Exponential Asymptotics in a Singular Limit for n-Level Scattering Systems

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Abstract

The singular limit $\varepsilon \to 0$ of the S-matrix associated with the equation $i\varepsilon d\psi(t)/dt = H(t)\psi(t)$ is considered, where the analytic generator $H(t) \in M_n(\mathbf{C})$ is such that its spectrum is real and non-degenerate for all $t \in \mathbf{R}$. Sufficient conditions allowing to compute asymptotic formulas for the exponentially small off-diagonal elements of the S-matrix as $\varepsilon \to 0$ are explicited and a wide class of generators for which these conditions are verified is defined. These generators are obtained by means of generators whose spectrum exhibits eigenvalue crossings which are perturbed in such a way that these crossings turn to avoided crossings. The exponentially small asymptotic formulas which are derived are shown to be valid up to exponentially small relative error, by means of a joint application of the complex WKB method together with superasymptotic renormalization. The application of these results to the study of quantum adiabatic transitions in the time dependent Schrödinger equation and of the semiclassical scattering properties of the multichannel stationary Schrödinger equation closes this paper. The results presented here are a generalization to n-level systems, $n \geq 2$, of results previously known for 2-level systems only.

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1 Introduction

Several problems of mathematical physics lead to the study of the scattering properties of linear ordinary differential equations in a singular limit

$$i\varepsilon\psi'(t) = H(t)\psi(t), \quad t \in \mathbf{R}, \quad \varepsilon \to 0, \tag{1.1}$$

where the prime denotes the derivative with respect to t, $\psi(t) \in \mathbf{C}^n$, $H(t) \in M_n(\mathbf{C})$, for all t. A system described by such an equation will be called a n-level system. Let us mention for example the study of the adiabatic limit of the time dependent Schrödinger equation or the semiclassical limit of the one-dimensional multichannel stationary Schrödinger equation at energies above the potential barriers, to which we will come back below. When the generator $H(t)$ is well behaved at $+\infty$ and $-\infty$, the scattering properties of the problem can be described by means of a matrix naturally associated with equation (1.1), the so-called S-matrix. This matrix relates the behavior of the solution $\psi(t)$ as $t \to -\infty$ to that of $\psi(t)$ as $t \to +\infty$. Assuming that the spectrum $\sigma(t)$ of $H(t)$ is real and non-degenerate,

$$\sigma(t) = \{e_1(t) < e_2(t) < \cdots < e_n(t)\} \in \mathbf{R}, \tag{1.2}$$

the S-matrix is essentially given by the identity matrix

$$S = \text{diag }(s_{11}(\varepsilon), s_{22}(\varepsilon), \cdots s_{nn}(\varepsilon)) + \mathcal{O}(\varepsilon^\infty), \quad \text{where } s_{jj}(\varepsilon) = 1 + \mathcal{O}(\varepsilon) \text{ as } \varepsilon \to 0, \tag{1.3}$$

provided $H(t)$ is C^∞, see e.g. [F1], [F2], [W]. Moreover, if $H(t)$ is assumed to be analytic, it was proven in various situations that the off-diagonal elements s_{jk} of S are exponentially decreasing [FF], [W], [F1], [F2], [JKP], [JP4]

$$s_{jk} = \mathcal{O}\left(\mathrm{e}^{-\kappa/\varepsilon}\right), \quad \forall j \neq k, \tag{1.4}$$

as $\varepsilon \to 0$. See also [JP1], [N], [M], [Sj] for corresponding results in infinite dimensional spaces. Since the physical information is often contained in these off-diagonal elements, it is of interest to be able to give an asymptotic formula for s_{jk}, rather then a mere estimate.

For 2-level systems (or systems reducible to this case, see [JP2], [J], [MN]), the situation is now reasonably well understood, at least under generic circumstances. Indeed, a rigorous study of the S-matrix associated with (1.1) when $n = 2$, under the hypotheses loosely stated above, is provided in the recent paper [JP4]. The treatment presented unifies in particular earlier results obtained either for the time dependent adiabatic schrödinger equation, see e.g [JP3] and references therein, or for the study of the above barrier reflexion in the semiclassical limit, see e.g. [FF],[O]. Further references are provided in [JP4]. As an intermediate result, the asymptotic formula

$$s_{jk} = g_{jk}\mathrm{e}^{-\Gamma_{jk}/\varepsilon}\left(1 + \mathcal{O}(\varepsilon)\right), \quad \varepsilon \to 0, \tag{1.5}$$

for $j \neq k \in \{1, 2\}$, with $g_{jk} \in \mathbf{C}$ and Re $\Gamma_{jk} > 0$ is proven in [JP4]. As is well known, to get an asymptotic formula for s_{jk}, one has to consider (1.1) in the complex plane, in particular in the vicinity of the degeneracy points of the analytic continuations of eigenvalues $\mathrm{e}_1(z)$ and $e_2(z)$. *Provided* the level lines of the multivalued function

$$\text{Im} \int_0^z e_1(z') - e_2(z')dz' = \text{cst}, \tag{1.6}$$

called Stokes lines, naturally associated with (1.1) behave properly in the complex plane, the so-called complex WKB method allows to prove (1.5). But more important, it is also shown in [JP4] how to improve (1.5) to an asymptotic formula accurate up to exponentially small relative error

$$s_{jk} = g^*_{jk}(\varepsilon)\mathrm{e}^{-\Gamma^*_{jk}(\varepsilon)/\varepsilon}\left(1+\mathcal{O}\left(\mathrm{e}^{-\kappa/\varepsilon}\right)\right), \quad \varepsilon \to 0, \tag{1.7}$$

with $g^*_{jk}(\varepsilon) = g_{jk}+\mathcal{O}(\varepsilon)$ and $\Gamma^*_{jk}(\varepsilon) = \Gamma_{jk}+\mathcal{O}(\varepsilon^2)$. This is achieved by using a complex WKB analysis jointly with the recently developed superasymptotic theory [Be], [N], [JP2]. Note that when given a generator, the principal difficulty in justifying formulas (1.5) and (1.7) is the verification that the corresponding Stokes lines (1.6) display the proper behavior *globally* in the complex plane, which may or may not be the case [JKP]. However, this condition is always satisfied when the complex eigenvalue degeneracy is close to the real axis, as shown in [J]. See also [MN] and [R] for recent related results.

For n-level systems, with $n \geq 3$, the situation is by no means as well understood. There are some results obtained with particular generators. In [D], [CH1], [CH2] and [BE], certain elements of the S-matrix are computed if $H(t) = H^*(t)$ depends linearly on t, $H(t) = A+tB$, for some particular matrices A and B. The choices of A and B are such that all components of the solution $\psi(t)$ can be deduced from the first one and an exact integral representation of this first component can be obtained. The integral representation is analyzed by standard asymptotic techniques and this leads to results which are valid for any $\varepsilon > 0$, as for the classical Landau-Zener generator. The study of the three-level problem when $H(t) = H^*(t) \in M_3(\mathbf{R})$ is tackled in the closing section of the very interesting paper [HP]. A non rigorous and essentially local discussion of the behavior of the level lines Im $\int_0^z e_j(z') - e_k(z')dz'$, $j \neq k = 1,2,3$, is provided and justifies in very favorable cases an asymptotic formula for some elements of the S-matrix. See also the review [So], where a non rigorous study of (1.1) is made close to a complex degeneracy point of a group of eigenvalues by means of an exact solution to a model equation. However, no asymptotic formula for s_{jk}, $j \neq k$, can be found in the literature for general n-level systems, $n \geq 3$. This is due to the fact that the direct generalization of the method used successfully for 2-level systems may lead to seemingly inextricable difficulties for $n = 3$ already. Indeed, with three eigenvalues, one has to consider three sets of level lines Im $\int_0^z e_j(z') - e_k(z')dz'$ to deal with (1.1) in the complex plane, and the conditions they have to fulfill in order that the limit $\varepsilon \to 0$ can be controlled may be incompatible for a given generator, see [F1], [F2] and [HP]. It should be mentioned however, that there are specific examples in which this difficult problem can be mastered. Such a result was recently obtained in the semiclassical study [Ba] of a particular problem of resonances for which similar considerations in the complex plane are required.

The goal of this paper is to provide some general insight on the asymptotic computation of the S-matrix associated with n-level systems, $n \geq 3$, based on a generalization the techniques which proved to be successful for 2-level systems. The content of this paper is twofold. On the one hand we set up a general framework in which asymptotic formulas for the exponentially small off-diagonal coefficients can be proven. On the other hand we actually prove such formulas for a wide class of n-level systems. In the first part of the paper, we give our definition of the S-matrix associated with equation (1.1) and explicit the symmetries it inherits from the symmetries of $H(t)$, for $t \in \mathbf{R}$ (proposition 2.1). Then we turn to the determination of the analyticity properties of the eigenvalues and eigenvectors of $H(z)$, $z \in \mathbf{C}$, which are at the root of the asymptotic formulas we derive later (lemma 3.1). The next step is the formulation of sufficient conditions adapted to the scattering situation we consider, under which a complex WKB analysis allows to prove a formula like (1.5) (proposition 4.1). The conditions stated are similar but not identical to those given in [JKP] or [HP]. As a final step, we show how to improve the asymptotic formula (1.5) to (1.7) by means of the superasymptotic machinery (proposition 5.2 and lemma 5.2). Then we turn to the second part of the paper, where we show that a wide class of generators fits into our framework and satisfy our conditions. These generators are obtained by perturbation of generators whose eigenvalues display degeneracies on the real axis, in the spirit of [J]. We prove that for these generators, in absence of any symmetry of the generator $H(t)$, one element per column at least in the S-matrix can be asymptotically computed (theorem 6.1). This is the main technical section of the paper. The major advantage of this construction is that it is sufficient to look at the behavior of the eigenvalues on the real axis to check if the conditions are satisfied. The closing section contains an application of our general results to the study of quantum adiabatic transitions in the time dependent Schrödinger equation and of the semiclassical scattering properties of the multichannel stationary Schrödinger equation. In particular, explicit use of the symmetries of the S-matrix is made to increase the number of its elements for which an asymptotic formula holds. In the latter application, further specific symmetry properties of the S-matrix are derived (lemma 7.1).

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2 Definition and properties of the S-matrix.

We consider the evolution equation

$$i\varepsilon\psi'(t) = H(t)\psi(t), \quad t \in \mathbf{R}, \ \ \varepsilon \to 0, \tag{2.1}$$

where the prime denotes the derivative with respect to t, $\psi(t) \in \mathbf{C}^n$, $H(t) \in M_n(\mathbf{C})$, for all t. We make some assumptions on the generator $H(t)$. The first one is the usual analyticity condition in this context.

H1 *There exists a strip*

$$S_\alpha = \{z \in \mathbf{C} | \, |\mathrm{Im}\, z| \leq \alpha\}, \quad \alpha > 0, \tag{2.2}$$

such that $H(z)$ is analytic for all $z \in S_\alpha$.

Since we are studying scattering properties, we need sufficient decay at infinity.

H2 *There exist two nondegenerate matrices $H(+), H(-) \in M_n(\mathbf{C})$ and $a > 0$ such that*

$$\lim_{t \to \pm\infty} |t|^{1+a} \sup_{|s| \leq \alpha} \|H(t+is) - H(\pm)\| < \infty. \tag{2.3}$$

We finally give a condition which has to do with the physics behind the problem.

H3 *For $t \in \mathbf{R}$, the spectrum of $H(t)$, denoted by $\sigma(t)$, is real and non-degenerate*

$$\sigma(t) = \{e_1(t) < e_2(t) < \cdots < e_n(t)\} \subset \mathbf{R} \tag{2.4}$$

and there exists $g > 0$ such that

$$\inf_{\substack{j \neq k \\ t \in \mathbf{R}}} |e_j(t) - e_k(t)| \geq g. \tag{2.5}$$

As a consequence of H3, for each $t \in \mathbf{R}$, there exists a complete set of projectors $P_j(t) = P_j^2(t) \in M_n(\mathbf{C})$, $j = 1, 2, \cdots, n$ such that

$$\sum_{j=1}^{n} P_j(t) \equiv \mathbf{I} \tag{2.6}$$

$$H(t) = \sum_{j=1}^{n} e_j(t) P_j(t) \tag{2.7}$$

and there exists a basis of $\mathbf{C}^n$ of eigenvectors of $H(t)$. We determine these eigenvectors $\varphi_j(t)$, $j = 1, 2, \cdots, n$ uniquely (up to a constant) by requiring them to satisfy

$$H(t)\varphi_j(t) = e_j(t)\varphi_j(t) \tag{2.8}$$
$$P_j(t)\varphi_j'(t) \equiv 0, \qquad j = 1, 2, \cdots, n. \tag{2.9}$$

Explicitly, if $\chi_j(t)$, $j = 1, 2, \cdots, n$ form a complete set of differentiable eigenvectors of $H(t)$, the eigenvectors

$$\varphi_j(t) = \mathrm{e}^{-\int_0^t \xi_j(t')dt'}\psi_j(t), \quad \text{s.t. } \varphi_j(0) = \psi_j(0) \tag{2.10}$$

with

$$\xi_j(t) = \frac{\langle\psi_j(t)|P_j(t)\psi_j'(t)\rangle}{\|\psi_j(t)\|^2}, \quad j = 1, \cdots, n \tag{2.11}$$

verify (2.9). That this choice leads to an analytic set of eigenvectors close to the real axis will be proven below. We expand the solution $\psi(t)$ along the basis just constructed, thus defining unknown coefficients $c_j(t)$, $j = 1, 2, \cdots, n$ to be determined,

$$\psi(t) = \sum_{j=1}^{n} c_j(t)\mathrm{e}^{-i\int_0^t e_j(t')dt'/\varepsilon}\varphi_j(t). \tag{2.12}$$

The phases $\mathrm{e}^{-i\int_0^t e_j(t')dt'/\varepsilon}$ (see H3) are introduced for convenience. By inserting (2.12) in (2.1) we get the following differential equation for the $c_j(t)$'s

$$c_j'(t) = \sum_{k=1}^{n} a_{jk}(t)\mathrm{e}^{i\Delta_{jk}(t)/\varepsilon}c_k(t) \tag{2.13}$$

where

$$\Delta_{jk}(t) = \int_0^t (e_j(t') - e_k(t'))dt' \tag{2.14}$$

and

$$a_{jk}(t) = -\frac{\langle\varphi_j(t)|P_j(t)\varphi_k'(t)\rangle}{\|\varphi_j(t)\|^2}. \tag{2.15}$$

Here $\langle\cdot|\cdot\rangle$ denotes the usual scalar product in $\mathbf{C}^n$. Our choice (2.9) implies $a_{jj}(t) \equiv 0$. It is also shown below that the $a_{jk}(t)$'s are analytic functions in a neighborhood of the real axis and that hypothesis H2 imply that they satisfy the estimate

$$\lim_{t\to\pm\infty} \sup_{j\neq k} |t|^{1+a}\,|a_{jk}(t)| < \infty. \tag{2.16}$$

As a consequence of this last property and of the fact that the eigenvalues are real by assumption, the following limits exist

$$\lim_{t\pm\infty} c_j(t) = c_j(\pm\infty). \tag{2.17}$$

We are now able to define the associated S-matrix, $S \in M_n(\mathbf{C})$, by the identity

$$S\begin{pmatrix} c_1(-\infty) \\ c_2(-\infty) \\ \vdots \\ c_n(-\infty) \end{pmatrix} = \begin{pmatrix} c_1(+\infty) \\ c_2(+\infty) \\ \vdots \\ c_n(+\infty) \end{pmatrix}. \tag{2.18}$$

Such a relation makes sense because of the linearity of the equation (2.13). It is a well known result that under our general hypotheses, the S-matrix satisfies

$$S = \mathbf{I} + \mathcal{O}(\varepsilon). \tag{2.19}$$

Note that the j^{th} column of the S-matrix is given by the solution of (2.13) at $t = \infty$ subjected to the initial conditions $c_k(-\infty) = \delta_{jk}$, $k = 1, 2, \cdots, n$.

