Partial Differential Equations/Mathematical Physics

Transition probability for multiple avoided crossings with a small gap through an exact WKB method and a microlocal approach

Probabilité de transition pour de multiples croisements évités avec un petit écart via la méthode BKW exacte et l'approche microlocale

Takuya Watanabe [a], Maher Zerzeri [b]

[a] *Department of Mathematical Sciences, Ritsumeikan University, 1-1-1 Noji Higashi, Kusatsu, Shiga, 525-8577, Japan*
[b] *LAGA, (UMR CNRS 7539), Institut Galilée, Université Paris Nord 13, 93430 Villetaneuse, France*

A R T I C L E I N F O

A B S T R A C T

In this Note, we study the adiabatic transition probability for a two-level system in the case of a finite number of avoided crossings. More precisely, we investigate a global change of bases of a first order differential system with respect to a semiclassical "adiabatic" parameter ($h \downarrow 0$) and an interaction parameter ($\varepsilon \downarrow 0$). We obtain its asymptotic behaviors by means of an exact WKB method and a microlocal analysis according to the interrelation of the two parameters.

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R É S U M É

Dans cette Note, nous intéressons à la probabilité de transition adiabatique d'un système à deux niveaux dans le cas d'un nombre fini de croisements évités. Plus précisément, nous étudions un changement global des bases d'un système différentiel du premier ordre par rapport à un paramètre semiclassique "adiabatique" ($h \downarrow 0$) et un paramètre d'interaction ($\varepsilon \downarrow 0$). Nous obtenons les différents comportements asymptotiques au moyen d'une méthode BKW exacte et une analyse microlocale en fonction de la corrélation entre les deux paramètres.

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1. Introduction

We consider the time-dependent Schrödinger equation:

$$ih\frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = H(t;\varepsilon)\psi(t), \quad \text{where } H(t;\varepsilon) := \begin{pmatrix} V(t) & \varepsilon \\ \varepsilon & -V(t) \end{pmatrix}, \text{ for all } t \in \mathbb{R}. \tag{1}$$

The potential V is a real-valued function on $\mathbb{R}$ and $\psi(t) = {}^t(\psi_1(t), \psi_2(t)) \in \mathbb{C}^2$. Here h is a semiclassical "adiabatic" parameter and ε is an interaction parameter of the gap at avoided crossing. The matrix $H(t;\varepsilon)$ has two real eigenvalues $\lambda_{\pm}(t;\varepsilon) := \pm\sqrt{V(t)^2 + \varepsilon^2}$ and the difference of these eigenvalues $g(t;\varepsilon) := \lambda_+ - \lambda_- \geqslant 2\varepsilon$ is strictly positive for all $t \in \mathbb{R}$.

The question is to study the transition probability between the energies of system (1), $\lambda_{\pm}(t;\varepsilon)$. The typical result is Landau–Zener formula, that is the transition probability is given by $P(\varepsilon;h) = \exp(-\frac{\pi\varepsilon^2}{vh})$, for $V(t) := vt$ ($v > 0$), see [13]. From this formula, the probability tends to 1 when $\varepsilon \downarrow 0$, while it decays exponentially when $h \downarrow 0$. From the viewpoint

of the so-called Adiabatic Theorem, the generalization of the Landau–Zener formula with respect to $h \downarrow 0$ for a fixed ε has been investigated by many authors (see [6] and references given therein), especially in [9] by means of a complex WKB method for multiple avoided crossings and in [10] by a microlocal theory. Remark that the adiabatic effect ($h \downarrow 0$) and the interaction effect ($\varepsilon \downarrow 0$) play the opposite roles in the transition probability.

In this Note, we want to study the asymptotic behavior of the transition probability when the two parameters h and ε tend to 0 simultaneously, where the potential V is short range (modulo an additive constant) and it vanishes in a finite number ($\geqslant 2$) of nondegenerate zeros, i.e., $V(t_k) = 0$ and $V'(t_k) \neq 0$ for $k = 1, \ldots, n$ with $n \geqslant 2$. The Landau–Zener formula says that the ratio of h and ε^2 must be very important. Specifically, there are three cases, as in [1] (see also [11]):

Case 1. $(\varepsilon, h) \downarrow (0, 0)$ and $\frac{h}{\varepsilon^2} \downarrow 0$. This regime was treated in [8] when V vanishes at only one point ($n = 1$), but for more general Hamiltonians. In Theorem 2.3 we get a small extension of this result in our simpler framework but with several avoided crossings ($n \geqslant 2$), by using the exact WKB method. This method was developed by C. Gérard and A. Grigis (see [4]). Note that in [12], the author has treated the case where V has one degenerate zero, the asymptotic behavior obtained depends strongly on the order of degeneracy.

