# Multilevel Landau-Zener formulae: adiabatic reduction on a complex path

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We consider, in the semi-classical (adiabatic) limit, evolution equations whose generators extend into a strip around real axis as a holomorphic family of operators (with respect to the time-variable). The asymptotic expansion of the  $\mathcal{S}$ -matrix associated to this evolution can be expressed in terms of simple quantities attached to the singularities for the spectrum of Hamiltonians from complex-time plane. We extend to many-level case the result from [26] which contains as limit cases both the Landau–Zener formula and Friedrichs–Hagedorn results for this problem.

#### Introduction

**General setting.** We study, in a separable complex Hilbert space  $\mathcal{H}$ , the limit  $\varepsilon \to 0$ ,  $\varepsilon \in \mathbb{R}_+$ , of the evolution operator, solution of the Schrödinger equation

$$i\varepsilon \frac{d}{ds}U_{\varepsilon}(s,s_0) = H(s)U_{\varepsilon}(s,s_0) \quad \text{with} \quad s,s_0 \in \mathbb{R}, \quad U_{\varepsilon}(s,s_0) = \mathbb{I}.$$
 (1)

It describes the dynamics of a time-dependent quantum system with the generator or the Hamiltonian H(s). In the adiabatic framework  $\varepsilon$  is the slowness parameter and s denotes the reduced time  $s = \varepsilon t$ .

This kind of limits, when the small parameter is in the front of the highest order derivative and reduce the equation order for  $\varepsilon = 0$ , is not tackled by standard perturbation methods and involves a strongly singular behavior for the solution

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of the differential equation at  $\varepsilon \to 0$ . The starting point of the method which we consider relies on the idea of getting information about  $U_{\varepsilon}(s, s_0)$  without actually integrating (1). Following [33] this can be realized by using a schema of reduction for the Schrödinger equation, to a subspace  $\mathcal{K}_{\varepsilon}(s_0)$  (almost) invariant under the evolution, i.e.,  $U_{\varepsilon}(s, s_0)\mathcal{K}_{\varepsilon}(s_0) \simeq \mathcal{K}_{\varepsilon}(s)$  or (see below a precise statement):

$$P_{\varepsilon}(s) \simeq U_{\varepsilon}(s, s_0) P_{\varepsilon}(s_0) U_{\varepsilon}^{-1}(s, s_0)$$
 (2)

(we denoted with  $\mathcal{P}_{\varepsilon}(s)$  the orthogonal projector onto  $\mathcal{K}_{\varepsilon}(s)$ ). The aim is to integrate the restriction of (1) to  $\mathcal{K}_{\varepsilon}(s_0)$ . This arguments relies upon the fact that the singularity of  $U_{\varepsilon}(s,s_0)$  at  $\varepsilon \to 0$  comes from one of its components called dynamical phase operator (for instance, see the exponential factor in (11)). It does not affect the subspaces  $\mathcal{K}_{\varepsilon}(s)$  which are regular at  $\varepsilon \to 0$ . For the construction of  $\mathcal{K}_{\varepsilon}(s)$  an equation without  $U_{\varepsilon}(s,s_0)$  is obtained differentiating (2) (the Heisenberg equation):

$$i\varepsilon \frac{d}{ds} \mathcal{P}_{\varepsilon}(s) \simeq [H(s), \mathcal{P}_{\varepsilon}(s)]$$
 (3)

We mention also the equivalent manner to formulate the invariance of  $\mathcal{P}_{\varepsilon}(s)$  under  $U_{\varepsilon}(s, s_0)$  by considering an exact intertwining evolution:

$$P_{\varepsilon}(s) = U_A(s, s_0) P_{\varepsilon}(s_0) [U_A(s, s_0)]^{-1}, \tag{4}$$

which turns (2) into

$$U_{\varepsilon}(s; s_0) \simeq U_A(s, s_0)$$
 (5)

(We send to (19), (34) for the precise form of (3), (5)). For such "adiabatic" evolutions we shall use a construction based on a generalization (given in [33]) of the Krein-Kato parallel transport, for which we consider a variant in Lemma 1.3. The restriction  $U_A(s,s_0)|_{\mathcal{K}_{\varepsilon}(s_0)}$  is simpler, being, e.g., trivially integrable when  $\dim \mathcal{K}=1$ .

A question of interest in adiabatic theory concern the transition probability between spectral subspaces of H(s) associated to parts of the spectrum separated by a gap. Thus the starting point in the construction of  $P_{\varepsilon}(s)$  was a spectral projector of H(s) corresponding to an isolated bounded part of the spectrum (let denote it  $\sigma_I(s)$ ). We assume for the spectrum of H:

$$\sigma(H(s)) = \sigma_I(s) \cup \sigma_{II}(s), \quad \inf_{s \in \mathbb{R}} \operatorname{dist}(\sigma_I(s)\sigma_{II}(s)) \ge d > 0.$$
 (i)

Let consider a continuity condition in s for  $\sigma_I(s)$ , for instance, we suppose the existence of a simple closed path  $\Gamma(s)$  in the rezolvent set of the Hamiltonian  $\Gamma(s) \subset \rho(H(s))$ , continuous in s, which encloses only  $\sigma_I(s)$ , with

$$\operatorname{dist}(\Gamma(s),\sigma(H(s))) \geq \frac{d}{2}.$$

This involves for  $P_{\sigma_I}$  the same regularity like that for H (we shall denote by  $P_{\sigma_{I,II}}$  the corresponding spectral projectors of H).

The fact that  $P_{\sigma_I}$  is invariant under  $U_{\varepsilon}(s, s_0)$  in the order  $o(\varepsilon)$ , i.e.,

$$P_{\sigma_I}(s) = U_{\varepsilon}(s, s_0) P_{\sigma_I}(s_0) U_{\varepsilon}(s_0, s) + o(\varepsilon)$$

is known as the Adiabatic Theorem, and it has a long history (see [2, 21, 30, 1]). For the study of the higher order solutions of (3) we mention the approaches from [25, 9, 38]. The higher orders are determined by the order of differentiability of the Hamiltonians family. For the indefinitely differentiable case the extension for complex times is important. We consider here the holomorphic case.

Let us extend (1) in the complex strip

$$\mathcal{S}_{\alpha} = \{ z \in \mathbb{C} | |Im \, z| < \alpha \}$$

where

$$H(z) \in B(\mathcal{H})$$
 (ii)

is an analytic family of bounded operators. We assume (i) for all  $z \in \mathcal{S}_{\alpha}$ .

As in most of physical situations we assume also the integrable decay condition

$$\sup_{z \in \mathcal{S}_{\alpha}, Re \, z \geq 0} (1 + |Re \, z|^{1+\beta}) ||H(z) - H_{\frac{r}{l}}|| < \infty \quad \text{for some} \quad H_{\frac{r}{l}} \in B(\mathcal{H}) \quad \text{(iii)}$$

(or a limiting approaching dominated by any  $b(Re\ z), b \in L^1(\mathbb{R})$ ).

The classical result states that (notice the assumption of self-adjointness on the real axis:

$$H(z) = H^*(\bar{z})$$
 (5')

the transition probability from  $\sigma_I(-\infty)$  to  $\sigma_{II}(\infty)$  is exponentially small:

$$\mathfrak{P}_{II,I}(+\infty,-\infty) := \lim_{\substack{s \to \infty \\ t_0 \to -\infty}} \|P_{\sigma_{II}}(s)U_{\varepsilon}(s,s_0)P_{\sigma_I}(s_0)\|^2 = \mathcal{O}(e^{-\frac{k}{\varepsilon}})$$
 (6)

(for some k > 0). We note that no assumption are made on the nature of the Hamiltonian spectrum except the gap condition. We mention [24] for initial formal methods to compute exponential tunneling for analytic Hamiltonians. For a rigorous approach we cite [17] which combines the first order in the construction of  $U_A(z, z_0)$  with a variant of the complex WKB method. In [33] there is a straightforward construction of the method (3)–(5) on the real axis. This fact allows one to cover the case when H(s) belongs to the Gevrey class, which "interpolates" between the  $\mathfrak{C}^{\infty}$  and the holomorphic case. It gives (6) for any reduced times and uses the concept of super-adiabatic evolution  $U_A(z, z_0)$  which verifies (5) up to exponentially small terms (see [18] for a similar construction). For a

better control of k in (6) we refer to [27] which by micro-local analysis techniques obtains

$$\mathfrak{P}_{II,I}(+\infty, -\infty) = \mathcal{O}(e^{-2\Sigma/\varepsilon}),$$
 (5")

with  $\Sigma$  arbitrary close to a positive constant  $\Sigma_0$  (which has a geometrical interpretation). We mention [32] for estimations of this type in the framework of [33].

The scattering operator associated to (1) is defined by the limit

$$\mathbb{S} = \lim_{\substack{t \to \infty \\ t_0 \to -\infty}} \exp(\frac{i}{\varepsilon} H_r s) U(s, s_0) \exp(-\frac{i}{\varepsilon} H_l s_0).$$

The goal is to express the asymptotic expansion of  $\mathbb{S}$  (in  $\varepsilon$ ) in terms of the local behavior spectrum of H(z). Let consider the *n*-dimensional case. We give the asymptotic expansion for

$$P_{\sigma_I}(\infty) \mathbb{S} P_{\sigma_I}(-\infty) \tag{7}$$

under the assumption

$$\operatorname{rank} P_{\sigma_I}(z) = n < \infty \tag{iv}$$

(let  $\sigma_I(H(z)) = \{h_i(z), i = 1, ..., n\}$ , with  $h_i(z)$  eigenvalues). The method covers also cases which violate the gap conditions of type (i) respectively (in the finite-dimensional framework (iv)) cases with crossing points at real arguments for  $h_i(s)$ . The idea (of the complex WKB method) is to remove in complex plane the path for the integration of  $U_{\varepsilon}(s;s_0)|_{\mathcal{K}_{\varepsilon}(s_0)}$  such that it avoids the degenerating points. Thus the gap condition is recovered but the difficulty become the loose of the self-adjointness of H(s). We shall see below the manner to avoid this inconvenience. We consider also the so called "quasi-crossing" case which covers the situation from many applications with small gaps between eigenvalues (with eigenvalue crossings in the complex plane close by the real axis). The interest of this situation comes from the double asymptotic expansion of S in the two small parameters:  $\varepsilon$  and the gap width.

As a by-product of the reduction method to  $\mathcal{K}_{\varepsilon}(s)$  the S-matrix

$$P_{\sigma_I}(+\infty) \mathbb{S} P_{\sigma_I}(-\infty) \tag{8}$$

can be obtained as the one given by an effective evolution in  $Ran P_{\sigma_I}(0)$  (see [26, 18]). The result hold up to exponentially small errors (see [28] for accurate results of type (5")). The only case where the asymptotic expansion (6) was computed is the 2-dimensional one (or reductible to it). In this article we consider the multidimensional one. For the 2 × 2 matrices case the leading term of the asymptotic expansion (6) is given by the so called Dykhine formula (see [20]

and also [6, 35] for previous results) which for small but finite gap (the quasicrossing case) gives the Landau–Zener formula [14] used by physicists since a long time in the computation of the non-adiabatic transition probability over a gap. The situation of a real crossing between the two eigenvalues is covered by the Fridrichs–Hagedorn result [10] obtained by techniques of stretching and matching for the asymptotic expansions of differential equation solutions. The method which we use covers as limit cases all these situations.

