Semiclassical approaches to generalizations of Landau-Zener formula for a two-level avoided crossing

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1 Introduction

The purpose of this article is to consider the background of our recent result [13] concerning generalizations of the Landau-Zener formula for a two-level avoided crossing. As in mentioned later, an asymptotic analysis of a 2×2 system with respect to two parameters contains various techniques of semiclassical analysis, for example, an exact WKB analysis, a semiclassical microlocal analysis and so on. In order to discuss this topic in a simple setting, we focus on the connection formula around an avoided crossing and compare each connection formula from the viewpoint of semiclassical approaches.

In a whole of this paper we treat the first order 2×2 system:

$$ih\frac{d}{dt}\psi(t) = H(t)\psi(t), \quad t \in \mathbb{R}, \tag{1.1}$$

$$H(t) = \begin{pmatrix} V(t) & \varepsilon \\ \varepsilon & -V(t) \end{pmatrix}, \tag{1.2}$$

where h, ε are small positive parameters and $V(t)$ is a real-valued smooth function. This equation (1.1) describes a time evolution of coupled quantum-states along two energies $\pm\sqrt{V(t)^2 + \varepsilon^2}$, which are eigenvalues of $H(t)$ with a gap $2\varepsilon > 0$. The zeros of $V(t)$ on $\mathbb{R}$ means the crossing points between $V(t)$ and $-V(t)$ and the small parameter ε does an interaction at the crossing points. Because of an interaction ε, we can intuitively understand the energies of the system avoid crossing at the zeros of $V(t)$. Such a situation is called avoided crossing and it is our interest in this paper.

Landau in [17] and Zener in [25] individually gave quantitively a transition between two energies by means of a transition probability, which is a square of the modulus of the off-diagonal of the change of basis of Jost solutions (see in §2.1). They consider the case where $V(t) = vt$ with $v > 0$, that is, $V(t)$ and $-V(t)$ cross each other only at the origin. Then the transition probability $\mathcal{P}(\varepsilon, h)$ is given by

$$\mathcal{P}(\varepsilon, h) = e^{-\frac{\pi\varepsilon^2}{vh}} \tag{1.3}$$

for any positive ε and h. This formula (1.3) is called *Landau-Zener formula*. For this case, as we show the proof in §2.2, we can reduce the equation (1.1) to the Weber's differential equation and apply the connection formula of the Weber's functions (i.e. the parabolic cylinder functions) to the connection formula around the avoided crossing at $t = 0$. From the viewpoint of the above strategy, the generalization of Landau-Zener formula in the context is to find the corresponding connection formula in the general setting.

We mention in §2.3 that the asymptotic analysis of (1.1) with respect to two small parameters ε and h involves technical difficulties. The parameter h is called adiabatic parameter, which plays a role of a semiclassical parameter. One can consult [9], [10], [19] on previous works under an adiabatic approximation, that is, to take a limit $h \to 0$ for a fixed ε. The second author and his collaborators have studied the two-parameter problems, that is, to take a limit $(\varepsilon, h) \to (0, 0)$. In this case, we must carry out various approaches depending on the relations between ε and h. Hence in this manuscript, we discuss semiclassical approaches to the connection formula near an avoided crossing along the following contents: In Section 2, we give the common setting and the strategy of deriving the connection formula through the Landau-Zener model, and also introduce the parameter regimes. We present in Section 3 the connection formula under an adiabatic regime and also under a non-adiabatic regime. In Section 4, we make a discussion on the comparison with these approaches and finally refer to the leading term of the asymptotic expansion of transition probability in each case.

2 Framework of generalizations of the Landau-Zener formula

2.1 Transition probability

In this subsection we give the definition of the transition probability, and state the conditions imposed on $V(t)$ throughout this manuscript.

Condition A. *The function $V(t) \in C^\infty(\mathbb{R}; \mathbb{R})$ has a limit $E_r \in \mathbb{R} \setminus \{0\}$ (resp. $E_\ell \in \mathbb{R} \setminus \{0\}$) as $t \to +\infty$ (resp. $-\infty$), and satisfies*

$$V - E_r \in L^1([0, +\infty)), \quad V - E_\ell \in L^1((-\infty, 0]), \quad V' \in L^1(\mathbb{R}).$$

Here we suppose $E_r > 0$ without loss of generality. Thanks to Condition A, one sees that there exist Jost solutions $J_\bullet^\pm(t)$ ($\bullet \in \{\ell, r\}$) which satisfy the asymptotic conditions:

$$J_r^+(t) \sim \exp\left[-\frac{i}{h}\sqrt{E_r^2 + \varepsilon^2}\, t\right] \begin{pmatrix} \cos\theta_r \\ \sin\theta_r \end{pmatrix} \quad \text{as } t \to +\infty,$$

$$J_r^-(t) \sim \exp\left[+\frac{i}{h}\sqrt{E_r^2 + \varepsilon^2}\, t\right] \begin{pmatrix} -\sin\theta_r \\ \cos\theta_r \end{pmatrix} \quad \text{as } t \to +\infty,$$

where $\tan 2\theta_r = \frac{\varepsilon}{E_r}$, $(0 < \theta_r < \frac{\pi}{2})$ and $J_\ell^\pm(t)$ behaves similar conditions as $t \to -\infty$. The construction of the Jost solutions can be consulted in [13]. One also sees that Jost solutions form orthonormal bases (J_r^+, J_r^-) and (J_ℓ^+, J_ℓ^-) on $\mathbb{C}^2$ for each $t \in \mathbb{R}$. Then we can introduce the scattering matrix $S(\varepsilon, h)$ as the change of basis of the pair of Jost solutions corresponding to the eigenvalues of $H(t;\varepsilon)$ at the infinity:

$$\left(J_\ell^+, J_\ell^-\right) = \left(J_r^+, J_r^-\right) S(\varepsilon, h), \quad S(\varepsilon, h) = \begin{pmatrix} s_{11}(\varepsilon, h) & s_{12}(\varepsilon, h) \\ s_{21}(\varepsilon, h) & s_{22}(\varepsilon, h) \end{pmatrix}. \tag{2.1}$$

And then we can define the transition probability $P(\varepsilon, h)$ as follows:

Definition 2.1. *The transition probability $P(\varepsilon, h)$ is defined by*

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

The target of this research is to study an asymptotic behavior of $P(\varepsilon, h)$ as both parameters ε and h tend to 0. The asymptotics of $P(\varepsilon, h)$ depends on the relation between ε and h and also on the local properties of $V(t)$ near an avoided crossing. Thus we assume the following condition:

Condition B. *The function $V(t)$ has only one zero at $t = 0$, which is of finite multiplicity.*

Although we treat in this paper the case where the number of zeros of $V(t)$ is one, we can consider the case where $V(t)$ has a finite number of zeros as in the references [15], [22], [13].

We can not obtain, at least in the adiabatic limit $h \to 0$, the scattering matrix $S(\varepsilon, h)$ directly by computing the Wronskian of Jost solutions, so that we must get a help of the connection formula of suitable solutions around an avoided crossing (i.e. a zero of $V(t)$) as in the next subsection,

2.2 Strategy in the Landau-Zener model

The Landau-Zener model, where $V(t) = vt$ with $v > 0$ constant, means that $V(t)$ and $-V(t)$ linearly cross each other at $t = 0$. This model makes clear the strategy of analyzing the connection formula. In this case, the modification of Jost solutions is required for the sake of the definition of the phase functions at infinity. As in Appendix of [21], the modified Jost solutions can be expressed by the Weber functions $D_\lambda(z), D_\lambda(-z), D_{-\lambda-1}(iz), D_{-\lambda-1}(-iz)$ and their derivatives, since the equation

$$ih\frac{d}{dt}\begin{pmatrix}\psi_1 \\ \psi_2\end{pmatrix} = \begin{pmatrix} vt & \varepsilon \\ \varepsilon & -vt \end{pmatrix}\begin{pmatrix}\psi_1 \\ \psi_2\end{pmatrix} \tag{2.2}$$

can be reduced into a single-valued equation (Weber equation)

$$\frac{d^2w}{dz^2} + \left(\lambda + \frac{1}{2} - \frac{z^2}{4}\right) w = 0, \tag{2.3}$$

where

$$w(z) = \psi_1\left(\left(\frac{h}{2v}\right)^{\frac{1}{2}} e^{-\frac{\pi}{4}i} z\right), \qquad \lambda = \frac{1}{2iv}\frac{\varepsilon^2}{h}.$$

The connection formula of the Weber functions is known in [23] as

$$\begin{pmatrix} D_\lambda(-z) \\ D_{-\lambda-1}(iz) \end{pmatrix} = \begin{pmatrix} e^{-\lambda\pi i} & -i\frac{\sqrt{2\pi}}{\Gamma(-\lambda)} e^{-\frac{\lambda\pi i}{2}} \\ \frac{\sqrt{2\pi}}{\Gamma(\lambda+1)} e^{-\frac{\lambda\pi i}{2}} & -e^{-\lambda\pi i} \end{pmatrix} \begin{pmatrix} D_\lambda(z) \\ D_{-\lambda-1}(-iz) \end{pmatrix}. \tag{2.4}$$

