered crossing points *A*, *A'*, *B* or *B'*.) As is indicated by a broken segment in figure 1, the portion of a new Stokes curve containing a virtual turning point 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 Stokes curves shown in figure 1.

Remark 2.1. As is expounded in section 3, figure 1 is obtained by the following procedure: we first draw the ordinary Stokes curves and then, to resolve *ordered* crossing points A, A', B and B' (without worrying about non-ordered crossing points C and C'), we locate the necessary



Figure 1. Stokes geometry of equation (2.1).

virtual turning points t_* and \tilde{t}_* by (2.15) and (2.16), and we add new Stokes curves passing through these virtual turning points to obtain figure 1, which is complete in the sense that no ordered crossing points remain. It is worth mentioning that, in the case of equation (2.1), instead of such a 'pragmatic' method (completely relying on computer-graphics), we can make use of the simple character of (2.1) to employ the following somewhat more 'axiomatic' method to obtain the same figure 1: for equation (2.1) we can analytically determine the location of all possible virtual turning points, that is, the *t*-coordinate of self-intersection points of a bicharacteristic chain (cf section 3), by the following equations:

$$\int_{t_{jk}}^{t} \rho_j \, \mathrm{d}t = \int_{t_{jk}}^{t} \rho_k \, \mathrm{d}t + n\varpi, \qquad (2.17)$$

where $(j, k) \in \{(1, 2), (1, 3), (2, 3)\}$, n runs over all (positive and negative) integers, and

$$\varpi = \int_{t_{13}}^{t_{12}} \rho_1 \, \mathrm{d}t + \int_{t_{12}}^{t_{23}} \rho_2 \, \mathrm{d}t + \int_{t_{23}}^{t_{13}} \rho_3 \, \mathrm{d}t \tag{2.18}$$

denotes the period of the equation (2.1). (For example, (2.15) (resp. (2.16)) is a special case of (2.17) with (j, k) = (1, 2) and n = -1 (resp. (j, k) = (2, 3) and n = -1). See section 3 and [AKT1, proposition 2.3].) Since all possible virtual turning points, i.e. solutions of (2.17), form a discrete subset of \mathbb{C}_t in this case (in general they become dense, as there are many periods; it is the reason why we cannot use this 'axiomatic' method for the general case), restricting our consideration to a compact set in \mathbb{C}_t , we can also draw all possible new Stokes curves numerically. The whole of the ordinary and possible new Stokes curves thus drawn fabricates a 'network of Stokes curves'. This mesh-like figure partitions each (ordinary or new) Stokes curve into infinitely many segments; here a segment means, by definition, a (connected) portion of a Stokes curve whose endpoint is a turning point or a crossing point of Stokes curves (or possibly a point at infinity). Note that on each Stokes curve of type (j, k) there is only one (ordinary or virtual) turning point of Stokes curves. We then determine whether each segment of a Stokes curve 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: A segment with an ordinary turning point as endpoint should be solid. (2.19*a*)

A segment with a virtual turning point as endpoint should be broken. (2.19b)

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 Γ_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 Γ_m^{\pm} (m = 1, 2) are all solid, at most one of Γ_3^{\pm} is broken (i.e. both of Γ_3^{\pm} are solid, or one is solid and the other is broken). Otherwise, both of Γ_3^{\pm} are solid, or both are broken. (2.19c)

In the case of equation (2.1), starting from segments neighbouring ordinary or virtual turning points, we can determine the attribute of being 'solid or broken' for all the segments of Stokes curves by applying these rules and, after erasing irrelevant segments from the figure, we obtain figure 1 where all crossing points of Stokes curves are non-ordered. In ending this Remark, we note the following: 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, provided that no pair of two (ordinary or virtual) turning points of the same type are connected by a Stokes curve (cf [AKT1]).

Since we deal with the connection problem along the real axis, the two new Stokes curves appearing in figure 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 the appendix, at each turning point t_{jk} equation (2.1) can be reduced to a Landau–Zener model for two levels

$$i\frac{d}{dz}\begin{pmatrix}\varphi_1\\\varphi_2\end{pmatrix} = \eta \left[\begin{pmatrix}-z & 0\\0 & z\end{pmatrix} + \sum_{m=0}^{\infty} \eta^{-(m+1)/2} \begin{pmatrix}0 & \mu_{m/2}\\\nu_{m/2} & 0\end{pmatrix}\right]\begin{pmatrix}\varphi_1\\\varphi_2\end{pmatrix} \quad (2.20)$$

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 (2.20) (to be more precise, when one crosses $\{\arg z = \pi/4\}$ anticlockwise), we have the connection formula

$$\varphi^{(+)} \mapsto \varphi^{(+)}, \qquad \varphi^{(-)} \mapsto \varphi^{(-)} - 2^{i\mu\nu/2}\eta^{i\mu\nu/2}\mu \frac{\sqrt{\pi}}{\Gamma(i\mu\nu/2+1)} e^{\pi(i+\mu\nu)/4}\varphi^{(+)}$$
(2.21)

for the following fundamental system of solutions of (2.20):

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

$$\varphi^{(-)} = \eta^{-1/2} \left\{ \begin{pmatrix} \frac{\eta^{-1/2}\mu_0}{2z} \\ 1 \end{pmatrix} + \cdots \right\} e^{-i\eta z^2/2} z^{-i\mu_0\nu_0/2} (1+\cdots).$$
(2.22)

(See [T1] or [T2].) We can thus expect that the same connection formula with (2.21) also holds for equation (2.1) on a Stokes curve emanating as a turning point when we adopt solutions which correspond to (2.22) through the reduction (part of) a fundamental system of solutions.