We mention that our results have the same expression for unbounded Hamiltonians. The assumptions should be modified as follows. The Hamiltonians H(z)are taken to be a family of closed operators defined on a common dense domain  $D \subset \mathcal{H}$ . The analyticity and decaying condition (iii) can be expressed in terms of graph norms. As was noticed in [17], the different graph norms on D, according to H(z), taken in different points z are equivalents. The analyticity and decaying condition of H(z) can be equally formulated (we recall for instance Theorem 1.3 from Chapter VII of [22]) for the resolvent  $R(z,\xi) = (H(z) - \xi)^{-1}, \xi \in \Gamma(z)$ (let  $\Gamma(z) \subset \rho(H(z'))$ ) be the rezolvent set of H(z'), for z' in a neighborhood of z). It should be set also for all  $z \in \mathcal{S}_{\alpha} \operatorname{diam}(\sigma_I(z)) = D(z) < D < \infty$ . For bounded Hamiltonians (5') is used only as  $\sigma(H(s)) \subset \mathcal{R}$  (for example, in the quantum scattering application from [7] the self-adjointness was considered with respect to a different scalar product). But in the unbounded case the condition that H(s),  $s \in \mathcal{R}$ , is a family of self-adjoint operators, defined on D and below bounded, ensures the existence and uniqueness of  $U(s, s_0)$  as unitary propagator, i.e., a two-parameter family of unitary operators, which leaves D invariant, is jointly strongly differentiable on D and verifies (1) – see the theorem of Kato and Yosida ([22, 42, 43]). Therefore the mentioned integration of  $U(z, z_0)$  for  $z, z_0$  on a complex path is not straightforwardly adaptable in the unbounded case. But using the reduction mentioned after (8) to the effective evolution corresponding to  $\sigma_I$  (see [18, 26]), we obtain in the unbounded case exactly the same expression of the results as for the bounded one. Thus, we restrict ourselves to the previous bounded case.

We also mention that the construction of  $\mathcal{K}_{\varepsilon}(s)$  from [33] does not involve differential equations and assume that Hamiltonians are a family of densely defined, closed operators acting in a Banach space. It is a local construction, in the sense that it involves only finite order derivatives of the Hamiltonian.

Improved complex WKB-type analysis. The S-matrix asymptotic expansion (6) for an complex extension of the Schrödinger equation (1) is an old subject in quantum theory. We cite [27] for a recent modern approach and mention [24] for an initial physical formulation. Extending H(s) holomorphically in  $S_{\alpha}$  (5') allows one to express  $\mathfrak{P}_{II,I}(+\infty, -\infty)$  (associated under (iii) to (1)), in terms of the geometry of the H(z)' spectrum at its singularities from complex-time plane.

We discuss a few arguments from [20] in order to note the progress brought to the classical complex WKB-type method (from [13]) by [26] (see Section V]. In [26] as an illustration of this improvement we find a short (see [14] for a different analysis in the unbounded case) derivation of Landau–Zener formula. By the same method we give in [7] (the time independent application from Part 2) an explicit simple realization of the existence results derived in [36] by micro-local analysis technique of [12].

To sketch this improvement let firstly recall for the complex extension of (1), that the spectral decomposition of H(z) describes a Riemann surface. For example, in the finite dimensional case, as the eigenvalues are solutions of the characteristic equation with the coefficients being analytic functions, this is a well known result for algebraic functions and by the Riesz formula it can be transposed for eigenprojectors (the branching points are among the points of degeneration, the crossings for eigenvalues). It is necessary to consider the multivaluesness of the spectral decomposition because the transition probabilities are defined with respect to the splittings of  $H_{r,l}$  spectrum and because, as we mentioned before, in the method which we use,  $\mathcal{K}_{\varepsilon}(s)$  is constructed from the spectral projector associated to an isolated part of the spectrum.

A consequence of this fact is that (as  $\mathcal{K}_{\varepsilon}(s)$ 's construction is local for reduced time in any complex domain  $\mathcal{D}$  where

$$\sigma(H(z)) = \sigma_I(z) \cup \sigma_{II}(z), \quad \inf_{z \in \mathcal{D}} \operatorname{dist}(\sigma_I(z), \sigma_{II}(z)) \ge d > 0 \tag{9}$$

holds) after restricting ourselves to sub-domains of  $\mathcal{S}_{\alpha}$  we shall be able to consider in (9) a splitting of the  $\sigma(H(z))$  which is different by the splitting on real axis, or cases which violates (i) on  $\mathbb{R}$ . Although the possible source of confusion this is the point of the exponentially small values for  $\mathfrak{P}_{II,I}(+\infty, -\infty)$  (see details below).

The operator H(z) (and by (1), also  $U(z, z_0)$ ) is an univalent function on  $S_{\alpha}$ . Therefore as a limit of an univalent analytic operator (see [26, Lemma 4.3])

$$\mathbb{S} = \lim_{\substack{Re \ z \to \infty \\ Re \ z_0 \to -\infty}} \exp(\frac{i}{\varepsilon} H_r z) U(z, z_0) \exp(-\frac{i}{\varepsilon} H_l z_0), \quad z, \ z_0 \in \mathcal{S}_{\alpha}.$$
 (10)

For the bidimensional problem, let us consider the ideas of the approach from [13] used in [20]. The evolution equation written in the form

$$i\varepsilon\psi'_{\varepsilon}(z) = H(z)\psi_{\varepsilon}(z), \quad \psi_{\varepsilon}(z) \in \mathbb{C}^2, \quad H(z) \in M_2(\mathbb{C})$$

(' denotes  $\frac{d}{dz}$ ) is decomposed into an orthogonal basis

$$H(z)n_{p,j}(z) = h_j(z)n_{p,j}(z)$$

(let denote with  $P_j(z)$  the spectral projectors for  $h_j(z)$ :  $H(z) = \sum_{j=1}^2 h_j(z) P_j(z)$  and decompose  $\psi_{\varepsilon}$  up to the dynamical phase

$$\psi_{\varepsilon}(z) = \sum_{j=1}^{2} c_{j}(z) \exp\left(-\frac{i}{\varepsilon} \int_{-\infty}^{z} dz' h_{j}(z')\right) n_{p,j}(z).$$
 (11)

The basis vectors are obtained by parallel transport in  $\mathcal{S}_{\alpha}$ :

$$n_{p,j}(z) = U_p(z, -\infty) n_{p,j}(-\infty) ,$$

$$\frac{d}{dz}U_p(z,z_0) = \left[\sum_{j=1}^2 P_j'(z)P_j(z)\right]U_p(z,z_0), \quad U_p(z_0,z_0) = \mathbb{I}.$$
 (12)

As  $U_p$  is multivalued (its generator is meromorphic on  $\mathcal{S}_{\alpha}$  and (12) has regular singular points at the eigenvalue crossings), the notation  $U_p(z_0, z_0) = \mathbb{I}$  is ambiguous because the evolutions after a closed path at  $z_0$  give a representation of the fundamental group of

$$S_{\alpha} \setminus \{ \text{the set of eigenvalue crossing points} \}$$
 (13)

at  $z_0$ .

The first step is to estimate  $c_j$  by WKB analysis for  $U(z, z_0)$  along a complex path  $\gamma$  above the "nearest" (see [20] for the discussion of this notion) branch point  $(\tilde{z} \text{ with } h_1(\tilde{z}) = h_2(\tilde{z}), Im \, \tilde{z} \geq 0)$ . We make the next considerations, supposing only one singularity in this situation. A technical aspect is the restriction of "dissipativity" for the path used in this analysis.

We denote by  $\sim$  the analytic continuation along  $\gamma$ , and for  $Im \tilde{z} \neq 0$  we denote "without  $\sim$ " the analytic continuation along  $\mathbb{R}$ . The result of the WKB analysis is (let consider  $h_2(-\infty) > h_1(-\infty)$ ):

$$|\tilde{c}_1(z) - c_1(-\infty)| = o(\varepsilon)$$
.

Therefore it follows from

$$ilde{\psi}_{arepsilon}(z) = \sum_{j=1}^{2} ilde{c}_{j} \exp \left( -rac{i}{arepsilon} \int\limits_{-\infty}^{z} dz' \, ilde{h}_{j}(z') 
ight) ilde{n}_{p,j}(z),$$

where  $\tilde{n}_{p,j}$  is the parallel transport on  $\gamma$  of  $\tilde{n}_{p,j}(-\infty) = n_{p,j}(-\infty)$  (orthonormal vectors):

$$\tilde{n}_{p,j}(z) = U_p(z, -\infty)\tilde{n}_{p,j}(-\infty)$$

that in order to calculate  $|\mathbb{S}_{2,1}| = ||P_2(\infty)\mathbb{S}P_1(-\infty)||$  all what is needed is  $||\tilde{n}_{p,1}(+\infty)||$ . Notice from (10) that  $\gamma$  is sufficient for the S-matrix element definition.

According to the remark after (9), we have

$$\tilde{h}_i(+\infty) = h_i(+\infty) \quad \text{and} \quad \tilde{P}_i(+\infty) = P_i(+\infty) \,.$$
 (14)

The classical argument for  $\|\tilde{n}_{p,1}(+\infty)\|$  calculus is to use (14) which gives

$$\tilde{n}_{p,1}(+\infty) = const \cdot n_{p,2}(+\infty) . \tag{15}$$

Because  $U_p(s, s_0)$ ,  $s, s_0 \in \mathbb{R}$  is unitary,  $n_{p,i}(+\infty)$  are orthonormal and the previous norm is given by |const|.

Although ingenious we observe a weakness of the argument. It requires the gap assumption (i) on  $\mathbb{R}$  (that is  $\inf_{s \in \mathbb{R}} [h_2(s) - h_1(s)] > 0$ ) or equivalently a pure imaginary singularity  $Im \tilde{z} > 0$ .

The fact pointed out in [26] is that the essence of the result does not rely on the previous motivation. Thus the same job (i.e., to compute  $\|\tilde{n}_{p,1}(+\infty)\|$ ) is realized as follows. We consider any known, differentiable family of orthonormal vectors in  $\tilde{P}_i$  (let us denote it by  $n_i$ ). For the complex factor  $\tilde{f}$  in

$$\tilde{n}_{p,1}(z) = \tilde{f}(z)n_1(z)$$
 (16)

we obtain from (12) the differential equation

$$\tilde{f}'(z) = \langle n_1, n_1' \rangle \tilde{f}(z)$$

which is integrable along  $\gamma$ . The real axis can be used finally in order to obtain local results for  $|\tilde{f}(+\infty)|$  (and also for  $Im \int_{-\infty}^{+\infty} \tilde{h}_1(z') dz'$  in (11)) by shifting  $\gamma$  to  $\mathbb{R}$ . This allows one to cover the case when  $\tilde{z} \in \mathbb{R}$ .

We observe that in (10) we use the fact that U is univalent whereas here multi-valueness of  $U_p$  was important. We mention also another implication of  $\sigma(H(s)) \subset \mathbb{R}$  for  $s \in \mathbb{R}$  in the simplification of the geometric setting from the proof for the existence of a dissipative path (see [7, Appendix 2]).

Therefore in both approaches the dependence of  $|\mathbb{S}_{21}|$  on the local behavior of H(z) at z is obtained. But the point is that after replacing the Hilbert space geometry at  $z = +\infty$  used in order to obtain (15) by that one used along  $\gamma$  in (16) it is shown that for the problem of interest the representation of fundamental group mentioned before (13) is not essential and can be avoided.

