GEOMETRICAL AND MATHEMATICAL ASPECTS OF THE ADIABATIC THEOREM OF QUANTUM MECHANICS

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Geometrical and Mathematical Aspects of the Adiabatic Theorem of Quantum Mechanics

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Abstract

This work is devoted to rigorous results about the adiabatic theorem of quantum mechanics. This theorem deals with the time dependent Schrödinger equation when the hamiltonian is a slowly varying function of time, characterizing the so-called adiabatic regime. Mathematically, the adiabatic theorem describes the solutions $\psi_\varepsilon(t)$ in an Hilbert space $\mathcal{H}$ of the rescaled Schrödinger equation

$$i\varepsilon \frac{d}{dt}\psi_\varepsilon(t) = H(t)\psi_\varepsilon(t)$$

in the limit $\varepsilon \to 0$. Suppose the hamiltonian possesses for any time t two spectral projectors, $P_1(t)$ and $P_2(t)$, which are spectrally isolated. Let us consider a normalized solution which belongs at time $t = -\infty$ to the spectral subspace $P_1(-\infty)\mathcal{H}$, i.e. which satisfies the boundary condition

$$\lim_{t\to-\infty} \|P_1(t)\psi_\varepsilon(t)\| = 1.$$

Then the transition probability $\mathcal{P}_{21}(\varepsilon)$ from $P_1(-\infty)\mathcal{H}$ to $P_2(+\infty)\mathcal{H}$ between the times $-\infty$ and $+\infty$ is defined by

$$\mathcal{P}_{21}(\varepsilon) = \lim_{t\to+\infty} \|P_2(t)\psi_\varepsilon(t)\|^2.$$

The adiabatic theorem states that $\mathcal{P}_{21}(\varepsilon)$ tends to zero in the limit $\varepsilon \to 0$. Our main concern is the study of the decay of $\mathcal{P}_{21}(\varepsilon)$ as $\varepsilon \to 0$. We first show that if $H(t)$ is an analytic unbounded operator then $\mathcal{P}_{21}(\varepsilon)$ decays exponentially fast to zero in the adiabaticity parameter ε:

$$\mathcal{P}_{21}(\varepsilon) = \mathcal{O}(\mathrm{e}^{-2\tau/\varepsilon})$$

for some positive constant τ.

Then we turn to two-level systems for which we have a finer control on the behaviour of $\mathcal{P}_{21}(\varepsilon)$ as $\varepsilon \to 0$. Indeed, in the generic case we give an explicit asymptotic formula for the transition probability $\mathcal{P}_{21}(\varepsilon)$ which reads

$$\mathcal{P}_{21}(\varepsilon) = \exp\{2\mathrm{Im}\theta_1\} \exp\left\{\frac{2}{\varepsilon}\mathrm{Im}\int_\gamma e_1(z)dz\right\}(1 + \mathcal{O}(\varepsilon)).$$

The prefactor $\exp\{2\mathrm{Im}\theta_1\}$ is of geometrical nature and the exponential decay rate $2\mathrm{Im}\int_\gamma e_1(z)dz$ is computed by means of the integral of the analytic continuation of the eigenvalue $e_1(t)$ along a suitable path γ in the complex plane. This expression constitutes a generalization of the so-called Dykhne formula which does not contain the geometric prefactor. Moreover, we improve this result and compute the leading term of $\mathcal{P}_{21}(\varepsilon)$ up to a correction of order $\mathcal{O}(\varepsilon^q)$, for any q, instead of $\mathcal{O}(\varepsilon)$. This result shows as well that the logarithm of $\mathcal{P}_{21}(\varepsilon)$ admits an asymptotic power series in ε up to any order. Finally we push the estimates to get the leading term of $\mathcal{P}_{21}(\varepsilon)$ up to a correction of order $\mathcal{O}(\mathrm{e}^{-\tau/\varepsilon})$. We consider also cases where the 2×2 hamiltonian possesses some symmetry, as the time reversal symmetry for example. In these situations, the leading term of $\mathcal{P}_{21}(\varepsilon)$ changes qualitatively since it is given by a decreasing exponential multiplying an oscillatory function of $1/\varepsilon$.

Then we come back to general systems driven by unbounded hamiltonians and study the case where $P_1(t)$ and $P_2(t)$ are both one-dimensional. These

projectors are thus associated with non-degenerate instantaneous eigenvalues $e_1(t)$ and $e_2(t)$ of the hamiltonian $H(t)$. We prove that, in this case too, an asymptotic formula for $\mathcal{P}_{21}(\varepsilon)$ exists, provided the two levels $e_1(t)$ and $e_2(t)$ are sufficiently isolated in the spectrum of $H(t)$. This formula turns out to be the same as the formula valid for two-level systems. Finally, we consider the situation frequently encountered in applications where the two levels $e_1(t)$ and $e_2(t)$ display an avoided crossing during the evolution. For an avoided crossing located at time $t = 0$, this means that the levels behave as

$$e_2(t) - e_1(t) \simeq \sqrt{a^2t^2 + 2c\delta t + b^2\delta^2}, \quad |t| \ll 1,$$

where $\delta \ll 1$. As a consequence, the gap between $e_1(t)$ and $e_2(t)$ is minimum for $t = t_0(\delta) \simeq -\frac{c\delta}{a^2}$ where its value is

$$e_2(t_0(\delta)) - e_1(t_0(\delta)) \simeq \delta\sqrt{b^2 - c^2/a^2} = \mathcal{O}(\delta).$$

In this case, we show that for ε and δ small enough, the above formula for $\mathcal{P}_{21}(\varepsilon)$ reduces to the well-known Landau-Zener formula

$$\mathcal{P}_{21}(\varepsilon) = \exp\left\{-\frac{\delta^2\pi}{\varepsilon 2}\left(\frac{b^2}{a} - \frac{c^2}{a^3}\right)(1 + \mathcal{O}(\delta))\right\}(1 + \mathcal{O}(\delta) + \mathcal{O}(\varepsilon)).$$

When $c = 0$ we recover the familiar Landau-Zener formula. This gives a rigorous mathematical status to a formula which has been widely applied for years in a variety of circumstances.

