Landau-Zener formulae from adiabatic transition histories

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Summary. We use recent results on precise coupling terms in the optimal superadiabatic basis in order to determine exponentially small transition probabilities in the adiabatic limit of time-dependent two-level systems. As examples, we discuss the Landau-Zener and the Rosen-Zener models.
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1 Introduction

Transitions between separated energy levels of slowly time-dependent quantum systems are responsible for many important phenomena in physics, chemistry and even biology. In the mathematical model the slow variation of the Hamiltonian is expressed by the smallness of the *adiabatic parameter* ε in the Schrödinger equation

$$\big(\mathrm{i}\partial_s - H(\varepsilon s)\big)\phi(t) = 0\,, \tag{1}$$

where $H(t)$ is a family of self-adjoint operator on a suitable Hilbert space. In order to see in (1) nontrivial effects from the time-variation of the Hamiltonian, one has to follow the solutions up to times s of order ε^{-1}. Alternatively one can transform (1) to the *macroscopic time scale* $t = \varepsilon s$, resulting in the equation

$$\big(\mathrm{i}\varepsilon\partial_t - H(t)\big)\phi(t) = 0\,, \tag{2}$$

and study solutions of (2) for times t of order one. Often one is interested in the situation where the Hamiltonian is time-independent for large negative and positive times. Then one can consider the scattering limit and the aim is to compute the scattering amplitudes. In the simplest and at the same time paradigmatic example the Hamiltonian is just a 2×2 matrix

$$H(t) = \begin{pmatrix} Z(t) & X(t) \\ X(t) & -Z(t) \end{pmatrix}\,,$$

which can be chosen real symmetric and traceless without essential loss of generality [Ber]. With this choice for $H(t)$, the Schrödinger equation (2) is just an ordinary differential equation for the $\mathbb{C}^2$-valued function $\phi(t)$. But even this simple system displays a very interesting behavior, of which we will give an informal description here in the introduction. The mathematical mechanism which generates this behavior will be explained in the main body of this paper.

We will assume that $H(t)$ has two distinct eigenvalues $\{E_+(t), E_-(t)\}$ for any t and approaches constant matrices as $t \to \pm\infty$. Then also the eigenvalues $\{E_+(t), E_-(t)\}$ and the orthonormal basis $\{v_+(t), v_-(t)\}$ of $\mathbb{R}^2$ consisting of the real eigenvectors of $H(t)$ have limits as $t \to \pm\infty$. By definition, the transition probability from the "upper" to the "lower" eigenstate is given by

$$P = \lim_{t\to\infty} |\phi_-(t)|^2 := \lim_{t\to\infty} |\langle v_-(t), \phi(t)\rangle_{\mathbb{C}^2}|^2, \tag{3}$$

where $\phi(t)$ is a solution of (2) with

$$\lim_{t\to-\infty} |\phi_-(t)|^2 = 1 - \lim_{t\to-\infty} |\phi_+(t)|^2 = 0. \tag{4}$$

Despite the presence of a natural small parameter, the adiabatic parameter $\varepsilon \ll 1$, it is far from obvious how to compute P even to leading order in ε. This is because the transition amplitudes connecting different energy levels are exponentially small with respect to ε, i.e. of order $\mathcal{O}(\mathrm{e}^{-c/\varepsilon})$ for some $c > 0$, and thus have no expansion in powers of ε.

The result of a numerical computation of $\phi_-(t)$ for a typical Hamiltonian $H(t)$ is displayed in Figure 1a). After rising to a value which is of order ε,

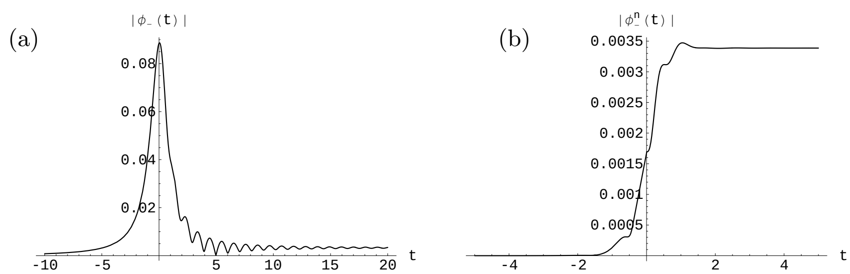

Fig. 1. *This figure shows the lower components of a numerical solution of (5) for $\varepsilon = 1/6$. In (a), the lower component in the adiabatic basis rises to a value order ε before approaching its exponentially small asymptotic value. In (b), the lower component in the optimal superadiabatic basis rises monotonically to its final value. Note the different axes scalings, as the asymptotic values in both pictures agree.*

$|\phi_-|$ falls off again and finally, in the regime where $H(t)$ is approximately constant, settles for a value of order $\mathrm{e}^{-c/\varepsilon}$.

It is no surprise that $\sup_{t\in\mathbb{R}} |\phi_-(t)|$ is of order ε: this is just a consequence of the proof of the adiabatic theorem [Ka], and in fact we perform the relevant calculation in Section 2. There we see that the size of $\phi_-(t)$ is determined by the size of the off-diagonal elements of the adiabatic Hamiltonian $H_{\mathrm{ad}}(t)$.

The latter is obtained by expressing (2) in the *adiabatic basis* $\{v_+(t), v_-(t)\}$. More precisely, let $U_0(t)$ be the orthogonal matrix that takes the adiabatic basis into the canonical basis. Then multiplication of (2) with $U_0(t)$ from the left leads to

$$\big(\mathrm{i}\varepsilon\partial_t - H_{\mathrm{ad}}(t)\big)\phi_{\mathrm{ad}}(t) := U_0(t)\,\big(\mathrm{i}\varepsilon\partial_t - H(t)\big)U_0^*(t)U_0(t)\phi(t) = 0, \qquad (5)$$

where $H_{\mathrm{ad}}(t) = \mathrm{diag}(E_+(t), E_-(t)) - \mathrm{i}\varepsilon U_0(t)\dot{U}_0^*(t)$. Clearly, the off-diagonal elements of the matrix H_{ad} are of order ε, and $\phi_-(t)$ is just the second component of $\phi_{\mathrm{ad}}(t)$. However, the $\mathcal{O}(\varepsilon)$ smallness of the coupling in the adiabatic Hamiltonian does not explain the exponentially small scattering regime in Figure 1a). In the adiabatic basis, there is no easy way to see why this effect should take place, although with some goodwill it may be guessed by a heuristic calculation to be presented in the next section.