A further improvement is to transpose the decomposition (11) in operator language and to use the tools of adiabatic reduction theory mentioned at the beginning. The assumptions and the results of complex WKB approach are recovered. But what is important that after replacing  $U_p(z, z_0)$  by  $U_{\varepsilon,A}(z, z_0)$  mentioned in (4), (5), (see the details below) the higher orders in  $\varepsilon$  are easy available.

Moreover, we mention the more general approach of the quasi-crossing case. Thus (see the 2-level situation) a single method for  $Im \tilde{z} = 0$  and  $Im \tilde{z} \neq 0$ 

cases, permits to describe small  $Im \tilde{z}$  ones by the next simple assumption on the Hamiltonian operator

$$H(z)H_0(z) + H_p(z) , (\mathbf{v})$$

where  $H_0$  has the eigenvalue crossing points on  $\mathbb{R}$  and  $H_p$  is a small perturbation (see the stronger condition on  $\sigma(H(z))$  imposed in [14] to avoid real crossing cases).

Let

$$\sup_{z \in \mathcal{S}_{\alpha}} |H_p(z)|| = \eta.$$

For an finite  $\eta$  example we mention [7, Section 2]. For such calculus we do not consider the terms which corresponds to the transition probability between  $\sigma_I$  and  $\sigma_{II}$ , by restricting (i) to

$$d^2 \gg \eta$$

or  $\sigma_I$  sufficiently isolated (see the precise result for k from (6) in [27, 32]). The physical interest for small values of  $\eta$  is given by the competition of the effects given by  $\varepsilon$  and  $\eta$ . Thus we obtain the asymptotic expansion also in  $\eta$ . A single result covers the limit cases mentioned above: Landau–Zener ( $\varepsilon \ll \eta$ ), Friedrichs Hagedorn ( $\eta = 0$ ) and the intermediate case ( $\eta \sim \varepsilon$ ). The case n = 2 with a single linear crossing was treated in [26]. We are interested in multilevel extensions to it (see also [19, 26] for the diagonal elements of the S-matrix in the non-degenerate case). We refer the reader to [14] for the Landau–Zener formula and to [10] for Friedrichs–Hagedorn result (see also [11] for an  $\eta = \eta(\varepsilon)$  situation).

In this article we restrict ourselves to a class (with respect to the topology of the eigenvalues crossings) of Hamiltonians for which the complex WKB-type method is directly applicable. The result was announced in [7]. It can be obtained also with the method of [20] (see [15]) but only for the non-degenerate case (in the framework of quantum scattering application from [7] this means only over barrier collision). In [8] we take advantage, among others ideas, from the previous mentioned improvements of the complex method and reconstruct the general argument of the reduction schema (2)–(5) in interdependence with the complex method. Via the point mentioned in (8) the construction is differentiated in subregions of  $S_{\alpha}$  solving a larger class of Hamiltonians.

#### 1. Multilevel adiabatic reduction method

Let  $\mathcal{D}$  be a simply connected domain in  $\mathcal{S}_{\alpha}$ , where the gap condition (i) holds. The projector from the next lemma verifies the Heisenberg equation up to exponentially small terms. The construction is achieved (see [33]) from a truncation of its formal asymptotic series into an  $\varepsilon$ -dependent order (the formal series becoming its proper asymptotic series).

**Lemma 1.1** (see [26, Lemma 3.3]. There exists the projector  $P_{\varepsilon}(z)$  such that

(i) at fixed z, in the sense of asymptotic series,

$$P_{\varepsilon}(z) = \sum_{j=0}^{\infty} E_j(z)\varepsilon^j \tag{17}$$

with

$$E_{0}(z) = P_{0}(z) = P_{I}(z) = \frac{1}{2\pi i} \oint_{\Gamma(z)} (\lambda - H(z))^{-1} d\lambda ,$$

$$E_{j}(z) = \frac{1}{2\pi} \oint_{\Gamma(z)} d\lambda (\lambda - H(z))^{-1} \left\{ Q_{0}(z) \left( \frac{d}{dz} E_{j-1}(z) \right) P_{0}(z) - P_{0}(z) \left( \frac{d}{dz} E_{j-1}(z) \right) Q_{0}(z) \right\} (\lambda - H(z))^{-1} + S_{j}(z) - 2P_{0}(z) S_{j}(z) P_{0}(z) , \quad (18)$$

where

$$Q_0(z) = 1 - P_0(z), \quad S_j(z) = \sum_{m=1}^{j-1} E_m(z) E_{j-m}(z)$$

(the path of integration is the contour  $\Gamma(z)$  surrounding  $\sigma_I(z)$  at finite distance by  $\sigma(z)$ );

(ii)  $P_{\varepsilon}$  checks the Heisenberg equation up to exponentially small errors:

$$\exists \varepsilon_0 > 0, \quad K < \infty, \quad k > 0, \quad \text{such that} \quad \forall z \in \mathcal{D}, \quad 0 < \varepsilon \le \varepsilon_0,$$

$$\|i\varepsilon \frac{d}{dz} P_{\varepsilon}(z) - [H(z), P_{\varepsilon}(z)]\| \le Kb(Re z) \exp\left(-\frac{k}{\varepsilon}\right) \tag{19}$$

(the function b is the decaying function from (iii)).

We note that  $E_i(z)$  before is the unique solution of

$$i\frac{d}{dz}E_j(z) = [H(z), E_{j+1}(z)],$$

$$E_j(z) = \sum_{m=0}^{j} E_m(z) E_{j-m}(z) ,$$

satisfying  $E_0(z) = P_0(z)$  or at the formal level series

$$\left(\sum_{j=0}^{\infty} E_j(z)\varepsilon^j\right) = \left(\sum_{j=0}^{\infty} E_j(z)\varepsilon^j\right)^2$$

and

$$i\varepsilon \frac{d}{dz} \left( \sum_{j=0}^{\infty} E_j(z) \varepsilon^j \right) = \left[ H(z), \sum_{j=0}^{\infty} E_j(z) \varepsilon^j \right].$$

An equivalent recurrence for this construction is given by

$$E_j(z) = \frac{1}{2\pi i} \int_{\Gamma(z)} q_j(z, \lambda) \, d\lambda \tag{19'}$$

with

$$q_{j}(z,\lambda) = -i(\lambda - H(z))^{-1} \frac{d}{dz} q_{j-1}(z,\lambda)$$
 and  $q_{0}(z,\lambda) = (\lambda - H(z))^{-1}$ 

(see [28, 40]).

We obtain  $E_j(z)$  analytic in D and  $P_{\varepsilon}(z) = P_{\varepsilon}^*(\bar{z})$  (in [7, Section 2] this self-adjointness is considered with respect to a different scalar product). As we mentioned all the theory is local in z (only finite order derivatives of the Hamiltonian are involved).

In the multilevel case we encounter the situation of more isolated bounded parts of the spectrum for which we want to make a similar construction. Thus, we consider the following gap assumption:

$$\sigma(H(z)) = \bigcup_{j=1}^{n} \sigma_{j}(z)$$
 with  $\min_{j \neq k} \inf_{z \in \mathcal{D}} \operatorname{dist}(\sigma_{j}(z), \sigma_{k}(z)) > 0$ 

(for an unbounded Hamiltonian we assume  $\sigma_j(z)$  to be uniformly bounded,  $j = \overline{1, n-1}$ ; apply the following lemma for  $P_{j,\varepsilon}$ ,  $j = \overline{1, n-1}$ , and take  $P_{n,\varepsilon} = I - \sum_{j=1}^{n-1} P_{j,\varepsilon}(z)$ ).

A construction for  $P_{j,\varepsilon}(z)$ ,  $j=1\ldots n$ , similar to the above is given by

**Theorem 1.** There exist the projectors  $P_{i,\varepsilon}(z)$  such that

(i) at fixed z, in the sense of asymptotic series

$$P_{j,\varepsilon}(z) = \sum_{i=0}^{\infty} E_{i,\sigma_j}(z) \varepsilon^i$$

with  $E_{i,\sigma_j}(z)$  supplied by Lemma 1.1 (or (19')) for  $\sigma_j(z)$ ;

(ii) ( $\exists$ )  $\varepsilon_0 > 0$ ,  $K < \infty$ , k > 0 such that ( $\forall$ ) $z \in \mathcal{D}$ ,  $0 < \varepsilon \le \varepsilon_0$ ,

$$||i\varepsilon \frac{d}{dz}P_{j,\varepsilon}(z) - [H(z), P_{j,\varepsilon}(z)]|| \le Kb(Re\,z)\exp\left(\frac{-k}{\varepsilon}\right);$$

(iii) 
$$P_{i,\varepsilon}(z)P_{j,\varepsilon}(z) = \delta_{i,j}P_{i,\varepsilon}(z);$$

(iv) 
$$\sum_{j=1}^{n} P_{j,\varepsilon}(z) = I.$$

Proof. In Lemma 1.1,  $P_{\varepsilon}(z)$  is constructed as a spectral projector (for the spectrum part which is near 1) of the operator ("almost" idempotent)  $T_{N_{\varepsilon}(z)}$  which is the truncation of the formal series (17) into the  $\varepsilon$  dependent order  $N_{\varepsilon} = \left[\frac{1}{c\varepsilon}\right]$  (with c constant)

$$T_{N_{\varepsilon}(z)} = \sum_{j=0}^{N_{\varepsilon}} E_j(z) \varepsilon^j$$
.

It verifies

$$||P_{\varepsilon}(z) - T_{N_{\varepsilon}(z)}|| \le Kb(Re\ z)e^{\frac{-k}{\varepsilon}}.$$
 (20)

Let  $\tilde{P}_{j,\varepsilon}(z)$  be the projectors given by this lemma for  $\sigma_j(z)$  making all the truncations in the same  $\varepsilon$ -dependent order supplied by

$$c = \sup_{i=\overline{1,n}} c_i$$

All the estimates remain valid with the same constants K and k in (20) (see [33]). Below we shall include generically in the same notation K all the multiplicative constants involved.

We have

$$\sum_{m=0}^{l} E_{m;\sigma_i} E_{l-m;\sigma_j} = 0 \quad for \quad i \neq j$$

(see [40]) which involves after estimates similar to those for (20) (see [33, Relations (2.50)-(2.52))]:

$$\|\tilde{P}_{i,\varepsilon}(z)\tilde{P}_{j,\varepsilon}(z)\| \le Kb(Re\,z)e^{\frac{-k}{2\varepsilon}} \quad for \quad i \ne j.$$
 (21)

Also,

$$\sum_{i=1}^{n} T_{N_{\varepsilon,\sigma_i}}(z) = T_{N_{\varepsilon,\sigma_1 \cup \sigma_2 \cup \dots \cup \sigma_n}}(z) = I$$

(the first equality from (19') and the second one from Lemma 1.1) implies

$$\|\sum_{i=1}^{n} \tilde{P}_{i,\varepsilon}(z) - I\| \le Kb(Re\ z)e^{\frac{-k}{\varepsilon}}.$$
 (22)

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Now from (21), (22), via a generalized Gram-Schmidt orthogonalization given in the following proposition, we obtain, after renoting k/2 by k, the required  $P_{i,\varepsilon}(z)$ .

For example, the Heisenberg equation up to the same errors is immediate using boundedness of H(z) and

$$\left\| \frac{d}{dz} (P_{i,\varepsilon}(z) - \tilde{P}_{i,\varepsilon}(z)) \right\| \le K b(Re \ z) e^{\frac{-k}{\varepsilon}}$$
.