For example, let us consider the turning point t_{12} . The explicit scheme for constructing the reduction to (2.20) near t_{12} described in the appendix tells us that (the top order part of)

the invariants μ and ν at t_{12} are respectively given by

$$\mu_0 = \sqrt{\frac{2}{b_2 - b_1}} c_{12}, \qquad \nu_0 = \sqrt{\frac{2}{b_2 - b_1}} \overline{c_{12}}$$
(2.23)

(cf (A.54) in the appendix). In particular,

$$\frac{i\mu_0 v_0}{2} = \frac{i|c_{12}|^2}{b_2 - b_1} \tag{2.24}$$

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

$$\begin{split} \psi_{0}^{(1)} &= \eta^{-1/2} \exp\left(\frac{\eta}{i} \int_{t_{12}}^{t} \rho_{1}(t) dt\right) \left(\sqrt{\frac{b_{2} - b_{1}}{2}}(t - t_{12})\right)^{\kappa_{12}} \\ &\times \left(\frac{\rho_{3} - \rho_{1}}{(\rho_{3} - \rho_{1})(t_{12})}\right)^{\kappa_{13}} (e^{(1)} + O(\eta^{-1/2})), \\ \psi_{0}^{(2)} &= \eta^{-1/2} \exp\left(\frac{\eta}{i} \int_{t_{12}}^{t} \rho_{2}(t) dt\right) \left(\sqrt{\frac{b_{2} - b_{1}}{2}}(t - t_{12})\right)^{-\kappa_{12}} \\ &\times \left(\frac{\rho_{3} - \rho_{2}}{(\rho_{3} - \rho_{2})(t_{12})}\right)^{\kappa_{23}} (e^{(2)} + O(\eta^{-1/2})) \end{split}$$
(2.25)

(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 (2.20) near t_{12} (cf (A.62) in the appendix). Hence it can be expected that the same connection formula with (2.21) 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

$$\psi_{0}^{(1)} = (2(b_{2} - b_{1}))^{-\kappa_{12}/2} \left(\frac{b_{3} - b_{2}}{b_{2} - b_{1}}a\right)^{-\kappa_{13}} e^{i\eta(a/(b_{2} - b_{1}))^{2}(b_{2} - b_{1}/2)} (1 + O(\eta^{-1/2}))\psi^{(1)},$$

$$\psi_{0}^{(2)} = e^{-i\pi\kappa_{12}} (2(b_{2} - b_{1}))^{\kappa_{12}/2} \left(\frac{b_{3} - b_{2}}{b_{2} - b_{1}}a\right)^{-\kappa_{23}} e^{i\eta(a/(b_{2} - b_{1}))^{2}(b_{2}/2)} (1 + O(\eta^{-1/2}))\psi^{(2)},$$
(2.26)

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:

$$\psi^{(1)} \longmapsto (1 + \alpha_{12}^{-} \alpha_{12}^{+}) \psi^{(1)} - \alpha_{12}^{-} \psi^{(2)}, \qquad \psi^{(2)} \longmapsto \psi^{(2)} - \alpha_{12}^{+} \psi^{(1)}, \quad (2.27)$$

where

$$\alpha_{12}^{\pm} = c_{12}^{\pm} \frac{i\sqrt{2\pi}}{\Gamma(1 \pm \kappa_{12})} (e^{\pm i\pi/2} (b_2 - b_1))^{-1/2} (2\eta)^{\pm \kappa_{12}} e^{(1/2 \mp 1)i\pi\kappa_{12}} \beta_{12}^{\pm 1},
\beta_{12} = e^{i\pi\kappa_{12}} (2(b_2 - b_1))^{-\kappa_{12}} \left(\frac{b_3 - b_2}{b_2 - b_1}a\right)^{\kappa_{23} - \kappa_{13}} e^{i\eta a^2/(2(b_2 - b_1))},
c_{12}^{+} = c_{12}, \qquad c_{12}^{-} = \overline{c_{12}}.$$
(2.28)

(In (2.28) 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 confusion.) In other words, if we let M_{12} denote

$$\begin{pmatrix} 1 + \alpha_{12}^{-} \alpha_{12}^{+} & -\alpha_{12}^{+} & 0\\ -\alpha_{12}^{-} & 1 & 0\\ 0 & 0 & 1 \end{pmatrix},$$
(2.29)

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

$$(\psi^{(1)}, \psi^{(2)}, \psi^{(3)}) \longmapsto (\psi^{(1)}, \psi^{(2)}, \psi^{(3)})M_{12}.$$
 (2.30)

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

$$\mu_0 = \sqrt{\frac{2}{b_3 - b_2}} c_{23}, \qquad \nu_0 = \sqrt{\frac{2}{b_3 - b_2}} \overline{c_{23}}, \qquad \frac{i\mu_0 \nu_0}{2} = \frac{i|c_{23}|^2}{b_3 - b_2} = \kappa_{23}, \tag{2.31}$$

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:

$$\psi^{(2)} \longmapsto (1 + \alpha_{23}^{-} \alpha_{23}^{+}) \psi^{(2)} - \alpha_{23}^{-} \psi^{(3)}, \qquad \psi^{(3)} \longmapsto \psi^{(3)} - \alpha_{23}^{+} \psi^{(2)}, \quad (2.32)$$

where

$$\begin{aligned} \alpha_{23}^{\pm} &= c_{23}^{\pm} \frac{i\sqrt{2\pi}}{\Gamma(1 \pm \kappa_{23})} (e^{\pm i\pi/2} (b_3 - b_2))^{-1/2} (2\eta)^{\pm \kappa_{23}} e^{(1/2 \mp 1)i\pi\kappa_{23}} \beta_{23}^{\pm 1}, \\ \beta_{23} &= e^{i\pi\kappa_{23}} (2(b_3 - b_2))^{-\kappa_{23}} a^{\kappa_{12} - \kappa_{13}}, \\ c_{23}^{\pm} &= c_{23}, \qquad c_{23}^{-} = \overline{c_{23}}. \end{aligned}$$

$$(2.33)$$

That is,

$$(\psi^{(1)}, \psi^{(2)}, \psi^{(3)}) \longmapsto (\psi^{(1)}, \psi^{(2)}, \psi^{(3)})M_{23},$$
 (2.34)

where

$$M_{23} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 + \alpha_{23}^{-} \alpha_{23}^{+} & -\alpha_{23}^{+} \\ 0 & -\alpha_{23}^{-} & 1 \end{pmatrix}.$$
 (2.35)