Denote the modified Jost solutions by $\tilde{J}^\bullet_\pm$ ($\bullet \in \{r, \ell\}$) and the change of basis of them by $\tilde{S}(\varepsilon, h)$ as $(\tilde{J}^\ell_+ \tilde{J}^\ell_-) = (\tilde{J}^r_+ \tilde{J}^r_-)\tilde{S}(\varepsilon, h)$. We can derive the connection formula $\tilde{S}(\varepsilon, h)$ from (2.4) as follows:

$$\tilde{S}(\varepsilon, h) = \begin{pmatrix} \frac{i}{\lambda^{\frac{1}{2}}} \left(\frac{h}{2v}\right)^\lambda \frac{\sqrt{2\pi}}{\Gamma(-\lambda)} e^{-\frac{\lambda\pi i}{2}} & e^{-\lambda\pi i} \\ e^{-\lambda\pi i} & \frac{1}{\lambda^{\frac{1}{2}}} \left(\frac{2v}{h}\right)^\lambda \frac{\sqrt{2\pi}}{\Gamma(-\lambda)} e^{-\frac{\lambda\pi i}{2}} \end{pmatrix}. \tag{2.5}$$

Hence we obtain the transition probability (i.e. Landau-Zener formula (1.3)):

$$\mathcal{P} = |e^{-\lambda\pi i}|^2 = e^{-\frac{\pi\varepsilon^2}{vh}}. \tag{2.6}$$

From the above argument, the following questions are crucial for the strategy of generalizations of the Landau-Zener formula.

Q.1 What are appropriate solutions corresponding to Weber functions?

Q.2 What is the connection formula (see (2.4)) between the appropriate solutions?

Q.3 What is the connection formula (see (2.5)) between the local change of basis of the original equation (1.1)?

2.3 Parameter regimes

Generalizations of Landau-Zener formula have been studied along the context of an adiabatic approximation $h \to 0$ for a fixed $\varepsilon > 0$. In this context the transition probability decays exponentially with respect to h and this fact consists of the adiabatic theorem in quantum dynamics (Bohr's correspondence principle in quantum mechanics). However, in the case of the two-parameter problem where $(\varepsilon, h) \to (0, 0)$, Landau-Zener formula claims that the transition probability tends to 1 as ε^2 goes to 0 faster than h. Hence, even if we take the adiabatic limit $h \to 0$, the transition probability does not decay exponentially against the adiabatic theorem depending on the relation between ε and h.

In the case where the zero of $V(t)$ is simple like the Landau-Zener model, we introduce the two regimes that both parameters ε and h tend to 0 with $h/\varepsilon^2 \to 0$ (resp. $\varepsilon^2/h \to 0$) called *adiabatic regime* (resp. *non-adiabatic regime*)

as in [2], [22]. The condition of the non-adiabatic regime implies that the speed of the confluence of so-called turning points is faster than the adiabatic effects (see §3.1). Hence we may roughly understand the adiabatic regime can be applied the exact WKB method to and the non-adiabatic regime can not be. The difference of these two regimes appears clearly in the connection formula as in the next section. Moreover we can consider the case where $V(t)$ has a zero of higher order and then see that two regimes are determined depending on the order of zero.

3 Connection formula around the avoided crossing

The purpose of this section is to investigate the connection formula around the avoided crossing under various regimes mentioned in §2.3. Here the connection formula means the asymptotic behavior of the change of basis over the zero of $V(t)$. We employ appropriate solutions near the origin under each regime.

3.1 Method of the exact WKB solution to 2×2 system in an adiabatic regime

The method of WKB approximations is useful for expressing appropriate solutions near the avoided crossing under the adiabatic limit $h \to 0$, and moreover, under the adiabatic regime $(\varepsilon, h) \to (0, 0)$ with $h/\varepsilon^2 \to 0$, an exact (complex) WKB method still works. In this subsection, we first treat the case where the multiplicity of the zero of $V(t)$ denoted by m satisfies $m = 1$, and at the end of this subsection we refer to the application of the exact WKB method to the general case where the zero is of finite order $m \geq 2$.

In order to apply the exact WKB method introduced by [8], [6], we assume only in this subsection an additional condition:

Condition C. *The function $V(t)$ is analytic in a complex domain $\mathcal{B}_{\sigma,\rho} \subset \mathbb{C}$ containing the origin, where $\mathcal{B}_{\sigma,\rho} := \{t \in \mathbb{C}\,;\, |\mathrm{Re}\, t| \leq \sigma,\ |\mathrm{Im}\, t| \leq \rho\}$ for positive constants σ, ρ.*

Fix an $\varepsilon > 0$ small. Under Condition C, there exist only two simple zeros of $V(t)^2 + \varepsilon^2$ in $\mathcal{B}_{\sigma,\rho}$, one of which is denoted by $\zeta(\varepsilon)$ with $\mathrm{Im}\, \zeta(\varepsilon) > 0$ and the other by $\overline{\zeta(\varepsilon)}$. One sees that $\zeta(\varepsilon)$ and $\overline{\zeta(\varepsilon)}$ are complex-valued crossing points between two energies $\pm\sqrt{V(t)^2 + \varepsilon^2}$, which are called turning points and crucial singular points in the exact WKB solutions. Note that $\zeta(\varepsilon)$ behaves like $\zeta(\varepsilon) \sim i\varepsilon/v$ as $\varepsilon \to 0$ and that both turning points $\zeta(\varepsilon)$ and $\overline{\zeta(\varepsilon)}$ converge to the origin, which is the crossing point of $V(t)$ and $-V(t)$.

We set the phase functions of the exact WKB solutions with a base point $a \in \mathcal{B}_{\sigma,\rho}$ as

$$z_a(t) := i \int_a^t \sqrt{V(s)^2 + \varepsilon^2} ds, \tag{3.1}$$

where the branch of the integrand $\sqrt{V(t)^2+\varepsilon^2}$ is taken as ε at $t=0$. The level set of the real part $z_a(t)$ is called Stokes lines emanating from $t=a$. The Stokes lines emanating from the turning points $\zeta(\varepsilon), \overline{\zeta(\varepsilon)}$ play an important role of characterizing a complex domain where the asymptotic expansion of the exact WKB solution corresponds to that of exact solutions. Now we illustrate with Figure 1 the location of the turning points $\zeta, \overline{\zeta}$, the Stokes lines (dashed lines), the branch cuts (waved lines) and the base points $r, \overline{r}, \ell, \overline{\ell} \in \tilde{\mathcal{B}}_{\sigma,\rho} := \mathcal{B}_{\sigma,\rho} \setminus \{\zeta, \overline{\zeta}\}$. near the origin in $\mathcal{B}_{\sigma,\rho}$. From [20], we admits the following proposition.

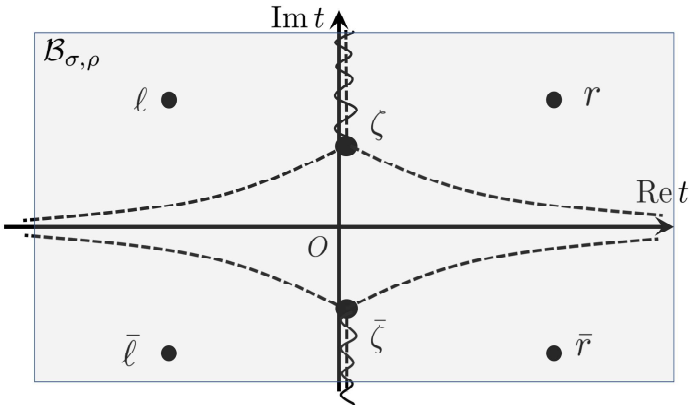

Figure 1: Configuration in $\mathcal{B}_{\sigma,\rho}$

Proposition 3.1. *Under Condition B, Condition C with $m=1$, and the above notations, we have the four exact WKB solutions given by*

$$\begin{aligned}
\Psi_+(t,\zeta,r;h) &= \exp\left[+\frac{z_\zeta(t)}{h}\right] M_+(z(t)) w_+(z(t),z(r);h) \quad := \Psi_+^r,\\
\Psi_-(t,\overline{\zeta},\overline{r};h) &= \exp\left[-\frac{z_{\overline{\zeta}}(t)}{h}\right] M_-(z(t)) w_-(z(t),z(\overline{r});h) \quad := \Psi_-^r,\\
\Psi_+(t,\zeta,\ell;h) &= \exp\left[+\frac{z_\zeta(t)}{h}\right] M_+(z(t)) w_+(z(t),z(\ell);h) \quad := \Psi_+^\ell,\\
\Psi_-(t,\overline{\zeta},\overline{\ell};h) &= \exp\left[-\frac{z_{\overline{\zeta}}(t)}{h}\right] M_-(z(t)) w_-(z(t),z(\overline{\ell});h) \quad := \Psi_-^\ell.
\end{aligned} \tag{3.2}$$

Here $M_\pm(z(t))$ are matrices of the forms:

$$M_\pm = \begin{pmatrix} K(z)^{-1} & K(z)^{-1} \\ \mp iK(z) & \pm iK(z) \end{pmatrix}, \quad K(z(t)) = \left(\frac{-iV(t)+\varepsilon}{-iV(t)-\varepsilon}\right)^{\frac{1}{4}}$$

and the amplitude $w_\pm(z(t),z(b))$ are the vector-valued functions determined by

a resummation based on an integral recurrence 2×2 *system of the variable* z *with base point* $z(b)$ $(b = r, \ell, \bar{r}, \bar{\ell})$.