Résumé

Ce travail est consacré aux résultats recents sur le théorème adiabatique de la mécanique quantique. Ce théorème traite de l'équation de Schrödinger dépendant du temps lorsque l'hamiltonien est une fonction lente du temps, caractérisant le régime dit adiabatique. Mathématiquement, le théorème adiabatique décrit les solutions $\psi_\varepsilon(t)$ dans un espace de Hilbert $\mathcal{H}$ de l'équation de Schrödinger écrite à l'aide d'un temps sans dimension

$$i\varepsilon\frac{d}{dt}\psi_\varepsilon(t) = H(t)\psi_\varepsilon(t)$$

dans la limite $\varepsilon \to 0$. On suppose que l'hamiltonien possède en tout temps t deux projecteurs spectraux $P_1(t)$ et $P_2(t)$ qui soient spectralement isolés. Considérons une solution normalisée qui appartient au temps $t = -\infty$ au sous espace spectral $P_1(-\infty)\mathcal{H}$, c'est-à dire, qui satisfait la condition de bord

$$\lim_{t\to-\infty} \|P_1(t)\psi_\varepsilon(t)\| = 1.$$

On définit alors la probabilité de transition $\mathcal{P}_{21}(\varepsilon)$ de $P_1(-\infty)\mathcal{H}$ à $P_2(+\infty)\mathcal{H}$ entre les temps $-\infty$ et $+\infty$ par

$$\mathcal{P}_{21}(\varepsilon) = \lim_{t\to+\infty} \|P_2(t)\psi_\varepsilon(t)\|^2.$$

Le théorème adiabatique affirme que $\mathcal{P}_{21}(\varepsilon)$ tend vers zéro dans la limite $\varepsilon \to 0$. Notre objectif principal est d'étudier la décroissance de $\mathcal{P}_{21}(\varepsilon)$ lorsque $\varepsilon \to 0$. On montre en premier lieu que si $H(t)$ est un opérateur analytique non-borné, alors $\mathcal{P}_{21}(\varepsilon)$ décroît exponentiellement vite vers zero dans le paramètre d'adiabaticité ε:

$$\mathcal{P}_{21}(\varepsilon) = \mathcal{O}(\mathrm{e}^{-2\tau/\varepsilon})$$

où τ est une constante positive.

On considère ensuite les systèmes à deux niveaux pour lesquels on a un contrôle plus fin du comportement de $\mathcal{P}_{21}(\varepsilon)$. En effet, dans le cas générique on donne une formule asymptotique explicite pour la probabilité de transition $\mathcal{P}_{21}(\varepsilon)$ qui s'écrit

$$\mathcal{P}_{21}(\varepsilon) = \exp\{2\mathrm{Im}\theta_1\}\exp\left\{\frac{2}{\varepsilon}\mathrm{Im}\int_\gamma e_1(z)dz\right\}(1+\mathcal{O}(\varepsilon)).$$

Le prefacteur $\exp\{2\mathrm{Im}\theta_1\}$ est de nature géometrique et le taux de décroissance exponentielle $2\mathrm{Im}\int_\gamma e_1(z)dz$ se calcule au moyen de l'intégrale du prolongement analytique de la valeur propre $e_1(t)$ le long d'un chemin γ judicieusement choisi dans le plan complexe. Cette expression constitue une généralisation de la formule dite de Dykhne qui ne contient pas le préfacteur géométrique. De plus, on améliore ce résultat par un calcul du terme dominant de $\mathcal{P}_{21}(\varepsilon)$ à une correction d'ordre $\mathcal{O}(\varepsilon^q)$ près, pour tout q, au lieu de $\mathcal{O}(\varepsilon)$. Ce résultat montre également que le logarithme de $\mathcal{P}_{21}(\varepsilon)$ admet un dévelopement asymptotique en puissances de ε d'ordre arbitraire. Finalement on pousse les estimations jusqu'à obtenir le terme dominant de $\mathcal{P}_{21}(\varepsilon)$ à une correction d'ordre $\mathcal{O}(\mathrm{e}^{-\tau/\varepsilon})$. On considère également des cas d'hamiltoniens 2×2 possédant une certaine

symétrie, par exemple la symétrie de renversement du temps. Dans ces situations le terme dominant de $\mathcal{P}_{21}(\varepsilon)$ change qualitativement puisqu'il est donné par une exponentielle décroissante multipliant une fonction oscillante de $1/\varepsilon$.