Indeed, from the analyticity of  $P_{i,\varepsilon}(z) - \tilde{P}_{i,\varepsilon}(z)$  in  $\mathcal{D}$  we get

$$\frac{d}{dz}(P_{i,\varepsilon} - \tilde{P}_{i,\varepsilon})(z) = -\frac{1}{2\pi i} \int_{|z-u|=\gamma} \frac{(P_{i,\varepsilon} - \tilde{P}_{i,\varepsilon})(u)}{(u-z)^2} du,$$

which implies (eventually in a smaller domain) the previous estimate.

For  $\delta := b(\operatorname{Re} z)e^{\frac{-k}{\varepsilon}}$ , we have the independent result:

**Proposition 1.2.** Let  $\delta > 0$  and  $\tilde{P}_{i,\delta}$ ,  $i = \overline{1, n}$ , be uniformly bounded projectors such that  $(\forall)\delta$  with  $0 < \delta < \tilde{\delta}$ :

$$\|\sum_{i=1}^n \tilde{P}_{i,\delta} - I\| \le \delta \quad and \quad \|\tilde{P}_{i,\delta}\tilde{P}_{j,\delta}\| \le \delta \quad (i \ne j).$$

Then  $(\exists) \delta_0 > 0$ , the projectors  $P_{i,\delta}$ ,  $i = \overline{1,n}$ , and a constant  $\tilde{K}$  such that  $(\forall) \delta$  with  $0 < \delta < \delta_0$ 

$$||P_{i,\delta} - \tilde{P}_{i,\delta}|| \le \tilde{K} \cdot \delta$$
 and  $\sum_{i=1}^{n} P_{i,\delta} = I, P_{i,\delta} P_{j,\delta} = \delta_{i,j} P_i$ .

Proof: Let us omit  $\delta$  in projector indices. We use the notation  $\tilde{K}$  generically for all constants involved. (In the previous theorem context all the estimates are uniform for  $z \in \mathcal{D}$ .) By the expression "for  $\delta$  small enough" we mean " $(\exists)\delta_0 > 0$  such that for any  $\delta$  with  $0 < \delta \leq \delta_0$ ".

We proceed by induction in n. The case n=2 is obvious by setting  $P_1 = \tilde{P}_1$  and  $P_2 = I - P_1$ .

For the general case we first orthogonalise  $\tilde{P}_1$  and  $\tilde{P}_2$ . The family of bounded operators  $T_{\delta} = (1 - \tilde{P}_2)\tilde{P}_1(1 - \tilde{P}_2)$  check  $\tilde{P}_2T_{\delta} = T_{\delta}\tilde{P}_2 = 0$  and  $||T_{\delta}^2 - T_{\delta}|| \leq \tilde{K}\delta$  for  $\delta$  small enough. On a contour that contains only the spectrum part of  $T_{\delta}$  which is near 1 we obtain the projector

$$\tilde{\tilde{P}} = \frac{1}{2\pi i} \int_{|z-1|=const} \frac{1}{z - T_{\delta}} dz \quad \text{with} \quad ||\tilde{\tilde{P}}_1 - \tilde{P}_1|| \le \tilde{K}\delta$$

(see, for example, [33, Proposition 3]). Also,  $\tilde{P}_2\tilde{\tilde{P}}_1=\tilde{\tilde{P}}_1\tilde{P}_2=0$  (because obviously  $\tilde{P}_2\frac{1}{z-T_\delta}=\frac{1}{z-T_\delta}\tilde{P}_2=\frac{\tilde{P}_2}{z}$ ). Therefore  $\tilde{P}_\delta=\tilde{\tilde{P}}_1+\tilde{P}_2$  is a projector.

Now from the induction assumption  $(\exists)P_{\delta}, P_{3}, \ldots, P_{n}$  associated to  $\tilde{P}_{\delta}, \tilde{P}_{3}, \ldots, \tilde{P}_{n}$  verifying the conditions of Proposition. For  $\delta$  small enough,  $||P_{\delta} - \tilde{P}_{\delta}|| < 1$ . Let  $M_{\delta}$  the Sz-Nagy transformation (see [22]) matrix corresponding to the pair  $\tilde{P}_{\delta}, P_{\delta}$ :

$$M_{\delta} = [I - (P_{\delta} - \tilde{P}_{\delta})^{2}]^{-1/2} [P_{\delta}\tilde{P}_{\delta} + (I - P_{\delta})(I - \tilde{P}_{\delta})], \qquad (23)$$

where  $(I-\mathcal{T})^{-1/2} = I + \sum_{k=1}^{\infty} \frac{(2k-1)!!}{k!2^k} T^k$ . It has the bounded inverse

$$M_{\delta}^{-1} = [\tilde{P}_{\delta}P_{\delta} + (I - \tilde{P}_{\delta})(I - P_{\delta})][I - (P_{\delta} - \tilde{P}_{\delta})^2]^{-1/2}$$

and verifies  $P_{\delta} = M_{\delta} \tilde{P}_{\delta} M_{\delta}^{-1}$ . Since for  $\delta$  small enough  $||M - I|| \leq \tilde{K} \cdot \delta$ ,  $||M^{-1} - I|| \leq \tilde{K} \cdot \delta$ , we finish the proof by setting

$$P_1 = M\tilde{\tilde{P}}_1 M^{-1}$$
 and  $P_2 = M\tilde{P}_2 M^{-1}$ .

Now we extend the Krein-Kato parallel transport from [33] to the many-level context by simple adaptation of one step from the recurrent construction of [31]:

#### Lemma 1.3. If

$$i\varepsilon \frac{d}{dz}U_A(z,z_0) = (H(z) - B_{\varepsilon}(z))U_A(z,z_0); \quad U_A(z,z_0) = I$$
 (24)

with

$$B_{\varepsilon}(z) = \sum_{j=1}^{n} P_{j,\varepsilon}(z) \left\{ i\varepsilon \frac{d}{dz} P_{j,\varepsilon}(z) - [H(z), P_{j,\varepsilon}(z)] \right\}$$

(exponentially small), then

$$P_{j,\varepsilon}(z) = U_A(z, z_0) P_{j,\varepsilon}(z_0) U_A^{-1}(z, z_0)$$

(exact intertwining).

We emphasize the before idea to looking for the asymptotic expansion of  $P_{\varepsilon}(z)$  in the  $\varepsilon$ -factorised form (17) and to construct the intertwining superadiabatic evolution  $U_A(z,z_0)$  independently. In the previous variants of the Adiabatic Reduction method [34] the utilization of  $U_A(z,z_0)$  directly in the  $P_{\varepsilon}$  construction brought inessential technicalities in the estimations from (19) (see [18] for such exponentially small results).

As long as  $U_{\varepsilon,A}(z,z_0)$  is close to  $U_{\varepsilon}(z,z_0)$ , we can obtain informations about S, using the superadiabatic evolution. The proof of (5) passes through the Gronwall

lemma-type argument (see [39]) and therefore uses the integration of the differential equation (24) along a path which we take (as we stated in introduction) in the complex plane. This proof is not straightforward because of the estimates of type  $||U_{\varepsilon}(z, z_0)||$  (a non-unitary operator for complex arguments) which presents difficulties similar to those of the method WKB complex.

Results of type adiabatic theorem

$$||P_{\sigma_{II}}(+\infty)\mathbb{S}P_{\sigma_I}(-\infty)|| = 0 + \mathcal{O}(Ke^{-\frac{k}{\varepsilon}})$$

are immediate (we replace  $U_{\varepsilon,A}(s,s_0)$  with  $U(s,s_0)$  along real axis when the evolution operators are unitary, and we also use  $\|P_{\varepsilon}(z) - P_0(z)\| \leq b(\operatorname{Re} z)\varepsilon$  as below). An explicit calculus of  $P_{\varepsilon}(\infty) \mathbb{S} P_{\varepsilon}(-\infty)$  can be realized when  $\operatorname{Ran} P_{\varepsilon}(z) = 1$  (by explicit integration of  $U_{\varepsilon,A}$  along the complex path of evolution).

For the general theory of adiabatic reduction (the construction of  $P_{\varepsilon}$  and  $U_{\varepsilon,A}$ ) we mention following [32], a few other topics which are contributed to clarify this problem. The general scheme can be viewed as an extension of a standard tool of the analytic theory of perturbations [22] to the time dependent case. It includes in a unitary approach ([31], in [3]) topics from the adiabatic theorem of quantum mechanics [29] and of the theory of spectral concentration [30], to the theory of adiabatic invariants for linear Hamiltonian system [4, 41] and the theory of simplifications and diagonalization of differential evolution equations [23].

#### 2. The complex WKB-type method

The reduced S-matrix  $P_{\sigma_I}(+\infty) \mathbb{S} P_{\sigma_I}(-\infty)$  is equal (up to exponentially small terms) with the S-matrix of another effective evolution operator acting in the n-dimensional space (fixed for instance to origin)  $Ran\ P_{\sigma_I}(0)$ . We refer the reader to [18, 26, 8] for details. In a few words, for this construction we first consider the iterative scheme from [33] in order to associate  $P_{\sigma_I,\varepsilon}(x)$  to  $P_{\sigma_I}(x)$  (Lemma 1.1) which are intertwined by the generalized parallel transport Krein-Kato (Lemma 1.3 for n=2)  $U_A(x,x_0)$  (exponentially close by the real evolution). We denote x the real variables to include time-independent situations. As for  $\varepsilon$  small enough  $\|P_{\sigma_I,\varepsilon}(x)-P_{\sigma_I}(x)\|<1$  the Sz-Nagy matrix (23) associated to them  $M_{\sigma_I,\varepsilon}$  is well defined, checking

$$P_{\sigma_I,\varepsilon}(x) = M_{\sigma_I,\varepsilon}(x) P_{\sigma_I}(x) M_{\sigma_I,\varepsilon}^{-1}(x) .$$

Finally, if  $A(x, x_0)$  is the parallel transport of  $P_{\sigma_I}(x)$ ,

$$i\frac{d}{dx}A(x,x_0) = i[\dot{P}_{\sigma_I}(x), P_{\sigma_I}(x)]A(x,x_0)$$

with

$$P_{\sigma_I}(x) = A(x, x_0) P_{\sigma_I}(x_0) A(x_0, x) ,$$

the desired effective evolution is given by

$$U_{\varepsilon,A}(x,x_0) = A(0,x)M_{\sigma_I,\varepsilon}^{-1}(x)U_A(x,x_0)M_{\sigma_I,\varepsilon}(x_0)A(x_0,0)$$
.

Its evolution equation

$$i\varepsilon \frac{d}{dx}U_{\varepsilon,A}(x,x_0) = H_{\varepsilon,A}(x)U_{\varepsilon,A}(x,x_0)$$

has the Hamiltonian

$$H_{\varepsilon,A}(x) = A(0,x)M_{\sigma_I,\varepsilon}^{-1}(x)(H(x) - B_{\varepsilon}(x))M_{\sigma_I,\varepsilon}(x)A_{1,2}(x,0)$$

$$-i\varepsilon A(0,x)[\dot{P}_{\sigma_I}(x)P_{\sigma_I}(x)]A(x,0) + i\varepsilon A(0,x)\frac{d}{dx}M_{\sigma_I,\varepsilon}^{-1}(x)M_{\sigma_I,\varepsilon}(x)A(x,0).$$

Therefore we can suppose  $\sigma_{II} = \emptyset$  (or  $\dim \mathcal{H} = n$ ) because if not, using the "change of representation" (given by  $M_{\sigma_{I},\varepsilon}(x)A(x,0)$ ), we reduce the problem to  $\operatorname{Ran} P_{\sigma_{I}}(0)$ . The only difference is the  $\varepsilon$ -dependence of  $H_{p}$ , but its expansion in  $\varepsilon$  has no contribution in the orders calculated. Also for  $\varepsilon$  small enough this dependence does not change the topology of eigenvalue crossings (see [8]).