In general, the S-matrix defined above has no particular properties besides that of being invertible. However, when the generator $H(t)$ satisfies some symmetry properties, the same is true for S. As such properties are important in applications, we show below that if $H(t)$ is self-adjoint with respect to some indefinite scalar product, then S is unitary with respect to another indefinite scalar product. Let $J \in M_n(\mathbf{C})$ be an invertible self-adjoint matrix. We define an indefinite metric on $\mathbf{C}^n$ by means of the indefinite scalar product

$$(\cdot, \cdot)_J = \langle \cdot | J \cdot \rangle. \tag{2.20}$$

It is easy to check that the adjoint $A^{\#}$ of a matrix A with respect to the $(\cdot, \cdot)_J$ scalar product is given by

$$A^{\#} = J^{-1} A^* J. \tag{2.21}$$

Proposition 2.1 *Let $H(t)$ satisfy H1, H2 and possess n distinct eigenvalues $\forall t \in \mathbf{R}$. Further assume $H(t)$ is self-adjoint with respect to the scalar product $(\cdot, \cdot)_J$,*

$$H(t) = H^{\#}(t) = J^{-1} H^*(t) J, \quad \forall t \in \mathbf{R}, \tag{2.22}$$

and the eigenvectors $\varphi_j(0)$ of $H(0)$ satisfy

$$(\varphi_j(0), \varphi_j(0))_J = \rho_j, \quad \rho_j \in \{-1, 1\}, \quad \forall j = 1, \cdots, n. \tag{2.23}$$

Then the eigenvalues of $H(t)$ are real $\forall t \in \mathbf{R}$ and the S-matrix is unitary with respect to the scalar product $(\cdot, \cdot)_R$, where $R = R^* = R^{-1}$ is the real diagonal matrix $R = \mathrm{diag}\ (\rho_1, \rho_2, \cdots, \rho_n)$,

$$S^{\#} = R S^* R = S^{-1}. \tag{2.24}$$

Remark:

The condition $(\varphi_j(0), \varphi_j(0))_J = \pm 1$ can always be satisfied by suitable renormalization provided $(\varphi_j(0), \varphi_j(0))_J \neq 0$.

The main interest of this proposition is that when the S-matrix possesses symmetries, some of its elements can be deduced from resulting identities, without resorting to their actual computations.

A simple proof of the proposition making use of notions discussed in the next section can be found in appendix. The above proposition can actually be used for the two main applications we deal with in section 7. Note that in specific cases, further symmetry property can be derived for the S-matrix, see section 7.

3 Analyticity properties

The generator $H(z)$ is analytic in S_α, hence the solution of the linear equation (2.1) $\psi(z)$ is analytic in S_α as well. However, the eigenvalues and eigenprojectors of $H(z)$ may have singularities in S_α. Let us recall some basic properties, the proofs of which can be found in [K]. The eigenvalues and eigenprojectors of a matrix analytic in a region of the complex plane have analytic continuations in that region with possible singularities located at points

Figure 1: The paths β, δ and η_0 in $S_\alpha \backslash \Omega$.

z_0 called exceptional points. In a neighborhood free of exceptional points, the eigenvalues are given by branches of analytic functions and their multiplicities are constant. One eigenvalue can therefore be analytically continued until it coincides at z_0 with one or several other eigenvalues. The set of such points defines the set of exceptional points. The eigenvalues may possess branching points at an exceptional z_0, where they are continuous, whereas the eigenprojectors are also multivalued but diverge as $z \to z_0$. Hence, by hypothesis H3, the n distinct eigenvalues $e_j(t)$ defined on the real axis are analytic on the real axis and possess multivalued analytic continuations in S_α, with possible branching points at the set of degeneracies Ω, given by

$$\Omega = \{z_0 |\ e_j(z_0) = e_k(z_0), \text{for some } k, j \text{ and some analytic continuation}\}. \tag{3.1}$$

By assumption H2, Ω is finite, by H3, $\Omega \cap \mathbf{R} = \emptyset$ and $\Omega = \overline{\Omega}$, due to Schwarz's principle. Similarly, the eigenprojectors $P_j(t)$ defined on the real axis are analytic on the real axis and possess multivalued analytic continuations in S_α, with possible singularities at Ω. To see more precisely what happens to these multivalued functions when we turn around a point $z_0 \in \Omega$, we consider the construction described in figure 1. Let f be a multivalued analytic function in $S_\alpha \backslash \Omega$. We denote by $f(z)$ the analytic continuation of $f(0)$ along some path $\beta \in S_\alpha \backslash \Omega$ from 0 to z. Then we perform the analytic continuation of $f(z)$ along a negatively oriented loop δ based at z around a unique point $z_0 \in \Omega$, and denote by $\widetilde{f}(z)$ the function we get when we come back at the starting point (if δ is positively oriented, the construction is similar). For later purposes, we define η_0 as the negatively oriented loop homotopic to the loop based at the origin encircling z_0 obtained by following β from 0 to z, δ from z back to z and β in the reverse sense from z back to the origin. We'll keep this notation in the rest of this section. It follows from the foregoing that if we perform the analytic continuation of the set of eigenvalues $\{e_j(z)\}_{j=1}^n$, along a negatively oriented loop around $z_0 \in \Omega$, we get the set $\{\widetilde{e}_j(z)\}_{j=1}^n$ with

$$\widetilde{e}_j(z) = e_{\sigma_0(j)}(z), \quad j = 1, \cdots, n, \tag{3.2}$$

where

$$\sigma_0 : \{1, 2, \cdots, n\} \to \{1, 2, \cdots, n\} \tag{3.3}$$

is a permutation which depends on η_0. Similarly, and with the same notations, we get for the analytic continuations of the projectors around z_0

$$\widetilde{P}_j(z) = P_{\sigma_0(j)}(z), \quad j = 1, \cdots, n. \tag{3.4}$$

Let us consider now the eigenvectors $\varphi_j(t)$. We define $W(t)$ as the solution of

$$\begin{aligned} W'(t) &= \sum_{j=1}^{n} P_j'(t)P_j(t)W(t) \\ &\equiv K(t)W(t), \quad W(0)=\mathbf{I}, \end{aligned} \tag{3.5}$$

where $t \in \mathbf{R}$. It is well known [K], [Kr], that $W(t)$ satisfies the intertwining identity

$$W(t)P_j(0) = P_j(t)W(t), \quad j=1,2,\cdots,n\ ,\ \forall t \in \mathbf{R}, \tag{3.6}$$

so that, if $\{\varphi_j(0)\}_{j=1}^{n}$ denotes a set of eigenvectors of $H(0)$, the vectors defined by

$$\varphi_j(t) = W(t)\varphi_j(0) \tag{3.7}$$

are eigenvectors of $H(t)$. Moreover, using the identity $Q(t)Q'(t)Q(t) \equiv 0$ which is true for any differentiable projector, it is easily checked that condition (2.9) is satisfied by these vectors. The generator $K(t)$ is analytic on the real axis and can be analytically continued in $S_\alpha\backslash\Omega$. Actually, $K(z)$ is single valued in $S_\alpha\backslash\Omega$. Indeed, let us consider the analytic continuation of $K(z)$ around $z_0 \in \Omega$. We get from (3.4) that

$$\widetilde{P}_j'(z) = P_{\sigma_0(j)}'(z), \tag{3.8}$$

so that

$$\begin{aligned} \widetilde{K}(z) &= \sum_{j=1}^{n} \widetilde{P}_j'(z)\widetilde{P}_j(z) = \sum_{j=1}^{n} P_{\sigma_0(j)}'(z)P_{\sigma_0(j)}(z) \\ &= \sum_{k=1}^{n} P_k'(z)P_k(z) = K(z). \end{aligned} \tag{3.9}$$

Consequently, $W(t)$ can be analytically continued in $S_\alpha\backslash\Omega$, where it is multivalued and satisfies both (3.5) and (3.6) with $z \in S_\alpha\backslash\Omega$ in place of $t \in \mathbf{R}$. Moreover, the relation between the analytic continuation $W(z)$ from 0 to some point $z \in S_\alpha\backslash\Omega$ and the analytic continuation $\widetilde{W}(z)$ is given by a monodromy matrix $W(\eta_0)$ such that

$$\widetilde{W}(z) = W(z)W(\eta_0), \tag{3.10}$$

where η_0 is the negatively oriented loop based at the origin which encircles $z_0 \in \Omega$ only, (see figure 1). Note also that the analytic continuation $W(z)$ is invertible in $S_\alpha\backslash\Omega$ and $W^{-1}(z)$ satisfies

$$W^{-1\prime}(z) = -W^{-1}(z)K(z), \quad W^{-1}(0) = \mathbf{I}. \tag{3.11}$$

As a consequence, the eigenvectors (3.7) possess multivalued analytic extensions in $S_\alpha\backslash\Omega$. Consider the relation

$$H(z)\varphi_j(z) = e_j(z)\varphi_j(z), \tag{3.12}$$

obtained by analytic continuation from 0 to some point $z \in S_\alpha\backslash\Omega$. When analytically continued along a negatively oriented loop around $z_0 \in \Omega$, it yields

$$\widetilde{H}(z)\widetilde{\varphi}_j(z) = H(z)\widetilde{\varphi}_j(z) = \widetilde{e}_j(z)\widetilde{\varphi}_j(z) = e_{\sigma_0(j)}(z)\widetilde{\varphi}_j(z). \tag{3.13}$$

Thus $\widetilde{\varphi}_j(z)$ is proportional to $\varphi_{\sigma_0(j)}(z)$ and we introduce the quantity $\theta_j(\eta_0) \in \mathbf{C}$ by the definition

$$\widetilde{\varphi}_j(z) = \mathrm{e}^{-i\theta_j(\eta_0)}\varphi_{\sigma_0(j)}(z), \quad j=1,2,\cdots,n\ . \tag{3.14}$$

This is equivalent to (see (3.10))

$$W(\eta_0)\widetilde{\varphi}_j(0) = \mathrm{e}^{-i\theta_j(\eta_0)}\varphi_{\sigma_0(j)}(0). \tag{3.15}$$

Let us consider the couplings (2.15). Using the definition (3.7), the invertibility of $W(t)$ and the identity (3.6), it's not difficult to see that we can rewrite

$$a_{jk}(t) = -\frac{\langle\varphi_j(0)|P_j(0)W(t)^{-1}K(t)W(t)\varphi_k(0)\rangle}{\|\varphi_j(0)\|^2}, \quad t \in \mathbf{R}, \tag{3.16}$$

which is analytic on the real axis and can be analytically continued in $S_\alpha\backslash\Omega$, where it is multivalued. Thus, the same is true for the coefficients $c_j(t)$ which satisfy the linear differential equation (2.13) and their analytic continuations satisfy the same equation with $z \in S_\alpha\backslash\Omega$ in place of $t \in \mathbf{R}$. We now come to the main identity of this section, regarding the coefficients $c_j(z)$. Let us denote by $c_j(z)$ the analytic continuation of $c_j(0)$ from 0 to some $z \in S_\alpha\backslash\Omega$. We perform the analytic continuation of $c_j(z)$ along a negatively oriented loop around $z_0 \in \Omega$ and denote by $\widetilde{c}_j(z)$ the function we get when we come back at the starting point z.

Lemma 3.1 *For any $j = 1, \cdots, n$, we have*

$$\widetilde{c}_j(z)e^{-i\int_{\eta_0} e_j(u)du/\varepsilon}e^{-i\theta_j(\eta_0)} = c_{\sigma_0(j)}(z) \tag{3.17}$$

where η_0, $\theta_j(\eta_0)$ and $\sigma_0(j)$ are defined as above.

Proof:
It follows from hypothesis H1 that $\psi(z)$ is analytic in S_α so that

$$\sum_{j=1}^{n} c_j(z)\mathrm{e}^{-i\int_0^z e_j(u)du/\varepsilon}\varphi_j(z) = \sum_{j=1}^{n} \widetilde{c}_j(z)\mathrm{e}^{-i\widetilde{\int_0^z e_j(u)du/\varepsilon}}\widetilde{\varphi}_j(z) =$$
$$\sum_{j=1}^{n} \widetilde{c}_j(z)\mathrm{e}^{-i\int_{\eta_0} e_j(u)du/\varepsilon}\mathrm{e}^{-i\int_0^z e_{\sigma_0(j)}(u)du/\varepsilon}\mathrm{e}^{-i\theta_j(\eta_0)}\varphi_{\sigma_0(j)}(z). \tag{3.18}$$

We conclude by the fact that $\{\varphi_j(z)\}_{j=1}^n$ is a basis. □

Remark:
It is straightforward to generalize the study of the analytic continuations around one singular point of the functions given above to the case where the analytic continuations are performed around several singular points, since Ω is finite. The loop η_0 can be rewritten as a finite succession of individual loops encircling one point of Ω only, so that the permutation σ_0 is given by the composition of a finite number of individual permutations. Thus the factors $\mathrm{e}^{-i\theta_j(\eta_0)}$ in (3.14) should be replaced by a product of such factors, each associated with one individual loop and the same is true for the factors $\exp(-i\int_{\eta_0} e_j(z)dz/\varepsilon)$ in lemma 3.1. This process is performed in the proof of theorem 6.1.

4 Complex WKB analysis

This section is devoted to basic estimates on the coefficients $c_j(z)$ in certain domains extending to infinity in both the positive and negative directions inside the strip S_α. We first consider what happens in neighborhoods of $\pm\infty$. It follows from assumption H1 by a direct application of the Cauchy formula that

$$\lim_{t\to\pm\infty} \sup_{|s|\leq\alpha} |t|^{1+a}\|H'(t+is)\| < \infty. \tag{4.1}$$

Figure 2: The path of integration for $\widetilde{\Delta}_{jk}(z)$ (the x's denote points of Ω).