A natural strategy to understand the exponentially small scattering amplitudes goes back to M. Berry [Ber]: the solution of (2) with initial condition (4) remains in the positive adiabatic subspace spanned by $v_+(t)$ only up to errors of order ε. Hence one should find a better subspace, the *optimal superadiabatic subspace*, in which the solution remains up to exponentially small errors for all times. Since we are ultimately interested in the transition probabilities, at the same time this subspace has to coincide with the adiabatic subspace as $t \to \pm\infty$. One way to determine the superadiabatic subspaces is to optimally truncate the asymptotic expansion of the true solution in powers of ε, as Berry [Ber] did. Alternatively one can look for a time-dependent basis of $\mathbb{C}^2$ such that the analogues transformation to (5) yields a Hamiltonian with exponentially small off-diagonal terms. To do so, one first constructs the n-th *superadiabatic basis* recursively from the adiabatic basis for any $n \in \mathbb{N}$. Let us write $U_\varepsilon^n(t)$ for the transformation taking the n-th superadiabatic basis into the canonical one. Then as in (5) the Schrödinger equation takes the form

$$\big(\mathrm{i}\varepsilon\partial_t - H_\varepsilon^n(t)\big)\phi^n(t) = 0\,, \qquad (6)$$

where

$$H_\varepsilon^n(t) = \begin{pmatrix} \rho_\varepsilon^n(t) & \varepsilon^{n+1}c_\varepsilon^n(t) \\ \varepsilon^{n+1}\bar{c}_\varepsilon^n(t) & -\,\rho_\varepsilon^n(t) \end{pmatrix} \quad \text{and} \quad \phi^n(t) = U_\varepsilon^n(t)\phi(t) = \begin{pmatrix} \phi_+^n(t) \\ \phi_-^n(t) \end{pmatrix}. \qquad (7)$$

Above, $\rho_\varepsilon^n = \frac{1}{2} + \mathcal{O}(\varepsilon^2)$. While the off-diagonal elements of H_ε^n indeed are of order ε^{n+1}, the *n-th superadiabatic coupling function* c_ε^n grows like $n!$ so that the function $n \mapsto \varepsilon^{n+1}c_\varepsilon^n$ will diverge for each ε as $n \to \infty$. However, for each $\varepsilon > 0$ there is an $n_\varepsilon \in \mathbb{N}$ such that $\varepsilon^{n+1}c_\varepsilon^n$ takes its minimal value for $n = n_\varepsilon$. This defines the *optimal superadiabatic basis*. In this basis the off-diagonal elements of $H_\varepsilon^n(t)$ are exponentially small for all t. As a consequence, also the lower component $\phi_-^n(t)$ of the solution with $\lim_{t\to-\infty}\phi_-^n(t) = \lim_{t\to-\infty}\phi_-(t) = 0$ is exponentially small, as illustrated in Figure 1b), and one can compute the scattering amplitude by first order perturbation theory.

Berry and Lim [Ber, BerLi] showed on a non-rigorous level that $\phi_-^n(t)$ is not only exponentially small in ε but has the universal form of an error function, a feature also illustrated in Figure 1b). A rigorous derivation of the optimal superadiabatic Hamiltonian and of the universal transition histories has been given recently in [BeTe$_1$] and [BeTe$_2$].

The aim of this note is to explain certain aspects of the results from [BeTe$_2$] and to show how to obtain scattering amplitudes from them. In Section 2 we basically give a more detailed and also more technical introduction to the problem of exponentially small non-adiabatic transitions. Section 3 contains a concise summary of the results obtained in [BeTe$_2$]. In order to apply these results to the scattering situation, we need some control on the time decay of the error estimates appearing in our main theorem. In Section 4 we use standard Cauchy estimates to obtain such bounds and give a general recipe for obtaining rigorous proofs of scattering amplitudes. We close with two examples, the Landau-Zener model and the Rosen-Zener model. While the Landau-Zener model displays, in a sense to be made precise, a generic transition point, the Rosen-Zener model is of a non-generic type, which is not covered by existing rigorous results.

2 Exponentially small transitions

From now on we study the Schrödinger equation (2) with the Hamiltonian

$$H_{\rm ph}(t) = \begin{pmatrix} Z(t) & X(t) \\ X(t) & -Z(t) \end{pmatrix} = \rho(t) \begin{pmatrix} \cos\theta_{\rm ph}(t) & \sin\theta_{\rm ph}(t) \\ \sin\theta_{\rm ph}(t) & -\cos\theta_{\rm ph}(t) \end{pmatrix} . \tag{8}$$

Thus $H_{\rm ph}(t)$ is a traceless real-symmetric 2×2-matrix, and the eigenvalues of $H_{\rm ph}(t)$ are $\pm\,\rho(t) = \pm\sqrt{X(t)^2+Z(t)^2}$. We assume that the gap between them does not close, i.e. that $2\rho(t)\geq g>0$ for all $t\in\mathbb{R}$. As to be detailed below, we assume that X and Z are real-valued on the real axis and analytic on a suitable domain containing the real axis. Moreover, in order to be able to consider the scattering limit it is assumed that $H_{\rm ph}(t)$ approaches limits $H_\pm$ sufficiently fast as $t\to\pm\infty$.