We specify the following notations. We denote by  $h_{0,i}(z)$ ,  $i = \overline{1, n}$ , the eigenvalues of  $H_0(z)$  in  $\sigma_{I,0}(z)$ , and we take  $\alpha$  small enough so that

$$\mathbb{R} \supset \{ z \in \mathbb{C} | h_{0,i}(z) = h_{0,j}(z), \quad i \neq j \}.$$
 (25)

We consider (5') also for  $H_0(z)$ , in addition to (iii) we claim

$$\sup_{z \in \mathcal{S}_{\alpha}} |Re \, z|^{1+\beta} ||H_p(z)|| < \infty ,$$

and we assume that

$$H_0(z)$$
 and  $H_p(z)$  are analytic in  $\mathcal{S}_{\alpha}$  for some  $\alpha > 0$ . (vi)

The analytic continuation of  $h_{0,i}(z)$  (their analyticity is obtained (under 25) from the Rellich theorem [37]) and the perturbation theory in  $H_p$ , give a consistent identification for  $h_{0,i}(z)$  and  $h_i(\pm\infty) := h_i^{l,r}$  (and thus for the S-matrix element  $\mathbb{S}_{i,j}$ ). To simplify the notations we shall use the same name (and notation) for the S-matrix elements as complex numbers given by the scalar product  $\mathbb{S}_{i,j} = \langle n_i(\infty), \mathbb{S} n_j(-\infty) \rangle$  between the normalized eigenvectors  $n_i(\pm\infty) = P_i(\pm\infty) n_i(\pm\infty)$  (see below a canonical choice of them) and the operator  $\mathbb{S}_{i,j} = P_i(\infty) \mathbb{S} P_i(-\infty)$ :

$$P_i(\infty) \mathbb{S} P_j(-\infty) n_j(-\infty) = \mathbb{S}_{i,j} n_i(\infty), \quad ||P_i(\infty) \mathbb{S} P_j(-\infty)|| = |\mathbb{S}_{i,j}|.$$

We resume the above assertions on the complex extension. In the proof that  $U_{\varepsilon,A}(z,z_0)$  is close to  $U_{\varepsilon}(z,z_0)$  (see (34)), we choose the mentioned integration path in the complex plane in order to avoid the crossing points on  $\mathbb R$  and therefore to recover the gap condition necessary for  $U_{\varepsilon,A}$  construction. The Hamiltonian H(z) (and therefore  $U_{\varepsilon}(z,z_0)$ ) is an univalent analytic operator in  $\mathcal{S}_{\alpha}$  while its spectral decomposition  $(h_i(z), i = \overline{1,n}, \sigma_{II}(z))$  and the corresponding eigenprojectors) are global multivalent analytic functions with branch points at the crossing points  $\{z \in \mathbb{C} | h_i(z) = h_j(z) \}$  for some  $i \neq j$ . This Riemann surface behavior determines the exponentially small results obtained for  $|\mathbb{S}_{i,j}|$ . Moreover, it permits to compute by the same method different elements of the  $\mathbb{S}$ -matrix (7) (let define them on the real axis for  $\eta = 0$  – see the remark after (vi)). For this we simply consider (topological) different dissipative path with respect to the branch points contained in the domain delimited by the path and the real axis.

The important technical point in the complex extension is that for the proof of (34) (see the discussion after Lemma 1.3) we can do estimations of type  $||U_{\varepsilon}(z,z_0)||$  (which otherwise blow-up in the limit  $\varepsilon \to 0$ ) if we restrict the evolution operators to the subspace corresponding to the least dissipative eigenvalue  $(h_1 \text{ in } (30), (31))$ . Thus (5) and hence adiabatic theorem – like results still hold true for non-self-adjoint Hamiltonians (see [34]). The existence of a complex path which verifies the technical requirement of dissipativity (characteristic for the complex WKB method) makes the method sensible to the behavior of Stokes lines (see [7, Appendix 2]). It impose constraints concerning the topology of the eigenvalues crossings and restrict the results only for linear crossing points. A straightforward approach along the Stokes lines ([16]) can supply results for higher order degeneracies but for example, the quasi-crossing case from below is not available.

The main condition, which we claim for the eigenvalue crossings, is

$$(\forall) r, \quad s = \overline{1,n} \quad \operatorname{card}\{x \in \mathbb{R} | h_{0,r}(x) = h_{0,s}(x)\} < 2 \,. \tag{cond 1}$$

We calculate the probability of "transition" after a crossing point from the S-matrix unitarity. A consequence is that we obtained only its module. A violation of (cond 1) would involve an interference of two such transition probabilities with the same order, hence the knowledge of their phases. It would generate the so called Stuckelberg oscillations (see [19] for less explicit results).

In this article we restrict ourselves to a first situation where the complex method gives directly any order of the S-matrix element (including the phase). We calculate  $S_{ii}$ , when all the crossings of  $h_i(x)$  with other eigenvalues are with positive slope (or all with negative slope):

$$\operatorname{sign}(h'_j(c) - h'_i(c)) = \operatorname{const}(\forall) c \in \mathbb{R} \text{ with } h_j(c) = h_i(c), \text{ for some } j \in \overline{1, n}, j \neq i.$$
(cond 2)

For the existence of the dissipative path in this case we extend the proof from ([7, Appendix 2; 14, 20] (if we consider  $\eta$  small enough) and we mention [7, Appendix 1] (for a finite  $\eta$ -example).

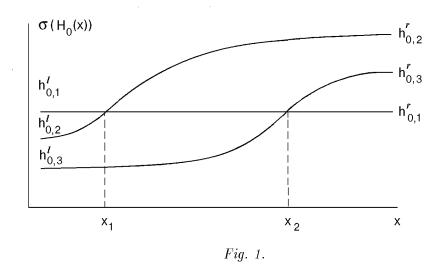
We illustrate the method in the following two cases: I – for several double eigenvalues crossing points and II – for one multiple crossing. Identical proofs are applicable to all their combinations according to (cond 2). Consider n=3 and  $h_1^l > h_2^l > h_3^l$ .

**Case I.** Let  $h_2^r > h_3^r > h_1^r$  and  $h_{0,2}(x) \neq h_{0,3}(x)$  for  $x \in \mathbb{R}$ . We assume that  $h_{0,1}(x)$  and  $h_{0,2}(x)$  (respectively  $h_{0,1}(x)$  and  $h_{0,3}(x)$ ) have a linear crossing at  $x_1$  (respectively  $x_2 > x_1$ ):

$$h'_{0,2}(x_1) - h'_{0,1}(x_1) = a > 0$$
,

$$h'_{0,3}(x_2) - h'_{0,1}(x_2) = b > 0$$
.

(See Fig. 1).



We calculate  $\mathbb{S}_{11}$ .

There exist the constants  $\varepsilon_0 > 0$ ,  $\eta_0 > 0$  such that for  $0 < \varepsilon \le \varepsilon_0$ ,  $0 \le \eta \le \eta_0$ ,

$$|\mathbb{S}_{11}|^2 = \exp\left\{-\frac{2\pi}{\varepsilon} \left[ \frac{1}{a} |H_{p,12}^{x_1} - i\varepsilon d_{12}^{x_1}|^2 + \frac{1}{b} |H_{p,13}^{x_2} - i\varepsilon d_{13}^{x_2}|^2 + o((\varepsilon + \eta)^3) \right] \right\} (25')$$

with the notations

$$H_{p,12}^{x_1} = \langle n_{0,1}(x_1), H_p(x_1) n_{0,2}(x_1) \rangle, \qquad (26)$$

$$H_{p,13}^{x_2} = \langle n_{0,1}(x_2), H_p(x_2) n_{0,3}(x_2) \rangle, \qquad (27)$$

$$d_{p,12}^{x_1} = \langle n_{0,1}(x), \frac{d}{dx} n_{0,2}(x) \rangle|_{x=x_1}, \qquad (28)$$

$$d_{p,13}^{x_2} = \langle n_{0,1}(x), \frac{d}{dx} n_{0,3}(x) \rangle|_{x=x_2}$$
(29)

(we send to (38), (39) for the choice of the eigenvectors). The value of  $\arg \mathbb{S}_{11}$  is given by (47). The previous expression contains as limit cases generalizations of the Landau–Zener formula and of the Friedrichs–Hagedorn result (see (48)–(50)).

Case II. We consider  $h_3^r > h_2^r > h_1^r$  and that all the three eigenvalues of  $H_0$  have a linear crossing at the origin with the slopes

$$h'_{0,2}(0) - h'_{0,1}(0) = \alpha > 0$$
 and  $h'_{0,3}(0) - h'_{0,2}(0) = \beta > 0$ .

(See Fig. 2).

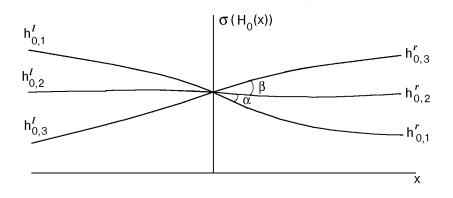


Fig. 2.

We calculate  $S_{33}$  (the only other matrix element given by the method is  $S_{11}$ ). There exist constants  $\varepsilon_0 > 0$ ,  $\eta_0 > 0$  such that for  $0 < \varepsilon \le \varepsilon_0$ ,  $0 \le \eta \le \eta_0$ ,

$$|\mathbb{S}_{33}|^2 = \exp\left\{-\frac{2\pi}{\varepsilon} \left[\frac{1}{\beta} |H_{p,32} - i\varepsilon d_{32}|^2 + \frac{1}{\alpha+\beta} |H_{p,31} - i\varepsilon d_{31}|^2 + o((\varepsilon+\eta)^3)\right]\right\}.$$

The argument  $arg \, \mathbb{S}_{33}$  is obtained from (47) if we replace 1 with 3. For  $|\mathbb{S}_{11}|^2$  we have a similar expression (see (51)) with the same argument as in Case I. The generalized Landau–Zener formula, Friedrichs–Hagedorn result, and the crossover regime are similar to Case I.

Adiabatic reduction along a complex path. Because all these cases violate (i) on  $\mathbb{R}$ , the step constrained to integrate a differential equation (the proof of (34)) is removed on a complex path in  $S_{\alpha}$ . As we noticed, because H(z)

is not self-adjoint the estimates involved in this lemma and therefore (5) are still true, if we restrict the evolution operator to one eigensubspace for which the path satisfies the global condition of dissipativity.