Furthermore, at t_{13} we have

$$\mu_0 = \sqrt{\frac{2}{b_3 - b_1}} c_{13}, \qquad \nu_0 = \sqrt{\frac{2}{b_3 - b_1}} \overline{c_{13}}, \qquad \frac{i\mu_0 \nu_0}{2} = \frac{i|c_{13}|^2}{b_3 - b_1} = \kappa_{13}, \tag{2.36}$$

and

$$\psi^{(1)} \longmapsto (1 + \alpha_{13}^{-} \alpha_{13}^{+}) \psi^{(1)} - \alpha_{13}^{-} \psi^{(3)}, \qquad \psi^{(3)} \longmapsto \psi^{(3)} - \alpha_{13}^{+} \psi^{(1)}, \quad (2.37)$$

where

$$\alpha_{13}^{\pm} = c_{13}^{\pm} \frac{i\sqrt{2\pi}}{\Gamma(1 \pm \kappa_{13})} (e^{\pm i\pi/2} (b_3 - b_1))^{-1/2} (2\eta)^{\pm \kappa_{13}} e^{(1/2 \mp 1)i\pi\kappa_{13}} \beta_{13}^{\pm 1},
\beta_{13} = e^{i\pi(-\kappa_{12} + \kappa_{23} + \kappa_{13})} (2(b_3 - b_1))^{-\kappa_{13}} \left(\frac{b_3 - b_2}{b_3 - b_1}a\right)^{-\kappa_{12} - \kappa_{23}} e^{i\eta a^2/(2(b_3 - b_1))},
c_{13}^{+} = c_{13}, \qquad c_{13}^{-} = \overline{c_{13}}.$$
(2.38)

That is,

$$(\psi^{(1)},\psi^{(2)},\psi^{(3)}) \longmapsto (\psi^{(1)},\psi^{(2)},\psi^{(3)})M_{13},$$
 (2.39)

where

$$M_{13} = \begin{pmatrix} 1 + \alpha_{13}^{-} \alpha_{13}^{+} & 0 & -\alpha_{13}^{+} \\ 0 & 1 & 0 \\ -\alpha_{13}^{-} & 0 & 1 \end{pmatrix}.$$
 (2.40)

The connection matrix \tilde{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:

$$\begin{pmatrix} e^{2i\pi(\kappa_{12}+\kappa_{13})} & \alpha_{23}^{-}\alpha_{13}^{+}e^{2i\pi\kappa_{12}} - \alpha_{12}^{+}e^{2i\pi\kappa_{23}} & -\alpha_{13}^{+}e^{2i\pi\kappa_{12}} + \alpha_{12}^{+}\alpha_{23}^{+} \\ -\alpha_{12}^{-}e^{2i\pi\kappa_{13}} & -\alpha_{12}^{-}\alpha_{23}^{-}\alpha_{13}^{+} + e^{2i\pi\kappa_{23}} & \alpha_{12}^{-}\alpha_{13}^{+} - \alpha_{23}^{+} \\ -\alpha_{13}^{-} & -\alpha_{23}^{-} & 1 \end{pmatrix}.$$
(2.41)

Finally, it follows from (2.13) and (2.41) that (the top order part of) the S-matrix for equation (2.1) becomes

$$\begin{pmatrix} e^{i\pi(\kappa_{12}+\kappa_{13})} & \alpha_{23}^{-}\alpha_{13}^{+}e^{i\pi(2\kappa_{12}-\kappa_{23})} - \alpha_{12}^{+}e^{i\pi\kappa_{23}} & -\alpha_{13}^{+}e^{2i\pi\kappa_{12}} + \alpha_{12}^{+}\alpha_{23}^{+} \\ -\alpha_{12}^{-}e^{i\pi\kappa_{13}} & -\alpha_{12}^{-}\alpha_{23}^{-}\alpha_{13}^{+}e^{i\pi(\kappa_{12}-\kappa_{23})} + e^{i\pi(\kappa_{12}+\kappa_{23})} & (\alpha_{12}^{-}\alpha_{13}^{+} - \alpha_{23}^{+})e^{i\pi\kappa_{12}} \\ -\alpha_{13}^{-}e^{i\pi(-\kappa_{12}+\kappa_{23})} & -\alpha_{23}^{-}e^{i\pi\kappa_{13}} & e^{i\pi(\kappa_{23}+\kappa_{13})} \end{pmatrix}.$$
(2.42)

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 recipe for finding a complete Stokes geometry

As Berk-Nevins-Roberts [BNR] first discovered, the 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 neighbourhood 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), 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.