Before proceeding we simplify (8) by switching to the *natural time scale*

$$\tau(t) = 2\int_0^t {\rm d}s\,\rho(s)\,. \tag{9}$$

Since $\rho(t)$ is assumed to be strictly positive, the map $t\mapsto\tau$ is a bijection of $\mathbb{R}$. In the natural time scale the Schrödinger equation (2) becomes

$$\big({\rm i}\varepsilon\partial_\tau - H_{\rm n}(\tau)\big)\phi(\tau) = 0 \tag{10}$$

with Hamiltonian

$$H_{\mathrm{n}}(\tau) = \tfrac{1}{2}\begin{pmatrix} \cos\theta_{\mathrm{n}}(\tau) & \sin\theta_{\mathrm{n}}(\tau) \\ \sin\theta_{\mathrm{n}}(\tau) & -\cos\theta_{\mathrm{n}}(\tau) \end{pmatrix}, \tag{11}$$

where $\theta_{\mathrm{n}}(\tau) = \theta_{\mathrm{ph}}(t(\tau))$. As a consequence we now deal with a Hamiltonian with constant eigenvalues equal to $\pm\frac{1}{2}$, which is completely defined through the single real-analytic function θ_{n}.

The transformation (5) to the adiabatic basis, i.e. the orthogonal matrix that diagonalizes $H_{\mathrm{n}}(\tau)$, is

$$U_0(\tau) = \begin{pmatrix} \cos(\theta_{\mathrm{n}}(\tau)/2) & \sin(\theta_{\mathrm{n}}(\tau)/2) \\ \sin(\theta_{\mathrm{n}}(\tau)/2) & -\cos(\theta_{\mathrm{n}}(\tau)/2) \end{pmatrix}. \tag{12}$$

Multiplying (10) from the left with $U_0(\tau)$ yields the Schrödinger equation in the *adiabatic representation*

$$\big(\mathrm{i}\varepsilon\partial_\tau - H^{\mathrm{a}}_\varepsilon(\tau)\big)\phi^{\mathrm{a}}(\tau) = 0\,, \tag{13}$$

where

$$H^{\mathrm{a}}_\varepsilon(\tau) = \begin{pmatrix} \frac{1}{2} & \frac{\mathrm{i}\varepsilon}{2}\theta'_{\mathrm{n}}(\tau) \\ -\frac{\mathrm{i}\varepsilon}{2}\theta'_{\mathrm{n}}(\tau) & -\frac{1}{2} \end{pmatrix} \qquad \text{and} \qquad \phi^{\mathrm{a}}(\tau) = U_0(\tau)\phi(\tau) = \begin{pmatrix} \phi_+(\tau) \\ \phi_-(\tau) \end{pmatrix}. \tag{14}$$

θ'_{n} is called the *adiabatic coupling function*.

The exponentially small scattering amplitude in Figure 1a) can be guessed by a heuristic calculation. We solve (13) for $\phi_-(\tau)$ using $\phi_+(\tau) = \mathrm{e}^{-\frac{\mathrm{i}\tau}{2\varepsilon}} + \mathcal{O}(\varepsilon)$, which holds according to the adiabatic theorem [Ka], and variation of constants, i.e.

$$\begin{aligned} \phi_-(\tau) &= \frac{\mathrm{i}}{\varepsilon}\,\mathrm{e}^{\frac{\mathrm{i}\tau}{2\varepsilon}} \int_{-\infty}^{\tau} \mathrm{d}\sigma\, \mathrm{e}^{-\frac{\mathrm{i}\sigma}{2\varepsilon}} \left(-\frac{\mathrm{i}\varepsilon}{2}\theta'_{\mathrm{n}}(\sigma)\right) \phi_+(\sigma) \\ &= \frac{1}{2}\,\mathrm{e}^{\frac{\mathrm{i}\tau}{2\varepsilon}} \int_{-\infty}^{\tau} \mathrm{d}\sigma\, \theta'_{\mathrm{n}}(\sigma)\, \mathrm{e}^{-\frac{\mathrm{i}\sigma}{\varepsilon}} \; + \mathcal{O}(\varepsilon)\,. \end{aligned} \tag{15}$$

Integration by parts yields

$$\phi_-(\tau) = \frac{\mathrm{i}\varepsilon}{2}\theta'_{\mathrm{n}}(\tau) - \frac{\mathrm{i}\varepsilon}{2}\,\mathrm{e}^{\frac{\mathrm{i}\tau}{2\varepsilon}} \int_{-\infty}^{\tau} \mathrm{d}\sigma\, \theta''_{\mathrm{n}}(\sigma)\, \mathrm{e}^{-\frac{\mathrm{i}\sigma}{\varepsilon}} \; + \mathcal{O}(\varepsilon)\,. \tag{16}$$

The first term in this expression is of order ε and not smaller. This strongly suggests that the $\mathcal{O}(\varepsilon)$ error estimate in the adiabatic theorem is optimal, which we have seen to be indeed the case. However, no conclusion can be inferred from (16) for the scattering regime $\tau \to \infty$ since θ'_{n} vanishes there.

The key to the heuristic treatment of the scattering amplitude is to calculate the integral in (15) not by integration by parts but by contour integration in the complex plane. For the sake of a simple argument let us assume here that θ_{n}' is a meromorphic function. Let τ_{c} be the location of the pole in the lower complex half plane closest to the real line and γ its residue, then from (15) and contour integration around the poles in the lower half plane we read off

$$\lim_{\tau\to\infty} |\phi_-(\tau)|^2 = \pi^2\gamma^2\,\mathrm{e}^{-\frac{2\mathrm{Im}\tau_{\mathrm{c}}}{\varepsilon}} + \mathcal{O}(\varepsilon^2)\,. \tag{17}$$

Strictly speaking (17) tells us nothing new: while the explicit term is exponentially small in ε, the error term is of order ε^2 and thus the statement is not better than what we know from the adiabatic theorem already. Nevertheless it turns out that the exponential factor appearing here actually yields the correct asymptotic behavior of the transition probability. Our heuristic argument also correctly attributes the dominant part of the transition to the pole of θ_{n}' closest to the real axis. The prefactor in (17), however, is wrong, the correct answer being

$$\lim_{\tau\to\infty} |\phi_-(\tau)|^2 = 4\sin^2\left(\frac{\pi\gamma}{2}\right)\mathrm{e}^{-\frac{2\mathrm{Im}\tau_{\mathrm{c}}}{\varepsilon}}\;\left(1+\mathcal{O}(\varepsilon^\alpha)\right) \tag{18}$$

for some $\alpha > 0$. Expression (18) is a generalization of the Landau-Zener formula and was first rigorously derived in [Jo].