For the previous evolution along a complex path  $\gamma$ , if we denote by

$$\Delta_{z_0}^1(z) := \int_{z_0}^z (h_1(u) - h_2(u)) \, du \,, \tag{30}$$

$$\Delta_{z_0}^2(z) := \int_{z_0}^z (h_1(u) - h_3(u)) \, du \,, \tag{31}$$

then the path  $\gamma$  is said to be dissipative for  $h_1(z)$  if

$$\operatorname{Im} \Delta^1_{z_0}(z) \quad \text{and} \quad \operatorname{Im} \Delta^2_{z_0}(z) \quad \text{are non---decreasing along} \quad \gamma \,. \tag{32}$$

In the applications (see [34]) with non-unitary evolution operators on the real axis (32) becomes  $(\forall)u \in \mathbb{R}$ ,  $Im\ h_1(u) \geq Im\ h_i(u)$ ,  $i=\overline{2,n}$  (the real and superadiabatical evolutions are close in the subspace corresponding to the eigenvalue with the largest imaginary part – the least dissipative). In the proof of the existence in our situation of such a path between  $\pm\infty$  (see [7, Appendix 2]) other implicit requirements for the path are a bound for  $\sup_{x\in\mathbb{R}}|\frac{d\gamma(x)}{dx}|$  and that it does not "pendulate" too much at the ends of the strip such that the integrals involved along the path to be convergent.

The problem along the complex path can be removed (see [26]) on the real axis. Let  $z(x) = x + i\gamma(x)$  be the dissipative path. We consider the evolution operators

$$U_{\gamma}(x,x_0) = \exp\left(\frac{i}{\varepsilon} \int_{x_0}^x h_1(z(u)) \left(1 + i \frac{d\gamma(u)}{du}\right) du\right) U(z(x), z_0(x_0))$$

(its generator  $H_{\gamma}(x)$  has the eigenvalues

$$h_{\gamma,1}(x) = 0$$
,  $h_{\gamma,j}(x) = (h_j(z(x)) - h_1(z(x))) \left(1 + i\frac{d\gamma(x)}{dx}\right)$ ,  $j = 2, 3$ ,

and

$$U_{\gamma,A}(x,x_0) = \exp\left(\frac{i}{\varepsilon} \int_{x_0}^x h_1(z(u)) \left(1 + i \frac{d\gamma(u)}{du}\right) du\right) U_A(z(x), z_0(x_0))$$

(we denote its evolution Hamiltonian by  $H_{\gamma}(x) - B_{\gamma,\varepsilon}(x)$ ). Let  $P_{\gamma,\varepsilon}(x) := P_{1,\varepsilon}(z(x))$ .

Defining  $\Omega_{\gamma}(x,x_0)$  by  $U_{\gamma}(x,x_0)=U_{\gamma,A}(x,x_0)\Omega_{\gamma}(x,x_0)$  with the integral equation

$$\Omega_{\gamma}(x, x_0) = I + i\varepsilon^{-1} \int_{x_0}^x U_{\gamma, A}^{-1}(u, x_0) B_{\gamma, \varepsilon}(x) U_{\gamma, A}(u, x_0) \Omega_{\gamma}(u, x_0) du$$
 (33)

for the next restriction to  $P_{\gamma,\varepsilon}(x_0)$  (see the intertwining property of  $U_{\gamma,A}(x,x_0)$ ):

$$P_{\gamma,\varepsilon}(x)U_{\gamma}(x,x_0)P_{\gamma,\varepsilon}(x_0) = P_{\gamma,\varepsilon}(x)U_{\gamma,A}(x,x_0)P_{\gamma,\varepsilon}(x_0)$$
$$\times [I + P_{\gamma,\varepsilon}(x_0)(\Omega_{\gamma}(x,x_0) - I)P_{\gamma,\varepsilon}(x_0)],$$

we have

**Lemma 2.1.** If  $\gamma$  is a dissipative path for  $h_1(z)$ , then for  $z, z_0 \in \gamma$ 

$$P_{1,\varepsilon}(z)U(z,z_0)P_{1,\varepsilon}(z_0) = P_{1,\varepsilon}(z)U_A(z,z_0)P_{1,\varepsilon}(z_0)(I+R(z,z_0;\varepsilon))$$
(34)

with  $||R(z, z_0; \varepsilon)|| \le K \exp(-\frac{k}{\varepsilon})$  for some  $K < \infty$ , k > 0 independent of  $z, z_0 \in \gamma$  (see [26, Lemma 5.1.] and also [34] for errors of order  $\varepsilon^k$ ).

In order to obtain the estimation of  $||R(z, z_0; \varepsilon)||$  (a Gronwall lemma-type estimate in (33)) they are used

$$||U_{\gamma,A}(x,x_0)P_{j,\varepsilon}(x_0)|| \le C|\exp(-i\Phi_{\gamma,j}(x,x_0;\varepsilon))|,$$
(35)

$$||P_{j,\varepsilon}(x_0)U_{\gamma,A}^{-1}(x,x_0)|| \le C|\exp(i\Phi_{\gamma,j}(x,x_0;\varepsilon))|,$$
 (36)

 $j = \overline{1,3}$  (see the intertwining property of  $U_A$  from Lemma 1.3), where

$$\Phi_{\gamma,j}(x,x_0;\varepsilon) = \frac{1}{\varepsilon} \int_{x_0}^x h_{\gamma,j}(u) \ du + o(1)$$

(see (45)).

This motivates the restriction to  $Ran P_{\gamma,\varepsilon}$  in (34) and involves the result by applying in the Gronwall lemma the estimations

$$||U_{\gamma,A}(x,x_0)|| \le const < \infty, \ x > x_0, \ \text{and} \ ||P_{\gamma,\varepsilon}(x_0)U_{\gamma,A}^{-1}(x,x_0)|| \le const.$$
(37)

Similarly [26], we consider the following families of analytic vectors:

• Eigenvectors of  $H_0(z)$ 

$$H_0(z)n_{0,j}(z) = h_{0,j}(z)n_{0,j}(z), \quad j = \overline{1,n},$$
 (38)

orthonormed on the real axis  $\langle n_{0,j}(x), n_{0,k}(x) \rangle = \delta_{j,k}, x \in \mathbb{R}$ , which are constructed for instance by parallel transport such that it avoids the eigenvalue crossing points (singularities of (12)).

•Eigenvectors of 
$$H_0^*(z)$$
 
$$m_{0,j}(z) = n_{0,j}(\bar{z})$$
 (39)

which are orthogonal to  $n_{0,j}(z)$  (see the analyticity of  $\overline{n_{0,j}(\bar{z})}$  and therefore of  $\langle m_{0,j}(z), n_{0,j}(z) \rangle$ ).

•Orthonormed eigenvectors of H(z)

$$n_j(z) = P_j(z)n_j(z)$$
 and  $m_j(z) = P_j^*(z)m_j(z)$ 

by simple projection and normalization of  $n_{0,j}(z)$  respective  $m_{0,j}(z)$  (for  $\eta$  small enough). Also we consider for  $\varepsilon$  small enough the projections

$$n_{i,\varepsilon}(z) = P_{i,\varepsilon}(z) n_i(z), \quad m_{i,\varepsilon}(z) = n_{i,\varepsilon}(\bar{z}), \quad j = \overline{1,3}.$$

In the both previous Cases I, II we have for the S-matrix elements:

$$\mathbb{S}_{11} = \langle n_1(\infty), \mathbb{S}n_1(-\infty) \rangle; \qquad \mathbb{S}_{11}n_1(-\infty) = P_{0,1}(\infty)\mathbb{S}P_{0,1}(-\infty)n_1(-\infty) =$$

$$= \lim_{\substack{\text{Re}z \to \infty \\ \text{Re}z_0 \to -\infty}} \exp\left(\frac{i}{\varepsilon}(h_{1,r}z - h_{1,l}z_0)\right) P_{0,1}(z)U(z,z_0)P_{0,1}(-\infty)n_{0,1}(-\infty)$$

$$= \lim_{\substack{\text{Re}z_0 \to -\infty \\ \text{Re}z \to \infty}} \exp\left(\frac{i}{\varepsilon}(h_{1,r}z - h_{1,l}z_0)\right) P_{1,\varepsilon}(z)U_A(z,z_0)P_{1,\varepsilon}(z_0)(\mathbb{I} + o(e^{-\frac{k}{\varepsilon}}))n_{1,\varepsilon}(-\infty).$$

$$(40)$$

In order to integrate this expression as well as to prove the estimates from (37) we obtain the explicit expression for  $U_A(z, z_0)$ .

By the intertwining property

$$P_{j,\varepsilon}(z) = U_A(z, z_0) P_{j,\varepsilon}(z_0) U_A^{-1}(z, z_0)$$

we have in the case  $Rank P_{i,\varepsilon}(z) = 1$  that

$$U_A(z, z_0) n_{i,\varepsilon}(z_0) = \lambda_i(z, z_0; \varepsilon) n_{i,\varepsilon}(z)$$
.

We consider only j = 1 ( $\lambda_j := \lambda$ ), the other ones used only in (37) being similar. Differentiate (see (24)) and take the scalar product with  $m_{1,\varepsilon}(z)$  to get (see [26]):

$$i\varepsilon \frac{d}{dz} \lambda_{j}(z, z_{0}; \varepsilon)$$

$$= \left(\frac{\langle m_{1,\varepsilon}(z), (H(z) - B_{\varepsilon}(z)) n_{1,\varepsilon}(z) \rangle}{\langle m_{1,\varepsilon}(z) n_{1,\varepsilon}(z) \rangle} - i\varepsilon \frac{\langle m_{1,\varepsilon}(z), \frac{d}{dz} n_{1,\varepsilon}(z) \rangle}{\langle m_{1,\varepsilon}(z) n_{1,\varepsilon}(z) \rangle}\right) \lambda_{j}(z, z_{0}; \varepsilon),$$

which involves

$$U_A(z, z_0) n_{1,\varepsilon}(z_0) = \exp\left(-i\Phi(z, z_0; \varepsilon) + o(e^{-\frac{k}{\varepsilon}})\right) n_{1,\varepsilon}(z)$$
(41)

with

$$\Phi(z, z_0; \varepsilon) = \varepsilon^{-1} \int_{z_0}^{z} \frac{\langle m_{1,\varepsilon}(u), H(u) n_{1,\varepsilon}(u) \rangle}{\langle m_{1,\varepsilon}(u) n_{1,\varepsilon}(u) \rangle} du - i \int_{z_0}^{z} \frac{\langle m_{1,\varepsilon}(u), \frac{d}{du} n_{1,\varepsilon}(u) \rangle}{\langle m_{1,\varepsilon}(u) n_{1,\varepsilon}(u) \rangle} du.$$
(42)

Now, along  $\gamma$ , by adiabatic perturbation theory with respect to  $\varepsilon$  and the usual perturbation theory with respect to  $H_p$ , we obtain the asymptotic expansion in  $\varepsilon$  and  $\eta$  of  $\Phi(z, z_0; \varepsilon)$  and the control of the remainder. We consider the low order contributions:

$$\Phi(z, z_0; \varepsilon) = \int_{z_0}^{z} \left\{ \varepsilon^{-1} h_1(u) \, du - i \langle m_1(u), \frac{d}{du} n_1(u) \rangle \right\}$$

$$-\varepsilon \langle m_1(u), P_1(u)E_1(u)(H(u) - h_1(u))E_1(u)P_1(u)n_1(u)\rangle \} du + o(\varepsilon^2).$$

From (18), by residue theorem, we have

$$E_1 = \frac{i}{h_2 - h_1} \left\{ P_2 P_1^{(1)} P_1 - P_1 P_1^{(1)} P_2 \right\} + \frac{i}{h_3 - h_1} \left\{ P_3 P_1^{(1)} P_1 - P_1 P_1^{(1)} P_3 \right\}.$$

We replace this relation,  $(P_1n_1)^{(1)}=n_1^{(1)}=P_1^{(1)}n_1+P_1n_1^{(1)}$  and the similar one for  $P_1^*m_1$  into the expression of  $\Phi(z,z_0;\varepsilon)$  and obtain

$$\Phi(z, z_0; \varepsilon) = \int_{z_0}^{z} \left\{ \varepsilon^{-1} h_1(u) - i \langle m_1(u), \frac{d}{du}(u) \rangle \right\}$$

$$-\varepsilon \left\langle \frac{d}{du} m_1(u), \left( \frac{P_2(u)}{h_2(u) - h_1(u)} + \frac{P_3(u)}{h_3(u) - h_1(u)} \right) \frac{d}{du} n_1(u) \right\rangle \right\} du + o(\varepsilon^2)$$
 (43)

with  $o(\varepsilon^2)$  uniform in z,  $z_0$  on the path of integration  $(z, z_0 \in \gamma)$ . The last assertion takes into account that  $E_m(z)$ ,  $m \ge 1$ , and  $R(z, z_0; \varepsilon)$  as well as their derivatives are O(b(Re z)).