On revient ensuite à des systèmes généraux gouvernés par des hamiltoniens non-bornés et on étudie le cas où $P_1(t)$ et $P_2(t)$ sont tous deux unidimensionnels. Ces projecteurs sont alors associés à des valeurs propres instantanées non dégénérées $e_1(t)$ et $e_2(t)$ de l'hamiltonien $H(t)$. On prouve dans ce cas également qu'une formule asymptotique pour $\mathcal{P}_{21}(\varepsilon)$ existe pour autant que les deux niveaux $e_1(t)$ et $e_2(t)$ soient suffisamment isolés dans le spectre de $H(t)$. Cette formule se révèle être identique à la formule valable pour les systèmes à deux niveaux. Finalement, on considère la situation que l'on rencontre fréquemment dans dans les applications dans laquelle les deux niveaux $e_1(t)$ et $e_2(t)$ présentent un "presque croisement" (avoided crossing) durant l'évolution. Pour un presque croisement situé en $t = 0$, cela signifie que les niveaux se comportent comme

$$e_2(t) - e_1(t) \simeq \sqrt{a^2t^2 + 2c\delta t + b^2\delta^2}, \quad |t| \ll 1,$$

où $\delta \ll 1$. Par conséquent, la lacune spectrale entre $e_1(t)$ et $e_2(t)$ est minimale en $t = t_0(\delta) \simeq -\frac{c\delta}{a^2}$ et vaut

$$e_2(t_0(\delta)) - e_1(t_0(\delta)) \simeq \delta\sqrt{b^2 - c^2/a^2} = \mathcal{O}(\delta).$$

Dans ce cas on montre que pour ε et δ suffisamment petits, la formule donnant $\mathcal{P}_{21}(\varepsilon)$ ci-dessus se réduit à la fameuse formule de Landau-Zener

$$\mathcal{P}_{21}(\varepsilon) = \exp\left\{-\frac{\delta^2\pi}{\varepsilon 2}\left(\frac{b^2}{a} - \frac{c^2}{a^3}\right)(1 + \mathcal{O}(\delta))\right\}(1 + \mathcal{O}(\delta) + \mathcal{O}(\varepsilon)).$$

Lorsque $c = 0$ on retrouve la forme usuelle de la formule de Landau-Zener. Ce résultat donne un statut mathématique à une formule largement appliquée depuis des années dans diverses circonstances.

Chapter 1

Introduction

1.1 Historical Account

Since the early days of quantum mechanics, the search for approximate solutions to the celebrated Schrödinger equation has been recognized as an important problem, since exact solutions were, and still are, rather scarce. This is the reason why we began to consider this equation in a variety of limits, corresponding to different physically relevant regimes, in order to study quantum physics through approximate but simple solutions obtained in these limits. Among the different cases under consideration, the so-called adiabatic regime has attracted physicists' as well as mathematicians' attention for a long time and it still does. This regime describes the evolution of a system in an environment characterized by a slowly varying time dependent hamiltonian. A typical example is the smooth switching on of a perturbation of a reference system. Mathematically we model that situation by considering a hamiltonian of the form $H(\varepsilon s)$ where s is the time and $1/\varepsilon$ is the characteristic time scale over which the hamiltonian changes a finite amount. Thus, the adiabatic regime corresponds to the limit $\varepsilon \to 0$ in the Schrödinger equation (with $\hbar = 1$)

$$i\frac{d}{ds}\varphi_\varepsilon(s) = H(\varepsilon s)\varphi_\varepsilon(s)\,, \quad \varphi_\varepsilon(0) = \varphi_0 \tag{1.1}$$

or in its equivalent rescaled version

$$i\varepsilon\frac{d}{dt}\psi_\varepsilon(t) = H(t)\psi_\varepsilon(t)\,, \quad \psi_\varepsilon(0) = \varphi_0 \tag{1.2}$$

obtained after introduction of the dimensionless time $t = \varepsilon s$. The presence of the small parameter ε in front of the time derivative in this last equation forbids a perturbative approach of its solutions through Dyson's series and makes the limit $\varepsilon \to 0$ singular.

The original statement already established by Born and Fock [BF] in 1928, is essentially that if $H(t)$ possesses an instantaneous energy level $e_1(t)$ isolated in the spectrum for all $t \in [t_1, t_2]$, then a system prepared in the eigenstate corresponding to $e_1(t_1)$ at time $t = t_1$ will evolve to an eigenstate corresponding to $e_1(t_2)$ at time $t = t_2$, in the limit $\varepsilon \to 0$. More precisely, if $\varphi_1(t)$ is the normalized instantaneous eigenstate associated with $e_1(t)$, characterized by the phase fixing condition

$$\langle\varphi_1(t)|\frac{d}{dt}\varphi_1(t)\rangle \equiv 0 \;\; \forall t \in [t_1, t_2], \tag{1.3}$$

the solution of (1.2) at time t_2 will be given by

$$\psi_\varepsilon(t_2) = \exp\left\{-\frac{i}{\varepsilon}\int_{t_1}^{t_2} e_1(t)dt\right\}\varphi_1(t_2) + \mathcal{O}(\varepsilon). \tag{1.4}$$

In particular, the transition probability $\mathcal{P}_{21}(\varepsilon)$ to any other eigenstate $\varphi_2(t_2)$ of $H(t_2)$ is of order ε^2 and vanishes in the limit $\varepsilon \to 0$.