The problem to solve when trying to rigorously treat exponentially small transitions and to arrive at the correct result (18) is to control the solution of (2) up to errors that are not only exponentially small in ε, but smaller than the leading order transition probability. As a consequence a naive perturbation calculation in the adiabatic basis will not do the job.

The classical approach [Jo] to cope with this is to solve (2) not on the real axis but along a certain path in the complex plane, where the lower component of the solution is always exponentially small. The comparison with the solution on the real line is made only in the scattering limit at $\tau = \pm\infty$. The trick is to choose the path in such a way that it passes through the relevant singularity of θ_{n}' in the complex plane. In a neighborhood of the singularity one can solve (13) explicitly and thereby determine the leading order contribution to the transition probability. Moreover, away from the transition point the path must be chosen such that the lower component $\phi_-(\tau)$ remains smaller than the exponentially small leading order contribution from the transition point for all τ along this path. There are two drawbacks of this approach: the technical one is that there are examples (see the Rosen-Zener model below), where such paths do not exist. On the conceptual side, this approach yields only the scattering amplitudes, but gives no information whatsoever about the solution for finite times.

Our approach is motivated by the findings of Berry [Ber] and of Berry and Lim [BerLi]. Instead of solving (13) along a path in the complex plane we solve the problem along the real axis but in a super-adiabatic basis instead of the adiabatic one, i.e. we solve (6) with the Hamiltonian (7) and the optimal $n(\varepsilon)$. While the off-diagonal elements of the Hamiltonian in the adiabatic basis are only of order ε, cf. (14), the off-diagonal elements of the Hamiltonian in the optimal superadiabatic basis are exponentially small, i.e. of order $\mathrm{e}^{-c/\varepsilon}$.

In order to control the exponentially small transitions, we will give precise exponential bounds on the coupling $\varepsilon^{n_\varepsilon+1}c_\varepsilon^{n_\varepsilon}(\tau)$ away from the transition regions and explicitly determine the asymptotic form of $c_\varepsilon(\tau)$ within each transition region. Since the superadiabatic bases agree asymptotically for $t \to \pm\infty$ with the adiabatic basis, the scattering amplitudes agree in all these bases. In the optimal superadiabatic basis the correct transition probabilities (18) now follow from a first order perturbation calculation analogous to the one leading to (17) in the adiabatic basis. However, in addition to the scattering amplitudes we obtain approximate solutions for all times, i.e. "histories of adiabatic quantum transitions" [Ber]. As is illustrated in Figure 1b), these are monotonous and asymptotically take the form of an error function.

3 The Hamiltonian in the super-adiabatic representation

In [BeTe$_2$] we formulate our results for the system (10) and (11). However, we have to keep in mind that (10) and (11) arise from the physical problem (2) and (8) through the transformation to the natural time scale (9). Therefore, to be physically relevant, the assumptions must be satisfied by all $\theta_{\rm n}$ arising from generic Hamiltonians of the form (8). As observed in [BerLi], see also [BeTe$_2$], for such $\theta_{\rm n}$ the adiabatic coupling function $\theta_{\rm n}'$ is real analytic and at its complex singularities z_0 closest to the real axis it has the form

$$\theta_{\rm n}'(z-z_0) = \frac{-\mathrm{i}\gamma}{z-z_0} + \sum_{j=1}^{N}(z-z_0)^{-\alpha_j}h_j(z-z_0), \tag{19}$$

where $|\mathrm{Im} z_0| > 0$, $\gamma \in \mathbb{R}$, $\alpha_j < 1$ and h_j is analytic in a neighborhood of 0 for $j = 1, \ldots, N$.

The following norms on the real line capture exactly the behavior (19) of the complex singularities of $\theta_{\rm n}'$. They are at the heart of the analysis in [BeTe$_2$].

Definition 1. *Let $\tau_{\rm c} > 0$, $\alpha > 0$ and $I \subset \mathbb{R}$ be an interval. For $f \in C^\infty(I)$ we define*

$$\|f\|_{(I,\alpha,\tau_{\rm c})} := \sup_{t\in I}\sup_{k\geq 0}\left|\partial^k f(t)\right| \frac{{\tau_{\rm c}}^{\alpha+k}}{\Gamma(\alpha+k)} \leq \infty \tag{20}$$

and

$$F_{\alpha,\tau_{\rm c}}(I) = \left\{ f \in C^\infty(I) : \|f\|_{(I,\alpha,\tau_{\rm c})} < \infty \right\}.$$

The connection of these norms with (19) relies on the Darboux Theorem for power series and is described in [BeTe$_2$]. Let us just note here that $\theta_{\rm n}'$ as given in (19) is an element of $F_{1,\tau_{\rm c}}(\{\tau_{\rm r}\})$ for $\tau_{\rm c} = \mathrm{Im}(z_0)$ and $\tau_{\rm r} = \mathrm{Re}(z_0)$, while the second term of (19) is in $F_{\beta,\tau_{\rm c}}(\{\tau_{\rm r}\})$ with $\beta = \max_j \alpha_j$. In order to control the transitions histories, the real line will be segmented into intervals I, which are either considered to be a small neighborhood of a transition point or to contain no transition point. Assumption 1 below thus applies to intervals without transition point and Assumption 2 generically holds near a transition point. In the rest of this section we drop the subscript n for the natural time scale in order not to overburden our notation.