Hence the same is true for the single valued matrix $K(z)$

$$\lim_{t\to\pm\infty} \sup_{|s|\leq\alpha} |t|^{1+a}\|K(t+is)\| < \infty. \tag{4.2}$$

Let $0 < T \in \mathbf{R}$ be such that

$$\min_{z\in\Omega} \text{Re } z > -T, \quad \text{and } \max_{z\in\Omega} \text{Re } z < +T. \tag{4.3}$$

All quantities encountered so far are analytic in $S_\alpha \cap \{z||\text{Re } z| > T\}$, and we denote by a "$\sim$" any analytic continuation in that set. As noticed earlier

$$\widetilde{W}'(z) = K(z)\widetilde{W}(z), \quad z \in S_\alpha \cap \{z||\text{Re } z| > T\} \tag{4.4}$$

so that it follows from (4.2) that the limits

$$\lim_{t\to\pm\infty} \widetilde{W}(t+is) = \widetilde{W}(\pm\infty) \tag{4.5}$$

exist uniformly in $s \in]-\alpha,\alpha[$. Consequently, see (3.16),

$$\lim_{t\to\pm\infty} |t|^{1+a} \sup_{|s|\leq\alpha} |\tilde{a}_{jk}(t+is)| < \infty, \quad \forall j,k \in \{1,\cdots,n\}. \tag{4.6}$$

Finally, for $|t| > T$, we can write

$$\begin{aligned} \text{Im } \widetilde{\Delta}_{jk}(t+is) &= \text{Im } \left(\int_\eta e_j(z)dz - \int_\eta e_k(z)dz \right) \\ &+ \int_0^s \text{Re } (e_{\sigma_j(j)}(t+is') - e_{\sigma_j(k)}(t+is'))ds', \end{aligned} \tag{4.7}$$

where this equation is obtained by deforming the path of integration from 0 to $z = t+is$ into a loop η based at the origin, which may encircle points of Ω, followed by the real axis from 0 to Re z and a vertical path from Re z to z, see figure 2. Hence we have

$$\sup_{z\in S_\alpha\cap\{z||\text{Re } z|>T\}} \text{Im } \widetilde{\Delta}_{jk}(z) < \infty, \tag{4.8}$$

which, together with (4.6) yields the existence of the limits

$$\lim_{t\to\pm\infty} \tilde{c}_j(t+is) = \tilde{c}_j(\pm\infty) \tag{4.9}$$

uniformly in $s \in]-\alpha,\alpha[$. We now define the domains in which useful estimates can be obtained.

Figure 3: The path β along which the analytic continuation of $\Delta_{jk}(t)$ in D_j is taken.

Definition: *Let $j \in \{1, \cdots, n\}$ be fixed. A* dissipative domain for the index j, *$D_j \subset S_\alpha \backslash \Omega$, is such that*

$$\sup_{z \in D_j} \text{Re } z = \infty, \quad \inf_{z \in D_j} \text{Re } z = -\infty, \tag{4.10}$$

and is defined by the property that for any $z \in D_j$ and any $k \in \{1, \cdots, n\}$, there exists a path $\gamma^k \subset D_j$ parameterized by $u \in]-\infty, t]$ which links $-\infty$ to z

$$\lim_{u \to -\infty} \text{Re } \gamma^k(u) = -\infty, \quad \gamma^k(t) = z \tag{4.11}$$

with

$$\sup_{z \in D_j} \sup_{u \in]-\infty, t]} \left| \frac{d}{du} \gamma^k(u) \right| < \infty \tag{4.12}$$

and satisfies the monotonicity condition

$$\text{Im } \widetilde{\Delta}_{jk}(\gamma^k(u)) \ \textit{ is a non decreasing function of } u \in]-\infty, t]. \tag{4.13}$$

Such a path is a dissipative path for $\{jk\}$. *Here $\widetilde{\Delta}_{jk}(z)$ is the analytic continuation of*

$$\Delta_{jk}(t) = \int_0^t (e_j(t') - e_k(t'))dt', \quad t \in \mathbf{R}, \tag{4.14}$$

in D_j along a path β described in figure 3 going from 0 to $-T \in \mathbf{R}$ along the real axis and then vertically up or down until it reaches D_j, where $T > 0$ is chosen as in (4.3).

Remark:

The finiteness of Ω insures the existence of such a path β.

Let $\widetilde{c}_k(z)$, $k = 1, 2, \cdots, n$, $z \in D_j$, be the analytic continuations of $c_k(t)$ along the same path β which are solutions of the analytic continuation of (2.13) in D_j along β

$$\widetilde{c}_k'(z) = \sum_{l=1}^{n} \widetilde{a}_{kl}(z) \mathrm{e}^{i\widetilde{\Delta}_{kl}(z)/\varepsilon} \widetilde{c}_l(z). \tag{4.15}$$

We take as initial conditions in D_j

$$\lim_{\text{Re } z \to -\infty} \widetilde{c}_k(z) = \lim_{t \to -\infty} c_k(t) = \delta_{jk}, \quad k = 1, \cdots, n. \tag{4.16}$$

and we define

$$x_k(z) = \widetilde{c}_k(z) \mathrm{e}^{i\widetilde{\Delta}_{jk}(z)/\varepsilon}, \quad z \in D_j, \ k = 1, \cdots, n. \tag{4.17}$$

Lemma 4.1 *In a dissipative domain for the index j we get the estimates*

$$\sup_{z\in D_j} |x_j(z)-1| = \mathcal{O}(\varepsilon) \tag{4.18}$$

$$\sup_{z\in D_j} |x_k(z)| = \mathcal{O}(\varepsilon), \quad \forall k \neq j. \tag{4.19}$$

Remark:
The real axis is a dissipative domain for all indices. In this case we have $\tilde{c}_j(t) \equiv c_j(t)$. Hence we get from the application of the lemma for all indices successively that

$$S = \mathbf{I} + \mathcal{O}(\varepsilon). \tag{4.20}$$

The estimates we are looking for are then just a direct corollary.

Proposition 4.1 *Assume there exists a dissipative domain D_j for the index j. Let η_j be a loop based at the origin which encircles all the degeneracies between the real axis and D_j and let σ_j be the permutation of labels associated with η_j, in the spirit of the remark ending the previous section. The loop η_j is negatively, respectively positively, oriented if D_j is above, respectively below, the real axis. Then the solution of (2.13) subjected to the initial conditions $c_k(-\infty) = \delta_{jk}$ satisfies*

$$\begin{aligned} c_{\sigma_j(j)}(+\infty) &= e^{-i\theta_j(\eta_j)} e^{-i\int_{\eta_j} e_j(z)dz/\varepsilon}(1+\mathcal{O}(\varepsilon)) &(4.21)\\ c_{\sigma_j(k)}(+\infty) &= \mathcal{O}\left(\varepsilon e^{\mathrm{Im}\int_{\eta_j} e_j(z)dz/\varepsilon + h_j(e_{\sigma_j(j)}(+\infty)-e_{\sigma_j(k)}(+\infty))/\varepsilon}\right), &(4.22)\end{aligned}$$

with $h_j \in [H_j^-, H_j^+]$, where $H_j^{\pm}$ is the maximum, respectively minimum, imaginary part of the points at $+\infty$ in D_j

$$H^+ = \lim_{t\to+\infty} \sup_{s|t+is\in D_j} s, \quad H^- = \lim_{t\to+\infty} \inf_{s|t+is\in D_j} s. \tag{4.23}$$

Thus we see that it is possible to get the (exponentially small) asymptotic behavior of the element $s_{\sigma_j(j),j}$ of the S-matrix, provided there exists a dissipative domain for the index j. The difficult part of the problem is of course to prove the existence of such domains D_j, which do not necessarily exist, and to have enough of them to compute the asymptotic of the whole S-matrix. This task is the equivalent for n-level systems to the study of the global behavior of the Stokes lines for 2-level systems. We postpone this aspect of the problem to the next section. Note that we also get from this result an exponential bound on the elements $s_{\sigma_j(k),j}$ of the S-matrix, $k \neq j$, which may or may not be useful. If η_j encircles no point of Ω, we cannot get the asymptotic behavior of $s_{\sigma_j(j),j}$ but we only get the exponential bounds. Since our main concern is asymptotic behaviors, we call the corresponding dissipative domain trivial.

Remark:
In contrast with the 2-level case, see [JP4], we have to work with dissipative domains instead of working with one dissipative path for all indices. Indeed, it is not difficult to convince oneself with specific 3-level cases that such a dissipative path may not exist, even when the eigenvalue degeneracies are close to the real axis. In return, we prove below the existence of dissipative domains in this situation.

Proof:
The asymptotic relation is a direct consequence of lemma 3.1, (4.9), (4.17) and the first part

of the lemma. The estimate is a consequence of the same equations, the second estimate of the lemma and the identity, for $t > T$,

$$\begin{aligned}\text{Im } \widetilde{\Delta}_{jk}(t+is) &= \text{Im } \left(\int_{\eta_j} e_j(z)dz - \int_{\eta_j} e_k(z)dz \right) \\ &+ \int_0^s \text{Re } (e_{\sigma_j(j)}(t+is') - e_{\sigma_j(k)}(t+is'))ds'. \end{aligned} \tag{4.24}$$

The path of integration from 0 to z for $\widetilde{\Delta}_{jk}(z)$ is deformed into the loop η_j followed by the real axis from 0 to Re z and a vertical path from Re z to z. It remains to take the limit $t \to +\infty$. □

Proof of lemma 4.1:

We rewrite equations (4.15) and (4.16) as an integral equation and perform an integration by parts on the exponentials

$$\begin{aligned}\widetilde{c}_k(z) &= \delta_{jk} - i\varepsilon \sum_{l=1}^n \frac{\widetilde{a}_{kl}(z)}{\widetilde{e}_k(z) - \widetilde{e}_l(z)} e^{i\widetilde{\Delta}_{kl}(z)/\varepsilon} \widetilde{c}_l(z) \\ &+ i\varepsilon \sum_{l=1}^n \int_{-\infty}^z \left(\frac{\widetilde{a}_{kl}(z')}{\widetilde{e}_k(z') - \widetilde{e}_l(z')} \right)' e^{i\widetilde{\Delta}_{kl}(z')/\varepsilon} \widetilde{c}_l(z')dz' \\ &+ i\varepsilon \sum_{l,m=1}^n \int_{-\infty}^z \frac{\widetilde{a}_{kl}(z')\widetilde{a}_{lm}(z')}{\widetilde{e}_k(z') - \widetilde{e}_l(z')} e^{i\widetilde{\Delta}_{km}(z')/\varepsilon} \widetilde{c}_m(z')dz'. \end{aligned} \tag{4.25}$$

Since all eigenvalues are distinct in $S_\alpha \backslash \Omega$, the denominators are always different from 0. Due to equation (4.9), the height above or below the real axis at which we start the integration is irrelevant, so that we can use the symbol $-\infty$ as lower integration bound. Note that the integrated term vanishes at $-\infty$. We have also used the identity

$$\widetilde{\Delta}_{kl}(z') + \widetilde{\Delta}_{lm}(z') \equiv \widetilde{\Delta}_{km}(z'). \tag{4.26}$$

In terms of the functions x_k we get, using the same identity,

$$\begin{aligned}x_k(z) &= \delta_{jk} - i\varepsilon \sum_{l=1}^n \frac{\widetilde{a}_{kl}(z)}{\widetilde{e}_k(z) - \widetilde{e}_l(z)} x_l(z) \\ &+ i\varepsilon \sum_{l=1}^n \int_{-\infty}^z \left(\frac{\widetilde{a}_{kl}(z')}{\widetilde{e}_k(z') - \widetilde{e}_l(z')} \right)' e^{i(\widetilde{\Delta}_{jk}(z) - \widetilde{\Delta}_{jk}(z'))/\varepsilon} x_l(z')dz' \\ &+ i\varepsilon \sum_{l,m=1}^n \int_{-\infty}^z \frac{\widetilde{a}_{kl}(z')\widetilde{a}_{lm}(z')}{\widetilde{e}_k(z') - \widetilde{e}_l(z')} e^{i(\widetilde{\Delta}_{jk}(z) - \widetilde{\Delta}_{jk}(z'))/\varepsilon} x_m(z')dz'. \end{aligned} \tag{4.27}$$

We introduce the quantity

$$|||x|||_j = \sup_{\substack{z \in D_j \\ l=1,\cdots,n}} |x_l(z)| \tag{4.28}$$

and consider for each k the equation (4.27) along the dissipative path $\gamma^k(u)$ described in the definition of D_j, such that

$$\left| e^{i(\widetilde{\Delta}_{jk}(\gamma^k(t)) - \widetilde{\Delta}_{jk}(\gamma^k(u)))/\varepsilon} \right| \leq 1 \tag{4.29}$$

when $u \leq t$ along that path. Due to the integrability of the $\widetilde{a}_{kl}(z)$ at infinity and the uniform boundedness of $d\gamma^k(u)/du$, we get the estimate

$$|x_k(z) - \delta_{kj}| \leq \varepsilon |||x|||_j A \tag{4.30}$$

for some constant A uniform in $z \in D_j$, hence

$$|||x|||_j \leq 1 + \varepsilon |||x|||_j A. \tag{4.31}$$

Consequently, for ε small enough

$$|||x|||_j \leq 2. \tag{4.32}$$

And the result follows. □

5 Superasymptotic improvement

All results above can be substantially improved by using the so-called superasymptotic renormalization method [Be], [N], [JP2]. The joint use of complex WKB analysis and superasymptotic renormalization is very powerful, as demonstrated recently in [JP4] for 2-level systems, and allows, roughly speaking, to replace all remainders $\mathcal{O}(\varepsilon)$ by $\mathcal{O}(\mathrm{e}^{-\kappa/\varepsilon})$, where $\kappa > 0$. We briefly show how to achieve this improvement in the case of n-level systems.