Figure 2. An example of a bicharacteristic chain.

$$b(\kappa, T; \alpha, c) = \left\{ (y, t) \in \mathbb{C}^{2}; y = i \int_{\alpha}^{t} \rho_{k_{1}} dt + c \right\}$$
$$\cup \left\{ (y, t) \in \mathbb{C}^{2}; y = i \int_{t^{(1)}}^{t} \rho_{k_{2}} dt + i \int_{\alpha}^{t^{(1)}} \rho_{k_{1}} dt + c \right\}$$
$$\cup \dots \cup \left\{ (y, t) \in \mathbb{C}^{2}; y = i \int_{t^{(n-1)}}^{t} \rho_{k_{n}} dt + i \sum_{l=1}^{n-2} \int_{t^{(l)}}^{t^{(l+1)}} \rho_{k_{l+1}} dt + i \int_{\alpha}^{t^{(1)}} \rho_{k_{1}} dt + c \right\}.$$
(3.1)

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 $(3.3)_{K,T}$. Here and in what follows we always assume condition (3.2) to avoid the degeneracy that a bicharacteristic chain contains a closed loop:

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

$$-\int_{t^{(0)}}^{\alpha} \rho_{k_0} dt + \int_{t^{(n-1)}}^{\alpha} \rho_{k_n} dt + \sum_{l=1}^{n-1} \int_{t^{(l-1)}}^{t^{(l)}} \rho_{k_l} dt \neq 0.$$
(3.2)

The equation

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

enjoys the following important property:

Reflecting the double turning point character of equation (1.1), 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



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

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 seem to exist infinitely many solutions (cf [AKT1, pp 82–3]).

Making use of this significant property of $(3.3)_{K,T}$, we now present a recipe 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 83–4]). To describe the procedure concretely, let us introduce the following diagram which schematically describes equation $(3.3)_{K,T}$; we call it a bicharacteristic diagram. The diagram is determined by (K, T), just as in the case of 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

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

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 labelled by k_l (l = 1, ..., n-1), two half lines respectively labelled by k_0 and k_n , and n points labelled by $t^{(l)}$ (l = 0, 1, ..., n-1), so that the line k_l and the line k_{l+1} are hinged by the point $t^{(l)}$ (l = 0, 1, ..., n-1). As a convention we let the half lines cross, and line segments are located in a linear order. To maintain the flavour of a bicharacteristic chain (cf figure 2), we draw line segments as curvilinear ones, but this is just a matter of taste (see figure 3).

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. It is clear that equation $(3.3)_{K_0,T_0}$ admits $t = t^{(0)}$ as a solution. Thus not only virtual but also ordinary turning points may be conventionally designated by a bicharacteristic diagram.

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})



Figure 4. Contraction of the diagram in figure 3.



Figure 5. Junction of bicharacteristic diagrams.

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, its contraction becomes the diagram shown in figure 4. Note also that the contraction procedure is a counterpart of the vanishing of the integral

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

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

The 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:

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

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

$$k_0 = 1, \quad k_n = 3, \quad k'_0 = 3 \quad \text{and} \quad k'_m = 2.$$
 (3.4')

To define the junction let k_{n+l} and $t^{(n+l)}$ respectively denote k'_l and $t'^{(l)}$ for l = 0, 1, ..., m - 1. This re-numbering is well-defined by 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) (cf figure 5). Note that contraction may often be applied to the resulting diagram. For example, if $t^{(0)} = t'^{(0)}$ in the example in figure 5, the resulting diagram may be contracted to the following:



The importance of the notion 'junction' lies in the following fact:

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 . (3.5)

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

$$\operatorname{Im}\left(\mathrm{i}(R_{1}(t) - R_{3}(t))\right) = \operatorname{Im}\left(\mathrm{i}(R_{1}(t_{*}) - R_{3}(t_{*}))\right),\tag{3.6}$$

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

$$\operatorname{Re}\left(R_{1}(t) - R_{3}(t)\right) = \operatorname{Re}\left(R_{1}(t_{*}) - R_{3}(t_{*})\right).$$
(3.7)

Similarly, σ_2 is given by

$$\operatorname{Re}\left(R_{3}(t) - R_{2}(t)\right) = \operatorname{Re}\left(R_{3}(t_{**}) - R_{2}(t_{**})\right),\tag{3.8}$$

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

$$R_1(t_*) - R_1(t^{(0)}) = R_3(t_*) - R_3(t^{(n-1)}) + \sum_{l=1}^{n-1} \left(R_{k_l}(t^{(l)}) - R_{k_l}(t^{(l-1)}) \right),$$
(3.9)

$$R_{3}(t_{**}) - R_{3}(t^{(n)}) = R_{2}(t_{**}) - R_{2}(t^{(n+m-1)}) + \sum_{l=1}^{m-1} \left(R_{k_{l+n}}(t^{(l+n)}) - R_{k_{l+n}}(t^{(l+n-1)}) \right).$$
(3.10)

On the other hand, σ is given by

$$\operatorname{Re}\left(R_{1}(t) - R_{2}(t)\right) = \operatorname{Re}\left(R_{1}(\tilde{t}_{*}) - R_{2}(\tilde{t}_{*})\right), \qquad (3.11)$$

where \tilde{t}_* satisfies

$$R_{1}(\tilde{t}_{*}) - R_{1}(t^{(0)}) = R_{2}(\tilde{t}_{*}) - R_{2}(t^{(n+m-1)}) + \sum_{l=1}^{n-1} \left(R_{k_{l}}(t^{(l)}) - R_{k_{l}}(t^{(l-1)}) \right) + R_{3}(t^{(n)}) - R_{3}(t^{(n-1)}) + \sum_{l=1}^{m-1} \left(R_{k_{l+n}}(t^{(l+n)}) - R_{k_{l+n}}(t^{(l+n-1)}) \right).$$
(3.12)

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

$$\operatorname{Re}\left(R_{1}(a) - R_{2}(a)\right) = \operatorname{Re}\left(R_{1}(t_{*}) - R_{3}(t_{*}) + R_{3}(t_{**}) - R_{2}(t_{**})\right).$$
(3.13)