Now, by standard perturbation theory (see, e.g., [5]), we have

$$h_{1} = h_{0,1} + \langle m_{0,1}, H_{p} n_{0,1} \rangle - \frac{1}{h_{0,2} - h_{0,1}} \langle m_{0,1}, H_{p} n_{0,2} \rangle \langle m_{0,2}, H_{p} n_{0,1} \rangle$$
$$- \frac{1}{h_{0,3} - h_{0,1}} \langle m_{0,1}, H_{p} n_{0,3} \rangle \langle m_{0,3}, H_{p} n_{0,1} \rangle + o(\eta^{3})$$
(44)

and

$$P_1 = P_{0,1} - \frac{1}{h_{0,2} - h_{0,1}} (P_{0,2}H_p P_{0,1} + P_{0,1}H_p P_{0,2})$$

$$-\frac{1}{h_{0,3}-h_{0,1}}(P_{0,3}H_pP_{0,1}+P_{0,1}H_pP_{0,3})+o(\eta^2).$$

As we claimed before, we expand the r.h.s. terms of (43) also in  $\eta$ . The insertion of the previous relation into (43) (note that  $\langle m_{0,j}; P_j(z) n_{0,j}(z) \rangle = 1 + o(\eta^2)$ ) gives for the second term

$$\langle m_1, n_1^{(1)} \rangle$$

$$= \langle m_{0,1}, n_{0,1}^{(1)} \rangle - \frac{1}{h_{0,2} - h_{0,1}} \left[ \langle m_{0,2}, H_p n_{0,1} \rangle \langle m_{0,1}, n_{0,2}^{(1)} \rangle + \langle m_{0,1}, H_p n_{0,2} \rangle \langle m_{0,2}, n_{0,1}^{(1)} \rangle \right]$$

$$- \frac{1}{h_{0,3} - h_{0,1}} \left[ \langle m_{0,3}, H_p n_{0,1} \rangle \langle m_{0,1}, n_{0,3}^{(1)} \rangle + \langle m_{0,1}, H_p n_{0,3} \rangle \langle m_{0,3}, n_{0,1}^{(1)} \rangle \right] + o(\eta^2) ,$$

and for the third term(only the first order in  $\eta$  is relevant when we expand in  $\varepsilon$  and  $\eta$ )

$$\langle m_1^{(1)}, \left( \frac{P_2}{h_2 - h_1} + \frac{P_3}{h_3 - h_1} \right) n_1^{(1)} \rangle$$

$$= -\frac{\langle m_{0,1} n_{0,2}^{(1)} \rangle \langle m_{0,2} n_{0,1}^{(1)} \rangle}{h_2 - h_1} - \frac{\langle m_{0,1} n_{0,3}^{(1)} \rangle \langle m_{0,3} n_{0,1}^{(1)} \rangle}{h_3 - h_1} + o(\eta)$$

(the first term was obtained in (44)). Therefore

$$\Phi(z, z_0; \varepsilon) = \frac{1}{\varepsilon} \left( \int_{z_0}^{z} \phi(u; \varepsilon) \, du + o((\varepsilon + \eta)^3) \right)$$
 (45)

with

$$\phi(\varepsilon) = h_{0,1} - i\varepsilon \langle m_{0,1} n_{0,1}^{(1)} \rangle + \langle m_{0,1}, H_p n_{0,1} \rangle$$

$$- \frac{1}{h_{0,2} - h_{0,1}} \left\{ \left[ \langle m_{0,1}, H_p n_{0,2} \rangle - i\varepsilon \langle m_{0,1} n_{0,2}^{(1)} \rangle \right] \left[ \langle m_{0,2}, H_p n_{0,1} \rangle - i\varepsilon \langle m_{0,2} n_{0,1}^{(1)} \rangle \right] \right\}$$

$$- \frac{1}{h_{0,3} - h_{0,1}} \left\{ \left[ \langle m_{0,1}, H_p n_{0,3} \rangle - i\varepsilon \langle m_{0,1} n_{0,3}^{(1)} \rangle \right] \left[ \langle m_{0,3}, H_p n_{0,1} \rangle - i\varepsilon \langle m_{0,3} n_{0,1}^{(1)} \rangle \right] \right\}.$$

#### The results.

#### Case I.

We point out the difference between the behavior for  $\text{Re}\,\sigma(H(z(x)))$  (see Fig. 3) and those of  $\sigma(H(z(x)))$ : the analytic continuation of  $h_1(z(x))$  intertwines between its limits  $h_1^l$  and  $h_1^r$ . For the proof of (25'), we repeat the method idea. In order to calculate  $\mathbb{S}_{11}$ , we use the superadiabatic evolution operator. It is integrated along a complex dissipative path (if we consider the restriction to

 $Ran P_{1,\varepsilon}$ ) where it differs by the real evolution operator with an exponentially small term. Thus, from (40) and (41) we obtain

$$\mathbb{S}_{11} = \lim_{\substack{\text{Re } z_0 \to -\infty \\ \text{Re } z \to \infty}} \exp\left\{-\frac{i}{\varepsilon} \left[ -(h_1^r z - h_1^l z_0) \right] \right\}$$

$$+ \int_{z_0}^{z} \phi(u;\varepsilon) du + o((\varepsilon + \eta)^3) \Big] \Big\} (1 + o(e^{-\frac{k''}{\varepsilon}}))$$

with the integral along the dissipative path  $\gamma$ . Now using the analyticity of the integrand in  $\mathcal{S}_{\alpha} \setminus \{x_1, x_2\}$  with simple poles in  $x_1, x_2$ , we can shift the contour of integration from  $\gamma$  to the real axis (note the compensation for vertical segments contributions).

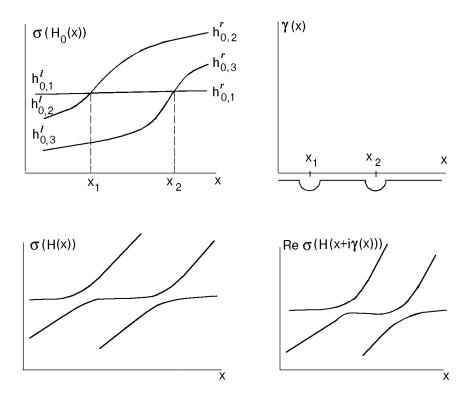


Fig. 3.

This allows one to use the self-adjointness of H(x),  $x \in \mathbb{R}$ , in order to obtain results for  $|\mathbb{S}_{i,j}|$  only in terms of the local behavior of the Hamiltonian at  $x_1, x_2$  (the singularities of the integrand). We use the standard formula  $\frac{1}{u} = \mathcal{P} + i\pi\delta(0)$ ,

where  $\mathcal{P}$  stands for the principal value integral, and we notice that for  $x \in \mathbb{R}$ ,  $m_{0,1}(x) = n_{0,1}(x)$ , which implies  $\operatorname{Re} \langle n_{0,1}(x), \frac{d}{dx} n_{0,1}(x) \rangle = 0$ . We obtain

$$|\langle n_{0,1}(\infty) \mathbb{S} n_{0,1}(-\infty) \rangle|^2 \equiv |\mathbb{S}_{11}|^2$$

$$= \exp\left\{-\frac{2\pi}{\varepsilon} \left[ \frac{1}{a} |H_{p,12}^{x_1} - i\varepsilon d_{12}^{x_1}|^2 + \frac{1}{b} |H_{p,13}^{x_2} - i\varepsilon d_{13}^{x_2}|^2 + o((\varepsilon + \eta)^3) \right] \right\}$$
(46)

with the notations from (26)-(29), and also

$$\arg \mathbb{S}_{11} = \varepsilon^{-1} \left\{ \int_{-\infty}^{0} \left( h_{0,1}(-\infty) - h_{0,1}(x) \right) dx + \int_{0}^{\infty} \left( h_{0,1}(\infty) - h_{0,1}(x) \right) dx - \int_{-\infty}^{\infty} \left\langle n_{0,1}(x), H_{p}(x) n_{0,1}(x) \right\rangle dx + i\varepsilon \int_{-\infty}^{\infty} \left\langle n_{0,1}(x), \frac{d}{dx} n_{0,1}(x) \right\rangle dx + \mathcal{P} \int_{-\infty}^{\infty} \frac{1}{h_{0,2}(x) - h_{0,1}(x)} |\langle n_{0,1}(x), (H_{p}(x) - i\varepsilon \frac{d}{dx}) n_{0,2}(x) \rangle|^{2} dx + \mathcal{P} \int_{-\infty}^{\infty} \frac{1}{h_{0,3}(x) - h_{0,1}(x)} |\langle n_{0,1}(x), (H_{p}(x) - i\varepsilon \frac{d}{dx}) n_{0,3}(x) \rangle|^{2} dx + o((\varepsilon + \eta)^{3}) \right\}.$$

$$(47)$$

For this general formula of the transition probability we consider the next limit cases. In the regime  $\varepsilon \ll \eta$  it becomes the following generalization of the classical Landau–Zener formula:

$$|\mathbb{S}_{11}|^2 = \exp\left\{-\frac{2\pi}{\varepsilon} \left[ \frac{1}{a} |H_{p,12}^{x_1}|^2 + \frac{1}{b} |H_{p,13}^{x_1}|^2 + o(\eta^3) \right] \right\} [1 + o(\varepsilon + \eta)], \tag{48}$$

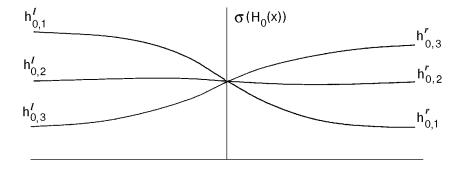
while for  $\eta = 0$  gives the following generalization of the Friedrich-Hagedorn result:

$$|\mathbb{S}_{11}|^2 = 1 - 2\pi\varepsilon \left(\frac{1}{a}|d_{12}^{x_1}|^2 + \frac{1}{b}|d_{13}^{x_2}|^2\right) + o(\varepsilon^2). \tag{49}$$

Similarly to [26], we note that in the crossover regime,  $\eta \sim \varepsilon$ , the Landau–Zener formula only gives  $|\mathbb{S}_{11}|^2 = 1 - o(\varepsilon)$ , while (46) gives

$$|\mathbb{S}_{11}|^2 = 1 - \frac{2\pi}{\varepsilon} \left( \frac{1}{a} |H_{p,12}^{x_1} - i\varepsilon d_{12}^{x_1}|^2 + \frac{1}{b} |H_{p,13}^{x_1} - i\varepsilon d_{13}^{x_2}|^2 \right) + o(\varepsilon^2) . \tag{50}$$





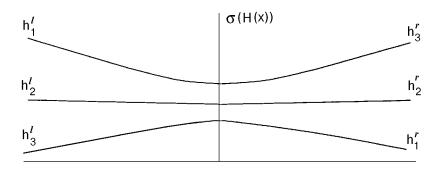


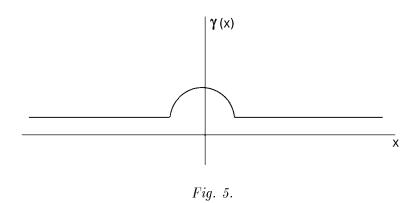
Fig. 4.