Note that, since the form of $K(z(t))$ is independent of the base point of the phase a, we omit the index a of $z_a(t)$ in the expression of $M_\pm(z(t))$ and $w_\pm(z(t), z(b))$. One of the kernels of two integral operators of the recurrence system is the derivative of $\log K(z)$ with respect to z and the other is the same derivative multiplied by the exponential factor $e^{\pm 2z/h}$. Consulting the references [6], [20], we see that the resummation goes well in a neighborhood of $t = b \in \tilde{\mathcal{B}}_{\sigma,\rho}$ and the four exact WKB solutions (3.2) are well-defined there. Moreover, if the integral path from the base point $z(b)$ to z is taken as the canonical curve introduced later, then the latter integral operator gains $\mathcal{O}(h)$.

We pick up one of the important properties of the exact WKB method, called Wronskian formula. In order to state the Wronskian formula, we introduce *canonical curves of type* $\pm$ in $\tilde{\mathcal{B}}_{\sigma,\rho}$ from a fixed point b to t along which $\pm \mathrm{Re}\, z_a(t)$ increase strictly, for a fixed $a \in \mathcal{B}_{\sigma,\rho}$. We set $\Sigma := \{\zeta, \bar{\zeta}\}$ and denote the Wronskian of two vector-valued functions f, g by $\mathcal{W}[f, g] := \det(fg)$.

Lemma 3.2. *If there exists a canonical curve of type* $+$ *from* b_+ *to* b_- *denoted by* γ*, there exist a function* $\mathcal{E}_\gamma(h)$ *depending on* γ *such that the Wronskian between any exact WKB solutions of type* $\pm$ *with the same base point of the phase satisfies*

$$\mathcal{W}[\Psi_+(t, a, b_+; h), \Psi_-(t, a, b_-; h)] = 2i + \mathcal{E}_\gamma(h) \tag{3.3}$$

for h *small enough, where* $\mathcal{E}_\gamma(h) = \mathcal{O}(h)$ *as* h *tends to* 0 *for a fixed* ε.

We can estimate $\mathcal{E}_\gamma(h)$ more precisely with some positive constant C as

$$|\mathcal{E}_\gamma(h)| \leq \frac{Ch}{\mathrm{dist}(\gamma; \Sigma)} \tag{3.4}$$

for h small enough, where $\mathrm{dist}(\gamma; \Sigma) = \inf_{t \in \gamma, \zeta \in \Sigma} |z_\zeta(t)|$. Remark that, if γ is close to turning points as $\varepsilon \to 0$, the Wronskian formula (Lemma 3.2) is broken down.

Our interest of this subsection is the connection formula between the four WKB solutions (3.2), which is the asymptotic formula of the change of basis $T_{\mathrm{local}}(\varepsilon, h)$ given by

$$(\Psi^\ell_+ \Psi^\ell_-) = (\Psi^r_+ \Psi^r_-) T_{\mathrm{local}}(\varepsilon, h), \qquad T_{\mathrm{local}}(\varepsilon, h) = \begin{pmatrix} \tau_{11} & \tau_{12} \\ \tau_{21} & \tau_{22} \end{pmatrix}. \tag{3.5}$$

The direct computation leads to the representation of $T_{\mathrm{local}}(\varepsilon, h)$ by means of the Wronskians of the solution (3.2) as follows:

$$T_{\mathrm{local}}(\varepsilon, h) = \begin{pmatrix} \dfrac{\mathscr{W}(\ell, \bar{r})}{\mathscr{W}(r, \bar{r})} & i \dfrac{\mathscr{W}(\hat{\bar{\ell}}, \bar{r})}{\mathscr{W}(r, \bar{r})} e^{z_{\bar{\zeta}}(\zeta)/h} \\ i \dfrac{\mathscr{W}(r, \hat{\ell})}{\mathscr{W}(r, \bar{r})} e^{z_{\bar{\zeta}}(\zeta)/h} & \dfrac{\mathscr{W}(r, \bar{\ell})}{\mathscr{W}(r, \bar{r})} \end{pmatrix}, \tag{3.6}$$

where $\mathscr{W}(b_+, b_-)$ stands for the Wronskian $\mathcal{W}[\Psi_+(t, a, b_+; h), \Psi_-(t, a, b_-; h)]$, and $\hat{\ell}$ (resp. $\hat{\bar{\ell}}$) is the same point as ℓ (resp. $\bar{\ell}$) after turning clockwise around ζ (resp. $\bar{\zeta}$) and passing through the branch cut on the upper (resp. lower) half plane. As in Figure 2 illustrating canonical curves as densely dashed lines, we can find canonical curves for the Wronskians in (3.6), although we need to look for such curves on the other Riemann surface. Hence from Lemma 3.2, we obtain the following asymptotics of the elements of $T_{\mathrm{local}}(\varepsilon, h)$:

Proposition 3.3. *Under Condition B with $m = 1$ and Condition C, the elements of $T_{\mathrm{local}}(\varepsilon, h)$ admit the asymptotic behavior*

$$|\tau_{11}| = |\tau_{22}| = 1 + \mathcal{O}\left(\frac{h}{\varepsilon^2}\right) \qquad \text{as} \quad \frac{h}{\varepsilon^2} \to 0, \tag{3.7}$$

$$|\tau_{12}| = |\tau_{21}| = e^{-\frac{1}{h}\operatorname{Im} A(\varepsilon)}(1 + \mathcal{O}(h)) \qquad \text{as} \quad h \to 0, \tag{3.8}$$

where $A(\varepsilon)$ is the action integral defined by the turning point $\zeta(\varepsilon)$ as follows:

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

with the branch of the integrand the same as $z_\zeta(t)$, that is, $\operatorname{Im} A(\varepsilon) > 0$.

From $\zeta(\varepsilon) = \mathcal{O}(\varepsilon)$, the action integral satisfies $A(\varepsilon) = \mathcal{O}(\varepsilon^2)$, so that the modulus of the off-diagonal entry decays exponentially as h/ε^2 tends to 0, called the adiabatic regime.

Remark 3.4. *This connection formula is guaranteed by the existence of the canonical curve between both base points of the exact WKB solutions in the Wronskian. In our setting, the turning points $\zeta(\varepsilon), \overline{\zeta(\varepsilon)}$ converge to the origin as $\varepsilon \to 0$. If the canonical curve is pinched by these turning points, the error of the Wronskian formula becomes worse (see the error term $\mathcal{E}_\gamma(h)$ in (3.4)). In particular, as $\varepsilon^2/h \to 0$, the Wronskian formula is no longer valid. This fact is the technical difficulty of two-parameter problem from the viewpoint of the exact WKB method.*

From the above remark, for example, the asymptotic expansion of the Wronskian $\mathscr{W}(r, \bar{\ell})$ is not uniform in ε, since the canonical curve from r to $\bar{\ell}$ is pinched by $\zeta, \bar{\zeta}$. Conversely, if the canonical curve is away from the turning points, the Wronskian formula is still true uniformly in small ε. In the case where the zero of $V(t)$ is simple, the asymptotics of the off-diagonal entry, which gives the transition probability, is $\mathcal{O}(h)$ uniformly in ε, since the canonical curve from r to $\bar{r}$ and also to $\hat{l}$ drawn by densely dashed line is not pinched by the turning points (see Figure 2).

We can extend the exact WKB method to a general case where there exist a finite number of zeros of $V(t)$ on $\mathbb{R}$. Then the scattering matrix (i.e. the change of basis of the Jost solutions) is given by the product of the local change of basis near each zero. The asymptotic expansion of the transition probability

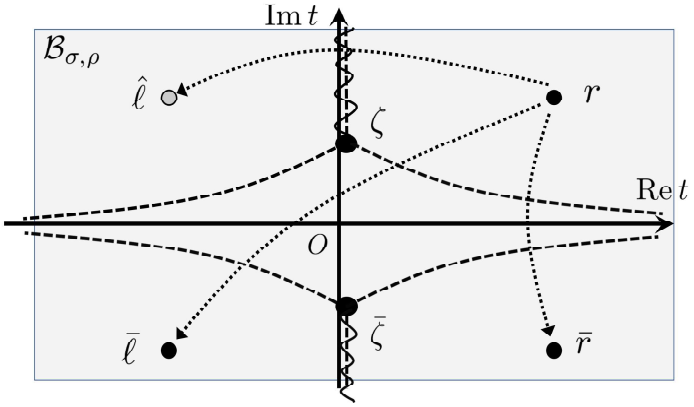

Figure 2: Canonical curves in $\mathcal{B}_{\sigma,\rho}$

obtained by the exact WKB method is valid under the adiabatic regime $h/\varepsilon^2 \to 0$. Therefore, as in the next subsection, we must find another approach in the non-adiabatic regime $\varepsilon^2/h \to 0$.