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

 $R_{1}(t_{*}) - R_{3}(t_{*}) + R_{3}(t_{**}) - R_{2}(t_{**})$ $= R_{1}(t^{(0)}) - R_{3}(t^{(n-1)}) + \sum_{l=1}^{n-1} \left(R_{k_{l}}(t^{(l)}) - R_{k_{l}}(t^{(l-1)}) \right)$ $+ R_{3}(t^{(n)}) - R_{2}(t^{(n+m-1)}) + \sum_{l=1}^{m-1} \left(R_{k_{l+n}}(t^{(l+n)}) - R_{k_{l+n}}(t^{(l+n-1)}) \right).$ (3.14)

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

$$\operatorname{Re}\left(R_{1}(a) - R_{2}(a)\right) = \operatorname{Re}\left(R_{1}(\tilde{t_{*}}) - R_{2}(\tilde{t_{*}})\right).$$
(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 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 6. 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.



Figure 6. Ordinary Stokes curves of example 3.1.



Figure 7. New Stokes curve resolving the ordered crossing points A and A'.

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

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

$$t+1 = \frac{t^2}{4} + \frac{1}{3}.$$
(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. (See figure 7 where, and in subsequent figures 8 and 10 also, a virtual turning point is designated by a small rectangle as in figure 1.)

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

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

In this region we observe three ordered crossing points, labelled respectively by B, E and F in figure 6. We first concentrate our attention on 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):



(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:

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



Figure 8. New Stokes curve resolving the ordered crossing point *B*.

We then see that a new Stokes curve of type (1, 2) passing through the virtual turning point $t = 2 - \sqrt{17/12}$ resolves the ordered crossings simultaneously (cf figure 8).

Let us now trace this new Stokes curve in $\{t \in \mathbb{C}; \text{Im } t > 0\}$. There it is of type (2 > 1) and its concrete form is shown in figure 8. 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):



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 (2.19c) in section 2 tells us, the (new) Stokes curve of type (2 > 1), i.e. of 'adjacent type' thus remains 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):



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

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

As shown in figure 9, we can then confirm that a new Stokes curve emanating from $t = 1 - \epsilon$ ($\epsilon > 0$) 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.

Now let us return 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):



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

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

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





Figure 9. New Stokes curve resolving the ordered crossing point *D*.

Extending this new Stokes curve beyond t_{**} , we are naturally led to the study of the configuration of ordinary Stokes curves in the region $\{t \in \mathbb{C}; \text{Re } t > 1, \text{Im } t > 0\}$. As we see in figure 6 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 10). Note that this new Stokes curve changes its type at t_{**} ; thus both F and G are simultaneously resolved by one new Stokes curve.

Finally let us study the ordered crossing point H in figure 6. 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):



Hence the defining equation of the required virtual turning point is

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



Figure 10. New Stokes curve resolving two ordered crossing points F and G simultaneously.

As this equation has one real solution $t_0 (= 1.3)$, 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 11). This fact can be immediately understood if we use bicharacteristic diagrams; for example, 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) 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):



This indicates that the new Stokes curve is actually an ordinary Stokes curve emanating from 1, and it is readily confirmed analytically. 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).

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 given by figure 12.



Figure 11. Three Stokes curves meeting at the point *b*.



Figure 12. Complete Stokes geometry of example 3.1.

For the reader's reference, we present two examples of completed Stokes geometry. We omit the explanations of how to obtain them. They are actually simpler to analyse 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 $\rho_3 = t^2 - 2$. The complete Stokes geometry is given by figure 13.

Example 3.3. $\rho_1 = 1 - 5t^2 + t^4$, $\rho_2 = -\frac{3}{2}t^2$ and $\rho_3 = -2$. The complete Stokes geometry is given by figure 14.



Figure 13. Complete Stokes geometry of example 3.2.

4. Computation of the transition probabilities: general case

In this section we present a general recipe for computing the transition probabilities from $t = -\infty$ to $+\infty$ 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

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

Since (1.5) entails the right-hand side of (4.1) being 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



Figure 14. Complete Stokes geometry of example 3.3.

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

But, as both t_* and \overline{t}_* are solutions of the same equation (4.1) and hence $\int_{t_*}^{\overline{t}_*} (\rho_{k_0} - \rho_{k_n}) dt = 0$ 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 $\int_{t_*}^{t} (\rho_{k_0} - \rho_{k_n}) dt$, we find

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

Therefore α is a turning point. Hence it lies on the real axis by assumption (1.5). In particular, $\int_{t_*}^{\alpha} (\rho_{k_0} - \rho_{k_n}) dt$ is real, while it is purely imaginary as α is on the new Stokes curve $\sigma \cup \overline{\sigma}$. Hence the integral $\int_{t_*}^{\alpha} (\rho_{k_0} - \rho_{k_n}) dt$ must be zero and, by the same reasoning as earlier, 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 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):

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

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 behaviour 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:

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

Here we are assuming that

$$\lambda_{jk}^{[n]} \stackrel{\text{def}}{=} \left. \frac{\mathrm{d}}{\mathrm{d}t} (\rho_k - \rho_j) \right|_{t = t_{jk}^{[n]}} > 0 \tag{4.6}$$

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:

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

where

$$c_{jk}^{+} = c_{jk}, \qquad c_{jk}^{-} = \overline{c_{jk}}, \qquad \kappa_{jk}^{[n]} = \frac{i|c_{jk}|^2}{\lambda_{ik}^{[n]}},$$
(4.8)