Let $H(z)$ satisfy H1, H2 and H3 in S_α and let

$$\widehat{S}_\alpha = S_\alpha \backslash \cup_{r=1,\cdots,p} (J_r \cup \overline{J_r}), \tag{5.1}$$

where each J_r is an open domain containing one point of Ω only in the open upper half plane. Hence, any analytic continuation $e_j(z)$ of $e_j(t)$, $t \in \mathbf{R}$, in $\widehat{S}_\alpha$ is isolated in the spectrum of $H(z)$ so that $e_j(z)$ is analytic and multivalued in $\widehat{S}_\alpha$, and the same is true for the corresponding analytic continuation $P_j(z)$ of $P_j(t)$, $t \in \mathbf{R}$. Let σ_r be the permutation associated with the loop ζ_r based at the origin which encircles J_r once, such that

$$\widetilde{e}_j(z) = e_{\sigma_r(j)}(z), \tag{5.2}$$

with the convention of section 3. The matrix $K(z)$ is analytic and single valued in $\widehat{S}_\alpha$. Consider the single valued analytic matrix

$$H_1(z, \varepsilon) = H(z) - i\varepsilon K(z), \quad z \in \widehat{S}_\alpha. \tag{5.3}$$

For ε small enough, the spectrum of $H_1(z,\varepsilon)$ is non degenerate $\forall z \in \widehat{S}_\alpha$ so that its eigenvalues $e_j^1(z,\varepsilon)$ and eigenprojectors $P_j^1(z,\varepsilon)$ are multivalued analytic functions in $\widehat{S}_\alpha$. Moreover, for ε small enough, the analytic continuations of $e_j^1(z,\varepsilon)$ and $P_j^1(z,\varepsilon)$ around J_r satisfy

$$\begin{aligned} \widetilde{e}_j^1(z) &= e^1_{\sigma_r(j)}(z) && (5.4)\\ \widetilde{P}_j^1(z) &= P^1_{\sigma_r(j)}(z), && (5.5) \end{aligned}$$

as can be easily deduced from (5.2) by perturbation theory. Consequently the matrix

$$K_1(z,\varepsilon) = \sum_{j=1}^{m} P_j^{1\prime}(z,\varepsilon) P_j^1(z,\varepsilon) \tag{5.6}$$

is analytic and single valued in $\widehat{S}_\alpha$. Defining the single valued matrix

$$H_2(z,\varepsilon) = H(z) - i\varepsilon K_1(z,\varepsilon), \quad z \in \widehat{S}_\alpha, \tag{5.7}$$

we can repeat the argument, for ε small enough. By induction we set for any $q \in \mathbf{N}$,

$$\begin{aligned} H_q(z,\varepsilon) &= H(z) - i\varepsilon K_{q-1}(z,\varepsilon) && (5.8)\\ K_{q-1}(z,\varepsilon) &= \sum_{j=1}^{m} P_j^{q-1\prime}(z,\varepsilon) P_j^{q-1}(z,\varepsilon), \quad z \in \widehat{S}_\alpha && (5.9) \end{aligned}$$

for ε is small enough. We have

$$H_q(z,\varepsilon)=\sum_{j=1}^{m} e_j^q(z,\varepsilon)P_j^q(z,\varepsilon), \tag{5.10}$$

where the eigenvalues and eigenprojections are multivalued in $\widehat{S}_\alpha$ and satisfy

$$\begin{aligned} \widetilde{e}_j^q(z,\varepsilon) &= e^q_{\sigma_r(j)}(z,\varepsilon) && (5.11)\\ \widetilde{P}_j^q(z,\varepsilon) &= P^q_{\sigma_r(j)}(z,\varepsilon), \quad j=1,\cdots,n, && (5.12)\end{aligned}$$

with the notations of (5.2). We quote from [JP4], [JP2] the main proposition regarding this construction.

Proposition 5.1 *Let $H(z)$ satisfy H1, H2 and H3 in S_α and let $\widehat{S}_\alpha$ be defined as above. Then there exist constants $c>0$, $\varepsilon^*>0$ and a real function $b(t)$ with $\lim_{t\rightarrow\pm\infty}|t|^{1+a}b(t)<\infty$, such that*

$$\begin{aligned} &\|K_q(z,\varepsilon)-K_{q-1}(z,\varepsilon)\|\leq b(\mathrm{Re}\ z)\varepsilon^q c^q q! && (5.13)\\ &\|K_q(z,\varepsilon)\|\leq b(\mathrm{Re}\ z), && (5.14)\end{aligned}$$

for all $z\in\widehat{S}_\alpha$, all $\varepsilon<\varepsilon^*$ and all $q\leq q^*(\varepsilon)\equiv[1/ec\varepsilon]$, where $[y]$ denotes the integer part of y and e is the basis of the neperian logarithm.

We can deduce from this that in $\widehat{S}_\alpha$

$$\begin{aligned} e_j^q(z,\varepsilon) &= e_j(z)+\mathcal{O}(\varepsilon^2 b(\mathrm{Re}\ z)) && (5.15)\\ P_j^q(z,\varepsilon) &= e_j(z)+\mathcal{O}(\varepsilon(\mathrm{Re}\ z)), \quad \forall q\leq q^*(\varepsilon). && (5.16)\end{aligned}$$

We introduce the notation $f^{q^*(\varepsilon)}\equiv f^*$ for any quantity f^q depending on the index q and we drop from now on the ε in the arguments of the functions we encounter. We define the multivalued analytic matrix $W_*(z)$ for $z\in\widehat{S}_\alpha$ by

$$W_*{}'(z)=K_*(z)W_*(z), \quad W_*(0)=\mathbf{I}. \tag{5.17}$$

Due to the above observations and proposition 5.1, $W_*(z)$ enjoys all properties $W(z)$ does, such as

$$\begin{aligned} &W_*(z)P_j^*(z)=P_j^*(0)W_*(z) && (5.18)\\ &\widetilde{W}^*(z)=W_*(z)W_*(\zeta_r) && (5.19)\end{aligned}$$

and, uniformly in s,

$$\lim_{t\pm\infty} W_*(t+is)=W_*(\infty). \tag{5.20}$$

Thus we define for any $z\in\widehat{S}_\alpha$ as set of eigenvectors of $H_*(z)$ by

$$\varphi_j^*(z)=W_*(z)\varphi_j^*(0), \tag{5.21}$$

where

$$H_*(0)\varphi_j^*(0)=e_j^*(0)\varphi_j^*(0), \quad j=1,\cdots,n, \tag{5.22}$$

and which satisfy

$$\widetilde{\varphi}_j^*(0)=\mathrm{e}^{-i\theta_j^*(\zeta_r)}\varphi^*_{\sigma_r(j)}(0), \tag{5.23}$$

with

$$\theta_j^*(\zeta_r) = \theta(\zeta_r) + \mathcal{O}(\varepsilon) \in \mathbf{C}. \tag{5.24}$$

Let us expand the solution of (2.1) on this multivalued set of eigenvectors as

$$\psi(z) = \sum_{j=1}^{n} c_j^*(z) \mathrm{e}^{-i\int_0^z e_j^*(z')dz'/\varepsilon} \varphi_j^*(z). \tag{5.25}$$

Since the analyticity properties of the eigenvectors and eigenvalues of $H_*(z)$ are the same as those enjoyed by the eigenvectors and eigenvalues of $H(z)$, we get as in lemma 3.1

$$\widetilde{c}_j^*(z)\mathrm{e}^{-i\int_{\zeta_r} e_j^*(u)du/\varepsilon}\mathrm{e}^{-i\theta_j^*(\zeta_r)} = c^*_{\sigma_r(j)}(z), \quad \forall z \in \widehat{S}_\alpha. \tag{5.26}$$

Substituting (5.25) in (2.1), we see that the multivalued coefficients $c_j^*(z)$ satisfy in $\widehat{S}_\alpha$ the differential equation

$$c_j^{*\prime}(z) = \sum_{k=1}^{n} a_{jk}^*(z)\mathrm{e}^{i\Delta_{jk}^*(z)/\varepsilon} c_k^*(z) \tag{5.27}$$

where

$$\Delta_{jk}^*(z) = \int_0^z e_j^*(z') - e_k^*(z')dz' \tag{5.28}$$

and

$$a_{jk}^*(z) = \frac{\langle \varphi_j^*(z)(0)|P_j^*(z)(0)W_*(z)^{-1}(K_{q^*-1}(z) - K_{q^*}(z))W_*(z)\varphi_k^*(0)\rangle}{\|\varphi_j^*(0)\|^2}, \tag{5.29}$$

to be compared with (3.16). The key point of this construction is that it follows from proposition 5.1 with $q = q^*(\varepsilon)$ that

$$|a_{jk}^*(z)| \leq 2b(\mathrm{Re}\ z)\mathrm{e}^{-\kappa/\varepsilon}, \quad \forall z \in \widehat{S}_\alpha \tag{5.30}$$

where $\kappa = 1/ec > 0$, and from (5.15) that

$$\mathrm{Im}\ \Delta_{jk}^*(z) = \mathrm{Im}\ \Delta_{jk}(z) + \mathcal{O}(\varepsilon^2), \tag{5.31}$$

uniformly in $z \in \widehat{S}_\alpha$. Thus, we deduce from (5.30) that the limits

$$\lim_{t\to\pm\infty} c_j^*(t+is) = c_j^*(\pm\infty), \quad j = 1, \cdots, n, \tag{5.32}$$

exist for any analytic continuation in $\widehat{S}_\alpha$. Moreover, along any dissipative path $\gamma^k(u)$ for $\{jk\}$, as defined above, we get from (5.31)

$$\left|\mathrm{e}^{i(\widetilde{\Delta}_{jk}^*(\gamma^k(t)) - \widetilde{\Delta}_{jk}^*(\gamma^k(u)))/\varepsilon}\right| = \mathcal{O}(1) \tag{5.33}$$

so that, reproducing the proof of lemma 4.1 we have

Lemma 5.1 *In a dissipative domain D_j, if $\widetilde{c}_k^*(-\infty) = c_k^*(-\infty) = \delta_{kj}$, then*

$$\widetilde{c}_j^*(z) = 1 + \mathcal{O}(e^{-\kappa/\varepsilon}) \tag{5.34}$$

$$e^{i\widetilde{\Delta}_{jk}(z)\varepsilon}\widetilde{c}_k^*(z) = \mathcal{O}\left(e^{-\kappa/\varepsilon}\right), \quad \forall k \neq j, \tag{5.35}$$

uniformly in $z \in \widehat{S}_\alpha$.

This lemma yields the improved version of our main result.

Proposition 5.2 *Under the conditions of proposition 4.1 and with the same notations. If* $c_k^*(-\infty)=\delta_{jk}$, *then*

$$\begin{aligned} c^*_{\sigma_j(j)}(+\infty) &= e^{-i\theta_j^*(\eta_j)} e^{-i\int_{\eta_j} e_j^*(z)dz/\varepsilon} \left(1+\mathcal{O}\left(e^{-\kappa/\varepsilon}\right)\right) && (5.36)\\ c^*_{\sigma_j(k)}(+\infty) &= \mathcal{O}\left(e^{-\kappa/\varepsilon} e^{\mathrm{Im}\int_{\eta_j} e_j(z)dz/\varepsilon + h_j(e_{\sigma_j(j)}(+\infty)-e_{\sigma_j(k)}(+\infty))/\varepsilon}\right). && (5.37)\end{aligned}$$

Note that we may or may not replace $e_j(z)$ by $e_j^*(z)$ in the estimate without altering the result. It remains to make the link between the S-matrix and the $c_k^*(+\infty)$'s of the proposition explicit. We define $\beta_j^{*\pm}$ by the relations ($H_*(z)$ and $H(z)$ coincide at $\pm\infty$),

$$\varphi_j^*(\pm\infty) = \mathrm{e}^{-i\beta_j^{*\pm}} \varphi_j(\pm\infty). \tag{5.38}$$

By comparison of (5.25) and (2.12) we deduce the lemma

Lemma 5.2 *If* $c_k(t)$ *and* $c_k^*(t)$ *satisfy* $c_k(-\infty)=c_k^*(-\infty)=\delta_{jk}$, *then, the element* kj *of the* S*-matrix is given by*

$$\begin{aligned} s_{kj} &= c_k(+\infty) = e^{-i(\beta_k^{*+}-\beta_j^{*-})} e^{-i\int_0^{+\infty} e_k^*(t')-e_k(t')dt'/\varepsilon} e^{-i\int_{-\infty}^0 e_j^*(t')-e_j(t')dt'/\varepsilon} c_k^*(+\infty)\\ &\equiv e^{-i\alpha_{kj}^*} c_k^*(+\infty), && (5.39)\end{aligned}$$

with $\beta_j^{*\pm}=\mathcal{O}(\varepsilon)$ *and* $\int_{\pm\infty}^0 e_j^*(t')-e_j(t')dt'/\varepsilon=\mathcal{O}(\varepsilon)$, *i.e.* $e^{-i\alpha_{kj}^*}=1+\mathcal{O}(\varepsilon)$.

Remarks:
i) Proposition 5.2 together with lemma 5.2 are the main results of the first part of this paper.
ii) As a direct consequence of these estimates on the real axis we have

$$s_{jk} = \mathcal{O}\left(\mathrm{e}^{-\kappa/\varepsilon}\right), \quad \forall k\neq j, \tag{5.40}$$

and

$$s_{jj} = \mathrm{e}^{-i\alpha_{jj}^*}\left(1+\mathcal{O}\left(e^{-\kappa/\varepsilon}\right)\right). \tag{5.41}$$

iii) It should be clear from the analysis just performed that all results obtained hold if the generator $H(z)$ in (2.1) is replaced by

$$H(z,\varepsilon) = H_0(z) + \mathcal{O}(\varepsilon b(\mathrm{Re}\ z)), \tag{5.42}$$

with $b(t)=\mathcal{O}(1/t^{1+a})$, provided $H_0(z)$ satisfies the hypotheses we assumed.

6 Avoided crossings

We now come to the second part of the paper in which we prove asymptotic formulas for the off-diagonal elements of the S-matrix, by means of the general set up presented above. To start with, we define a class of n-level systems for which we can prove the existence of one non trivial dissipative domains for all indices. They are obtained by means of systems exhibiting degeneracies of eigenvalues on the real axis, hereafter called real crossings, which we perturb in such a way that these degeneracies are lifted and turn to avoided crossings on the real axis. When the perturbation is small enough, this process moves the eigenvalue degeneracies off the real axis but they remain close to the place where the real crossings occurred. This method was used successfully in [J] to deal with 2-level systems. We do not attempt to list all cases in which dissipative domains can be constructed by means of this technique but rather present a wide class of examples which are relevant in the theory of quantum adiabatic transitions and in the theory of multichannel semiclassical scattering, as described below.

Let $H(t,\delta) \in M_n(\mathbf{C})$ satisfy the following assumptions.

H4 For each fixed $\delta \in [0,d]$, the matrix $H(t,\delta)$ satisfies H1 in a strip S_α independent of δ and $H(z,\delta)$, $\partial/\partial z H(z,\delta)$ are continuous as a functions of two variables $(z,\delta) \in S_\alpha \times [0,d]$. Moreover, it satisfies H2 uniformly in $\delta \in [0,d]$, with limiting values $H(\pm,\delta)$ which are continuous functions of $\delta \in [0,d]$.