Case 2. $(\varepsilon, h) \downarrow (0, 0)$ and $\frac{h}{\varepsilon^2} \sim C$ where C is some strictly positive constant. This case was treated by G.-A. Hagedorn. In fact, he considered a more general setting than Landau–Zener model and his result is a natural extension of the Landau–Zener formula in the case where one avoided crossing is nondegenerate. See [5, p. 435, formula (1.7)]. The proof of G.-A. Hagedorn is essentially based on the properties of "parabolic cylinder functions" as in Zener's paper.

Case 3. $(\varepsilon, h) \downarrow (0, 0)$ and $\frac{\varepsilon^2}{h} \downarrow 0$. This regime is our main interest in this Note. This case is more involved than the others. In fact, from the mathematical point of view and more precisely WKB method, the problem of the confluence of turning points happens when $\frac{\varepsilon^2}{h} \downarrow 0$. In Theorem 2.6, we show that the asymptotic expansion of the transition probability depends on the parity of the number of zeros of the potential V and we give a precise expression of $C_n(\varepsilon; h)$ the prefactor of $\frac{\pi \varepsilon^2}{h}$, see (4). Moreover, we derive a kind of a Bohr–Sommerfeld quantization condition when the prefactor $C_n(\varepsilon; h)$ vanishes, see Remark 2.9.

2. Hypotheses and statements

In this section we give the precise assumptions and we state the results. The potential V is smooth, real-valued on $\mathbb{R}$ and satisfies the following assumptions:

(A1) V extends holomorphically in the sector $\mathcal{S} = \{t \in \mathbb{C}; \ |\mathrm{Im}\, t| < \langle \mathrm{Re}\, t \rangle \tan \alpha_0$, for some $\alpha_0 \in \,]0, \frac{\pi}{2}[$.
(A2) There exist E_r, E_l in $\mathbb{R}^*$ and $\delta > 1$ s.t., $V(t) = \begin{cases} E_r + \mathcal{O}(|t|^{-\delta}) & \text{as } \mathrm{Re}\, t \to +\infty \text{ in } \mathcal{S}, \\ E_l + \mathcal{O}(|t|^{-\delta}) & \text{as } \mathrm{Re}\, t \to -\infty \text{ in } \mathcal{S}. \end{cases}$

Under the analyticity condition (A1) and the boundaries conditions (A2), we define four *Jost solutions* $J^r_\pm(t)$ and $J^l_\pm(t)$ uniquely defined by the asymptotic conditions: $J^r_+(t) \sim \exp[+\frac{i}{h}\sqrt{E_r^2 + \varepsilon^2}\,t]\,{}^t(-\sin\theta_r \ \cos\theta_r)$ as $\mathrm{Re}\, t \to +\infty$ in $\mathcal{S}$ and $J^r_-(t) \sim \exp[-\frac{i}{h}\sqrt{E_r^2 + \varepsilon^2}\,t]\,{}^t(\cos\theta_r \ \sin\theta_r)$ as $\mathrm{Re}\, t \to +\infty$ in $\mathcal{S}$, where $\tan 2\theta_r = \frac{\varepsilon}{E_r}$ $(0 < \theta_r < \frac{\pi}{2})$ and the similar formulas for $J^l_\pm(t)$ as $\mathrm{Re}\, t \to -\infty$ in $\mathcal{S}$. The pairs of Jost solutions (J^r_+, J^r_-) and (J^l_+, J^l_-) are orthonormal bases on $\mathbb{C}^2$ for any fixed t.

Definition 2.1. The scattering matrix S is defined as the change of bases of Jost solutions:

$$\left(J^l_+ \ J^l_-\right) = \left(J^r_+ \ J^r_-\right) S(\varepsilon; h), \qquad S(\varepsilon; h) = \begin{pmatrix} s_{11}(\varepsilon; h) & s_{12}(\varepsilon; h) \\ s_{21}(\varepsilon; h) & s_{22}(\varepsilon; h) \end{pmatrix}.$$

The matrix S is unitary and independent of t. Then $|s_{11}(\varepsilon; h)|^2 + |s_{21}(\varepsilon; h)|^2 = 1$.

Definition 2.2. The transition probability $P(\varepsilon; h)$ is defined by $P(\varepsilon; h) := |s_{21}(\varepsilon; h)|^2 = |s_{12}(\varepsilon; h)|^2$.