This first approximation, known as the adiabatic theorem in text books, is often invoked in physics in a form or another to reduce a complicated time dependent quantum mechanical problem to the study of an effective hamiltonian acting in an instantaneous eigenspace of the complete hamiltonian driving the system. We make use of the fact that in this approximation the transitions out of the eigenspace under consideration must be small with respect to the transitions between the eigenstates belonging to that subspace, provided the corresponding energy levels are isolated in the spectrum. However, this reduction process is only a first step, often implicit, and the physically interesting quantities are given by the transition probabilities to be computed in the reduced system. This is the case for example in the theory of electronic transitions in slow atomic collisions. The motion of one excited electron in the field created by two slowly moving atoms can sometimes be reduced to the study of a two-level system driven by a slowly varying time dependent hamiltonian. The probability of a charge transfer from one atom to the other during the slow collision is then given by the corresponding transition probability $\mathcal{P}_{21}(\varepsilon)$ from one level to the other in the adiabatic limit $\varepsilon \to 0$, where ε is proportional to the relative velocity of the atoms (see for example the monograph [NU] and the reviews [So], [Na], [C]). It is thus important in this physical context to obtain accurate formulae for $\mathcal{P}_{21}(\varepsilon)$, and not only bounds, when ε is small but finite. Indeed, shortly after the establishment of the adiabatic theorem, Landau [La], Zener [Z], Majorana [M] and Rosen and Zener [RZ] gave explicit formulae for transition probabilities in the adiabatic limit for two-level systems, to be applied in similar physical contexts.

Let $e_1(t)$ and $e_2(t)$ be the eigenvalues of a 2×2 hamiltonian displaying an avoided crossing with closest approach of order δ at time $t = 0$:

$$e_2(t) - e_1(t) = \sqrt{a^2t^2 + b^2\delta^2} + \mathcal{O}(t^2). \tag{1.5}$$

If δ is small but finite, the Landau-Zener formula states that the transition probability from one level to the other is given by

$$\mathcal{P}_{21}(\varepsilon) \simeq \exp\left\{-\frac{\delta^2\pi b^2}{\varepsilon 2a}\right\} \quad \text{as } \varepsilon \to 0. \tag{1.6}$$

This formula has been obtained by Zener [Z] and Majorana [M] in the case of a particular two-level hamiltonian for which they found an analytic solution of the Schrödinger equation. It was derived independently by Landau [La] who introduced the remarkable idea of integrating the Schrödinger equation in the complex plane on a path surrounding the complex eigenvalue crossing point $z_0 \simeq i\frac{b\delta}{a}$, thus making explicit use of the analyticity of the hamiltonian.

The formula given in [RZ] also results from an exact solution of the Schrödinger equation and displays an exponentially decaying behaviour as $\varepsilon \to 0$ as well. This result together with the Landau-Zener formula gave credit to a folk adiabatic theorem saying that

> "*the transition probability out of a spectral subspace of the hamiltonian is exponentially small in the adiabaticity parameter, provided this subspace is spectrally isolated by a gap and the hamiltonian is analytic in time*".

This folk adiabatic theorem, in turn, gave an a posteriori justification to the reduction process which leads from the complete problem to a reduced two-dimensional problem.

In 1960, following the original idea of Landau, Dykhne [D] derived a generalization of the Landau-Zener formula for analytic real symmetric hamiltonians without assuming avoided crossings between the energy levels. He proposed the following formula for the transition probability

$$\mathcal{P}_{21}(\varepsilon) \simeq \exp\left\{\frac{2}{\varepsilon}\mathrm{Im}\int_{\zeta}(e_1(z)-e_2(z))dz\right\} \quad \text{as } \varepsilon \to 0 \tag{1.7}$$

where ζ is a path in the complex plane leading from the real axis to a complex eigenvalue crossing point z_0 (i.e. such that $e_1(z_0) = e_2(z_0)$). Further generalizations and other exact results can also be found in the chemical physics literature.

The Landau-Zener and Dykhne formulae have been used with success for years in atomic and molecular physics mainly [NU], [So], [Na] but also in nuclear physics [Thi], in solid state physics [Wi] or in laser physics [BH], [Kam] for example. A more recent field of application for the adiabatic approximation is the theory of the quantum Hall effect discovered by von Klitzing et. al. [vKDP]. Indeed, when it had been recognized that the adiabatic theorem could contribute to understand this phenomenon [Tho], more general versions of it, to which we shall come back, were introduced and used to explain some aspects of the quantum Hall effect [Ku], [ASY].

There has been also a sudden regain of interest in the adiabatic theorem for itself among physicists when in 1984 Berry [B1] pointed out that if it was applied to hamiltonians satisfying $H(t_1) = H(t_2)$, it could generate a phase factor having non trivial geometrical meaning. The point is that when the hamiltonians coincide at t_1 and t_2, the initial condition $\varphi_1(t_1)$ and the eigenvector $\varphi_1(t_2)$ appearing in the approximate solution

$$\psi_\varepsilon(t_2) = \exp\left\{-\frac{i}{\varepsilon}\int_{t_1}^{t_2} e_1(t)dt\right\}\varphi_1(t_2) + \mathcal{O}(\varepsilon) \tag{1.8}$$

must coincide up to a phase $\exp\{-i\beta\}$ which is determined by the condition (1.3). Thus we have

$$\psi_\varepsilon(t_2) = \exp\left\{-\frac{i}{\varepsilon}\int_{t_1}^{t_2} e_1(t)dt\right\}\exp\{-i\beta\}\,\psi_\varepsilon(t_1) + \mathcal{O}(\varepsilon) \tag{1.9}$$

where the geometrical meaning of the phase $\exp\{-i\beta\}$ has been clearly exposed by Simon in [Si]. The discovery of this geometrical phase has been confirmed experimentally by Delacretaz et. al. [DGWWZ]. We shall not investigate this geometrical aspect of the adiabatic theorem and we refer the reader to [SW] for more details and references on the subject. Another aspect of the adiabatic theorem we shall not consider here is the study of the decay of the transition probability with ε when the instantaneous energy level $e_1(t)$ experiences crossings with other levels during the evolution. Born and Fock [BF] showed that the adiabatic theorem was still true for a certain type of crossings, although the transition probability decays to zero with ε more slowly in these cases. The most recent and complete investigation of this problem is the work of Hagedorn [H1] who gives an asymptotic expansion of the solution of the Schrödinger equation in the adiabatic limit, in the case of real eigenvalue crossings.