Moreover we can develop the exact WKB method into the case where the zero is of finite order denoted by m. In this case, turning points exist around the origin like the power roots of order $2m$. Denoting them by $\zeta_1(\varepsilon), \ldots, \zeta_m(\varepsilon)$ and their complex conjugates, we have

$$\zeta_k(\varepsilon) \sim \left(\frac{m!}{V^{(m)}(0)}\right)^{\frac{1}{m}} e^{\frac{(2k-1)\pi i}{2m}} \varepsilon^{\frac{1}{m}} \qquad (\varepsilon \to 0).$$

The exact WKB method remains valid even in this case. Taking ρ suitably small, then even if m is larger than 2 we can find a similar configuration in $\mathcal{B}_{\sigma,\rho}$ to the case $m = 2$, that is, there exist only four turning points in the box $\mathcal{B}_{\sigma,\rho}$ as Figure 3. According to [20], one sees that these turning points closest to the real axis determine the leading term of the asymptotic expansion of the transition probability. We skip the details of the argument but give the asymptotics of the elements of T_{local} as follows:

Proposition 3.5. *Under Condition B with $m \geq 2$ and Condition C, the elements of $T_{\mathrm{local}}(\varepsilon, h)$ have the asymptotic behavior*

$$|\tau_{11}| = |\tau_{22}| = 1 + \mathcal{O}\left(\frac{h}{\varepsilon^{\frac{m+1}{m}}}\right) \tag{3.9}$$

$$|\tau_{12}| = |\tau_{21}| = \left|e^{\frac{i}{h}A_1(\varepsilon)} + (-1)^{m+1} e^{\frac{i}{h}A_m(\varepsilon)}\right| + \mathcal{O}\left(\frac{h}{\varepsilon^{\frac{m+1}{m}}} e^{-\frac{1}{h}\alpha(\varepsilon)}\right) \tag{3.10}$$

as $h/\varepsilon^{\frac{m+1}{m}} \to 0$, where $A_k(\varepsilon)$ is defined similarly and behaves when $\varepsilon \to 0$ as

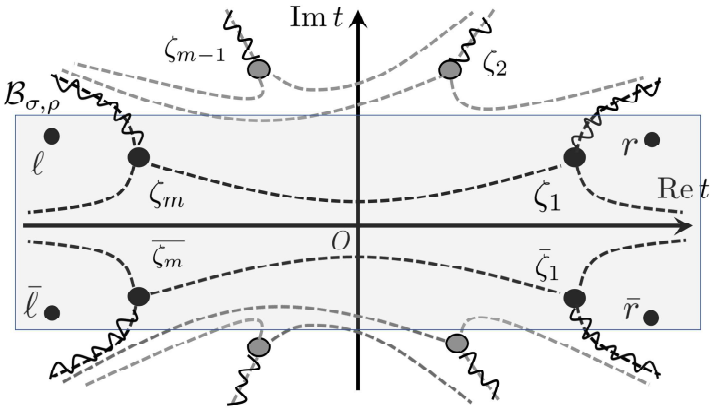

Figure 3: Configuration in $\mathcal{B}_{\sigma,\rho}$

follows:

$$A_k(\varepsilon) = 2\int_0^{\zeta_k(\varepsilon)} \sqrt{V(t)^2+\varepsilon^2}\, dt = \mathcal{O}(\varepsilon^{\frac{m+1}{m}}), \tag{3.11}$$

and $\alpha(\varepsilon) := \min\{\mathrm{Im}A_1(\varepsilon), \mathrm{Im}A_m(\varepsilon)\}$.

The asymptotic behavior (3.11) implies that $|\tau_{21}|$ is exponentially small with respect to $\varepsilon^{\frac{m+1}{m}}/h \ll 1$ as well as the case $m = 1$. However the Wronskian formula, which gives the transition probability, does not have asymptotic expansions uniformly in ε even if the the number of the zero of $V(t)$ on $\mathbb{R}$ is only one. As in Figure 4, the canonical curves from the intermideate point δ to $\bar{\delta}$ cannot help being pinched by the turning points ζ_1, ζ_m and their complex conjugates gathering at the origin.

3.2 Method of the solution to microlocal normal form in a non-adiabatic regime

In this subsection, we assume that the zero of $V(t)$ is simple and consider the non-adiabatic regime: $(\varepsilon, h) \to (0,0)$ with $\varepsilon^2/h \to 0$. As we mentioned in the previous subsection, the Wronskian formula in the exact WKB method does not work in the non-adiabatic regime. The aim of this subsection is to introduce a microlocal normal form, called branching model, and its solutions along the context of [22].

The original equation (1.1) is of the following form:

$$P_0\psi(t) = \begin{pmatrix} hD_t + V(t) & \varepsilon \\ \varepsilon & hD_t - V(t) \end{pmatrix} \psi(t) = 0, \tag{3.12}$$

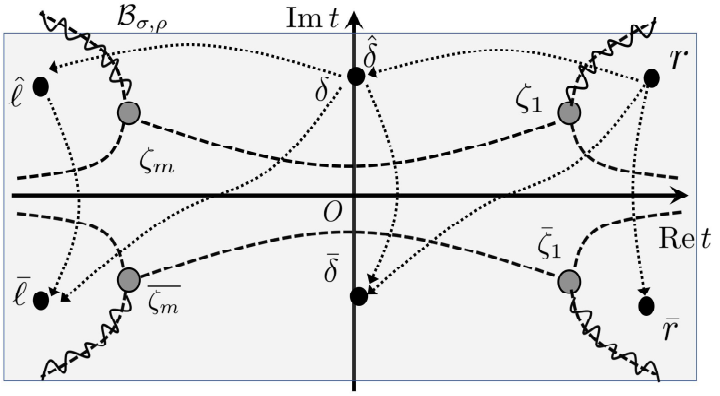

Figure 4: Canonical curves in $\mathcal{B}_{\sigma,\rho}$

where $D_t = \frac{1}{i}\frac{d}{dt}$, can be transformed into so-called *branching model* (microlocal normal form) of the first order 2×2 system:

$$Q\phi(y) = \begin{pmatrix} \sqrt{2}y & \mu \\ \mu & \sqrt{2}\mu D_y \end{pmatrix} \phi(y) = 0, \tag{3.13}$$

where $\mu = \varepsilon^2/h$ is a crucial small parameter of the non-adiabatic regime. This model was introduced in a single-valued case by Helffer-Sjöstrand [11] (see also März [18]). A 2×2 system depending only on one parameter was studied first by Kaidi-Rouleux [16], and also by Fermanian Kammerer-Gérard [4], Colin de Verdière[3], Fujiié-Lasser-Nédélec [6] in other settings.

The branching model (3.13) has a couple of solutions

$$\phi^{\vdash}(y) = Y(y) y^{\frac{i}{2}\mu} \begin{pmatrix} -\frac{\mu}{\sqrt{2}y} \\ 1 \end{pmatrix}, \qquad \phi^{\dashv}(y) = Y(-y)|y|^{\frac{i}{2}\mu} \begin{pmatrix} -\frac{\mu}{\sqrt{2}y} \\ 1 \end{pmatrix}, \tag{3.14}$$

where $Y(y)$ is the Heaviside function. The properties of these distributions can be found in [7]. Moreover the differential operator Q commutes with the operator $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathcal{C}\mathcal{F}_\mu$, where $\mathcal{C}$ is an operator of taking its complex conjugate, that is, $\mathcal{C}\phi(y) = \overline{\phi(y)}$, and $\mathcal{F}_\mu$ is a semi-classical Fourier transform:

$$\mathcal{F}_\mu[u](\xi) = \frac{1}{\sqrt{2\pi\mu}} \int_{\mathbb{R}} e^{-\frac{i}{\mu}x\xi} u(x) dx. \tag{3.15}$$

Then the functions $\phi^{\perp}(y)$ and $\phi^{\top}(y)$ given by

$$\phi^{\perp}(y) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathcal{C}\mathcal{F}_\mu \phi^{\vdash}(y), \qquad \phi^{\top}(y) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathcal{C}\mathcal{F}_\mu \phi^{\dashv}(y) \tag{3.16}$$

are also solutions of (3.13). Computing $\phi^{\perp}(y)$, $\phi^{\top}(y)$ by using the property $\mathcal{C}\mathcal{F}_{\mu} = \mathcal{F}_{\mu}^{-1}\mathcal{C}$, we obtain the relation between the pairs $(\phi^{\vdash}, \phi^{\dashv})$ and $(\phi^{\perp}, \phi^{\top})$.