H5 *For each $t \in \mathbf{R}$ and each $\delta \in [0,d]$, the spectrum of $H(t,\delta)$, denoted by $\sigma(t,\delta)$, consists in n real eigenvalues*

$$\sigma(t,\delta) = \{e_1(t,\delta), e_2(t,\delta), \cdots, e_n(t,\delta)\} \subset \mathbf{R} \tag{6.1}$$

which are distinct when $\delta > 0$

$$e_1(t,\delta) < e_2(t,\delta) < \cdots < e_n(t,\delta). \tag{6.2}$$

When $\delta = 0$, the functions $e_j(t,0)$ are analytic on the real axis and there exists a finite set of crossing points $\{t_1 \leq t_2 \leq \cdots \leq t_p\} \in \mathbf{R}$, $p \geq 0$, such that

i) $\forall t < t_1$,

$$e_1(t,0) < e_2(t,0) < \cdots < e_n(t,0). \tag{6.3}$$

ii) $\forall j < k \in \{1,2,\cdots,n\}$, there exists at most one t_r with

$$e_j(t_r,0) - e_k(t_r,0) = 0, \tag{6.4}$$

and if such a t_r exists we have

$$\frac{\partial}{\partial t}\left(e_j(t_r,0) - e_k(t_r,0)\right) > 0. \tag{6.5}$$

iii) $\forall j \in \{1,2,\cdots,n\}$, the eigenvalue $e_j(t,0)$ crosses eigenvalues whose indices are all superior to j or all inferior to j.

Remarks:

i) The parameter δ can be understood as a coupling constant controlling the strength of the perturbation.

ii)The eigenvalues $e_j(t,0)$ are assumed to be analytic on the real axis, because of the degeneracies on the real axis. However, if $H(t,\delta)$ is self adjoint for any $\delta \in [0,d]$, this follows from a theorem of Rellich, see [K].

iii) We give in figure 4 an example of pattern of crossings with the corresponding pattern of avoided crossings for which the above conditions are fulfilled.

iv) The crossings are assumed to be generic in the sense that the derivative of $e_j - e_k$ are non zero at the crossing t_r.

v) The crossing points $\{t_1, t_2, \cdots, t_p\}$ need not be distinct, which is important when the eigenvalues possess symmetries. However, for each $j = 1,\cdots,n$, the eigenvalue $e_j(t,\delta)$ experiences avoided crossings with $e_{j+1}(t,\delta)$ and/or $e_{j-1}(t,\delta)$ at a subset of distinct points $\{t_{r_1},\cdots,t_{r_j}\} \subseteq \{t_1,t_2,\cdots,t_p\}$.

We now state the main lemma of this section regarding the analyticity properties of the perturbed levels and the existence of dissipative domains for all indices in this perturbative context.

Figure 4: A pattern of eigenvalue crossings (bold curves) with the corresponding pattern of avoided crossings (fine curves) satisfying H5.

Lemma 6.1 *Let $H(t, \delta)$ satisfy H4 and H5. We can choose $\alpha > 0$ small enough so that the following assertions are true for sufficiently small $\delta > 0$:*
i) Let $\{t_{r_1}, \cdots, t_{r_j}\}$ be the set of avoided crossing points experienced by $e_j(t, \delta)$, $j = 1, \cdots, n$. For each j, there exists a set of distinct domains $J_r \in S_\alpha$, where $r \in \{r_1, \cdots, r_j\}$,

$$J_r = \{z = t + is| \, 0 \leq |t - t_r| < L, \, 0 < g < s < \alpha'\}, \tag{6.6}$$

with L small enough, $\alpha' < \alpha$ and $g > 0$ such that $e_j(-\infty, \delta)$ can be analytically continued in

$$S_\alpha^j = S_\alpha \backslash \cup_{r=r_1,\cdots,r_j} (J_r \cup \overline{J_r}). \tag{6.7}$$

ii) Let t_r be an avoided crossing point of $e_j(t, \delta)$ with $e_k(t, \delta)$, $k = j \pm 1$. Then the analytic continuation of $e_j(t_r, \delta)$ along a loop based at $t_r \in \mathbf{R}$ which encircles J_r once yields $\widetilde{e}_j(t_r, \delta)$ back at t_r with

$$\widetilde{e}_j(t_r, \delta) = e_k(t_r, \delta). \tag{6.8}$$

iii) For each $j = 1, \cdots, n$, there exists a dissipative domain D_j above or below the real axis in $S_\alpha \cap \{z = t + is| \, |s| \geq \alpha'\}$. The permutation σ_j associated with these dissipative domains (see proposition 4.1) are all given by $\sigma_j = \sigma$ where σ is the permutation which maps the index of the k^{th} eigenvalue $e_j(\infty, 0)$ numbered from the lowest one on k, for all $k \in \{1, 2, \cdots, n\}$.

Remarks:
i) In part ii) the same result is true along a loop encircling $\overline{J_r}$.
ii) The dissipative domains D_j of part iii) are located above (respectively below) all the sets J_r (resp. $\overline{J_r}$), $r = 1, \cdots, p$.
iii) The main interest of this lemma is that the sufficient conditions required for the existence of dissipative domains in the complex plane can be deduced from the behavior of the eigenvalues on the *real* axis.
iv) We emphasize that more general types of avoided crossings than those described in H5 may lead to the existence of dissipative domains for *certain* indices but we want to get dissipative domains for *all* indices. For example, if part iii) of H5 is satisfied for certain indices only, then part iii) of lemma 6.1 is satisfied for those indices only.

v) Note also that there are patterns of eigenvalue crossings for which there exist no dissipative domain for some indices. For example, if $e_j(t,0)$ and $e_k(t,0)$ display two crossings, it is not difficult to see from the proof of the lemma that no dissipative domains can exist for j or k.

We postpone the proof of this lemma to the end of the section and go on with its consequences. By applying the results of the previous section we get

Theorem 6.1 *Let $H(t,\delta)$ satisfy H4 and H5. If $\delta>0$ is small enough, the elements $\sigma(j)j$ of the S-matrix, with $\sigma(j)$ defined in lemma 6.1, are given in the limit $\varepsilon\rightarrow 0$ for all $j=1,\cdots,n$, by*

$$s_{\sigma(j)j}=\prod_{k=j}^{\sigma(j)\mp 1} e^{-i\theta_k(\zeta_k)}e^{-i\int_{\zeta_k}e_k(z,\delta)dz/\varepsilon}\left(1+\mathcal{O}(\varepsilon)\right),\quad \sigma(j)\begin{cases}>j\\<j\end{cases}\tag{6.9}$$

where, for $\sigma(j)>j$ (respectively $\sigma(j)<j$), ζ_k, $k=j,\cdots,\sigma(j)\mp 1$, denotes a negatively (resp. positively) oriented loop based at the origin which encircles the set J_r (resp. $\overline{J_r}$ corresponding to the avoided crossing between $e_k(t,\delta)$ and $e_{k+1}(t,\delta)$ (resp. $e_{k-1}(z,\delta)$)) at t_r, $\int_{\zeta_k}e_k(z,\delta)dz$ denotes the integral along ζ_k of the analytic continuation of $e_k(0,\delta)$ and $\theta_k(\zeta_k)$ is the corresponding factor defined by (3.14), see figure 5.

More accurately, with the notations of section 5, we have the improved formula

$$s_{\sigma(j)j}=e^{-i\alpha^*_{\sigma(j)j}}\prod_{k=j}^{\sigma(j)\mp 1} e^{-i\theta^*_k(\zeta_k)}e^{-i\int_{\zeta_k}e^*_k(z,\delta)dz/\varepsilon}\left(1+\mathcal{O}\left(e^{-\kappa/\varepsilon}\right)\right),\quad \sigma(j)\begin{cases}>j\\<j\end{cases}\tag{6.10}$$

The element $\sigma(l)j$, $l\neq j$, are estimated by

$$s_{\sigma(l)j}=\mathcal{O}\left(\varepsilon e^{h(e_{\sigma(j)}(\infty,\delta)-e_{\sigma(l)}(\infty,\delta))/\varepsilon}\prod_{k=j}^{\sigma(j)\mp 1} e^{\mathrm{Im}\int_{\zeta_k}e_k(z,\delta)dz/\varepsilon}\right),\quad \sigma(j)\begin{cases}>j\\<j\end{cases}\tag{6.11}$$

where h is strictly positive (resp. negative) for $\sigma(j)>j$ (respectively $\sigma(j)<j$).

Remarks:
i) As the eigenvalues are continuous at the degeneracy points, we have that

$$\lim_{\delta\rightarrow 0}\mathrm{e}^{-i\int_{\zeta_k}e_k(z,\delta)dz}=0,\quad \forall k=1,\cdots,p.\tag{6.12}$$

ii) The remainders $\mathcal{O}(\varepsilon)$ depend on δ but it should be possible to get estimates which are valid as both ε and δ tend to zero, in the spirit of [J], [MN] and [R].
iii) This result shows that one off-diagonal element per column of the S-matrix at least can be computed asymptotically. However, it is often possible to get more elements by making use of symmetries of the S-matrix. Moreover, if there exist dissipative domains going above or below other eigenvalue degeneracies further away in the complex plane, other elements of the S-matrix can be computed.
iv) Finally, note that all starred quantities in (6.10) depend on ε.
Proof: The first thing to determine is whether the loops ζ_k are above or below the real axis. Since the formulas we deduce from the complex WKB analysis are asymptotic formulas, it suffices to choose the case which yields exponential decay of $s_{\sigma(j)j}$. It is readily checked in the proof of lemma 6.1 below that if $\sigma(j)>j$, D_j is above the real axis and if $\sigma(j)<j$, D_j is below the real axis. Then it remains to explain how to pass from the loop η_j given in proposition 4.1 to the set of loops ζ_k, $k=j,\cdots,\sigma(j)-1$. We briefly deal with the case

Figure 5: The loops η_j and ζ_k, $k = j, \cdots, \sigma(j) - 1$.

$\sigma(j) > j$, the other case being similar. It follows from lemma 6.1 that we can deform η_j into the set of loops ζ_k, each associated with one avoided crossing, as described in figure 5. Thus we have

$$\int_{\eta_j} = \sum_{k=j}^{\sigma(j)-1} \int_{\zeta_k} \tag{6.13}$$

for the decay rate and, see 3.10,

$$W(\eta_j) = W(\zeta_{\sigma(j)-1}) \cdots W(\zeta_{j+1}) W(\zeta_j) \tag{6.14}$$

for the prefactors. Let ν_j be a negatively oriented loop based at t_r which encircles J_r as described in lemma 6.1. Consider now the loop ζ_j associated with this avoided crossing and deform it to the path obtained by going from 0 to t_r along the real axis, from t_r to t_r along ν_j and back from t_r to the origin along the real axis. By the point ii) of the lemma we get

$$\widetilde{e}_j(0, \delta) = e_{j+1}(0, \delta) \tag{6.15}$$

along ζ_j, and, accordingly (see (3.14)),

$$\widetilde{\varphi}_j(0, \delta) = \mathrm{e}^{-i\theta_j(\zeta_j)} \varphi_{j+1}(0, \delta). \tag{6.16}$$

This justifies the first factor in the formula. By repeating the argument at the next avoided crossings, keeping in mind that we get $e_{j+1}(0, \delta)$ at the end of ζ_j and so on, we get the final result. The estimate on $s_{\sigma(l)j}$ is obtained by direct application of lemma 6.1. □

Proof of lemma 6.1: In the sequel we shall denote "$\frac{\partial}{\partial t}$" by a "$\prime$". We have to consider the analyticity properties of $\widetilde{e}_j(z, \delta)$ and define domains in which every point z can be reached from $-\infty$ by means of a path $\gamma(u)$, $u \in]-\infty, t]$, $\gamma(t) = z$ such that Im $\widetilde{\Delta}_{jk}(\gamma(u), \delta)$ is non decreasing in u for certain indices $j \neq k$ when $\delta > 0$ is fixed. Note that by Schwarz's principle if $\gamma(u)$ is dissipative for $\{jk\}$, then $\overline{\gamma(u)}$ is dissipative for $\{kj\}$. When $\gamma(u) = \gamma_1(u) + i\gamma_2(u)$ is differentiable, saying that $\gamma(u)$ is dissipative for $\{jk\}$ is equivalent to

$$\begin{aligned}&\text{Re } (\widetilde{e}_j(\gamma(u), \delta) - \widetilde{e}_k(\gamma(u), \delta))\dot{\gamma}_2(u) + \text{Im } (\widetilde{e}_j(\gamma(u), \delta) - \widetilde{e}_k(\gamma(u), \delta))\dot{\gamma}_1(u) \geq 0 \\ &\forall u \in]-\infty, t]\end{aligned} \tag{6.17}$$

where "$\dot{}$" denotes the derivative with respect to u. Moreover, if the eigenvalues are analytic in a neighborhood of the real axis, we have the relation in that neighborhood

$$\text{Im }(\tilde{e}_j(t+is,\delta)-\tilde{e}_k(t+is,\delta))=\int_0^s \text{Re }(\tilde{e}'_j(t+is',\delta)-\tilde{e}'_k(t+is',\delta))ds', \tag{6.18}$$

which is a consequence of the Cauchy-Riemann identity. We proceed as follows. We construct dissipative domains above and below the real axis when $\delta=0$ and we show that they remain dissipative for the perturbed quantities $\widetilde{\Delta}_{jk}(z,\delta)$ provided δ is small enough. We introduce some quantities to be used in the construction. Let $C_r\in\{1,\cdots,n\}^2$ denote the set of distinct couples of indices such that the corresponding eigenvalues experience one crossing at $t=t_r$. Similarly, $N\in\{1,\cdots,n\}^2$ denotes the set of couples of indices such that the corresponding eigenvalues never cross.
Let $I_r=[t_r-L,t_r+L]\in\mathbf{R}$, $r=1,\cdots,p$, with L so small that

$$\min_{r\in\{1,\cdots,p\}}\ \min_{\{jk\}\in C_r,\, j<k}\ \inf_{t\in I_r}(e'_j(t,0)-e'_k(t,0))\equiv 4c>0. \tag{6.19}$$

This relation defines the constant c and we also define b by

$$\min_{r\in\{1,\cdots,p\}}\ \min_{\{jk\}\in C_r,\, j<k}\ \inf_{t\in\mathbf{R}\setminus I_r}|e_j(t,0)-e_k(t,0)|\geq 4b>0 \tag{6.20}$$

$$\min_{\{jk\}\in N,\, j<k}\ \inf_{t\in\mathbf{R}}|e_j(t,0)-e_k(t,0)|\geq 4b>0. \tag{6.21}$$

We further introduce

$$I_r^\alpha=\{z=t+is|t\in I_r, |s|\leq\alpha\},\quad r=1,\cdots,p. \tag{6.22}$$

Then we choose α small enough so that the only points of degeneracy of eigenvalues in S_α are on the real axis and

$$\min_{r\in\{1,\cdots,p\}}\ \min_{\{jk\}\in C_r,\, j<k}\ \inf_{z\in I_r^\alpha}\text{Re }(e'_j(z,0)-e'_k(z,0))>2c>0 \tag{6.23}$$

$$\min_{r\in\{1,\cdots,p\}}\ \min_{\{jk\}\in C_r,\, j<k}\ \inf_{z\in S_\alpha\setminus I_r^\alpha}|\text{Re }(e_j(z,0)-e_k(z,0))|>2b>0 \tag{6.24}$$

$$\min_{\{jk\}\in N,\, j<k}\ \inf_{z\in S_\alpha}|\text{Re }(e_j(z,0)-e_k(z,0))|>2b>0. \tag{6.25}$$

That this choice is always possible is a consequence of the analyticity of $e_j(z,0)$ close to the real axis and of the fact that we can work essentially in a compact, because of hypothesis H4. Let $a(t)$ be integrable on $\mathbf{R}$ and such that

$$\frac{a(t)}{2}>\max_{j<k\in\{1,\cdots,n\}}\ \sup_{|s|\leq\alpha}\left|\text{Re }(e'_j(t+is,0)-e'_k(t+is,0))\right|. \tag{6.26}$$

It follows from H4 that such functions exist.