1.2 Mathematical Aspects

These rapid successes of the adiabatic theorem in physical applications are to be contrasted with the rather slow process which gave a rigorous mathematical status to some of its aspects. Indeed, it was only in 1950 that Kato [Kat1] gave a rigorous and expected generalization of the result obtained by Born and Fock. This generalization consists in enlarging the class of hamiltonians for which the adiabatic theorem holds, by removing some technical restrictions on their spectrum. Kato's work was important from a physical point of view since the main result of Born and Fock had been derived under the assumption that the spectrum of the hamiltonian was discrete and non degenerate. These hypotheses on the spectrum are physically too restrictive as most spectra encountered in applications contain a continuous part and degeneracies of eigenvalues can occur as the result of some symmetry of the hamiltonian. Nevertheless, the adiabatic theorem was expected to hold true under the sole hypothesis that the eigenvalue of interest $e_1(t)$ was isolated in the spectrum for $t \in [t_1, t_2]$. It was argued that the nature of that spectrum far from $e_1(t)$ should not influence in an essential way the solution of the Schrödinger equation with initial condition at $t = t_1$ in the eigenspace associated with $e_1(t_1)$. Kato proved that it was indeed the case. Let $\mathcal{H}$ be the Hilbert space which describes the system and let $P_1(t)$ be the spectral projector associated with $e_1(t)$. We suppose $e_1(t)$ to be finitely degenerate and isolated in the spectrum of the hamiltonian $H(t)$ for any $t \in [t_1, t_2]$. We denote by $U_\varepsilon(t, t_1)$ the *physical evolution* associated with the equation

$$i\varepsilon \frac{d}{dt} U_\varepsilon(t, t_1) = H(t) U_\varepsilon(t, t_1), \quad U_\varepsilon(t_1, t_1) = \mathbb{I} \tag{1.10}$$

so that the solution of (1.2) is given by

$$\psi_\varepsilon(t) = U_\varepsilon(t, t_1)\varphi_0. \tag{1.11}$$

Kato introduced in [Kat1] a unitary operator $W(t, t_1)$, solution of the equation

$$i\frac{d}{dt} W(t, t_1) = i[\frac{d}{dt} P_1(t), P_1(t)] W(t, t_1), \quad W(t_1, t_1) = \mathbb{I}, \tag{1.12}$$

which he showed to have the intertwining relation

$$W(t, t_1) P_1(t_1) = P_1(t) W(t, t_1). \tag{1.13}$$

Performing an integration by parts on the dynamical phase, he obtained the estimate

$$\left\{ U_\varepsilon(t, t_1) - \exp\left\{ -\frac{i}{\varepsilon} \int_{t_1}^t e_1(t')dt' \right\} W(t, t_1) \right\} P_1(t_1) = \mathcal{O}(\varepsilon) \quad \forall t \in [t_1, t_2]. \tag{1.14}$$

These last two expressions mean that if $\psi_\varepsilon(t_1) = \varphi_0$ is in the eigenspace $P_1(t_1)\mathcal{H}$, i.e. $P_1(t_1)\varphi_0 = \varphi_0$, then $\psi_\varepsilon(t)$ will be in $P_1(t)\mathcal{H}$ for any $t \in [t_1, t_2]$, up to an error of order ε since they lead to

$$\psi_\varepsilon(t) \equiv U_\varepsilon(t, t_1)\varphi_0 = \exp\left\{ -\frac{i}{\varepsilon} \int_{t_1}^t e_1(t')dt' \right\} W(t, t_1)\varphi_0 + \mathcal{O}(\varepsilon) \tag{1.15}$$

where

$$W(t, t_1)\varphi_0 = P_1(t) W(t, t_1)\varphi_0. \tag{1.16}$$

As a corollary, we obtain again that the transition probability $\mathcal{P}_{21}(\varepsilon)$ to any state $\varphi_2(t)$ which is not in $P_1(t)\mathcal{H}$, i.e. such that $P_1(t)\varphi_2(t) = 0$, is given by $\mathcal{P}_{21}(\varepsilon) = \mathcal{O}(\varepsilon^2)$. When we apply Kato's result to a case where the eigenspace $P_1(t)\mathcal{H}$ is one dimensional, we come back to the approximation (1.4) of Born and Fock since it can be shown that $W(t, t_1)\varphi_0 \equiv \varphi_1(t)$ satisfies condition (1.3) on the phases of the instantaneous eigenstates. We shall call $W(t, t_1)$ the *parallel transport* operator in the sequel, according to its geometrical meaning in the setting studied by Berry [B1].