Proposition 3.6. *Let R be a 2×2 matrix such that $(\phi^{\perp}\phi^{\top}) = (\phi^{\vdash}\phi^{\dashv})R$. Then R is of the form: $R = \begin{pmatrix} p & -q \\ q & -p \end{pmatrix}$ with*

$$p = \gamma e^{\frac{\pi\mu}{4}}, \qquad q = \gamma e^{-\frac{\pi\mu}{4}}, \qquad \gamma = \frac{1}{i\sqrt{\pi\mu}}\mu^{-\frac{i\mu}{2}}\Gamma\left(1 - \frac{i\mu}{2}\right). \tag{3.17}$$

The proof of Proposition 3.6 is done by the direct computation that the semiclassical Fourier transform of solutions $\phi^{\perp}(y), \phi^{\top}(y)$ are reduced to the integral expressions of the Gamma functions. From the reflection property of the Gamma function:

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin \pi z} = \frac{2\pi i}{e^{i\pi z} - e^{-i\pi z}} \qquad (z \in \mathbb{C} \setminus \mathbb{Z})$$

and thanks to $q/p = e^{-\frac{\pi\mu}{2}} \in \mathbb{R}$, the constants γ, p and q satisfy

$$|\gamma|^2 = \left(e^{\frac{\pi}{2}\mu} - e^{-\frac{\pi}{2}\mu}\right)^{-1}, \quad |p|^2 - |q|^2 = 1, \quad \frac{p^2 - q^2}{p} = \frac{1}{\bar{p}}. \tag{3.18}$$

The change of basis R in Proposition 3.6 gives the connection formula of the appropriate solutions replacing the exact WKB solutions. The relation between the solutions of the branching model (3.13) and those of the original equation is given by Proposition 3.9 based on the following microlocal reduction.

First, the following lemma guarantees the existence of a local smooth change of variables which allows us to replace $V(t)$ by a linear function near the crossing point.

Lemma 3.7. *There exist a small neighborhood $\mathcal{U}$,$\tilde{\mathcal{U}}$ of the origin and a change of variables $f : \mathcal{U} \to \tilde{\mathcal{U}}$ such that $f(0) = 0$, $f'(0) = 1$ and $f(t)f'(t) = V(t)$ for any $t \in \mathcal{U}$.*

Note that the function f is determined independently from the parameters ε and h. The proof of this lemma can be done by constructing $f(t)$ concretely for t in a small neighborhood of $t = 0$ as follows:

$$f(t) = t\left(1 + 2t\int_0^1\int_0^1 s^2(1-\sigma)V''(ts\sigma)d\sigma ds\right)^{\frac{1}{2}}. \tag{3.19}$$

Putting $\psi_1(z) := \psi(f^{-1}(\sqrt{h}\,t))$, we see that the equation (3.12) becomes

$$P_1\psi_1(z) = \begin{pmatrix} D_z + z & \sqrt{\mu}(f^{-1})'(\sqrt{h}z) \\ \sqrt{\mu}(f^{-1})'(\sqrt{h}z) & D_z - z \end{pmatrix}\psi_1(z) = 0. \tag{3.20}$$

Recall that $\mu = \varepsilon^2/h \to 0$ implies that $\varepsilon \to 0$ uniformly with respect to $h \in (0, h_0]$ for some fixed $h_0 > 0$. Notice that (3.20) is a regular perturbation problem of order $\sqrt{\mu}$.

Second, we apply the Neumann lemma to (3.20). According to Lemma 11 in [22], there exists a C^∞-matrix $M(z;\sqrt{\mu},h) = \mathrm{Id} + \sum_{k\geq 1} \mu^{\frac{k}{2}} M_k(z;h)$ such that the equation (3.20) becomes

$$P_2\psi_2(z) = \begin{pmatrix} D_z + z & \sqrt{\mu} \\ \sqrt{\mu} & D_z - z \end{pmatrix} \psi_2(z) = 0, \qquad z \in I, \tag{3.21}$$

where $\psi_2(z) := M(z;\sqrt{\mu},h)\psi_1(z)$.

Now, by using a change of scaling $x = \sqrt{\mu}z$, we can regard the equation (3.21) as a semi-classical problem with respect to μ.

$$P_3\psi_3(x) = \begin{pmatrix} \mu D_x + x & \mu \\ \mu & \mu D_x - x \end{pmatrix} \psi_3(x) = 0, \qquad x \in \sqrt{\mu}I, \tag{3.22}$$

where $\psi_3(x) := \psi_2(x/\sqrt{\mu})$.

Finally, we employ the so-called Egorov type theorem by means of the Fourier integral operator. Let $U_{\frac{\pi}{4}}$ be the Fourier integral (metaplectic) operator associated with the rotation $\pi/4$ on the phase space $T^*\mathbb{R}$:

$$\kappa_{\frac{\pi}{4}} \ : \ T^*\mathbb{R} \ni (x,\xi) \longmapsto \frac{1}{\sqrt{2}}(x-\xi, x+\xi) \in T^*\mathbb{R}.$$

The Fourier integral operator $U_{\frac{\pi}{4}}$ is given, in the book of Helffer-Sjöstrand [11], by

$$U_{\frac{\pi}{4}}[u](x) = \frac{e^{\frac{\pi}{8}i}2^{\frac{1}{4}}}{\sqrt{2\pi\mu}} \int_{\mathbb{R}} e^{\frac{i}{\mu}(-\frac{x^2}{2}+\sqrt{2}xy-\frac{y^2}{2})} u(y)\, dy$$

for u in the space of tempered distributions. We notice that the microsupport of $U[u]$ is given by the canonical transformation $\kappa_{\frac{\pi}{4}}$ of the microsupport of u.

Lemma 3.8. *We denote the symbols of the diagonal entries of P_3 and Q by*

$$\begin{aligned} p_1(x,\xi) &= \xi + x, & p_2(x,\xi) &= \xi - x, \\ q_1(y,\eta) &= \sqrt{2}y, & q_2(y,\eta) &= \sqrt{2}\eta. \end{aligned}$$

Then the operators

$$P_3 = \begin{pmatrix} p_1^w(x,\mu D_x) & \mu \\ \mu & p_2^w(x,\mu D_x) \end{pmatrix}, \qquad Q = \begin{pmatrix} q_1^w(y,\mu D_y) & \mu \\ \mu & q_2^w(y,\mu D_y) \end{pmatrix}$$

satisfy

$$U_{\frac{\pi}{4}}^{-1} p_j^w(x,\mu D_x) U_{\frac{\pi}{4}} = (p \circ \kappa_{\frac{\pi}{4}})^w(y,\mu D_y) = q_j(y,\mu D_y), \quad (j=1,2).$$

Let $\chi \in C_0^\infty(\mathbb{R})$ be identically equal to 1 near I. Then we put

$$\phi(y) = U_{\frac{\pi}{4}}^{-1}\left[\chi\left(\frac{x}{\sqrt{\mu}}\right)\psi_3(x)\right](y).$$

The equation (3.22) is equivalent to

$$Q\phi(y) = -i\sqrt{\mu}U_{\frac{\pi}{4}}^{-1}\left[\chi'\left(\frac{x}{\sqrt{\mu}}\right)\psi_3(x)\right](y). \tag{3.23}$$

The right-hand side of (3.23) is of $\mathcal{O}(\mu^\infty)$ uniformly on $\sqrt{\mu}I$.

Summing up, we obtain the following proposition:

Proposition 3.9. *There exist $h_0 > 0$ small enough and $c_0 > 0$ independent of ε and h such that the equation (3.12) has a solution given by, as $\varepsilon^2/h \to 0$,*

$$\psi(t;\varepsilon,h) = M\left(\frac{\varepsilon}{h}f(t);\frac{\varepsilon}{\sqrt{h}},h\right)U_{\frac{\pi}{4}}[\phi]\left(\frac{\varepsilon}{h}f(t)\right) + \mathcal{O}\left(\left(\frac{\varepsilon^2}{h}\right)^\infty\right), \tag{3.24}$$

uniformly on $h \in (0,h_0]$ and $t \in \{|t| \le c_0\sqrt{h}\}$, where ϕ is a solution of (3.23), and f and M are given in the above reduction.

To obtain the colinear relations between the appropriate solutions $U_{\frac{\pi}{4}}[\phi^\bullet]$ ($\bullet = \vdash, \dashv, \perp, \top$) and exact WKB solutions, we study the microsupports of them on the annulus in the phase space. Note that, on the annulus of radius $\mathcal{O}(h)$ in the corresponding complex plane, we can treat the exact WKB solutions away from turning points, since they are $\mathcal{O}(\varepsilon^2)$. Comparing the microsupports of $U_{\frac{\pi}{4}}[\phi]$ with those of the exact WKB solutions, computing the asymptotics of $U_{\frac{\pi}{4}}[\phi]$ by the stationary phase method with respect to $\mu = \varepsilon^2/h$, and also combining the asymptotics of R in Proposition 3.6, we can find the connection formula of T_{local} given in (3.5) under the non-adiabatic regime as follows:

Proposition 3.10. *Suppose Condition B with $m = 1$. There exist $\mu_0 > 0$ and $h_0 > 0$ small enough such that for any ε and h with $\frac{\varepsilon^2}{h} \in (0,\mu_0]$ and $h \in (0,h_0]$ the transfer matrix $T_{\mathrm{local}}(\varepsilon,h)$ has the following asymptotic behavior:*

$$T_{\mathrm{local}}(\varepsilon,h) = \begin{pmatrix} e^{i\vartheta}\dfrac{1}{\bar{p}} & \dfrac{1}{i}\dfrac{q}{p} \\ \dfrac{1}{i}\dfrac{q}{p} & \mathcal{C}\left(e^{i\vartheta}\dfrac{1}{\bar{p}}\right) \end{pmatrix}\left(1 + \mathcal{O}\left(\sqrt{h}\right) + \mathcal{O}\left(\frac{\varepsilon}{\sqrt{h}}\right)\right), \tag{3.25}$$

where p, q are given by (3.17), $\vartheta = \frac{3\pi}{4} + \frac{\varepsilon^2}{h}\log\frac{\varepsilon^2}{h}$ and $\mathcal{C}$ stands for the operator of taking the complex conjugate.