Let $r\in\{1,\cdots,p\}$ and $\gamma_2(u)$ be a solution of

$$\begin{cases}\dot{\gamma}_2(u)=-\frac{\gamma_2(u)a(u)}{b} & u\in]-\infty,t_r-L]\\ \dot{\gamma}_2(u)=0 & u\in]t_r-L,t_r+L[\\ \dot{\gamma}_2(u)=+\frac{\gamma_2(u)a(u)}{b} & u\in[t_r+L,\infty[\end{cases} \tag{6.27}$$

with $\gamma_2(t_r)>0$. Then $\gamma_2(u)>0$ for any u, since

$$\begin{cases}\gamma_2(u)=\gamma_2(t_r)\mathrm{e}^{-\int_{t_r-L}^u a(u')du'/b} & u\in]-\infty,t_r-L]\\ \gamma_2(u)=\gamma_2(t_r) & u\in]t_r-L,t_r+L[\\ \gamma_2(u)=\gamma_2(t_r)\mathrm{e}^{\int_{t_r+L}^u a(u')du'/b} & u\in[t_r+L,\infty[\end{cases} \tag{6.28}$$

and since $a(u)$ is integrable, the limits

$$\lim_{u\to\pm\infty}\gamma_2(u)=\gamma_2(\pm\infty) \tag{6.29}$$

exist. Moreover, we can always choose $\gamma_2(t_r)>0$ sufficiently small so that $\gamma^r(u)\equiv u+i\gamma_2(u)\in S_\alpha$, for any real u. Let us verify that this path is dissipative for all $\{jk\}\in C_r$, $j<k$. For $u\in]-\infty,t_r-L]$, we have, using

$$\text{Re }(e_j(z,0)-e_k(z,0))<-2b<0,\quad \forall z\in S_\alpha\cap\{z|\text{Re }z\le t_r-L\} \tag{6.30}$$

and

$$|\text{Im }(e_j(t+is,0)-e_k(t+is,0))|<|s|\sup_{s'\in[0,s]}\left|\text{Re }(e_j'(t+is',0)-e_k'(t+is',0))\right|, \tag{6.31}$$

(see (6.18)), and the definition (6.26)

$$\begin{aligned}&\text{Re }(e_j(\gamma^r(u),0)-e_k(\gamma^r(u),0))\dot\gamma_2(u)+\text{Im }(e_j(\gamma^r(u),0)-e_k(\gamma^r(u),0))\dot\gamma_1(u)=\\&-\text{Re }(e_j(\gamma^r(u),0)-e_k(\gamma^r(u),0))\frac{\gamma_2(u)a(u)}{b}+\text{Im }(e_j(\gamma^r(u),0)-e_k(\gamma^r(u),0))>\\&2\gamma_2(u)a(u)-\gamma_2(u)a(u)/2>\gamma_2(u)a(u)>0.\end{aligned} \tag{6.32}$$

Similarly, when $u\ge t_r+L$ we get, using

$$\text{Re }(e_j(z,0)-e_k(z,0))>2b>0,\quad \forall z\in S_\alpha\cap\{z|\text{Re }z\ge t_r+L\}, \tag{6.33}$$

$$\begin{aligned}&\text{Re }(e_j(\gamma^r(u),0)-e_k(\gamma^r(u),0))\dot\gamma_2(u)+\text{Im }(e_1(\gamma^r(u),0)-e_k(\gamma^r(u),0))\dot\gamma_1(u)=\\&\text{Re }(e_j(\gamma^r(u),0)-e_k(\gamma^r(u),0))\frac{\gamma_2(u)a(u)}{b}+\text{Im }(e_j(\gamma^r(u),0)-e_k(\gamma^r(u),0))>\\&2\gamma_2(u)a(u)-\gamma_2(u)a(u)/2>\gamma_2(u)a(u)>0.\end{aligned} \tag{6.34}$$

Finally, for $s\in[t_r-L,t_r+L]$, we have with (6.23)

$$\begin{aligned}&\text{Im }(e_j(\gamma^r(u),0)-e_k(\gamma^r(u),0))=\int_0^{\gamma_2(u)}\text{Re }(e_j'(t'+is,0)-e_k'(t'+is,0))\ge\\&\gamma_2(u)2c>\gamma_2(u)c>0.\end{aligned} \tag{6.35}$$

Thus, $\gamma^r(u)$ is dissipative for all $\{jk\}\in C_r$, $j<k$. Note that the last estimate shows that it is not possible to find a dissipative path for $\{jk\}\in C_r$, $j<k$ below the real axis.

Consider now $\{jk\}\in N$, $j<k$ and let $\gamma_2(u)$ be a solution of

$$\dot\gamma_2(u)=-\frac{\gamma_2(u)a(u)}{b},\quad \gamma_2(0)>0,\ u\in]-\infty,+\infty[, \tag{6.36}$$

i.e.

$$\gamma_2(u)=\gamma_2(0)\mathrm{e}^{-\int_0^u a(u')du'/b}. \tag{6.37}$$

As above, we have $\gamma_2(u)>0$ for any u and we can choose $\gamma_2(0)>0$ small enough so that $\gamma^+(u)\equiv u+i\gamma_2(u)\in S_\alpha$ for any $u\in\mathbf{R}$. Since

$$\text{Re }(e_j(z,0)-e_k(z,0))>-2b\quad\forall z\in S_\alpha \tag{6.38}$$

we check by a computation analogous to (6.32) that $\gamma^+(u)$ is dissipative for $\{jk\}\in N$, $j<k$. Similarly, one verifies that if $\gamma_2(u)$ is the solution of

$$\dot\gamma_2(u)=\frac{\gamma_2(u)a(u)}{b},\quad \gamma_2(0)<0,\ u\in]-\infty,+\infty[\tag{6.39}$$

Figure 6: The dissipative domain D and some dissipative paths.

with $|\gamma_2(0)|$ small enough, the path $\gamma^-(u) \equiv u + i\gamma_2(u)$ below the real axis is in S_α for any $u \in \mathbf{R}$ and is dissipative for $\{jk\} \in N$, $j < k$ as well.

Finally, the complex conjugates of these paths yield dissipative paths above and below the real axis for $\{jk\} \in N$, $j > k$.

We now define the dissipative domains by means of their borders. Let $\gamma^+(u)$ and $\gamma^-(u)$, $u \in \mathbf{R}$, two dissipative paths in S_α defined as above with $|\gamma_2^-(0)|$ sufficiently small so that $\overline{\gamma^-}$ is below γ^+. We set

$$D = \{z = t + is | 0 < -\gamma_2^-(t) \leq s \leq \gamma_2^+(t),\, t \in \mathbf{R}\}. \tag{6.40}$$

Let $z \in D$, and $j \in \{1, \cdots, n\}$ be fixed. By assumption H5, the set X_j of indices k such that $\{jk\} \in C_r$ for some $r \in \{1, \cdots, p\}$ consists in values k satisfying $j < k$ or it consists in values k satisfying $j > k$. Let us assume the first alternative takes place. Now for any $k \in \{1, \cdots, n\}$, there are three cases.
1) If $k \in X_j$, then there exists a dissipative path $\gamma^r \in D$ for $\{jk\} \in C_r$, $j < k$ constructed as above which links $-\infty$ to z. It is enough to select the initial condition $\gamma_2(t_r)$ suitably, see figure 6.
2) Similarly, if $j < k \notin X_j$, there exists a dissipative path $\gamma^+ \in D$ for $\{jk\}$ constructed as above which links $-\infty$ to z obtained by a suitable choice of $\gamma_2(0)$.
3) Finally, if $k > j$, we can take as a dissipative path for $\{jk\}$, the path $\overline{\gamma^-} \in D$ constructed as above which links $-\infty$ to z with suitable choice of $\gamma_2(0)$. Hence D is dissipative for the index j, when $\delta = 0$. If j is such that the set X_j consists in points k with $k > j$, a similar argument with the complex conjugates of the above paths shows that the domain $\overline{D}$ below the real axis is dissipative for j when $\delta = 0$.

Let us show that these domains remain dissipative when $\delta > 0$ is not too large. We start by considering the analyticity properties of the perturbed eigenvalues $e_j(z, \delta)$, $\delta > 0$. Let $0 < \alpha' < \alpha$ be such that

$$I_r^{\alpha'} \cap (D \cup \overline{D}) = \emptyset, \quad \forall r = 1, \cdots, p. \tag{6.41}$$

The analytic eigenvalues $e_j(z, 0)$, $j \in \{1, \cdots, n\}$, are isolated in the spectrum of $H(z, 0)$ for any $z \in \widetilde{S}_\alpha$, where

$$\widetilde{S}_\alpha = S_\alpha \backslash \cup_{r=1,\cdots,p} I_r^{\alpha'}. \tag{6.42}$$

For any $j = 1, \cdots, n$ we get from perturbation theory [K], that the analytic continuations $\widetilde{e}_j(z, \delta)$ of $e_j(t_1 - L, \delta)$ in $\widetilde{S}_\alpha$ are all distinct in $\widetilde{S}_\alpha$, provided δ is small enough. This is due to the fact that assumption H5 implies the continuity of $H(z,\delta)$ in δ uniformly in $z \in S_\alpha$, as is easily verified. More precisely, for any fixed index j, the eigenvalue $e_j(t,\delta)$ experiences avoided crossings at the points $\{t_{r_1},\cdots,t_{r_j}\}$. We can assume without loss of generality that

$$I_k^{\alpha'} \cap I_l^{\alpha'} = \emptyset, \quad \forall k \neq l \in \{r_1,\cdots,r_j\}. \tag{6.43}$$

Hence, for $\delta > 0$ small enough, the analytic continuation $\widetilde{e}_j(z,\delta)$ is isolated in the spectrum of $H(z,\delta)$, uniformly in $z \in S_\alpha \backslash \cup_{r=r_1,\cdots,r_j} I_r^{\alpha'}$. Since by assumption H5 there is no crossing of eigenvalues on the real axis when $\delta > 0$, there exists a $0 < g < \alpha'$, which depends on δ, such that $\widetilde{e}_j(z,\delta)$ is isolated in the spectrum of $H(z,\delta)$, uniformly in $z \in S_\alpha^j$, where

$$S_\alpha^j = S_\alpha \backslash \cup_{r=r_1,\cdots,r_j} (J_r \cup \overline{J_r}) \tag{6.44}$$

and

$$J_r = I_r^{\alpha'} \cap \{z |\, \mathrm{Im}\ z > g\}, \quad r = 1,\cdots,p. \tag{6.45}$$

Hence the singularities of $\widetilde{e}_j(z,\delta)$ are located in $\cup_{r=r_1,\cdots,r_j}(J_r \cup \overline{J_r})$, which yields the first assertion of the lemma.

Consider a path ν_r from $t_r - L$ to $t_r + L$ which goes above J_r, where t_r is an avoided crossing between $e_j(t,\delta)$ and $e_k(t,\delta)$, $k = j \pm 1$. By perturbation theory again, $e_j(t_r - L,\delta)$ and $e_k(t_r - L,\delta)$ tend to $e_{j'}(t_r - L, 0)$ and $e_{k'}(t_r - L, 0)$ as $\delta \to 0$, for some $j', k' \in 1,\cdots,n$, whereas $e_j(t_r + L,\delta)$ and $e_k(t_r + L,\delta)$ tend to $e_{k'}(t_r + L, 0)$ and $e_{j'}(t_r + L, 0)$ as $\delta \to 0$, see figure 4. Now, the analytic continuations of $e_j(t_r - L,\delta)$ and $e_k(t_r - L,\delta)$ along ν_r, $\widetilde{e}_j(z,\delta)$ and $\widetilde{e}_k(z,\delta)$ tend to the analytic functions $\widetilde{e}_{j'}(z,0) = e_{j'}(z,0)$ and $\widetilde{e}_{k'}(z,0) = e_{k'}(z,0)$ as $\delta \to 0$, for all $z \in \nu_r$. Thus, we deduce that for δ small enough

$$\widetilde{e}_j(t_r + L,\delta) \equiv e_k(t_r + L,\delta), \tag{6.46}$$

since we know that $\widetilde{e}_j(t_r + L,\delta) = e_{\sigma(j)}(t_r + L,\delta)$, for some permutation σ. Hence the point iii) of the lemma follows.

Note that the analytic continuations $\widetilde{e}_j(z,\delta)$ are single valued in $\widetilde{S}_\alpha$. Indeed, the analytic continuation of $e_j(t_r - L,\delta)$ along $\overline{\nu_r}$, denoted by $\widehat{e}_j(z,\delta)$, $\forall z \in \overline{\nu_r}$, is such that

$$\widehat{e}_j(t_r + L,\delta) = \overline{\widetilde{e}_j(t_r + L,\delta)} = \widetilde{e}_j(t_r + L,\delta) = e_k(t_r + L,\delta), \tag{6.47}$$

due to Schwarz's principle. We further require δ to be sufficiently small so that the following estimates are satisfied

$$\min_{r\in\{1,\cdots,p\}} \min_{\substack{\{jk\}\in C_r \\ j<k}} \inf_{z\in\widetilde{S}_\alpha\backslash I_r^\alpha} |\mathrm{Re}\ (\widetilde{e}_j(z,\delta) - \widetilde{e}_k(z,\delta))| > b > 0 \tag{6.48}$$

$$\min_{\substack{\{jk\}\in N \\ j<k}} \inf_{z\in\widetilde{S}_\alpha} |\mathrm{Re}\ (\widetilde{e}_j(z,\delta) - \widetilde{e}_k(z,\delta))| > b > 0 \tag{6.49}$$

$$\max_{j<k\in\{1,\cdots,n\}} \sup_{\mathrm{Im}\ z|\, z\in\widetilde{S}_\alpha} \left|\mathrm{Re}\ (\widetilde{e}_j'(z,\delta) - \widetilde{e}_k'(z,\delta))\right| < a(\mathrm{Re}\ z). \tag{6.50}$$

and, in the compacts $\widetilde{I}_r^\alpha = I_r^\alpha \backslash I_r^{\alpha'}$,

$$\begin{aligned}&\min_{r\in\{1,\cdots,p\}} \min_{\substack{\{jk\}\in C_r \\ j<k}} \inf_{z\in\widetilde{I}_r^\alpha} |\mathrm{Im}\ (\widetilde{e}_j(z,\delta) - \widetilde{e}_k(z,\delta))| > \\ &\frac{1}{2} \min_{r\in\{1,\cdots,p\}} \min_{\substack{\{jk\}\in C_r \\ j<k}} \inf_{z\in\widetilde{I}_r^\alpha} |\mathrm{Im}\ (\widetilde{e}_j(z,0) - \widetilde{e}_k(z,0))| > |\mathrm{Im}\ z| c\end{aligned} \tag{6.51}$$

$$\begin{aligned}&\max_{r\in\{1,\cdots,p\}} \max_{j<k\in\{1,\cdots,n\}} \sup_{z\in\widetilde{I}_r^\alpha} |\mathrm{Im}\ (\widetilde{e}_j(z,\delta) - \widetilde{e}_k(z,\delta))| < \\ &2 \max_{r\in\{1,\cdots,p\}} \max_{j<k\in\{1,\cdots,n\}} \sup_{z\in\widetilde{I}_r^\alpha} |\mathrm{Im}\ (\widetilde{e}_j(z,0) - \widetilde{e}_k(z,0))| < |\mathrm{Im}\ z| a(\mathrm{Re}\ z).\end{aligned} \tag{6.52}$$

The simultaneous requirements (6.26) and (6.50) is made possible by the continuity properties of $H'(z,\delta)$ and the uniformity in δ of the decay at $\pm\infty$ of $H(z,\delta)$ assumed in H4 together with the fact that $a(t)$ can be replaced by a multiple of $a(t)$ if necessary, to satisfy both estimates. The condition on δ is given by the first inequalities in (6.51) and (6.52), whereas the second ones are just recalls.