Since we discuss the transition probability under the case where nondegenerate avoided crossing happens finite times, we assume the crossing condition which realizes the above situation:

(A3) The potential V has a finite number of zeros $t_1 > \cdots > t_n$ on $\mathbb{R}$ and the order of every zero is 1.

From now on, we set $v_k := |V'(t_k)| > 0$ for $k = 1, \ldots, n$. We can assume that $V'(t_1) > 0$ without loss of generality. Notice that the sign of $V(t)$ for $t < t_n$ changes depending on the parity of n.

For each k $(k = 1, \ldots, n)$, there exist *two simple turning points* $\zeta_k(\varepsilon)$ and $\overline{\zeta_k(\varepsilon)}$, that is, simple zeros in $\mathcal{S}$ of $2\sqrt{-\det H(t; \varepsilon)}$ close to t_k, where $\det H(t; \varepsilon) := -V(t)^2 - \varepsilon^2$. They behave like $\zeta_k(\varepsilon) \sim t_k + \frac{i}{v_k}\varepsilon$ as $\varepsilon \downarrow 0$. For $k = 1, \ldots, n$ we define the action integral $A_k(\varepsilon)$ by

$$A_k(\varepsilon) = 2 \int_{t_k}^{\zeta_k(\varepsilon)} \sqrt{V(t)^2 + \varepsilon^2}\, dt, \tag{2}$$

where each integration path is the complex segment from t_k to $\zeta_k(\varepsilon)$ and the branch of the square root is ε at $t = t_k$. On this branch, $\operatorname{Im} A_k(\varepsilon) = \frac{\pi \varepsilon^2}{2 v_k} + \mathcal{O}(\varepsilon^4)$ is positive. We also define action integrals by

$$R_{j,k}(\varepsilon) = 2 \int_{t_k}^{t_j} \sqrt{V(t)^2 + \varepsilon^2}\, dt, \quad \text{for } 1 \leqslant j \leqslant k \leqslant n. \tag{3}$$

Since $t_j \geqslant t_k$ for $j \leqslant k$ then $R_{j,k}(\varepsilon)$ is positive and behaves like $R_{j,k}(\varepsilon) = \mathcal{A}_{j,k} + \mathcal{O}(\varepsilon^2)$ as $\varepsilon \downarrow 0$, where $\mathcal{A}_{j,k}$ stands for the area enclosed by $V(t)$ and $-V(t)$, that is $\mathcal{A}_{j,k} = 2 \int_{t_k}^{t_j} |V(t)|\, dt$. Notice that all these actions are independent of h.

Theorem 2.3. *Assume* (A1), (A2) *and* (A3). *Then the transition probability $P(\varepsilon; h)$ is given by*

$$P(\varepsilon; h) = \left| \sum_{k \in \Lambda} (-1)^k e^{\frac{i}{h}(A_k(\varepsilon) - R_{1,k}(\varepsilon))} \right|^2 + \mathcal{O}\left(\frac{h}{\varepsilon^2} e^{-\frac{2\alpha(\varepsilon)}{h}} \right), \quad \text{as } (\varepsilon, h) \downarrow (0,0) \text{ and } \frac{h}{\varepsilon^2} \downarrow 0,$$

where $\alpha(\varepsilon) = \min_{k \in \Lambda} \operatorname{Im} A_k(\varepsilon) > 0$, see (2), *and Λ is the set of $k \in \{1, 2, \dots, n\}$ which attains $\max\{v_1, \dots, v_n\}$.*

Remark 2.4. In the case of one avoided nondegenerate crossing (i.e., $n = 1$) we have only one transfer matrix (see Proposition 3.1, identity (6)) and we take the off-diagonal entry. Then the error in Theorem 2.3 is $\mathcal{O}(h)$ uniformly with respect to ε which recover the previous results of [8,11,12] in our setting.

Remark 2.5. Theorem 2.3 implies that the asymptotic behavior of $P(\varepsilon; h)$ decays exponentially and its decay rate is characterized by the maximum of $(v_p)_{p=1,\dots,n}$.