Assumption 1: *For a compact interval I and $\delta \geq 0$ let $\theta'(\tau) \in F_{1,\tau_\mathrm{c}+\delta}(I)$.*

Assumption 2: *For γ, τ_r, $\tau_\mathrm{c} \in \mathbb{R}$ let*

$$\theta_0'(t) = \mathrm{i}\,\gamma\left(\frac{1}{\tau - \tau_\mathrm{r} + \mathrm{i}\tau_\mathrm{c}} - \frac{1}{\tau - \tau_\mathrm{r} - \mathrm{i}\tau_\mathrm{c}}\right)$$

be the sum of two complex conjugate first order poles located at $\tau_\mathrm{r} \pm \mathrm{i}\tau_\mathrm{c}$ with residues $\mp\,\mathrm{i}\gamma$. On a compact interval $I \subset [\tau_\mathrm{r} - \tau_\mathrm{c}, \tau_\mathrm{r} + \tau_\mathrm{c}]$ with $\tau_\mathrm{r} \in I$ we assume that

$$\theta'(\tau) = \theta_0'(\tau) + \theta_\mathrm{r}'(\tau) \quad \textit{with} \quad \theta_\mathrm{r}'(\tau) \in F_{\alpha,\tau_\mathrm{c}}(I) \tag{21}$$

for some γ, $\tau_\mathrm{c}, \tau_\mathrm{r} \in \mathbb{R}$, $0 < \alpha < 1$.

It turns out that under Assumption 2 the optimal superadiabatic basis is given as the $n_\varepsilon^{\mathrm{th}}$ superadiabatic basis where $0 \leq \sigma_\varepsilon < 2$ is such that

$$n_\varepsilon = \frac{\tau_\mathrm{c}}{\varepsilon} - 1 + \sigma_\varepsilon \qquad \text{is an even integer.} \tag{22}$$

The two main points of the following theorem are: outside the transition regions, the off-diagonal elements of the Hamiltonian in the optimal superadiabatic basis are bounded by (24), while within each transition region they are asymptotically equal to $g(\varepsilon,\tau)$ as given in (ii).

Theorem 1. (i) *Let H satisfy Assumption 1. Then there exists $\varepsilon_0 > 0$ such that for all $\varepsilon \in (0, \varepsilon_0]$ and all $\tau \in I$ the elements of the superadiabatic Hamiltonian (7) and the unitary $U_\varepsilon^{n_\varepsilon}(\tau)$ with n_ε as in (22) satisfy*

$$\left|\rho_\varepsilon^{n_\varepsilon}(\tau) - \frac{1}{2}\right| \leq \varepsilon^2 \phi_1\Big(\|\theta'\|_{(I,1,\tau_\mathrm{c}+\delta)}\Big) \tag{23}$$

$$\left|\varepsilon^{n_\varepsilon+1} c_\varepsilon^{n_\varepsilon}(\tau)\right| \leq \sqrt{\varepsilon}\,\mathrm{e}^{-\frac{\tau_\mathrm{c}}{\varepsilon}(1+\ln\frac{\tau_\mathrm{c}+\delta}{\tau_\mathrm{c}})} \phi_1\Big(\|\theta'\|_{(I,1,\tau_\mathrm{c}+\delta)}\Big) \tag{24}$$

and

$$\|U_\varepsilon^{n_\varepsilon}(\tau) - U_0(\tau)\| \leq \varepsilon \phi_1\Big(\|\theta'\|_{(I,1,\tau_\mathrm{c}+\delta)}\Big)\,. \tag{25}$$

Here $\phi_1 : \mathbb{R}^+ \to \mathbb{R}^+$ is a locally bounded function with $\phi_1(x) = \mathcal{O}(x)$ as $x \to 0$ which is independent of I and δ.

(ii) *Let H satisfy Assumption 2 and define*

$$g(\varepsilon,\tau) = 2\mathrm{i}\sqrt{\tfrac{2\varepsilon}{\pi\tau_\mathrm{c}}}\,\sin\left(\tfrac{\pi\gamma}{2}\right)\,\mathrm{e}^{-\frac{\tau_\mathrm{c}}{\varepsilon}}\,\mathrm{e}^{-\frac{(\tau-\tau_\mathrm{r})^2}{2\varepsilon\tau_\mathrm{c}}}\,\cos\left(\tfrac{\tau-\tau_\mathrm{r}}{\varepsilon} - \tfrac{(\tau-\tau_\mathrm{r})^3}{3\varepsilon{\tau_\mathrm{c}}^2} + \tfrac{\sigma_\varepsilon\tau}{\tau_\mathrm{c}}\right).$$

There exists $\varepsilon_0 > 0$ *and a constant* $C < \infty$ *such that for all* $\varepsilon \in (0, \varepsilon_0]$ *and all* $\tau \in I$

$$\left|\varepsilon^{n_\varepsilon+1} c_\varepsilon^{n_\varepsilon}(\tau) - g(\varepsilon,\tau)\right| \le C\varepsilon^{\frac{3}{2}-\alpha} \mathrm{e}^{-\frac{\tau_\mathrm{c}}{\varepsilon}} . \tag{26}$$

Furthermore, the assertions of part (i) hold with $\delta = 0$.

Remark 1. In [BeTe$_2$] we show in addition that the error bounds in Theorem 1 are locally uniform in the parameters α, γ and τ_c. This generality is not needed here and thus omitted from the statement.

In order to pass to the scattering limit it is now necessary to show that the errors in part (i) of Theorem 1, i.e. in the regions away from the transition points, are integrable.