See Fig. 4. In the situations without multiple crossing points, in fact the many-level problem can be decomposed in 2-level problems. The possibility of the separations (in different manners on different sectors of the real axis) of an isolated 2-level part of the entire spectrum permits to apply there the reduction idea from (8) (see [8]). But in Case II, in order to separate at least one eigenvalue, we are obligated to use a complex path. We compute only  $\mathbb{S}_{11}$  and  $\mathbb{S}_{33}$  when the dissipative path is under or over the origin (when  $h_1$ , respectively,  $h_3$  are eigenvalues dissipative with respect to the two others). The distribution of the others transition probabilities remains an open question.

For the  $S_{33}$  calculus, the path  $z = x + i\gamma(x)$  dissipative for  $h_3(z)$  with respect to  $h_1(z)$  and  $h_2(z)$ , is above the real axis  $\gamma(x) > 0$  (see Fig. 5). The method exposed is applicable completely similar with Case I for

$$|\mathbb{S}_{33}|^2 = \exp\left\{-\frac{2\pi}{\varepsilon} \left[\frac{1}{\beta} |H_{p,32} - i\varepsilon d_{32}|^2 + \frac{1}{\alpha+\beta} |H_{p,31} - i\varepsilon d_{31}|^2 + o((\varepsilon+\eta)^3)\right]\right\}$$

and  $\arg S_{33}$  (the same as in (47) if we substitute  $1 \leftrightarrow 3$ ).



For  $S_{11}$  with a path  $x+i\gamma(x)$  below the real axis  $\gamma(x)<0$  (see Fig. 6), we obtain the result

$$|\mathbb{S}_{11}|^2 = \exp\left\{-\frac{2\pi}{\varepsilon} \left[ \frac{1}{\alpha} |H_{p,12} - i\varepsilon d_{12}|^2 + \frac{1}{\alpha + \beta} |H_{p,13} - i\varepsilon d_{13}|^2 + o((\varepsilon + \eta)^3) \right] \right\}$$
(51)

with the same  $\arg S_{11}$  like in Case 1. The extensions of Landau–Zener formula, Friedrichs–Hagedorn result and the crossover regime are similar to Case I.

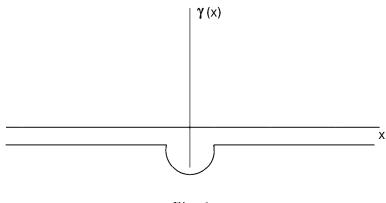


Fig. 6.

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#### References

[1] J.E. Avron, R. Seiler, and L.G. Yaffe, Adiabatic theorems and applications to the quantum hall effect. — Commun. Math. Phys. (1987), v. 110, p. 33-49.

- [2] M. Born and V. Fock, Beweis des Adiabatensatzes. Zeit. Phys. (1928), Bd. 51, S. 165-180.
- [3] A. Boutet de Monvel et. al. (Eds.), Recent developments in quantum mechanics. Kluver, Dordrecht (1991).
- [4] A. Boutet de Monvel and G. Nenciu, On the theory of adiabatic invariants for linear Hamiltonian systems. C. R. Acad. Sci. Paris (1990), v. 310, p. 807-810.
- [5] N. Dunford and J. Schwartz, Linear operators. I. Interscience, New York (1958).
- [6] A.M. Dykhne, Adiabatic perturbation of discrete spectrum states. Soviet Phys. JETP (1962), v. 14, p. 941–943.
- [7] G. Firica, Refined Landau-Zener formulae: multilevel systems and semi-classical limit of quantum scattering on the line, Preprint-Jussieu (May, 1995) (a preliminary version of Section 2 in: Fortschr. Phys. (1995), v.43, No. 2, p.99-137).
- [8] G. Firica, Refined Landau-Zener formulae: multilevel adiabatic reduction method (to appear).
- [9] L.M. Garrido, Generalized adiabatic invariance. J. Math. Phys. (1964), v. 5, p. 335-362.
- [10] G. Hagedorn, Adiabatic expansion near eigenvalue crossings. Ann. Phys. (1989), v. 196, p. 278–295.
- [11] G. Hagedorn, Proof of the Landau-Zener formula in an adiabatic limit with small eigenvalue gaps. Commun. Math. Phys. (1991), v. 136, p. 433-449.
- [12] B. Helffer and J. Sjöstrand, Semi-classical analysis of Harper's equation III. Bull. Soc. Math. France, Mémoire (1990), No. 39.
- [13] J.-T. Hwang and P. Pechukas, The adiabatic theorem in the complex plane and the semi-classical calculation of non-adiabatic transition amplitudes. — J. Chem. Phys. (1977), v. 67, p. 4640-4653.
- [14] A. Joye, Proof of Landau-Zener formula. Asympt. Anal. (1994), v. 9, p. 209-258.
- [15] A. Joye, Exponential asymptotic in a singular limit for n-level scattering systems. Preprint CPT-95/P.3216, CNRS Luminy, Marseilles (June, 1995).
- [16] A. Joye, Non-trivial prefactors in adiabatic transition probabilities induced by high order complex degeneracies. Preprint C.N.E.S. Luminy, Marseilles (1993).
- [17] A. Joye and Ch.-E. Pfister, Exponentially small adiabatic invariant for the Schrödinger equation. Commun. Math. Phys. (1991), v. 140, p. 15-41.
- [18] A. Joye and Ch.-E. Pfister, Super-adiabatic evolution and adiabatic transition probability between two non-degenerate levels isolated in the spectrum. J. Math. Phys. (1993), v. 34, p. 454-479.
- [19] A. Joye and Ch.-E. Pfister, Semi-classical asymptotic beyond all orders for simple scattering systems. Preprint, CNRS Luminy, Marseilles (1993).

- [20] A. Joye, H. Kunz, and Ch.-E. Pfister, Exponential decay and geometric aspect of transition probabilities in the adiabatic limit. Ann. Phys. (1991), v. 208, p. 299–332.
- [21] T. Kato, On the adiabatic theorem of quantum mechanics. J. Phys. Soc. Japan (1950), v. 5, p. 435-439.
- [22] T. Kato, Perturbation theory for linear operators. Springer, Berlin-Heidelberg-New York (1976).
- [23] S. G. Krein, Linear differential equations in Banach spaces. Trans. of Math. Monographs, Providence (1971), v. 29.
- [24] L. D. Landau and E. M. Lifschitz, Quantum mechanics. Pergamon, Oxford (1965), 2-nd ed.
- [25] A. Lenard, Adiabatic invariance to all orders. Ann. Phys. (1959), v. 6, p. 261-276.
- [26] Ph.A. Martin and G. Nenciu, Semi-classical inelastic S-matrix for one-dimensional N-states systems. Rev. Math. Phys. (1995), v. 7, p. 193-242.
- [27] A. Martinez, Precise exponential estimates in adiabatic theory. J. Math. Phys. (1994), v. 35, p. 3889-3915.
- [28] A. Martinez and G. Nenciu, On adiabatic reduction theory. Preprint Université Paris Nord (1994).
- [29] G. Nenciu, On the adiabatic theorem of quantum mechanics. J. Phys. (1980), v. A 13, p. L15-L18.
- [30] G. Nenciu, Adiabatic theorems and spectral concentration. Commun. Math. Phys. (1981), v. 82, p. 121-135.
- [31] G. Nenciu, Asymptotic invariant subspaces, adiabatic theorems and bloc diagonalization, p. 133-149 in [3].
- [32] G. Nenciu, Exponential estimates in linear adiabatic theory: dependence on the gap. Report No.7. Inst. Mitag-Leffer (1992/1993).
- [33] G. Nenciu, Linear adiabatic theory. Exponential estimates. Commun. Math. Phys. (1993), v. 152, p. 479-496.
- [34] G. Nenciu and G. Rasche, On the adiabatic theorem for non-self-adjoint Hamiltonians. J. Phys. A: Math. Gen. (1992), v. 25, p. 5741-5751.
- [35] V.L. Pokrovskii and I.M. Khalatnikov, On the problem of above-barrier reflection of high-energy particles. Soviet Phys. JETP (1961), v. 13, p. 1207-1210.
- [36] T. Ramond, Semi-classical study of quantum scattering on the line. Preprint Université Paris Nord (1995).
- [37] F. Rellich, Perturbation theory of eigenvalue problem. Gordon and Brecht (Science Publishers), New York-London-Paris (1969).
- [38] S.J. Sancho, m'th order adiabatic invariance. Proc. Phil. Soc. London (1966), v. 89, p. 1-5.

- [39] G. Sansone and G. Conté, Nonlinear differential equations. Pergamon, Oxford (1964).
- [40] J. Sjöstrand, Projecteurs adiabatiques du point de vue pseudo-differentiel. C. R. Acad. Sci. Paris (1993), t. 317, ser. 1, p. 217-220.
- [41] W. Wasow, Topics in the theory of linear differential equations having singularities with respect to a parameter, Ser. Math. Pures et Apliqus, IRMA, Strasbourg (1978).
- [42] M.Reed, B.Simon, Methods of modern mathematical physics. (v. II) Fourier analysis, self-adjointness. Acad. Press, New York (1975).
- [43] K. Yosida, Functional analysis. Grundlagen der Math. Wissenschaften, Bd. 123. Springer, Berlin-Heidelberg-New York.

## Многоуровневые формулы Ландау-Зенера: адиабатическая редукция вдоль комплексного пути

#### Габриэль Фирика

В квазиклассическом (адиабатическом) пределе рассматриваются эволюционные уравнения, генераторы которых продолжаются в полосу около вещественной оси как голоморфное семейство операторов (по отношению к переменной времени). Асимптотическое разложение \$\mathbb{S}\-\mathbb{M}\mathbb{M}\mathbb{T}\mathbb{D}\m

### Багаторівневі формули Ландау-Зенера: адіабатична редукція вздовж комплексного шляху

#### Габріель Фіріка

У квазікласичній (адіабатичній) границі розглядаються еволюційні рівняння, генератори яких продовжуються у смугу поблизу дійсної осі як голоморфна сім'я операторів (відносно змінної часу). Асимптотичний розклад S-матриці, що пов'язана з цією еволюцією, може бути виражено у термінах простих величин, які асоційовані з сінгулярностями спектру гамільтоніанів з комплексної площини змінної часу. Мы продовжуємо на багаторівневий випадок результат [26], що вміщує як граничні випадки формули Ландау-Зенера, так і результати Фрідріхса-Хагедорна для цієї задачі.