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

$$\begin{split} \psi_{0}^{(j)} &= \eta^{-1/2} \exp\left(\frac{\eta}{\mathbf{i}} \int_{t_{jk}^{[n]}}^{t} \rho_{j}(t) \, \mathrm{d}t + \frac{1}{\mathbf{i}} \int_{t_{jk}^{[n]}}^{t} \left(|c_{jk}|^{2} \left(\frac{1}{\rho_{j} - \rho_{k}} + \frac{1}{\lambda_{jk}^{[n]}(t - t_{jk}^{[n]})}\right)\right) \\ &+ \frac{|c_{jl}|^{2}}{\rho_{j} - \rho_{l}} \right) \mathrm{d}t \right) \left(\frac{\lambda_{jk}^{[n]}(t - t_{jk}^{[n]})^{2}}{2}\right)^{\kappa_{jk}^{[n]}/2} (e^{(j)} + O(\eta^{-1/2})), \\ \psi_{0}^{(k)} &= \eta^{-1/2} \exp\left(\frac{\eta}{\mathbf{i}} \int_{t_{jk}^{[n]}}^{t} \rho_{k}(t) \, \mathrm{d}t + \frac{1}{\mathbf{i}} \int_{t_{jk}^{[n]}}^{t} \left(-|c_{jk}|^{2} \left(\frac{1}{\rho_{j} - \rho_{k}} + \frac{1}{\lambda_{jk}^{[n]}(t - t_{jk}^{[n]})}\right) \right. \\ &+ \frac{|c_{kl}|^{2}}{\rho_{k} - \rho_{l}} \right) \mathrm{d}t \right) \left(\frac{\lambda_{jk}^{[n]}(t - t_{jk}^{[n]})^{2}}{2} \right)^{-\kappa_{jk}^{[n]}/2} (e^{(k)} + O(\eta^{-1/2})), \end{split}$$
(4.9)

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

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

where

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

Note that the WKB solutions (4.9) correspond to the solutions (2.22) of the Landau–Zener model (2.20) for two levels through the reduction to (2.20) 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:

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

$$\begin{pmatrix} N^{+,(1)} & 0 & 0 \\ 0 & N^{+,(2)} & 0 \\ 0 & 0 & N^{+,(3)} \end{pmatrix}^{-1} M^{[N]} \cdots M^{[1]} \begin{pmatrix} N^{-,(1)} & 0 & 0 \\ 0 & N^{-,(2)} & 0 \\ 0 & 0 & N^{-,(3)} \end{pmatrix}$$
(4.13)

describes the S-matrix for 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 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

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

Then φ should satisfy

$$i\frac{d}{dt}\varphi = \eta \left((1+\eta^{-1/2}P_{1/2})^{-1}(H_0+\eta^{-1/2}H_{1/2})(1+\eta^{-1/2}P_{1/2}) - i\eta^{-3/2}(1+\eta^{-1/2}P_{1/2})^{-1}\frac{dP_{1/2}}{dt} \right)\varphi$$

= $\eta (H_0+\eta^{-1/2}(H_{1/2}+[H_0,P_{1/2}])+\cdots)\varphi,$ (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

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

 $\psi = R(t, \eta)\varphi$, $R(t, \eta) = 1 + \eta^{-1/2}R_{1/2}(t) + \dots = (1 + \eta^{-1/2}P_{1/2})(1 + \eta^{-1}P_1) \dots$ (A.4) which transforms equation (1.1) into

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

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

(where each $\psi_{m/2}^{(j)}(t)$ 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 transformation (A.4).

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

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

$$R_{1} = \begin{pmatrix} 0 & \frac{c_{23}c_{13}}{(\rho_{2}-\rho_{1})(\rho_{2}-\rho_{3})} & \frac{c_{12}c_{23}}{(\rho_{3}-\rho_{1})(\rho_{3}-\rho_{2})} \\ \frac{c_{23}\overline{c_{13}}}{(\rho_{1}-\rho_{2})(\rho_{1}-\rho_{3})} & 0 & \frac{\overline{c_{12}}c_{13}}{(\rho_{3}-\rho_{1})(\rho_{3}-\rho_{2})} \\ \frac{\overline{c_{12}}\overline{c_{23}}}{(\rho_{1}-\rho_{2})(\rho_{1}-\rho_{3})} & \frac{c_{12}\overline{c_{13}}}{(\rho_{2}-\rho_{1})(\rho_{2}-\rho_{3})} & 0 \end{pmatrix},$$
(A.8)

$$H_0 = \begin{pmatrix} \rho_1 & 0 & 0\\ 0 & \rho_2 & 0\\ 0 & 0 & \rho_3 \end{pmatrix}, \tag{A.9}$$

$$\tilde{H}_{1} = \begin{pmatrix} \frac{|c_{12}|^{2}}{\rho_{1} - \rho_{2}} + \frac{|c_{13}|^{2}}{\rho_{1} - \rho_{3}} & 0 & 0\\ 0 & \frac{|c_{12}|^{2}}{\rho_{2} - \rho_{1}} + \frac{|c_{23}|^{2}}{\rho_{2} - \rho_{3}} & 0\\ 0 & 0 & \frac{|c_{13}|^{2}}{\rho_{3} - \rho_{1}} + \frac{|c_{23}|^{2}}{\rho_{3} - \rho_{2}} \end{pmatrix},$$
(A.10)