Then it remains to check that the paths γ^r, γ^+ and γ^- defined above satisfy the dissipativity condition (6.17) for the corresponding indices. This is not difficult, since the above estimates are precisely designed to preserve inequalities such as (6.32), (6.34) and (6.35). However, it should not be forgotten that in the sets $I_r^{\alpha'}$ the eigenvalues may be singular so that (6.18) cannot be used there. So when checking that a path parameterized as above by $u \in \mathbf{R}$ is dissipative, it is necessary to consider separately the case $u \in \mathbf{R}\backslash(\cup_{r=1,\cdots,p} I_r)$, where we proceed as above with (6.48), (6.49), (6.50) and (6.18) and the case $u \in \cup_{r=1,\cdots,p} I_r$, where we use use (6.51) and (6.52) instead of (6.18) as follows. If $u \in I_r$ for r such that t_r is a crossing point for $e_j(t,0)$ and $e_j(t,0)$, one takes (6.51) to estimate Im $(\widetilde{e}_{j'}(z,\delta) - \widetilde{e}_{k'}(z,\delta))$ for the corresponding indices j' and k', and if t_r is not a crossing point for $e_j(t,0)$ and $e_j(t,0)$, one uses (6.52) to estimate Im $(\widetilde{e}_{j'}(z,\delta) - \widetilde{e}_{k'}(z,\delta))$. Consequently, the domains D and $\overline{D}$ defined above keep the same dissipativity properties when $\delta > 0$ is small enough.

Let us finally turn to the determination of the associated permutation σ. As noticed earlier, the eigenvalues $\widetilde{e}_j(z,\delta)$ are continuous in δ, uniformly in $z \in \widetilde{S}_\alpha$. Hence, since the eigenvalues $e_j(z,0)$ are analytic in S_α, we have

$$\lim_{\delta\to 0} \widetilde{e}_j(\infty,\delta) = e_j(\infty,0) \quad j = 1,2,\cdots,n. \tag{6.53}$$

Whereas we have along the real axis (see figure 4),

$$\lim_{\delta\to 0} e_{\sigma(j)}(\infty,\delta) = e_j(\infty,0), \tag{6.54}$$

with σ defined in the lemma, from which the result follows. □

7 Applications

Let us consider the time-dependent Schrödinger equation in the adiabatic limit. The relevant equation is then (2.1) where $H(t) = H^*(t)$ is the time-dependent self-adjoint hamiltonian. Thus we can take $J = \mathbf{I}$ in proposition 2.1 to get

$$H(t) = H^*(t) = H^{\#}(t). \tag{7.1}$$

The norm of an eigenvector being positive, it remains to impose the gap hypothesis in H3 to fit in the framework and we deduce that the S-matrix is unitarity, since $R = \mathbf{I}$. In this context, the elements of the S-matrix describe the transitions between the different levels between $t = -\infty$ and $t = +\infty$ in the adiabatic limit.

We now specify a little more our concern and consider a three-level system, i.e. $H(t) = H^*(t) \in M_3(\mathbf{C})$. We assume that $H(t)$ satisfies the hypotheses of corollary 6.1 with an extra parameter δ which we omit in the notation and displays two avoided crossings at $t_1 < t_2$, as shown in figure 7. The corresponding permutation σ is given by

$$\sigma(1) = 3, \quad \sigma(2) = 1, \quad \sigma(3) = 2. \tag{7.2}$$

By corollary 6.1, we can compute asymptotically the elements s_{31}, s_{12}, s_{23} and s_{jj}, $j = 1,2,3$. Using the unitarity of the S-matrix, we can get some more information. Introducing

$$\Gamma_j = \left| \text{Im} \int_{\zeta_j} e_j(z)dz \right|, \quad j = 1,2, \tag{7.3}$$

Figure 7: The pattern of avoided crossings in the adiabatic context.

where ζ_j is in the upper half plane, with the notation of section 6, it follows that

$$s_{31} = \mathcal{O}\left(\mathrm{e}^{-(\Gamma_1+\Gamma_2)/\varepsilon}\right), \quad s_{12} = \mathcal{O}\left(\mathrm{e}^{-\Gamma_1/\varepsilon}\right), \quad s_{23} = \mathcal{O}\left(\mathrm{e}^{-\Gamma_2/\varepsilon}\right) \tag{7.4}$$

and

$$s_{jj} = 1 + \mathcal{O}(\varepsilon), \quad j = 1, 2, 3. \tag{7.5}$$

Expressing the fact that the first and second columns as well as the second and third rows are orthogonal, we deduce

$$s_{21} = -\overline{s_{12}}\frac{s_{11}}{\overline{s_{22}}}\left(1 + \mathcal{O}\left(\mathrm{e}^{-2\Gamma_2/\varepsilon}\right)\right) \tag{7.6}$$

$$s_{32} = -\overline{s_{23}}\frac{s_{33}}{\overline{s_{22}}}\left(1 + \mathcal{O}\left(\mathrm{e}^{-2\Gamma_1/\varepsilon}\right)\right). \tag{7.7}$$

Finally, the estimate in corollary 6.1 yields

$$s_{13} = \mathcal{O}\left(\varepsilon \mathrm{e}^{-|h|(e_2(\infty,\delta)-e_1(\infty,\delta))/\varepsilon}\mathrm{e}^{-\Gamma_2/\varepsilon}\right) = \mathcal{O}\left(\mathrm{e}^{-(\Gamma_2+\Gamma_2+K)/\varepsilon}\right) \tag{7.8}$$

where $K > 0$, since we have that $\Gamma_j \to 0$ as $\delta \to 0$. Hence we get

$$S = \begin{pmatrix} s_{11} & s_{12} & \mathcal{O}\left(\mathrm{e}^{-(\Gamma_2+\Gamma_2+K)/\varepsilon}\right) \\ -\overline{s_{12}}\frac{s_{11}}{\overline{s_{22}}}\left(1 + \mathcal{O}\left(\mathrm{e}^{-2\Gamma_2/\varepsilon}\right)\right) & s_{22} & s_{23} \\ s_{31} & -\overline{s_{23}}\frac{s_{33}}{\overline{s_{22}}}\left(1 + \mathcal{O}\left(\mathrm{e}^{-2\Gamma_1/\varepsilon}\right)\right) & s_{33} \end{pmatrix} \tag{7.9}$$

where all s_{jk} above can be computed asymptotically up to exponentially small relative error, using (6.10).

The smallest asymptotically computable element s_{13} describes the transition from $e_1(-\infty,\delta)$ to $e_3(+\infty,\delta)$. The result we get for this element is in agreement with the rule of the thumb claiming that the transitions take place locally at the avoided crossings and can be considered as independent. Accordingly, we can only estimate the smallest element of all, s_{13}, which describes the transition from $e_3(-\infty,\delta)$ to $e_1(+\infty,\delta)$, for which the avoided crossings are not encountered in "right order", as discussed in [HP]. It is possible however to get an asymptotic expression for this element in some cases. When the unperturbed levels $e_2(z,0)$ and $e_3(z,0)$ possess a degeneracy point in S_α and when there exists a dissipative domain for the index 3 of the unperturbed eigenvalues going above this point, one can convince oneself that s_{13} can be computed asymptotically for δ small enough, using the techniques presented above.

Our second application is the study of the semi-classical scattering properties of the multichannel stationnary Schrödinger equation with energy above the potential barriers. The relevant equation is then

$$-\varepsilon^2 \frac{d^2}{dt^2}\Phi(t) + V(t)\Phi(t) = E\Phi(t), \tag{7.10}$$

where $t \in \mathbf{R}$ has the meaning of a space variable, $\Phi(t) \in \mathbf{C}^m$ is the wave function, $\varepsilon \to 0$ denotes Planck's constant, $V(t) = V^*(t) \in M_m(\mathbf{C})$ is the matrix of potentials and the spectral parameter E is kept fixed and large enough so that

$$U(t) \equiv E - V(t) > 0. \tag{7.11}$$

Introducing

$$\psi(t) = \begin{pmatrix} \Phi(t) \\ i\varepsilon\Phi(t) \end{pmatrix} \in \mathbf{C}^{2m}, \tag{7.12}$$

we cast equation (7.10) into the equivalent form (2.1) for $\psi(t)$ with generator

$$H(t) = \begin{pmatrix} \mathbf{O} & \mathbf{I} \\ U(t) & \mathbf{O} \end{pmatrix} \in M_{2m}(\mathbf{C}). \tag{7.13}$$

It is readily verified that

$$H(t) = J^{-1}H^*(t)J \tag{7.14}$$

with

$$J = \begin{pmatrix} \mathbf{O} & \mathbf{I} \\ \mathbf{I} & \mathbf{O} \end{pmatrix}. \tag{7.15}$$

Concerning the spectrum of $H(t)$, it should be remarked that if the real and positive eigenvalues of $U(t)$, $k_j^2(t)$, $j = 1, \cdots, m$ associated with the eigenvectors $u_j(t) \in \mathbf{C}^m$ are assumed to be distinct, i.e.

$$0 < k_1^2(t) < k_2^2(t) < \cdots < k_m^2(t), \tag{7.16}$$

then the spectrum of the generator $H(t)$ given by (7.13) consists in $2m$ real distinct eigenvalues

$$-k_m(t) < -k_{m-1}(t) < \cdots < -k_1(t) < k_1(t) < k_2(t) < \cdots < k_m(t) \tag{7.17}$$

associated with the $2m$ eigenvectors

$$\begin{aligned} &\chi_j^{\pm}(t) = \begin{pmatrix} u_j(t) \\ \pm k_j(t)u_j(t) \end{pmatrix} \in \mathbf{C}^{2m}, \\ &H(t)\chi_j^{\pm}(t) = \pm k_j(t)\chi_j^{\pm}(t). \end{aligned} \tag{7.18}$$

We check that

$$(\chi_j^{\pm}(0), \chi_j^{\pm}(0))_J = \pm 2k_j(0)\|u_j(0)\| \neq 0, \quad j = 1, \ldots, m \tag{7.19}$$

where $\|u_j(0)\|$ is computed in $\mathbf{C}^m$, so that proposition 2.1 applies. Before dealing with its consequences, we further explicit the structure of S. Adopting the notation suggested by (7.17) and (7.18) we write

$$H(t) = \sum_{j=1}^{n} k_j(t)P_j^+(t) - \sum_{j=1}^{n} k_j(t)P_j^-(t) \tag{7.20}$$

$$\psi(t) = \sum_{j=1}^{n} c_j^+(t)\varphi_j^+(t)\mathrm{e}^{-i\int_0^t k_j(t')dt'/\varepsilon} + \sum_{j=1}^{n} c_j^-(t)\varphi_j^-(t)\mathrm{e}^{i\int_0^t k_j(t')dt'/\varepsilon} \tag{7.21}$$

and introduce

$$\mathbf{c}^{\pm}(t) = \begin{pmatrix} c_1^{\pm}(t) \\ c_2^{\pm}(t) \\ \vdots \\ c_m^{\pm}(t) \end{pmatrix} \in \mathbf{C}^m. \tag{7.22}$$

Hence we have the block structure

$$S\begin{pmatrix} \mathbf{c}^+(-\infty) \\ \mathbf{c}^-(-\infty) \end{pmatrix} \equiv \begin{pmatrix} S_{++} & S_{+-} \\ S_{-+} & S_{--} \end{pmatrix} \begin{pmatrix} \mathbf{c}^+(-\infty) \\ \mathbf{c}^-(-\infty) \end{pmatrix} = \begin{pmatrix} \mathbf{c}^+(+\infty) \\ \mathbf{c}^-(+\infty) \end{pmatrix} \tag{7.23}$$

where $S_{\sigma\tau} \in M_m(\mathbf{C})$, $\sigma, \tau \in \{+,-\}$.

Let us turn to the symmetry properties of S. We get from (7.19) and proposition 2.1 that

$$\begin{pmatrix} S_{++} & S_{+-} \\ S_{-+} & S_{--} \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{I} & \mathbf{O} \\ \mathbf{O} & -\mathbf{I} \end{pmatrix} \begin{pmatrix} S_{++} & S_{+-} \\ S_{-+} & S_{--} \end{pmatrix}^{*} \begin{pmatrix} \mathbf{I} & \mathbf{O} \\ \mathbf{O} & -\mathbf{I} \end{pmatrix} = \begin{pmatrix} S_{++}^* & -S_{-+}^* \\ -S_{+-}^* & S_{--}^* \end{pmatrix}. \tag{7.24}$$

In terms of the blocks $S_{\sigma\tau}$, this is equivalent to

$$S_{++}S_{++}^* - S_{+-}S_{+-}^* = \mathbf{I} \tag{7.25}$$

$$S_{++}S_{-+}^* - S_{+-}S_{--}^* = \mathbf{O} \tag{7.26}$$

$$S_{--}S_{--}^* - S_{-+}S_{-+}^* = \mathbf{I}. \tag{7.27}$$

The block S_{++} describes the transmission coefficients associated with a wave traveling from the right and S_{-+} describes the associated reflexion coefficients. Similarly, S_{--} and S_{+-} are related to the transmission and reflexion coefficients associated with a wave incoming from the left. It should be noted that in case of equation (7.10) another convention is often used to define an S-matrix, see [F1], for instance. This gives rise to a different S-matrix with similar interpretation. However it is not difficult to establish a one-to-one correspondence between the two definitions. If the matrix of potentials $V(t)$ is real symmetric, we have further symmetry in the S-matrix.