Theorem 2.6. *Assume* (A1), (A2) *and* (A3). *Then the transition probability $P(\varepsilon; h)$ is given by*

$$P(\varepsilon; h) = \begin{cases} 1 - C_n(\varepsilon; h) \pi \frac{\varepsilon^2}{h} + \mathcal{O}(\varepsilon^2) + \mathcal{O}(\frac{\varepsilon^4}{h^2}) & \text{if } n \text{ is odd}, \\ C_n(\varepsilon; h) \pi \frac{\varepsilon^2}{h} + \mathcal{O}(\varepsilon^2) + \mathcal{O}(\frac{\varepsilon^4}{h^2}) & \text{if } n \text{ is even}, \end{cases}$$

as $(\varepsilon, h) \downarrow (0,0)$ and $\frac{\varepsilon^2}{h} \downarrow 0$. Here $C_1(\varepsilon; h) = \frac{1}{v_1}$ and $C_n(\varepsilon; h)$ for $n \geqslant 2$ is given by

$$C_n(\varepsilon; h) = \sum_{j=1}^{n} \frac{1}{v_j} + \sum_{1 \leqslant j < k \leqslant n} \frac{2}{\sqrt{v_j v_k}} \cos\left[\frac{\mathcal{A}_{j,k}}{h} + \frac{1}{2}\left(\frac{1}{v_j} + \frac{1}{v_k} \right) \frac{\varepsilon^2}{h} \log \frac{1}{h} \right]. \tag{4}$$

Remark 2.7. When $n = 1$, we recover the Landau–Zener formula.

Remark 2.8. The asymptotic expansions of $P(\varepsilon; h)$ as $\frac{\varepsilon^2}{h} \downarrow 0$ depending on the parity of n imply that the time evolutions of the eigenstates propagate along potentials $\pm V(t)$ instead of the energy of system $\lambda_\pm(t; \varepsilon)$.

Remark 2.9. Notice that v_k does not determine the decay rate of the transition probability. In fact the prefactor $C_n(\varepsilon; h)$ for $n \geqslant 2$ may vanish, while $C_1(\varepsilon; h)$ does not. For example, take $n = 2$ and $v_1 = v_2$. Under the assumption that the leading term of $C_2(\varepsilon; h)$ vanishes, we obtain $P(\varepsilon; h) = \mathcal{O}(\frac{\varepsilon^4}{h^2} \log \frac{1}{h}) + \mathcal{O}(\varepsilon^2)$, as $(\varepsilon, h) \downarrow (0,0)$ and $\frac{\varepsilon^2}{h} \log \frac{1}{h} \downarrow 0$. This assumption is equivalent to $\frac{\mathcal{A}_{1,2}}{h} = (2N + 1)\pi + \mathcal{O}(\frac{\varepsilon^2}{h} \log \frac{1}{h})$ for some integer N. We may understand this condition as a Bohr–Sommerfeld quantization condition for the simple well potential.

3. Outline of the proofs

We decompose the scattering matrix $S(\varepsilon; h)$ into the transfer matrices $T_r(\varepsilon; h)$, $T_l(\varepsilon; h)$, $T_{j,j+1}(\varepsilon; h)$ ($j = 1, \dots, n-1$) and $T_k(\varepsilon; h)$ ($k = 1, \dots, n$) (see, for example, [2]), which are the local change of bases between the exact WKB solutions with the valid asymptotic expansions for h small enough in the canonical region, see [4]. In the following we denote by $\operatorname{diag}(a, b)$ the diagonal matrix of order 2 such that the entries $a_{11} = a$, $a_{22} = b$ and $a_{12} = 0 = a_{21}$. The diagonals matrices $T_r(\varepsilon; h)$ and $T_l(\varepsilon; h)$, which connect Jost solutions and exact WKB solutions are given by: (for $p \in \{r, l\}$)

$$T_p(\varepsilon; h) = \left[\mathrm{diag}(a_p, \overline{a_p})\right]\left(1 + \mathcal{O}(h)\right) \quad \text{with} \quad a_p(\varepsilon; h) = \exp\left[\frac{i}{2h}\left(\mathbf{A}_p(\varepsilon) + R_p(\varepsilon)\right)\right], \tag{5}$$

as $h \downarrow 0$ uniformly with respect to $\varepsilon \in (0, \varepsilon_0]$, for some $\varepsilon_0 > 0$, where $\mathbf{A}_r = A_1$ and $\mathbf{A}_l = A_n$. Here $R_r(\varepsilon)$ and $R_l(\varepsilon)$ are some real-valued actions associated to $\pm\infty$. Similarly $T_{k,k+1}(\varepsilon; h)$, which is the phase shift of WKB solutions between adjacent avoided crossings, is of the form: $T_{j,j+1}(\varepsilon; h) = [\mathrm{diag}(a_j, \overline{a_j})](1 + \mathcal{O}(h))$ with $a_j(\varepsilon; h) = \exp[\frac{i}{2h}(A_j(\varepsilon) - A_{j+1}(\varepsilon) + R_{j,j+1}(\varepsilon))]$ as $h \downarrow 0$ uniformly with respect to $\varepsilon \in (0, \varepsilon_0]$, for some $\varepsilon_0 > 0$. Here $R_{j,j+1}$ is given by (3). For $k = 1, \ldots, n$, the matrix $T_k(\varepsilon; h)$ is the connection near k-th avoided crossing. The essential point of the proofs is to calculate $T_k(\varepsilon; h)$ depending on the interrelationship between h and ε^2.