3.3 Method of the fundamental solution to the diagonal in a non-adiabatic regime

In the case where a non-adiabatic regime, that is, ε with some power tends to 0 faster than h, we must adopt other approaches instead of the exact WKB method. When $V(t)$ has the zero with a finite multiplicity m larger than 1, that is $V(t)$ and $-V(t)$ have a tangential intersection, the microlocal approach

introduced in the previous subsection is not applied immediately. Recalling that the connection formula by the exact WKB method (3.9) is valid under the adiabatic regime $h/\varepsilon^{\frac{m+1}{m}} \to 0$, we regard the regime $\varepsilon^{\frac{m+1}{m}}/h \to 0$ as the non-adiabatic regime in the case of the zero of higher order. Hence our interest in this subsection is to find suitable solutions near the origin and the connection formula between the bases composed by those solutions under the non-adiabatic regime $\varepsilon^{\frac{m+1}{m}}/h \to 0$.

The approach by means of fundamental solutions, which we introduce in this subsection, is based on the works of [24] in a single-valued Schrödinger equation, of [5] in a 2×2 system of Schrödinger equations with a transversal crossing of the potentials, of [1] in a similar system with tangential crossings and in particular of [12] in a first order 2×2 system with a tangential crossing. Here we give the idea of these methods of fundamental solutions along the our recent work [13].

We precede this approach with the construction of solutions to (1.1) under the non-adiabatic regime. Let I be a small interval containing 0. For any continuous function u and for any point $s_0 \in I$, we define an integral operator $K = K(u, s_0)$ by

$$K(u, s_0)f(t) := \frac{i}{h}u(t)\int_{s_0}^{t} \frac{f(s)}{u(s)}ds. \tag{3.26}$$

If $u^{\pm}$ satisfy respectively

$$\left(\frac{h}{i}\frac{d}{dt} \pm V(t)\right)u^{\pm} = 0 \quad \text{on} \quad I, \tag{3.27}$$

the operators $K^{\pm} := K(u^{\pm}, s^{\pm})$ for any $s^{\pm} \in I$ are fundamental solutions:

$$\left(\frac{h}{i}\frac{d}{dt} \pm V(t)\right)K^{\pm}f = f \quad \text{for} \quad f \in C(I), \tag{3.28}$$

where $C(I)$ is the Banach space of continuous functions on I equipped with the norm $\|f\|_{C(I)} := \sup_I |f(x)|$. Our equation (1.1) turns into the integral system:

$$\begin{cases} \psi_1(t) = -\varepsilon K^{+}\psi_2(t), \\ \psi_2(t) = -\varepsilon K^{-}\psi_1(t). \end{cases} \tag{3.29}$$

Notice that $K^{\pm}$ are independent of ε. Let us fix

$$u^{\pm}(t) = e^{\mp\frac{i}{h}\int_0^t V(s)ds}.$$

For the choice of the endpoints s^{+} and s^{-}, we have the following proposition:

Proposition 3.11. *For any s^{-}, $s^{+} \in I$, we have*

$$\begin{aligned} &\left\|(K^{\mp}K^{\pm})^k u^{\mp}\right\|_{C(I)} = \mathcal{O}(h^{-\frac{2km}{m+1}}), \\ &\left\|K^{\pm}(K^{\mp}K^{\pm})^k u^{\mp}\right\|_{C(I)} = \mathcal{O}(h^{-\frac{(2k+1)m}{m+1}}), \end{aligned} \tag{3.30}$$

where we consider the Banach space of continuous functions on I with the sup norm $\|f\|_{C(I)} := \sup_I |f(x)|$.

The proof of Proposition 3.11 follows the next lemma based on the degenerate stationary phase method (see e.g. [14]):

Lemma 3.12. *On a compact interval $I \subset \mathbb{R}$, the integral*

$$\mathcal{I}_I(h) := \int_I \exp\left(\frac{2i}{h}\int_{t_0}^t V(s)ds\right) dt \tag{3.31}$$

is estimated as $\mathcal{O}(h)$ as $h \to 0$ when V does not vanish on I. If t_0 is the unique zero in I of V, one has

$$\mathcal{I}_I(h) = \omega_m h^{\frac{1}{m+1}} + \mathcal{O}(h^{\frac{2}{m+1}}), \tag{3.32}$$

where ω_m is given by

$$\omega_m = \frac{2}{m+1}\Gamma\left(\frac{1}{m+1}\right)\left(\frac{(m+1)!}{2|V^{(m)}(t_0)|}\right)^{\frac{1}{m+1}} \eta_m, \tag{3.33}$$

with

$$\eta_m := \begin{cases} \cos\left(\dfrac{\pi}{2(m+1)}\right) & m : \textit{even}, \\ \exp\left(\dfrac{\mathrm{sgn}(V^{(m)}(t_0))\pi i}{2(m+1)}\right) & m : \textit{odd}. \end{cases} \tag{3.34}$$

From Proposition 3.11, we construct the solutions w^+ and w^- by

$$w^+ = w^+(K^+, K^-, u^+) := \begin{pmatrix} \displaystyle\sum_{k\geq 0}(\varepsilon^2 K^+K^-)^k u^+ \\ -\varepsilon K^- \displaystyle\sum_{k\geq 0}(\varepsilon^2 K^+K^-)^k u^+ \end{pmatrix}, \tag{3.35}$$

and

$$w^- = w^-(K^+, K^-, u^-) := \begin{pmatrix} -\varepsilon K^+ \displaystyle\sum_{k\geq 0}(\varepsilon^2 K^-K^+)^k u^- \\ \displaystyle\sum_{k\geq 0}(\varepsilon^2 K^-K^+)^k u^- \end{pmatrix}. \tag{3.36}$$

Examining the fundamental solutions more precisely in the proof of Proposition 3.11, the integral factors of $|K^{\pm}u^{\mp}(t)|$ respectively are estimated as $\mathcal{O}(h)$ if the integral region of $K^{\pm}$ does not contain $t = 0$. Hence we have

$$w^+ = \begin{pmatrix} u^+ + \mathcal{O}(\varepsilon^2/h) \\ \mathcal{O}(\varepsilon) \end{pmatrix} \quad \text{on} \quad I \cap \{\pm t > 0\} \tag{3.37}$$

if $\pm s^- > 0$ and

$$w^- = \begin{pmatrix} \mathcal{O}(\varepsilon) \\ u^- + \mathcal{O}(\varepsilon^2/h) \end{pmatrix} \quad \text{on} \quad I \cap \{\pm t > 0\} \tag{3.38}$$

if $\pm s^+ > 0$. These asymptotic behaviors imply that the construction by means of the iteration with fundamental solutions gives not only local solutions near an avoided crossing but also those away from an avoided crossing.

Let $\delta > 0$ be a small constant independent of ε and h, and set

$$I_L := [-\delta, 0], \quad I_R := [0, \delta], \quad K_L^{\pm} = K(u^{\pm}, -\delta), \quad K_R^{\pm} = K(u^{\pm}, +\delta), \tag{3.39}$$

(i.e., $s_R^{\pm} = +\delta$, $s_L^{\pm} = -\delta$). From Proposition 3.11, we can define four solutions $w_S^{\pm}$ on I_S for $S = L, R$ by

$$w_S^{\pm} := w^{\pm}(K_S^+, K_S^-, u^{\pm}). \tag{3.40}$$

One sees that for $S = L, R$ each (w_S^+, w_S^-) is a basis of the solution space on I_S and that the property of the symmetricity:

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \overline{w_S^-} = w_S^+ \tag{3.41}$$

holds. Let T_{local} be the change of basis as

$$(w_L^+, w_L^-) = (w_R^+, w_R^-) T_0. \tag{3.42}$$

Then we obtain the connection formula:

Theorem 1. *The 2×2-matrix $T_0 = T(\varepsilon, h)$ admits the following asymptotic formula:*

$$T_0 = \mathrm{Id} - i\mu_m T_{\mathrm{sub}} + \mathcal{O}(\mu_m^2 + \mu_m h^{\frac{1}{m+1}}) \tag{3.43}$$

with $\mu_m := \varepsilon h^{-\frac{m}{m+1}}$ and

$$T_{\mathrm{sub}} = \begin{pmatrix} 0 & \omega_m \\ \overline{\omega}_m & 0 \end{pmatrix}. \tag{3.44}$$

Here, the constant ω_m is given in Lemma 3.12.