Lenard [Len] made an important step in 1959 concerning the study of the decay with ε of the transition probability out of a spectral subspace. Let us denote by $\mathcal{P}_{21}(\varepsilon)$ the transition probability from one spectral subspace $P_1(t_1)\mathcal{H}$ of $H(t_1)$ to any other spectral subspace $P_2(t_2)\mathcal{H}$ of $H(t_2)$ between the times t_1 and t_2. Lenard showed that if $H(t)$ is a non degenerate n-level hamiltonian for any $t \in [t_1, t_2]$ satisfying $\frac{d^n}{dt^n}H(t_1) = 0$ for all n, then the transition probability admits an asymptotic expansion in powers of ε:

$$\mathcal{P}_{21}(\varepsilon) = a_2\varepsilon^2 + a_3\varepsilon^3 + \cdots + a_n\varepsilon^n + \mathcal{O}(\varepsilon^{n+1}) \quad \forall n. \tag{1.17}$$

An important feature of this asymptotic expansion is that its first N terms vanish if $\frac{d^n}{dt^n}H(t_2) = 0$ for all $n \leq N$, yielding a transition probability of order ε^{N+1}. In particular, if $\frac{d^n}{dt^n}H(t_2) = 0$ for any n, the transition probability is smaller than any power of ε

$$\mathcal{P}_{21}(\varepsilon) = \mathcal{O}(\varepsilon^n) \quad \forall n. \tag{1.18}$$

Lenard obtained this result by considering the projector

$$Q_\varepsilon(t) \equiv U_\varepsilon(t, t_1)P_1(t_1)U_\varepsilon^{-1}(t, t_1) \tag{1.19}$$

solution of the Heisenberg equation of motion

$$i\varepsilon\frac{d}{dt}Q_\varepsilon(t) = [H(t), Q_\varepsilon(t)], \quad Q_\varepsilon(t_1) = P_1(t_1). \tag{1.20}$$

Inserting in (1.20) an a priori expansion of the solution in powers of ε with unknown matrix coefficients, he could solve the resulting equations for the coefficients, order by order. The link between $Q_\varepsilon(t_2)$ and $\mathcal{P}_{21}(\varepsilon)$ is furnished by the general relation

$$\mathcal{P}_{21}(\varepsilon) = \|P_2(t_2)U_\varepsilon(t_2, t_1)P_1(t_1)\|^2 = \|P_2(t_2)Q_\varepsilon(t_2)\|^2. \tag{1.21}$$

In 1964, Garrido [G] generalized the results of Lenard under the same assumptions on the hamiltonian by means of an iterative scheme generating hamiltonians $H_0 \equiv H, H_1, \cdots, H_q$. His recurrent construction allowed Garrido to show that to any (one-dimensional) spectral projector $P_1(t)$ of $H(t)$ corresponds a spectral projector $P_{q,1}(t)$ of the hamiltonian $H_q(t)$, such that if the solution of the Schrödinger equation (1.2) is in $P_{q,1}(t_1)\mathcal{H}$ at $t = t_1$, it will be in $P_{q,1}(t_2)$ at $t = t_2$ up to order ε^{q+1}, for any $q \geq 0$, provided ε is small enough. Moreover, when all the derivatives of $H(t)$ vanish at time t_1, $P_{q,1}(t_1) = P_1(t_1)$ so that we recover the result of Lenard [Len]. Similarly, when all the derivatives of $H(t)$ vanish at time t_2 as well, we get $\mathcal{P}_{21}(\varepsilon) = \mathcal{O}(\varepsilon^n)$. Another generalization of this last result had been previously established in 1962 by Sancho [Sa] who showed that the estimate (1.18) still holds when $P_1(t)$ is a finite dimensional projector associated with the eigenvalue $e_1(t)$ which is isolated in the spectrum of $H(t)$ for any time $t \in [t_1, t_2]$, provided the same conditions on the derivatives of H are satisfied. Kato's generalization of the formulation of the original adiabatic theorem together with the improvements in the bounds on the transition probability by Lenard, Garrido and Sancho gave further credit to the folk adiabatic theorem on the exponential decay of the transition probability mentioned earlier. At that point, it remains essentially two steps to take, one of qualitative nature and the other of rather technical character, before a mathematical proof of such a theorem in the setting used by physicists could be given. The qualitative step is to extend the same kind of results to cases where $P_1(t)$ is a spectral projector of $H(t)$ corresponding essentially to several different eigenvalues which may cross each other but which are otherwise isolated from the rest of the spectrum for any time $t \in [t_1, t_2]$. This is typically the situation encountered in the reduction process from complete problems to effective simpler problems described in the previous section. The second step, of a more mathematical nature is to prove that the transition probability $\mathcal{P}_{21}(\varepsilon)$, shown to be smaller than any power of ε, is actually exponentially decreasing with ε, under suitable conditions, that is

$$\mathcal{P}_{21}(\varepsilon) = \mathcal{O}(\exp\{-2\tau/\varepsilon\}) \quad \text{as} \quad \varepsilon \to 0. \tag{1.22}$$

1.2.1 Adiabatic Evolution

The extension of the adiabatic theorem to the general cases just described was first demonstrated by Nenciu [Ne1] in 1980 for bounded hamiltonians. Later, in 1987, Avron, Seiler and Yaffe [ASY] showed that this extension held for unbounded hamiltonians as well and applied it to deal with the quantum Hall effect. The main hypothesis on the hamiltonian $H(t)$ is that its spectrum $\sigma(t)$ must be composed of two parts $\sigma_1(t)$ and $\sigma_2(t)$ separated by a finite gap g for any time $t \in [t_1, t_2]$, i.e.