4 The scattering regime

We will treat the scattering regime by using first order perturbation theory on the equation in the optimal superadiabatic basis. As in (15), variation of constants yields

$$\phi_-^{n_\varepsilon}(\tau) = \frac{\mathrm{i}}{\varepsilon}\, \mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\int_{-\infty}^{\tau} \mathrm{d}\sigma\, \rho(\sigma)} \int_{-\infty}^{\tau} \mathrm{d}\sigma\, \mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}\int_{-\infty}^{\sigma} \mathrm{d}\nu\, \rho(\nu)}\, c(n_\varepsilon,\sigma)\, \phi_+^{n_\varepsilon}(\sigma)\,, \tag{27}$$

where we put $c(n_\varepsilon,\tau) = \varepsilon^{n_\varepsilon+1} c_\varepsilon^{n_\varepsilon}(\tau)$. We now replace $\rho_\varepsilon^{n_\varepsilon}(\tau)$ and $c(n_\varepsilon,\tau)$ in (27) by the explicit asymptotic values given in Theorem 1, and use the adiabatic approximation $\phi_+^{n_\varepsilon}(\tau) = \mathrm{e}^{-\frac{\mathrm{i}\tau}{2\varepsilon}} + \mathcal{O}(\varepsilon)$. To this end we assume that θ_n' has k poles of the form (19) at distance τ_c from the real axis and none closer to the real axis. Let $g_j(\varepsilon,\tau)$ be the associated coupling functions of Theorem 1 for $j = 1, \ldots, k$ and

$$f_1(\tau) = \left|\rho_\varepsilon^{n_\varepsilon}(\tau) - \frac{1}{2}\right|, \quad f_2(\tau) = c(n_\varepsilon,\tau) - \sum_{j=1}^{k} g_j(\varepsilon,\tau), \quad f_3(\tau) = \phi_+^{n_\varepsilon}(\tau) - \mathrm{e}^{-\frac{\mathrm{i}\tau}{2\varepsilon}} .$$

Then

$$\mathrm{e}^{\frac{i}{\varepsilon}\int_{-\infty}^{\tau} \mathrm{d}\sigma\, \rho(\sigma)} = \mathrm{e}^{\frac{\mathrm{i}\tau}{2\varepsilon}} \left(1 + \mathcal{O}\left(\varepsilon \underbrace{\int_{-\infty}^{\tau} \mathrm{d}\sigma\, f_1(\sigma)}_{=:F_1(\tau)}\right)\right)$$

and

$$\phi_-^{n_\varepsilon}(\tau) = \frac{\mathrm{i}}{\varepsilon}\, \mathrm{e}^{\frac{\mathrm{i}\tau}{2\varepsilon}} \Big(1 + \mathcal{O}(\varepsilon F_1(\tau))\Big) \int_{-\infty}^{\tau} \mathrm{d}\sigma\, \mathrm{e}^{-\frac{\mathrm{i}\sigma}{2\varepsilon}} \Big(1 + \mathcal{O}(\varepsilon F_1(\sigma))\Big) \times$$
$$\left(\sum_{j=1}^{k} g_j(\varepsilon,\sigma) - f_2(\sigma)\right) \phi_+^{n_\varepsilon}(\sigma)$$

$$
\begin{aligned}
&= \frac{\mathrm{i}}{\varepsilon}\,\mathrm{e}^{\frac{\mathrm{i}\tau}{2\varepsilon}} \int_{-\infty}^{\tau} \mathrm{d}\sigma\, \mathrm{e}^{-\frac{\mathrm{i}\sigma}{\varepsilon}} \sum_{j=1}^{k} g_j(\varepsilon,\sigma) \\
&\quad + \mathcal{O}\left((\|F_1\|_\infty + \varepsilon^{-1}\|f_3\|_\infty) \int_{-\infty}^{\tau} \mathrm{d}\sigma |c(n_\varepsilon,\sigma)| + \varepsilon^{-1} \int_{-\infty}^{\tau} \mathrm{d}\sigma |f_2(\sigma)| \right).
\end{aligned}
$$

Assuming integrability of the error terms in (23) and (24), the following lemma can be established by straightforward computations.

Proposition 1. *Let $\theta'_{\mathrm{n}}(\tau)$ be as above and let $\tau \mapsto \|\theta'_{\mathrm{n}}\|_{(\{\tau\},1,\tau_{\mathrm{c}}+\delta)}$ be integrable outside of some bounded interval and for some $\delta > 0$. Then*

$$
\phi_-^{n_\varepsilon}(\tau) = \frac{\mathrm{i}}{\varepsilon}\,\mathrm{e}^{\frac{\mathrm{i}\tau}{2\varepsilon}} \int_{-\infty}^{\tau} \mathrm{d}\sigma\, \mathrm{e}^{-\frac{\mathrm{i}\sigma}{\varepsilon}} \sum_{j=1}^{k} g_j(\varepsilon,\sigma) + \mathcal{O}(\varepsilon^{\frac{1}{2}-\alpha}\mathrm{e}^{-\frac{\tau_{\mathrm{c}}}{\varepsilon}}).
$$

Note that the leading term in Proposition 1 is of order $\mathrm{e}^{-\frac{\tau_{\mathrm{c}}}{\varepsilon}}$. Thus for $\alpha \geq \frac{1}{2}$ the estimate is too weak. However, a more careful analysis of the error near the transition points allows one to replace $\varepsilon^{\frac{1}{2}-\alpha}$ by $\varepsilon^{1-\alpha}$ in Proposition 1, see [BeTe3], and thus to obtain a nontrivial estimate for all $\alpha < 1$.

Since the functions $g_j(\varepsilon,\tau)$ are explicitly given in Theorem 1, the leading order expression for $\phi_-^{n_\varepsilon}(\tau)$ can be computed explicitly as well. A simple computation, c.f. [BeTe1], yields for $k = 1$ that

$$
\begin{aligned}
\phi_-^{n_\varepsilon}(\tau) &= \frac{\mathrm{i}}{\varepsilon}\,\mathrm{e}^{\frac{\mathrm{i}\tau}{2\varepsilon}} \int_{-\infty}^{\tau} \mathrm{d}\sigma\, \mathrm{e}^{-\frac{\mathrm{i}\sigma}{\varepsilon}}\, g(\varepsilon,\sigma) + \mathcal{O}(\varepsilon^{\frac{1}{2}-\alpha}\mathrm{e}^{-\frac{\tau_{\mathrm{c}}}{\varepsilon}}) \\
&= \sin\left(\frac{\pi\gamma}{2}\right) \mathrm{e}^{-\frac{\tau_{\mathrm{c}}}{\varepsilon}}\,\mathrm{e}^{\frac{\mathrm{i}\tau}{2\varepsilon}} \left(\mathrm{erf}\left(\frac{\tau}{\sqrt{2\varepsilon\tau_{\mathrm{c}}}}\right) + 1 \right) + \mathcal{O}(\varepsilon^{\frac{1}{2}-\alpha}\mathrm{e}^{-\frac{\tau_{\mathrm{c}}}{\varepsilon}}).
\end{aligned}
$$