The case when $\frac{h}{\varepsilon^2} \downarrow 0$: we can apply the connection formula near a simple turning point guaranteed by the exact WKB method (see [12]) and then we obtain the following:

Proposition 3.1. *For* $k = 1, \ldots, n$, *we have*:

$$T_k(\varepsilon; h) = \begin{pmatrix} 1 + \mathcal{O}(\frac{h}{\varepsilon^2}) & (-1)^{k-1} i e^{iA_k(\varepsilon)/h}(1 + \mathcal{O}(h)) \\ (-1)^{k-1} i e^{iA_k(\varepsilon)/h}(1 + \mathcal{O}(h)) & 1 + \mathcal{O}(\frac{h}{\varepsilon^2}) \end{pmatrix}, \tag{6}$$

as $(\varepsilon, h) \downarrow (0, 0)$ *and* $\frac{h}{\varepsilon^2} \downarrow 0$, *where the action* A_k *is given by* (2).

Computing the appropriate product of these transfer matrices obtained in (5) and (6), we get Theorem 2.3.

The case when $\frac{\varepsilon^2}{h} \downarrow 0$: The last connection formula among exact WKB solutions is not valid for the reason why the two turning points accumulate to the zero of $V(t)$ each other as $\varepsilon \downarrow 0$. Hence instead of the exact WKB solutions, we employ the solutions of the normal form: $\begin{pmatrix} t & \frac{\varepsilon}{\sqrt{2}} \\ \frac{\varepsilon}{\sqrt{2}} & \frac{h}{i}\frac{d}{dt} \end{pmatrix} \phi(t) = 0$, which is microlocally equivalent to (1) up to the translation: $t \mapsto t - t_k$ and the scaling: $t \mapsto \sqrt{v_k}t$ with respect to h small enough near the origin of the phase space. This is guaranteed by Egorov type theorem through the Fourier integral operator U: $U[u](t) = \frac{e^{\frac{\pi}{8}i}2^{\frac{1}{4}}}{\sqrt{2\pi h}} \int_{\mathbb{R}} e^{i(-t^2 + 2\sqrt{2}ts - s^2)/2h} u(s)\, ds$, $u \in \mathbf{S}(\mathbb{R})$, which is associated with the rotation $\frac{\pi}{4}$ on the phase space as in [7]. The advantage of the normal form is that we can get two bases of solutions and their change of bases explicitly. Moreover we have the collinear relation between each WKB solution and each "corresponding" normal form solution by comparing their microsupport, see [3]. The ratio of them can be computed by the stationary phase method. Hence we obtain, through the change of bases of the normal form solutions, the following:

Proposition 3.2. *For* $k = 1, \ldots, n$, *we have*: $T_k(\varepsilon; h) = \begin{pmatrix} -\gamma_k^{-1} e^{-\frac{\pi\varepsilon^2}{4v_kh}} & ie^{-\frac{\pi\varepsilon^2}{2v_kh}} \\ -ie^{-\frac{\pi\varepsilon^2}{2v_kh}} & (\overline{\gamma_k})^{-1} e^{-\frac{\pi\varepsilon^2}{4v_kh}} \end{pmatrix}(1 + \mathcal{O}(h) + \mathcal{O}(\frac{\varepsilon^2}{h}))$, *as* $(\varepsilon, h) \downarrow (0, 0)$ *and* $\frac{\varepsilon^2}{h} \downarrow 0$,

where $\gamma_k = \frac{1}{i\varepsilon}\sqrt{\frac{v_kh}{\pi}} h^{-\frac{i\varepsilon^2}{2v_kh}} \Gamma(1 - \frac{i\varepsilon^2}{2v_kh})$. *Here* Γ *stands for Gamma function.*

By an algebraic computation, we express and identify the entries of the scattering matrix. Note that in the odd case it is useful to rewrite $P(\varepsilon; h)$ as $1 - |s_{11}(\varepsilon; h)|^2$ in order to get the explicit expression of the prefactor $C_n(\varepsilon; h)$. This ends the proof of Theorem 2.6.

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