$$\sigma(t) = \sigma_1(t) \cup \sigma_2(t) \text{ and } \inf_{t\in[t_1,t_2]} \text{dist}[\sigma_1(t), \sigma_2(t)] \geq g > 0 \tag{1.23}$$

where $\sigma_1(t)$ is bounded. The projector $P_1(t)$ corresponding to $\sigma_1(t)$ is then given by a Riesz formula and the nature of the spectrum included in $\sigma_1(t)$ does not matter. The idea is essentially to build an approximation of the evolution operator $U_\varepsilon(t, t_1)$, similar to the one given by Kato when $P_1(t)$ is associated with one eigenvalue $e_1(t)$, which was essentially

$$U_\varepsilon(t, t_1) = \exp\left\{-\frac{i}{\varepsilon}\int_{t_1}^{t} e_1(t')dt'\right\} W(t, t_1) + \mathcal{O}(\varepsilon). \tag{1.24}$$

We shall call such an approximation an *adiabatic evolution*. The point here is to find an expression which is an equivalent of the dynamical phase factor $\exp\left\{-\frac{i}{\varepsilon}\int_{t_1}^{t} e_1(t')dt'\right\}$ when $e_1(t)$ is replaced by $\sigma_1(t)$. Such an expression is provided by the unitary operator $\Phi_\varepsilon(t, t_1)$, which we shall call *dynamical phase operator*, defined by the equation

$$i\varepsilon\frac{d}{dt}\Phi_\varepsilon(t, t_1) = W^{-1}(t, t_1)H(t)W(t, t_1)\Phi_\varepsilon(t, t_1), \quad \Phi_\varepsilon(t_1, t_1) = \mathbb{I} \tag{1.25}$$

where W is the parallel transport defined by (1.12). By performing an integration by parts on this dynamical phase operator, in the spirit of the original proof by Born and Fock, Avron Seiler and Yaffe established the estimate

$$U_\varepsilon(t, t_1) = W(t, t_1)\Phi_\varepsilon(t, t_1) + \mathcal{O}(\varepsilon). \tag{1.26}$$

The unitary operator $W\Phi_\varepsilon$ is thus an adiabatic evolution operator which approximates the physical evolution up to an error of order ε. This formula implies that the transition probability $\mathcal{P}_{21}(\varepsilon)$ to any other spectral subspace $P_2(t)\mathcal{H}$ satisfies $\mathcal{P}_{21}(\varepsilon) = \mathcal{O}(\varepsilon^2)$ because of the intertwining property (1.13) and the relation

$$[\Phi_\varepsilon(t, t_1), P_1(t_1)] = 0 \quad \forall t \in [t_1, t_2]. \tag{1.27}$$

Moreover Nenciu [Ne2] and Nenciu and Rasche [NR] generalized the ideas of Garrido when $H(t)$ satisfies the sole gap assumption just mentioned. They introduced another hierarchy of hamiltonians $\{H_q\}$, $q \geq 0$ for which they could prove a similar result to the one obtained by Garrido. As before, when all the derivatives of $H(t)$ vanish at t_1 and t_2, we have $\mathcal{P}_{21}(\varepsilon) = \mathcal{O}(\varepsilon^n)$, for any n ([Ne2], [ASY], [NR]).

On the other hand, results concerning the actual exponential decay of the transition probability with ε were rather scarce and not quite satisfactory as far as mathematical rigour is concerned. Moreover, essentially two-level systems were treated in these works and there was a complete lack of rigorous results for general systems.

We would like to stress that although we presented this aspect of the problem as a technical one, it has a definite importance in the physics involved. Indeed, suppose the adiabatic theorem is invoked to reduce a problem to the study of a two-level system, for which the physically relevant transition probability from one level to the other turns out to be exponentially decreasing in the adiabatic limit. It is then necessary that the discarded transition probability out of the two-dimensional subspace considered decreases exponentially as well, so that the former probability actually gives the leading behaviour in the adiabatic limit.

This was the major motivation to begin this study which is focused mainly on the exponential suppression of transition probabilities in the adiabatic limit.

1.2.2 Adiabatic Invariants

As a final remark before describing the content of this work, we can replace these considerations in the broader frame of the search for adiabatic invariants of a dynamical system. Consider a dynamical system depending on a parameter ε

$$\frac{d}{dt}X = F(X, \varepsilon t) \tag{1.28}$$

where X belongs to some functional space. An *adiabatic invariant* of this system is a function $I(X(t), \varepsilon)$ such that

$$|I(X(t), \varepsilon) - I(X(0), \varepsilon)| \to 0 \quad \text{as} \quad \varepsilon \to 0. \tag{1.29}$$

In the case of a classical system driven by a time dependent hamiltonian of the form $H(p, q, \varepsilon t)$, an adiabatic invariant is a function $I(p(t), q(t), \varepsilon)$ such that

$$|I(p(t), q(t), \varepsilon) - I(p(0), q(0), \varepsilon)| \to 0 \quad \text{as} \quad \varepsilon \to 0. \tag{1.30}$$