For more than one transition point the same computation reveals interference effects, c.f. [BeTe3]. In the limit $\tau \to \infty$ we recover the Landau-Zener formula for the transition probability:

$$
|\phi_-^{n_\varepsilon}(\infty)|^2 = 4\sin^2\left(\frac{\pi\gamma}{2}\right) \mathrm{e}^{-\frac{2\tau_{\mathrm{c}}}{\varepsilon}} + \mathcal{O}(\varepsilon^{\frac{1}{2}-\alpha}\mathrm{e}^{-\frac{2\tau_{\mathrm{c}}}{\varepsilon}}). \tag{28}
$$

Proposition 1 yields the transition histories as well as the transition probabilities in the scattering limit for a large class of Hamiltonians under the assumption that $\|\theta'_{\mathrm{n}}\|_{(\{\tau\},1,\tau_{\mathrm{c}}+\delta)}$ is integrable at infinity for some $\delta > 0$. At first sight it might seems hard to establish integrability of this norm, since it involves derivatives of θ'_{n} of all orders. However, the following proposition shows that $\|\theta'_{\mathrm{n}}\|_{(\{\tau\},1,\tau_{\mathrm{c}}+\delta)}$ can be bounded by the supremum of the function θ'_{n} in a ball around τ with radius slightly larger than $\tau_{\mathrm{c}} + \delta$.

Proposition 2. *Let $\alpha > 0$ and $r > 0$. Assume for some $\delta > 0$ that f is analytic on*

$$
B_{r+\delta} = \{z \in \mathbb{C} : |z| \leq r + \delta\}.
$$

Then

$$\|f\|_{(\{0\},\alpha,r)} \leq \frac{r^\alpha}{\mathrm{e}\ln\left((r+\delta)/r\right)} \sup_{z\in B_{r+\delta}} |f(z)|\,.$$

Proof. Put $M = \sup_{z\in B_{r+\delta}} |f(z)|$. By the Cauchy formula,

$$\partial_t^k f(0) = k! \oint_{|z|=r+\delta} \mathrm{d}z\, \frac{f(z)}{z^{k+1}} \leq 2\pi\, k!\, M(r+\delta)^{-k}.$$

Therefore

$$\partial_t^k f(0) \frac{r^{\alpha+k}}{\Gamma(\alpha+k)} \leq M r^\alpha \frac{\Gamma(1+k)}{\Gamma(\alpha+k)} \left(\frac{r}{r+\delta}\right)^k. \tag{29}$$

The k-dependent part of the right hand side above is obviously maximal for $\alpha = 0$, and then is equal to $\phi(k) := k(r/(r+\delta))^k$. $\phi(k)$ is maximal at $k = 1/\ln((r+\delta)/r)$ with value $1/(\mathrm{e}\ln((r+\delta)/r)$, and the claim follows by taking the supremum over k in (29).

Hence, integrability of $\|\theta_\mathrm{n}'\|_{(\{\tau\},1,\tau_\mathrm{c}+\delta)}$ follows if we can establish sufficient decay of $\sup_{|z-\tau|<\tau_\mathrm{c}+2\delta} |f(z)|$ as $\tau \to \infty$. We will demonstrate how to do this for two simple examples. More elaborate examples including interference effects can be found in [BeTe$_3$]. We will use the transformation formula

$$\theta_\mathrm{n}'(\tau(t)) = \frac{\theta_\mathrm{ph}'(t)}{2\rho(t)} = \frac{1}{2\rho(t)} \frac{\mathrm{d}}{\mathrm{d}t} \arctan\left(\frac{X}{Z}\right)(t) = \frac{X'Z - Z'X}{2\rho^3}(t). \tag{30}$$

Example 1 (Landa-Zener model). The paradigmatic example is the Landau-Zener Hamiltonian

$$H(t) = \begin{pmatrix} a & t \\ t & -a \end{pmatrix},$$

which is explicitly solvable [Ze] and for which the transition probabilities are well-known. Nevertheless it is instructive to exemplify our method on this simple model. We have $X(t) = t$ and $Z(t) = a > 0$. Thus $\rho^2(t) = a^2 + t^2$, and the transformation to the natural time scale reads

$$\tau(t) = 2\int_0^t \sqrt{a^2+s^2}\,\mathrm{d}s. \tag{31}$$

From (30) one reads off that complex zeros of ρ give rise to complex singularities of θ_n'. In the Landau-Zener model, ρ has two zeros at $t_\mathrm{c} = \pm\mathrm{i}a$. Thus (31) yields $\tau_\mathrm{c} = \frac{a^2\pi}{2}$, and expansion of $\theta_\mathrm{n}'(\tau)$ around τ_c shows $\gamma = \frac{1}{3}$ and $\alpha = \frac{1}{3}$, cf. [BerLi, BeTe$_2$]. We now apply Proposition 1 in order to pass to the scattering limit. According to Proposition 2 we need to control the decay of $|\theta_\mathrm{n}'|$ in a finite strip around the real axis for large $|\tau|$. From (31) one reads off that

$$|\tau(t)| \leq 2\cdot 2|t|\sqrt{a^2+|t|^2} \leq 4(a^2+|t|^2),$$

and thus $|t^2| \geq |\tau|/4 - a^2$. From (30) and the estimates above we infer for $|\tau|$ sufficiently large that

$$|\theta_{\mathrm{n}}'(\tau)| = \frac{a}{2|a^2 + t(\tau)^2|^{3/2}} \leq \frac{a}{2(|t(\tau)|^2 - a^2)^{3/2}} \leq \frac{a}{2(|\tau|/4 - 2a^2)^{3/2}}.$$