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

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 $e_k^{(j)} = \delta_{jk}$, we find that (2.1) has the following WKB solutions:

$$\psi^{(j)} = \eta^{-1/2} \exp\left(\frac{\eta}{i} \int^{t} \left(\rho_{j}(t) + \eta^{-1} \left(\frac{|c_{kj}|^{2}}{\rho_{j} - \rho_{k}} + \frac{|c_{lj}|^{2}}{\rho_{j} - \rho_{l}}\right) + O(\eta^{-3/2})\right) dt\right)$$

$$\times (e^{(j)} + O(\eta^{-1/2}))$$

$$= \eta^{-1/2} \exp\left(\frac{\eta}{i} \int^{t} \rho_{j}(t) dt\right) (\rho_{k} - \rho_{j})^{-\kappa_{kj}} (\rho_{l} - \rho_{j})^{-\kappa_{lj}} (e^{(j)} + O(\eta^{-1/2})).$$
(A.12)

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 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:

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

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

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

and a change of variables defined by

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

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 (2.20) for two levels at a turning point z = 0:

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

where

$$H_{0}(z) = \begin{pmatrix} -z & 0 \\ 0 & z \end{pmatrix}, \qquad H_{1/2}(z) = \begin{pmatrix} 0 & b_{1/2}(z) \\ c_{1/2}(z) & 0 \end{pmatrix},$$

$$H_{j/2}(z) = \begin{pmatrix} a_{j/2}(z) & b_{j/2}(z) \\ c_{j/2}(z) & d_{j/2}(z) \end{pmatrix} \qquad (j \ge 2).$$
(A.18)

First, we consider the following transformation

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

with

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

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

1

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

where

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

and

$$\tilde{H}_{1}(z) = \begin{pmatrix} a_{1} + \frac{s}{p}b_{1/2} - \frac{r}{q}c_{1/2} - 2\frac{rs}{pq}z - i\frac{p'}{p} & \frac{q}{p}b_{1} \\ \frac{p}{q}c_{1} & d_{1} - \frac{s}{p}b_{1/2} + \frac{r}{q}c_{1/2} + 2\frac{rs}{pq}z - i\frac{q'}{q} \end{pmatrix}.$$
 (A.23)

Hence, if we require

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

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

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

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

$$pq = \exp\left(\frac{1}{i}\int_{0}^{z} (a_{1}+d_{1}) \,\mathrm{d}z\right),\tag{A.28}$$

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

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

and choosing r and s so that they satisfy (A.24) and (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

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

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

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 already been converted to a canonical form (2.20) for $j \le n - 1$ and the diagonal components of $H_{n/2}(z)$ vanish, (A.31) transforms equation (A.17) into

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

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

$$b_{n/2} - (p_{(n-1)/2} - q_{(n-1)/2})\mu_{1/2} - 2r_{n/2}z,$$
(A.34)

$$c_{n/2} + (p_{(n-1)/2} - q_{(n-1)/2})v_{1/2} + 2s_{n/2}z,$$
(A.35)

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

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

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

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

$$p_{(n-1)/2} + q_{(n-1)/2} = \frac{1}{i} \int_0^\infty (a_{(n+1)/2} + d_{(n+1)/2}) \, \mathrm{d}z, \tag{A.38}$$

$$(b_{n/2} - b_{n/2}(0))v_{1/2} + (c_{n/2} - c_{n/2}(0))\mu_{1/2}$$

$$-z\left[(a_{(n+1)/2} - d_{(n+1)/2}) - i\frac{\mathrm{d}}{\mathrm{d}z}(p_{(n-1)/2} - q_{(n-1)/2})\right] = 0, \tag{A.39}$$

$$p_{(n-1)/2}(0) = q_{(n-1)/2}(0) = 0$$
(A.40)

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

$$b_{n/2} - (p_{(n-1)/2} - q_{(n-1)/2})\mu_{1/2} - 2r_{n/2}z = b_{n/2}(0),$$
(A.41)

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

then 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

$$T(z, \eta) = T_0(z) + \eta^{-1/2} T_{1/2}(z) + \eta^{-1} T_1(z) + \cdots$$

= $(P_0 + \eta^{-1/2} Q_{1/2})(1 + \eta^{-1/2} P_{1/2} + \eta^{-1} Q_1) \cdots,$ (A.44)

which reduces equation (A.17) to a Landau–Zener model (2.20) 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 blockdiagonalized near a turning point, say, $t_{12} = a/(b_2 - b_1)$ by the following:

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

$$S_{1} = \begin{pmatrix} 0 & 0 & \frac{c_{12}c_{23}}{(\rho_{3}-\rho_{1})(\rho_{3}-\rho_{2})} \\ 0 & 0 & \frac{c_{12}c_{13}}{(\rho_{3}-\rho_{1})(\rho_{3}-\rho_{2})} \\ -\frac{c_{12}c_{23}}{(\rho_{3}-\rho_{1})(\rho_{3}-\rho_{2})} & -\frac{c_{12}c_{13}}{(\rho_{3}-\rho_{1})(\rho_{3}-\rho_{2})} & 0 \end{pmatrix}.$$
 (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

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

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

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

where

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

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

$$H_{1} = -\sqrt{\frac{2}{b_{2} - b_{1}}} \begin{pmatrix} \frac{|c_{13}|^{2}}{\rho_{3} - \rho_{1}} & \frac{\overline{c_{23}}c_{13}}{\rho_{3} - \rho_{2}} \\ \frac{c_{23}\overline{c_{13}}}{\rho_{3} - \rho_{1}} & \frac{|c_{23}|^{2}}{\rho_{3} - \rho_{2}} \end{pmatrix},$$
(A.52)

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

(Here each ρ_j is regarded as a function of the new variable z.) System (A.47) can be transformed into a Landau–Zener model (2.20) for two levels with the invariants