We remark that, from the relation (3.41), the matrix T_0 satisfies the following symmetry

$$T_0 = \begin{pmatrix} \tau_1 & -\tau_2 \\ \overline{\tau_2} & \overline{\tau_1} \end{pmatrix}. \tag{3.45}$$

The proof of this theorem is based on the degenerate stationary phase method (Lemma 3.12) of the oscillatory integrals coming from the composition of the fundamental solutions $K^{\pm}$. The ε-independence of the fundamental solutions implies that the local solutions $w_S^{\pm}$ correspond to $\pm V(t)$ but not to the energies $\pm\sqrt{V(t)^2 + \varepsilon^2}$. We recall that each entry of the change of basis T_0 can be expressed by the Wronskian and also that the Wronskian is independent of the variable t. Thanks to the definition of the bases (w_R^+, w_R^-) and (w_L^+, w_L^-), more precisely to the construction of the solutions, one sees that there exist 2×2 constant matrices A_R, A_L such that

$$(w_R^+(0), w_R^-(0)) = \mathrm{Id} + A_R, \qquad (w_L^+(0), w_L^-(0)) = \mathrm{Id} + A_L. \tag{3.46}$$

Hence the change of basis T_0 can be represented by

$$T_0 = (\mathrm{Id} + A_R)^{-1}(\mathrm{Id} + A_L). \tag{3.47}$$

The representation (3.47) implies that the connection formula can be derived from computations of asymptotic behaviors of $w_S^{\pm}(0)$ with respect to ε and h with the regime $\varepsilon^{\frac{m+1}{m}}/h = (\mu_m)^{\frac{m+1}{m}} \to 0$. From Lemma 3.12, we obtain

$$A_S = -\frac{i}{2}\varepsilon h^{-\frac{m}{m+1}} \begin{pmatrix} 0 & \omega_m \\ \overline{\omega}_m & 0 \end{pmatrix} + \mathcal{O}((\varepsilon h^{-\frac{m}{m+1}})^2). \tag{3.48}$$

This is the idea of the proof of Theorem 1.

By matching the asymptotic behaviors of the local solutions $w_S^{\pm}$ on suitable subinterval of I_S for $S = L, R$, (3.37), (3.38) with those of the exact WKB solutions $\Psi_{\pm}^r, \Psi_{\pm}^{\ell}$, we have the following relations

$$w_R^+ = -i\Psi_-^r, \qquad w_R^- = -\Psi_+^r,$$
$$w_L^+ = \begin{cases} \Psi_+^{\ell} & (m : \text{odd}), \\ -i\Psi_-^{\ell} & (m : \text{even}), \end{cases} \qquad w_L^- = \begin{cases} -i\Psi_-^{\ell} & (m : \text{odd}), \\ -\Psi_+^{\ell} & (m : \text{even}). \end{cases}$$

Hence we obtain

Proposition 3.13. *Suppose Condition B with $m \geq 2$. As $(\varepsilon, h) \to (0,0)$ with $\mu_m = \varepsilon h^{-\frac{m}{m+1}} \to 0$, the following holds.*

$$T_{\mathrm{local}} = \begin{pmatrix} 1 & -\omega_m\mu_m \\ \overline{\omega_m}\mu_m & 1 \end{pmatrix} \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}^{[m]_2} + \mathcal{O}(\mu_m^2 + \mu_m h^{\frac{1}{m+1}}), \tag{3.49}$$

where ω_m is given in Lemma 3.12 and $[m]_2$ stands for m (mod 2).

4 Comparison among the connection formulae

Let us enumerate the connection formula as $(\varepsilon, h) \to (0,0)$ depending on each regime.

(A) Landau-Zener model (i.e. $V(t) = vt$): We have

$$\tilde{S}(\varepsilon, h) = \begin{pmatrix} \frac{i}{\lambda^{\frac{1}{2}}} \left(\frac{h}{2v}\right)^{\lambda} \frac{\sqrt{2\pi}}{\Gamma(-\lambda)} e^{-\frac{\lambda\pi i}{2}} & e^{-\lambda\pi i} \\ e^{-\lambda\pi i} & \frac{1}{\lambda^{\frac{1}{2}}} \left(\frac{2v}{h}\right)^{\lambda} \frac{\sqrt{2\pi}}{\Gamma(-\lambda)} e^{-\frac{\lambda\pi i}{2}}, \end{pmatrix} \tag{4.1}$$

where $\lambda = \varepsilon^2/2ivh$.

(Btra) Linearly crossing (i.e. transversal intersection) model under the adiabatic regime $h/\varepsilon^2 \to 0$: Denoting the entries of $T_{\mathrm{local}}(\varepsilon, h)$ by $(\tau_{jk}(\varepsilon, h))_{1 \leq j,k \leq 2}$, we get

$$|\tau_{11}| = |\tau_{22}| = 1 + \mathcal{O}\left(\frac{h}{\varepsilon^2}\right) \qquad \text{as} \quad \frac{h}{\varepsilon^2} \to 0, \tag{4.2}$$

$$|\tau_{12}| = |\tau_{21}| = e^{-\frac{1}{h}\mathrm{Im}\, A(\varepsilon)}(1 + \mathcal{O}(h)) \qquad \text{as} \quad h \to 0. \tag{4.3}$$

(Btan) Tangentially crossing (i.e. tangential intersection) model under the adiabatic regime $h/\varepsilon^{\frac{m+1}{m}} \to 0$: Putting $T_{\mathrm{local}}(\varepsilon, h) = (\tau_{jk}(\varepsilon, h))_{1\le j,k\le 2}$, we have

$$\begin{aligned} |\tau_{11}| &= |\tau_{22}| = 1 + \mathcal{O}\left(\frac{h}{\varepsilon^{\frac{m+1}{m}}}\right) \\ |\tau_{12}| &= |\tau_{21}| = \left| e^{\frac{i}{h}A_1(\varepsilon)} + (-1)^{m+1} e^{\frac{i}{h}A_m(\varepsilon)} \right| + \mathcal{O}\left(\frac{h}{\varepsilon^{\frac{m+1}{m}}} e^{-\frac{1}{h}\alpha(\varepsilon)}\right) \end{aligned} \tag{4.4}$$

as $h/\varepsilon^{\frac{m+1}{m}} \to 0$, where $\alpha(\varepsilon) := \min\{\mathrm{Im}A_1(\varepsilon), \mathrm{Im}A_m(\varepsilon)\}$.

(Ctra) Linearly crossing (i.e. transversal intersection) model under the non-adiabatic regime $\varepsilon^2/h \to 0$: Then we get

$$T_{\mathrm{local}}(\varepsilon, h) = \begin{pmatrix} e^{i\vartheta}\dfrac{1}{\overline{p}} & \dfrac{1}{i}\dfrac{q}{p} \\ \dfrac{1}{i}\dfrac{q}{p} & e^{-i\vartheta}\dfrac{1}{p} \end{pmatrix} \left(1 + \mathcal{O}\left(\sqrt{h}\right) + \mathcal{O}\left(\frac{\varepsilon}{\sqrt{h}}\right)\right), \tag{4.5}$$

where p, q, ϑ are the same as Proposition 3.10.

(Ctan) Tangentially crossing (i.e. tangential intersection) model under the non-adiabatic regime $\varepsilon^{\frac{m+1}{m}}/h \to 0$: We obtain, as $\mu_m = \varepsilon h^{-\frac{m}{m+1}} \to 0$,

$$T_{\mathrm{local}} = \begin{pmatrix} 1 & -\omega_m\mu_m \\ \overline{\omega_m}\mu_m & 1 \end{pmatrix} \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}^{[m]_2} + \mathcal{O}(\mu_m^2 + \mu_m h^{\frac{1}{m+1}}), \tag{4.6}$$

where ω_m is given in Lemma 3.12 and $[m]_2$ stands for m (mod 2).

In addtion, we summarize the answers of the questions in §2.2 as in Table 1.

	Q.1	Q.2	Q.3
L-Z model	Weber functions	(2.4)	(2.5)
adiabatic $m = 1$	exact WKB sol.'s (3.2)	(3.6)	Prop.3.3
adiabatic $m \ge 2$	exact WKB sol.'s (3.2)	[20]	Prop.3.5
non-adiabatic $m = 1$	sol.'s to BM (3.13)	Prop.3.6	Prop.3.10
non-adiabatic $m \ge 2$	sol.'s to IS (3.29)	Thm.1	Prop.3.13

Table 1: Comparison among the semiclassical approaches

Actually one more connection between such local solutions and Jost solutions is required for a study of the scattering matrix, however the matrices enumerated as above are essentially the same as the scattering matrix in the sense of the modulus of each entry. Therefore we can derive the transition probability from the off-diagonal term in each connection formula. In fact, if we suppose that $V(t) = vt$ in the case $m = 1$, we find the Landau-Zener formula in the square of the modulus of the off-diagonal entry as follows:

(A) From $\lambda = \varepsilon^2/2ivh$, one sees

$$|e^{-\lambda\pi i}|^2 = \left|e^{-(\frac{\varepsilon^2}{2ivh})\pi i}\right|^2 = e^{-\frac{\pi\varepsilon^2}{vh}}. \tag{4.7}$$

(Btra) In this case, the turning point $\zeta(\varepsilon) = i\varepsilon/v$ and the action integral $A(\varepsilon)$ is computed explicitly as

$$A(\varepsilon) = 2\int_0^{i\varepsilon/v} \sqrt{((vt)^2+\varepsilon^2}\, dt = \frac{2i\varepsilon}{v}\int_0^1 \sqrt{1-s^2}\, ds = \frac{\pi i}{2v}\varepsilon^2, \tag{4.8}$$

so that the Landau-Zener formula appears in the leading term of $|\tau_{21}|^2$;

$$|e^{-\frac{1}{h}\operatorname{Im} A(\varepsilon)}|^2 = \left|e^{-\frac{1}{h}(\frac{\pi}{2v}\varepsilon^2)}\right|^2 = e^{-\frac{\pi\varepsilon^2}{vh}}.$$

(Ctra) From the definition of p, q, i.e. (3.17), we have

$$\left|i\frac{q}{p}\right|^2 = \left|i\frac{\gamma e^{-\frac{\pi\mu}{4}}}{\gamma e^{\frac{\pi\mu}{4}}}\right|^2 = e^{-\frac{\pi}{2}\mu} = e^{-\frac{\pi\varepsilon^2}{vh}}, \tag{4.9}$$

where $\mu = \varepsilon^2/h$, that is, μ stands for $(\mu_1)^2$ under the notation of μ_m.