Consequently, Proposition 2 yields for every $r, \delta > 0$ and $\tau \in \mathbb{R}$ sufficiently large that

$$\|\theta_{\mathrm{n}}'\|_{(\{\tau\},1,r)} \leq \frac{r}{\mathrm{e}\ln((r+\delta)/r)} \frac{a}{((|\tau| - r - \delta)/4 - 2a^2)^{3/2}}.$$

Thus $\tau \mapsto \|\theta_{\mathrm{n}}'\|_{(\{\tau\},1,r)}$ is integrable at infinity for any $r > 0$, and in particular for $r = \tau_{\mathrm{c}} + 2\delta$. According to (28), we have therefore shown the classical Landau-Zener formula

$$|\phi_{-}^{n_\varepsilon}(\infty)|^2 = \mathrm{e}^{-\frac{a^2\pi}{\varepsilon}} + \mathcal{O}(\varepsilon^{\frac{1}{6}} \mathrm{e}^{-\frac{a^2\pi}{\varepsilon}}).$$

For the Landau-Zener model, the transition probabilities can also be proved by the method of [Jo]. There, the anti-Stokes lines, i.e. the level lines $\mathrm{Im}(\tau(t)) = \mathrm{Im}(\tau(t_{\mathrm{c}}))$, play an essential role. In particular, the method requires that an anti-Stokes line emanating from the critical point t_{c} of τ stays in a strip of finite width around the real axis as $\mathrm{Re}(t) \to \pm\infty$. As shown in Figure 2, this is the case in the present example.

The previous example also shows a useful general strategy: One can use (30) in order to find upper bounds on $\tau(t)$, which in turn yield lower bounds on the inverse function $t(\tau)$. These can then be used in (30) to estimate the decay at infinity of θ_{n}' in a strip around the real axis. It is clear that this strategy also works in cases where the Hamiltonian is not given in closed form. Of course, things are much easier when we know θ_{n}' explicitly. This is the case in the following example.

Example 2 (Rosen-Zener model). In this model $X(t) = \frac{1}{2(t^2+1)}$ and $Z(t) = \frac{t}{2(t^2+1)}$. Therefore $\tau(t) = \mathrm{arsinh}(t)$, $\tau_{\mathrm{c}} = \mathrm{Im}(\mathrm{arsinh}(\mathrm{i})) = \pi$, and (30) yields $\theta_{\mathrm{n}}'(\tau) = 1/\cosh(\tau)$ in the natural time scale. It is immediate that $|\theta_{\mathrm{n}}'(\tau)| \leq c\exp(-|\tau|)$ for large $|\tau|$ in each fixed strip around the real axis, and that $\gamma = 1$. Since θ_{n}' is meromorphic, $0 < \alpha$ can be chosen arbitrarily small. In summary, Propositions 1 and 2 yield

$$|\phi_{-}^{n_\varepsilon}(\infty)|^2 = 4\mathrm{e}^{-\frac{\pi}{\varepsilon}} + \mathcal{O}(\varepsilon^{\frac{1}{2}-\alpha} \mathrm{e}^{-\frac{\pi}{\varepsilon}}).$$

Although the Rosen-Zener example is very easy in our picture, it is not clear how to prove it using the methods of [Jo]. The reason is that there are no anti-Stokes lines emanating from the singularity of θ_{n}' and staying in a bounded strip around the real axis as $\mathrm{Re}(t) \to \pm\infty$. In fact, the only relevant anti-Stokes line remains on the imaginary axis, cf. Figure 2.

(a)

(b)

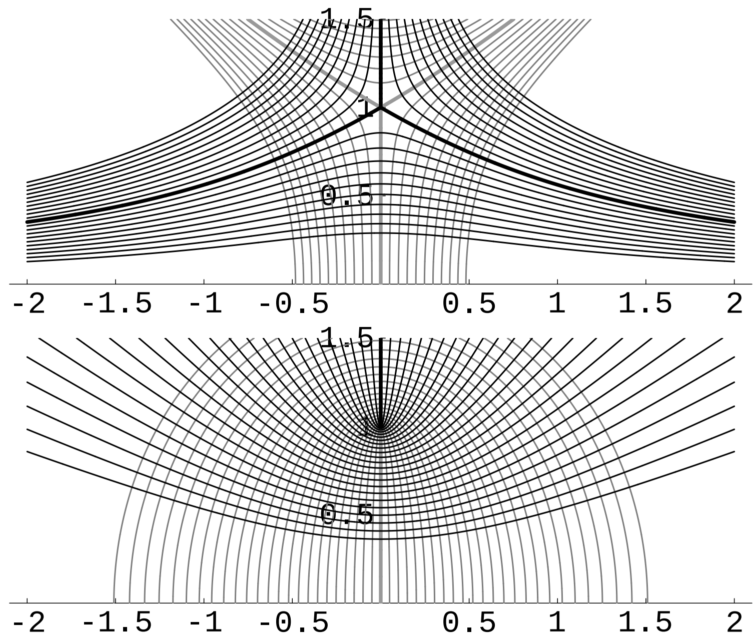

Fig. 2. *This figure shows the Stokes and anti-Stokes lines for $\tau(t)$ in the Landau-Zener model (Figure 2a) and the Rosen-Zener model (Figure 2b). Level lines of* $\mathrm{Re}\tau(t)$ *are grey, while the lines of* $\mathrm{Im}\tau(t)$ *are black. The fat lines correspond to the Stokes and anti-Stokes lines emanating from the critical point* t_{c} *of $\tau(t)$ in the upper complex half-plane. In both examples,* $t_{\mathrm{c}} = \mathrm{i}$. *While in the Landau-Zener model, two anti-Stokes lines remain in a finite strip around the real axis, the anti-Stokes line of the Rosen-Zener model remains on the imaginary axis.*

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