Lemma 7.1 *Let S given by (7.23) be the S-matrix associated with (7.10) under condition (7.11). If we further assume $V(t) = \overline{V(t)}$, then, taking $\varphi_j^{\pm}(0) \in \mathbf{R}^{2m}$, $j = 1, \cdots, m$, in (7.21), we get*

$$S_{++} = \overline{S_{--}}, \quad S_{+-} = \overline{S_{-+}}. \tag{7.28}$$

The corresponding results for the S-matrix defined in [F1] are derived in [MN]. The proof of this lemma can be found in appendix. We consider now (7.10) the case $U(t) = U^*(t) = \overline{U(t)} \in M_2(\mathbf{R})$, which describes a two-channel Schrödinger equation. We assume that the four-level generator $H(t)$ displays three avoided crossings at $t_1 < t_2$, two of which take place at the same point t_1, because of the symmetry of the eigenvalues, as in figure 8. By lemma

Figure 8: The pattern of avoided crossings in the semiclassical context.

7.1, it is enough to consider the blocks S_{++} and S_{+-}. The transitions corresponding to elements of these blocks which we can compute asymptotically are from level 1^+ to level 2^+ and from level 2^- to level 1^+. They correspond to elements s_{21}^{++} and s_{12}^{+-} respectively. With the notations

$$\Gamma_j = \left| \mathrm{Im} \int_{\zeta_j} k_1(z)dz \right|, \quad j = 1, 2, \tag{7.29}$$

where ζ_j is in the upper half plane, we have the estimates

$$s_{21}^{++} = \mathcal{O}\left(\mathrm{e}^{-\Gamma_1/\varepsilon}\right), \quad s_{12}^{+-} = \mathcal{O}\left(\mathrm{e}^{-(\Gamma_1+\Gamma_2)/\varepsilon}\right), \quad s_{jj}^{++} = 1 + \mathcal{O}(\varepsilon), \quad j = 1, 2. \tag{7.30}$$

It follows from (7.26) and lemma 7.1 that the matrix $S_{++}S_{+-}^T$ is symmetric. Hence

$$s_{11}^{++}s_{21}^{+-} + s_{12}^{++}s_{22}^{+-} = s_{21}^{++}s_{11}^{+-} + s_{22}^{++}s_{12}^{+-}, \tag{7.31}$$

whereas we get from (7.25)

$$s_{11}^{++}\overline{s_{21}^{++}} + s_{12}^{++}\overline{s_{22}^{++}} = s_{11}^{+-}\overline{s_{21}^{+-}} + s_{12}^{+-}\overline{s_{22}^{+-}}. \tag{7.32}$$

The only useful estimate we get with corollary 6.1 is

$$s_{22}^{+-} = \mathcal{O}\left(\mathrm{e}^{-(\Gamma_1+\Gamma_2+K)/\varepsilon}\right), \quad K > 0, \tag{7.33}$$

which yields together with (7.30) in (7.31)

$$s_{21}^{+-} = s_{21}^{++}s_{11}^{+-}/s_{11}^{++} + \mathcal{O}\left(\mathrm{e}^{-(\Gamma_1+\Gamma_2)/\varepsilon}\right). \tag{7.34}$$

Thus, from (7.32) and (5.40) for s_{11}^{+-},

$$s_{12}^{++} = -\overline{s_{21}^{++}}\,\overline{\frac{s_{11}^{++}}{s_{22}^{++}}}\left(1 + \mathcal{O}\left(\mathrm{e}^{-\kappa/\varepsilon}\right)\right), \tag{7.35}$$

with

$$0 < \kappa < \min(\Gamma_1, \Gamma_2). \tag{7.36}$$

Summarizing, we have

$$S_{++} = \begin{pmatrix} s_{11}^{++} & -\overline{s_{21}^{++}}\frac{s_{11}^{++}}{s_{22}^{++}}\left(1+\mathcal{O}\left(\mathrm{e}^{-\kappa/\varepsilon}\right)\right) \\ s_{21}^{++} & s_{22}^{++} \end{pmatrix} \tag{7.37}$$

and

$$S_{+-} = \begin{pmatrix} \mathcal{O}\left(\mathrm{e}^{-\kappa/\varepsilon}\right) & s_{12}^{+-} \\ \mathcal{O}\left(\mathrm{e}^{-\kappa/\varepsilon}\right) & \mathcal{O}\left(\mathrm{e}^{-(\Gamma_1+\Gamma_2+K)/\varepsilon}\right) \end{pmatrix}, \tag{7.38}$$

where all elements $s_{jk}^{\sigma\tau}$ can be asymptotically computed up to exponentially small relative corrections using (6.10). We get no information on the first column of S_{+-} but the estimate (5.40) where necessarily, (7.36) holds. However, if there exists one or several other dissipative domains for certain indices, it is then possible to get asymptotic formulas for the estimated terms.

A Proof of proposition 2.1

A direct consequence of the property

$$H(t) = H^{\#}(t) = J^{-1}H^*(t)J \tag{A.1}$$

is the relation $\sigma(H(t)) = \overline{\sigma(H(t))}$. Thus, if $\sigma(H(0)) \subset \mathbf{R}$, then $\sigma(H(t)) \subset \mathbf{R}$, for all $t \in \mathbf{R}$, since the analytic eigenvalues are assumed to be distinct and nondegenerate for all $t \in \mathbf{R}$. Let $e_j(0)$ be the eigenvalue associated with $\varphi_j(0)$. Then, due to the property $H(0) = H^{\#}(0)$

$$(\varphi_j(0), H(0)\varphi_k(0))_J = e_k(0)(\varphi_j(0), \varphi_k(0))_J = \overline{e_j(0)}(\varphi_j(0), \varphi_k(0))_J, \tag{A.2}$$

for any $j,k = 1,\cdots,n$. For $j = k$ we get from the assumption $(\varphi_j(0), \varphi_j(0))_J \neq 0$ that $e_j(0) \in \mathbf{R}$ and from the fact that the eigenvalues of $H(0)$ are distinct

$$(\varphi_j(0), \varphi_k(0))_J = 0, \quad j \neq k. \tag{A.3}$$

The resulting reality of $e_j(t)$ for all $t \in \mathbf{R}$ and $j = 1,\cdots,n$ yields together with (A.1)

$$P_j(t) = J^{-1}P_j^*(t)J. \tag{A.4}$$

Hence, using the fact that the P_j^* are projectors,

$$\begin{aligned} K(t) &= \sum_{j=1}^n P_j{}'(t)P_j(t) = \sum_{j=1}^n (J^{-1}P_j^*(t)J)'J^{-1}P_j^*(t)J = J^{-1}\sum_{j=1}^n P_j^{*\prime}(t)P_j^*(t)J \\ &= -J^{-1}\sum_{j=1}^n P_j^*(t)P_j^{*\prime}(t)J = -J^{-1}K^*(t)J. \end{aligned} \tag{A.5}$$

Let $\Phi, \Psi \in \mathbf{C}^n$ and $W(t)$ be defined by (see (3.5))

$$W'(t) = K(t)W(t), \quad W(0) = \mathbf{I}. \tag{A.6}$$

Then we have

$$\begin{aligned} (W(t)\Phi, W(t)\Psi)_J' &= \langle W'(t)\Phi|JW(t)\Psi\rangle + \langle W(t)\Phi|JW'(t)\Psi\rangle \\ &= \langle K(t)W(t)\Phi|JW(t)\Psi\rangle + \langle W(t)\Phi|JK(t)W(t)\Psi\rangle \\ &= \langle W(t)\Phi|J(J^{-1}K^*(t)J + K(t))W(t)\Psi\rangle \equiv 0. \end{aligned} \tag{A.7}$$

Thus, in the indefinite metric, the scalar products of the eigenvectors of $H(t)$, $\varphi_j(t) = W(t)\varphi_j(0)$ (see (3.7)), are constants

$$(\varphi_j(t), \varphi_k(t))_J \equiv (\varphi_j(0), \varphi_k(0))_J. \tag{A.8}$$

We can then normalize the $\varphi_j(0)$ in such a way that

$$(\varphi_j(t), \varphi_k(t))_J = (\varphi_j(0), \varphi_k(0))_J = \delta_{jk}\rho_j \tag{A.9}$$

with $\rho_j \in \{+1, -1\}$. Let $\psi(t)$ and $\chi(t)$ be two solutions of (2.1). By a argument similar to the one above using (A.1), we deduce

$$(\chi(t), \psi(t))_J \equiv (\chi(0), \psi(0))_J. \tag{A.10}$$

Inserting the decompositions

$$\psi(t) = \sum_{j=1}^{n} c_j(t)\mathrm{e}^{-i\int_0^t e_j(t')dt'/\varepsilon}\varphi_j(t) \tag{A.11}$$

$$\chi(t) = \sum_{j=1}^{n} d_j(t)\mathrm{e}^{-i\int_0^t e_j(t')dt'/\varepsilon}\varphi_j(t) \tag{A.12}$$

in this last identity yields

$$\begin{aligned}\sum_{j,k=1}^{n} \overline{d}_k(t)c_j(t)(\varphi_k(t), \varphi_j(t))_J\mathrm{e}^{i\int_0^t(e_k(t')-e_j(t'))/\varepsilon dt'} &= \sum_j \overline{d}_j(t)\rho_j c_j(t) \\ \equiv \sum_{j=1}^{n} \overline{d}_j(0)\rho_j c_j(0) = \sum_{j=1}^{n} \overline{d}_j(\pm\infty)\rho_j c_j(\pm\infty).\end{aligned} \tag{A.13}$$

Since the initial conditions for the coefficients

$$c_j(-\infty) = \delta_{jk}\,, \quad d_j(-\infty) = \delta_{jl} \tag{A.14}$$

imply

$$c_j(+\infty) = s_{jk}\,, \quad d_j(+\infty) = s_{jl}, \tag{A.15}$$

we get from (A.13), introducing the matrix $R = \mathrm{diag}\,(\rho_1, \rho_2, \cdots, \rho_n) \in M_n(\mathbf{C})$,

$$R = S^* R S, \tag{A.16}$$

which is equivalent to the assertion $S^{-1} = RS^*R$. □

B Proof of lemma 7.1

Let $G = G^* = G^{-1}$ be given in block structure by

$$G = \begin{pmatrix} \mathbf{I} & \mathbf{O} \\ \mathbf{O} & -\mathbf{I} \end{pmatrix} \in M_{2m}(\mathbf{C}) \tag{B.1}$$

and $H(t)$ be given by (7.13) with $U(t) = \overline{U(t)} = U^*(t)$. Since

$$GH(t)G = -H(t)\,, \quad \overline{H(t)} = H(t)\,, \tag{B.2}$$

and the eigenvalues of $H(t)$ are real, it is readily verified that

$$GP_j^{\pm}(t)G = P_j^{\mp}(t)\,, \quad \overline{P_j^{\pm}(t)} = P_j^{\pm}(t)\,,\ j = 1,\cdots,m. \tag{B.3}$$

Hence

$$K(t) = \sum_{\substack{j=1\\ \tau=\pm}}^{m} P_j^{\tau\prime}(t)P_j^{\tau}(t) = \overline{K(t)} = GK(t)G, \tag{B.4}$$

from which follows that the solution $W(t)$ of

$$W'(t) = K(t)W(t)\,, \quad W(0) = \mathbf{I} \tag{B.5}$$

satisfies

$$W(t) = \overline{W(t)} = GW(t)G. \tag{B.6}$$

As the matrix of potentials $U(0)$ is real symmetric, its eigenvectors $u_j(0)$ may be chosen real, so that we can assume that

$$\varphi_j^{\pm}(0) = \begin{pmatrix} u_j(0) \\ \pm k_j(0)u_j(0) \end{pmatrix} \in \mathbf{R}^{2m}. \tag{B.7}$$

Thus it follows from the foregoing that

$$\varphi_j^{\pm}(t) = W(t)\varphi_j^{\pm}(0) \in \mathbf{R}^{2m} \quad \forall t \in \mathbf{R} \tag{B.8}$$

and satisfies

$$G\varphi_j^{\pm}(t) = GW(t)GG\varphi_j^{\pm}(0) = W(t)G\varphi_j^{\pm}(0) = \varphi_j^{\mp}(t). \tag{B.9}$$

Finally, the main consequence of (B.2) is that if $\psi(t)$ is a solution of

$$i\varepsilon\psi'(t) = H(t)\psi(t), \tag{B.10}$$

then $\varphi(t) = G\overline{\psi(t)}$ is another solution, as easily verified. Thus we can write with (7.21),(B.8) and (B.9) that

$$\begin{aligned} \varphi(t) &= \sum_{j=1}^{m} d_j^{+}(t)\varphi_j^{+}(t)\mathrm{e}^{-i\int_0^t k_j(t')dt'/\varepsilon} + \sum_{j=1}^{m} d_j^{-}(t)\varphi_j^{-}(t)\mathrm{e}^{i\int_0^t k_j(t')dt'/\varepsilon} \\ &= \sum_{j=1}^{m} \overline{c_j^{+}(t)}\varphi_j^{-}(t)\mathrm{e}^{i\int_0^t k_j(t')dt'/\varepsilon} + \sum_{j=1}^{m} \overline{c_j^{-}(t)}\varphi_j^{+}(t)\mathrm{e}^{-i\int_0^t k_j(t')dt'/\varepsilon}, \end{aligned} \tag{B.11}$$

i.e.

$$\begin{aligned} d_j^{+}(t) &= \overline{c_j^{-}(t)} \\ d_j^{-}(t) &= \overline{c_j^{+}(t)}\,, \quad \forall j = 1,\cdots,m\,,\ \forall t \in \mathbf{R}. \end{aligned} \tag{B.12}$$

Finally, using the definition (7.23) and the above property for $t = \pm\infty$, we get for any $\mathbf{d}^{\pm}(-\infty) \in \mathbf{C}^m$

$$\begin{pmatrix} \mathbf{d}^{+}(+\infty) \\ \mathbf{d}^{-}(+\infty) \end{pmatrix} = \begin{pmatrix} S_{++} & S_{+-} \\ S_{-+} & S_{--} \end{pmatrix} \begin{pmatrix} \mathbf{d}^{+}(-\infty) \\ \mathbf{d}^{-}(-\infty) \end{pmatrix} = \begin{pmatrix} \overline{S_{--}} & \overline{S_{-+}} \\ \overline{S_{+-}} & \overline{S_{++}} \end{pmatrix} \begin{pmatrix} \mathbf{d}^{+}(-\infty) \\ \mathbf{d}^{-}(-\infty) \end{pmatrix}, \tag{B.13}$$

from which the result follows. □

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