A similar consideration for the case of the tangential crossings (Btan) and (Ctan) with $V(t) = v_m t^m/m!$ $(v > 0)$ leads us to a generalized Landau-Zener formula under the adiabatic and non-adiabatic regimes.

(Btan) According to [20], the action integrals $A_1(\varepsilon)$ and $A_m(\varepsilon)$ can be computed explicitly as

$$A_1(\varepsilon) = C_m e^{\frac{\pi i}{2m}}\varepsilon^{\frac{m+1}{m}}, \qquad C_m = \frac{\sqrt{\pi}\Gamma(\frac{1}{2m})}{(m+1)\Gamma(\frac{m+1}{2m})}\left(\frac{m!}{v_m}\right)^{\frac{1}{m}} \tag{4.10}$$

and $A_m(\varepsilon) = -\overline{A_1(\varepsilon)}$. Then one sees that $\operatorname{Im} A_1(\varepsilon) = \operatorname{Im} A_m(\varepsilon)$ holds. We have the leading term of the transition probability P_0:

$$P_0 = 4\sin^2\left(C_m(\cos\frac{\pi}{2m})\frac{\varepsilon^{\frac{m+1}{m}}}{h} + \frac{m}{2}\pi\right)e^{-2C_m(\sin\frac{\pi}{2m})\varepsilon^{\frac{m+1}{m}}/h}. \tag{4.11}$$

Notice that the prefactor of P_0 oscillates faster as $h/\varepsilon^{\frac{m+1}{m}} \to 0$ and the quantity of P_0 is estimated by exponentially small factor. This fact is consistent with the adiabatic theorem (Bohr's correspondence principle).

(Ctan) In this case, the transition probability depends on the parity of m. More precisely the leading term of the transition probability P_0 is given by

$$P_0 = \begin{cases} 1-\gamma_m\left(\dfrac{\varepsilon}{h^{\frac{m}{m+1}}}\right)^2 & \text{if } m \text{ is odd,} \\ \gamma_m\left(\dfrac{\varepsilon}{h^{\frac{m}{m+1}}}\right)^2 & \text{if } m \text{ is even,} \end{cases} \tag{4.12}$$

where

$$\gamma_m = \frac{4}{(m+1)^2}\left(\frac{(m+1)!}{2v_m}\right)^{\frac{2}{m+1}}\Gamma\left(\frac{1}{m+1}\right)^2 \times\left(1+\frac{1-(-1)^m}{2}\sin^2(\frac{\pi}{2(m+1)})\right). \tag{4.13}$$

The formula (4.12) implies that the contribution to the transition probability issues from $\pm V(t)$ not from energies $\pm\sqrt{V(t)^2+\varepsilon^2}$. This difference also appears in the phase function of the local solutions which consist of the bases near the avoided crossing.

Remark 4.1. *While the formula* (4.12) *with* (4.13) *in the case where* $m = 1$ *corresponds to the Landau-Zener formula, the formula* (4.11) *does not so. More precisely the decay rate is same but the multiplication prefactor is not. This difference arises from the fact that the turning points (i.e. zeros of* $V(t)^2+\varepsilon^2$*) are crucial in the adiabatic regime whereas the crossing point (i.e. the zero of* $V(t)$*) is so in the non-adiabatic regime.*

Although, in this manuscript, we treat only the case where the number of the zeros of $V(t)$ on $\mathbb{R}$ is one, we can naturally extend this problem to the case where $V(t)$ has a finite number of zeros as in [15], [22]. Since the scattering matrix can be expressed by the products of the local change of basis near each avoided crossing, these connection formulae enumerated in this subsection are an essential part of such further generalizations. Finally we remark that the interaction effects between the avoided crossings can be found in the non-adiabatic regimes as in [22], [13].

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References

[1] M. Assal, S. Fujiié and K. Higuchi, *Semiclassical resonance asymptotics for systems with degenerate crossings of classical trajectories*, Preprint on arXiv:2211.1165.

[2] Y. Colin de Verdière, M. Lombardi and J. Pollet, *The microlocal Landau-Zerner formula*, Ann. Inst. H. Poincaré, **71**(1999), no. 1, 95–127.

[3] Y. Colin de Verdière, *The level crossing problem in semi-classical analysis. I. The symmetric case. Proceedings of the International Conference in Honor of Frédéric Pham (Nice, 2002).* Ann. Inst. Fourier (Grenoble) **53**(2003), no. 4, 1023–1054.

[4] C. Fermanian-Kammerer and P. Gérard, *Mesures semi-classiques et croisement de modes. (French) [Semiclassical measures and eigenvalue crossings]* Bull. Soc. Math. France **130**(2002), no. 1, 123–168.

[5] S. Fujiié, A. Martinez and T. Watanabe, *Widths of resonances above an energy-level crossing*, J. Funct. Anal. **280**(2021), no. 6, 48 pages.

[6] S. Fujiié, C. Lasser and L. Nédélec, *Semiclassical resonances for a two-level Schrödinger operator with a conical intersection*, Asymptot. Anal. **65**(2009), no. 1-2, 17–58.

[7] I.-M. Guelfand and G.-E. Chilov, *Les distributions. (French)*, Traduit par G. Rideau. Collection Universitaire de Mathématiques, VIII Dunod, Paris 1962.

[8] C. Gérard and A. Grigis, *Precise estimates of tunneling and eigenvalues near a potential barrier*, J. Diff. Equations **42**(1988), 149–177.

[9] G.-A. Hagedorn, *Molecular propagation through electron energy level crossings.* Mem. Amer. Math. Soc. **111**(1994), no. 536.

[10] G.-A. Hagedorn and A. Joye, *Recent results on non-adiabatic transitions in Quantum mechanics*, Recent advances in differential equations and mathematical physics, Contemp. Math., **412**, Amer. Math. Soc., Providence, RI, 2006, 183–198.

[11] B. Helffer and J. Sjöstrand, *Semiclassical analysis for Harper's equation. III. Cantor structure of the spectrum*, Mém. Soc. Math. France, no. 39(1989), 1–124.

[12] K. Higuchi, *Local scattering matrix for a degenerate avoided-crossing in non-coupled regime*, in preparation.

[13] K. Higuchi and T. Watanabe, *Two-level adiabatic transition probability for small avoided crossings generated by tangential intersections*, In preparation.

[14] L. Hörmander, *The analysis of linear partial differential operators. I: Distribution theory and Fourier analysis*, Grundlehren der Mathematischen Wissenschaften, **256**(1983). Berlin Heidelberg-New York -Tokyo: Springer-Verlag. IX

[15] A. Joye, G. Mileti and C.-E. Pfister, *Interferences in adiabatic transition probabilities mediated by Stokes lines*, Phys. Rev. A. **44**(1991), 4280–4295.

[16] N. Kaidi and M. Rouleux, *Forme normale d'un hamiltonien à deux niveaux près d'un point de branchement (limite semi-classique).* C. R. Acad. Sci. Paris Sér. I Math. **317**(1993), no. 4, 359–364.

[17] L.D. Landau, *Collected papers of L. D. Landau*, Pergamon Press, 1965.

[18] C. März, *Spectral asymptotic near the potential maximum for the Hill's equation*, Asymptot. Anal. **5**(1992), 221–267.

[19] S. Teufel, *Adiabatic perturbation theory in quantum dynamics*, Lecture Notes in Mathematics 1821. Springer-Verlag, Berlin, Heidelberg, New York, 2003.

[20] T. Watanabe, *Adiabatic transition probability for a tangential crossing*, Hiroshima Math. J. **36**(2006), no. 3, 443–468.

[21] T. Watanabe, *Exact WKB approach to 2-level adiabatic transition problems with a small spectral gap*, Tohoku Mathematical Publications **37**(2012). 1–68.

[22] T. Watanabe and M. Zerzeri, *Landau-Zener formula in a "non-adiabatic" regime for avoided crossings*, Anal. Math. Phys. **11**(2021), no. 82, 47.

[23] E.T. Whittaker and G.N. Watson, *A course of modern analysis 4th ed.*, Cambridge University Press. (1927).

[24] D.R. Yafaev, D. R. *The semiclassical limit of eigenfunctions of the Schrödinger equation and the Bohr-Sommerfeld quantization condition, revisited*, St. Petersbg. Math. J. **22**(2011), No. 6, 1051-1067.

[25] C. Zener, *Non-Adiabatic Crossing of Energy Levels*, Proc. R. Soc. London A, **137**(1932), 696–702.

J. Chem. Phys. **97**(1992), 1892–1904.

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