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

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

by transformation (A.43) with

$$T_0 = \begin{pmatrix} \rho_{13}^{\kappa_{13}} & 0\\ 0 & \rho_{23}^{\kappa_{23}} \end{pmatrix}, \tag{A.56}$$

$$T_{1/2} = \begin{pmatrix} \frac{1(c_{12}c_{23}c_{13}+c_{12}-c_{23}c_{13})}{a(b_3-b_2)}\rho_{13}^{\kappa_{13}}\log\rho_{13} & -\frac{c_{12}}{\sqrt{2(b_2-b_1)}}\frac{1}{z}(\rho_{13}^{\kappa_{13}}-\rho_{23}^{\kappa_{23}}) \\ -\frac{c_{12}}{\sqrt{2(b_2-b_1)}}\frac{1}{z}(\rho_{13}^{\kappa_{13}}-\rho_{23}^{\kappa_{23}}) & -\frac{i(c_{12}c_{23}c_{13}+c_{12}-c_{23}c_{13})}{a(b_3-b_2)}\rho_{23}^{\kappa_{23}}\log\rho_{23} \end{pmatrix},$$
(A.57)

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

$$\frac{\overline{c_{23}}c_{13}\sqrt{b_2 - b_1}}{\sqrt{2}a(b_3 - b_2)} \frac{1}{z} (\rho_{13}^{\kappa_{13}} - \rho_{23}^{\kappa_{23} - 1}) - \frac{ic_{12}(c_{12}c_{23}\overline{c_{13}} + \overline{c_{12}}\ \overline{c_{23}}c_{13})}{a\sqrt{2(b_2 - b_1)}(b_3 - b_2)} \frac{1}{z} (\rho_{13}^{\kappa_{13}}\log\rho_{13} - \rho_{23}^{\kappa_{23}}\log\rho_{23}),$$
(A.58)

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

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

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

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

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 system (2.1), letting $\psi_0^{(j)}$ (j = 1, 2) denote a WKB solution (2.25) 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 (2.22):

$$\psi_{0}^{(1)} = S(t,\eta) \exp\left(\frac{\eta}{2i} \int_{t_{12}}^{t} (\rho_{1} + \rho_{2}) dt\right) \begin{pmatrix} T(z,\eta)\varphi^{(+)} \\ 0 \end{pmatrix} \Big|_{z=z(t)} (1 + O(\eta^{-1})),$$

$$\psi_{0}^{(2)} = S(t,\eta) \exp\left(\frac{\eta}{2i} \int_{t_{12}}^{t} (\rho_{1} + \rho_{2}) dt\right) \begin{pmatrix} T(z,\eta)\varphi^{(-)} \\ 0 \end{pmatrix} \Big|_{z=z(t)} (1 + O(\eta^{-1})).$$
(A.62)

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References

[AKT1]	Aoki T, Kawai T and Takei Y 1994 New turning points in the exact WKB analysis for higher order ordinary
	differential equations Analyse algébrique des perturbations singulières, I. Méthodes résurgentes vol 1
	(Paris: Hermann) pp 69–84

- [AKT2] Aoki T, Kawai T and Takei Y 1998 On the exact WKB analysis for the third order ordinary differential equations with a large parameter Asian J. Math. 2 625–40
- [BNR] Berk H L, Nevins W M and Roberts K V 1982 New Stokes' line in WKB theory J. Math. Phys. 23 988–1002
 [BE] Brundobler S and Elser V 1993 S-matrix for generalized Landau–Zener problem J. Phys. A: Math. Gen. 26 1211–27
- [CH] Carroll C E and Hioe F T 1986 Transition probabilities for the three-level Landau–Zener model J. Phys. A: Math. Gen. 19 2061–73
- [CLP] Colin de Verdière Y, Lombardi M and Pollet J 1999 The microlocal Landau–Zener formula Ann. Inst. Henri Poincaré 71 95–127
- [DDP] Delabaere E, Dillinger H and Pham F 1993 Résurgence de Voros et périodes des courbes hyperelliptiques Ann. Inst. Fourier (Grenoble) 43 163–99
- [H] Hagedorn G A 1991 Proof of the Landau–Zener formula in an adiabatic limit with small eigenvalue gaps Commun. Math. Phys. 136 433–49
- [J1] Joye A 1994 Proof of the Landau–Zener formula Asymptotic Anal. 9 209–58
- [J2] Joye A 1997 Exponential asymptotics in a singular limit for n-level scattering systems SIAM J. Math. Anal. 28 669–703
- [JP] Joye A and Pfister C-E 2000 Complex WKB method for 3-level scattering systems Asymptotic Anal. 23 91–109
- [KKO] Kashiwara M, Kawai T and Oshima T 1974 Structure of cohomology groups whose coefficients are microfunction solution sheaves of systems of pseudo-differential equations with multiple characteristics, I Proc. Japan Acad. 49 420–5
- [L] Landau L 1965 A theory of energy transfer II Collected Papers of L D Landau (Oxford: Pergamon) pp 63–6 (Engl. transl. 1932 Zur Theorie der Energieübertragung II Phys. Z. Sowjet. 2 46–51)
- [P] Pham F 1988 Resurgence, quantized canonical transformations, and multi-instanton expansions Algebraic Analysis vol 2 (New York: Academic) pp 699–726
- [T1] Takei Y 2000 An explicit description of the connection formula for the first Painlevé equation Toward the Exact WKB Analysis of Differential Equations, Linear or Non-Linear (Kyoto: Kyoto University Press) pp 271–96
- [T2] Takei Y On a double turning point problem for systems of linear ordinary differential equations in preparation
- [V] Voros A 1983 The return of the quartic oscillator—the complex WKB method Ann. Inst. Henri Poincare 39 211–338
- [W] Wasow W 1965 Asymptotic Expansions for Ordinary Differential Equations (New York: Interscience)
- [Z] Zener C 1932 Non-adiabatic crossing of energy levels Proc. R. Soc. 137 696–702