An important example is provided by the one-dimensional harmonic oscillator whose frequency varies slowly with time. The corresponding hamiltonian reads

$$H(p, q, \varepsilon t) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2(\varepsilon t)q^2 \tag{1.31}$$

and the adiabatic invariant for this system is given by

$$I(p(t), q(t), \varepsilon) = \frac{H(p(t), q(t), \varepsilon t)}{\omega(\varepsilon t)}, \tag{1.32}$$

provided $\omega(\varepsilon t) > 0$ for any time t (see [A], paragraph 20). For this linear dynamical system, it is even possible to obtain an exponential estimate for the total change $\Delta I(\varepsilon)$ of the adiabatic invariant

$$\Delta I(\varepsilon) = |I(p(+\infty), q(+\infty), \varepsilon) - I(p(-\infty), q(-\infty), \varepsilon)| = \mathcal{O}(\exp\{-\tau/\varepsilon\}) \tag{1.33}$$

when $\omega(t)$ possesses an analytic extension in a strip including the real axis and tends sufficiently rapidly to definite limits at $\pm\infty$. With these notions we see that the transition probability

$$\mathcal{P}_{21}(\varepsilon) = \|P_2(t)U_\varepsilon(t, 0)P_1(0)\|^2 \tag{1.34}$$

is an adiabatic invariant of the dynamical system

$$i\varepsilon\frac{d}{dt}U_\varepsilon(t,0) = H(t)U_\varepsilon(t,0), \quad U_\varepsilon(0,0) = \mathbb{I}. \tag{1.35}$$

In relation with the KAM theorem of classical mechanics Nekhoroshev [Nek] studied in details what he calls nearly integrable systems, i.e. systems governed by hamiltonians of the form

$$H = H_0(I) + \varepsilon H_1(I,\varphi,\varepsilon t) \tag{1.36}$$

where φ and I denote the canonical angle action variables of the system. When $\varepsilon = 0$, the system is integrable and I is a constant of the motion by virtue of the equation $\frac{d}{dt}I = -\frac{\partial H_0(I)}{\partial\varphi} \equiv 0$, whereas for ε positive but small, $I(t,\varepsilon)$ stay close to their initial value. The quantity $I(t,\varepsilon)$ is not quite an adiabatic invariant in the sense given above, but it shares the same general properties of an adiabatic invariant. Indeed, Nekhoroshev investigated the decay with ε of the difference $|I(t,\varepsilon) - I(0,\varepsilon)|$ and showed that under suitable smoothness assumptions on the hamiltonian

$$|I(t,\varepsilon) - I(0,\varepsilon)| \leq \varepsilon^b \quad \forall t \in [0, \exp\{1/\varepsilon^a\}] \tag{1.37}$$

where a and b depend on $H_0(I)$. Put in another way, this means that

$$|I(t,\varepsilon) - I(0,\varepsilon)| \leq \varepsilon^b \exp\{-1/\varepsilon^a\}\, t. \tag{1.38}$$

Thus obtaining of an exponential estimate on the transition probability $\mathcal{P}_{21}(\varepsilon)$ amounts to prove an estimate of the type (1.38) for $\|P_2(t)U_\varepsilon(t,0)P_1(0)\|$. We shall call such results in our quantum setting "Nekhoroshev type estimates" although the dynamical systems corresponding to (1.36) and (1.35) are rather different.

1.2.3 Reader's Guide

Before coming to the description of the main results of this work, we would like to draw the reader's attention to the following fact. From now on, we drop the historical point of view to adopt a more synthetic presentation of the most recent contributions to the adiabatic theorem which were obtained by several authors. In the notes at the end of the introduction we restore the chronology and make precise the links between these results.

1.3 Iterative Scheme

Let us now describe more precisely the two main ideas which will underlie most of this work and lead to our main results. The first essential tool we use is another recurrent construction of hamiltonians $H_0(t) \equiv H(t), H_1(t), \cdots, H_q(t), \cdots$, which is simple and local. By this we mean that $H_q(t)$ is computed directly from $H_{q-1}(t)$, without solving any differential equation.

Let $H(t)$ be a smooth hamiltonian, bounded from below, whose spectrum $\sigma(t)$ consists of two distinct parts $\sigma_1(t)$ and $\sigma_2(t)$, separated by a finite gap $g > 0$, as above. We denote by $P(t)$ the spectral projector corresponding to the bounded part $\sigma_1(t)$ of the spectrum. We have seen in the foregoing that the projector $Q_\varepsilon(t)$ solution of the Heisenberg equation of motion

$$i\varepsilon\frac{d}{dt}Q_\varepsilon(t) = [H(t), Q_\varepsilon(t)], \quad Q_\varepsilon(t_1) = P(t_1) \tag{1.39}$$

can provide direct information on the transition probability. Let us look at this equation more closely. Since its solution is a projector, it satisfies

$$Q_\varepsilon(t)Q'_\varepsilon(t)Q_\varepsilon(t) = 0 \tag{1.40}$$

where "$'$" means "$\frac{d}{dt}$", which is a direct consequence of the property $Q^2_\varepsilon(t) = Q_\varepsilon(t)$. By means of this identity, it is then possible to express the Heisenberg equation under the form

$$[H(t) - i\varepsilon[Q'_\varepsilon(t), Q_\varepsilon(t)], Q_\varepsilon(t)] = 0. \tag{1.41}$$

We shall try to find an approximate solution of this equation for $Q_\varepsilon(t)$ in the limit $\varepsilon \to 0$. The leading order in (1.41) will vanish if we replace $Q_\varepsilon(t)$ by the approximation $P_0(t) = P(t)$, since we obviously have $[H(t), P(t)] = 0$. Thus we write

$$Q_\varepsilon(t) = P_0(t) + \varepsilon R_1(t,\varepsilon), \tag{1.42}$$

where $R_1(t,\varepsilon)$ is a rest. We are hopeful that it will be of order 1 in ε. Inserting this expression for $Q_\varepsilon(t)$ in (1.41), we obtain

$$[H(t) - i\varepsilon[P'_0(t), P_0(t)] + \mathcal{O}(\varepsilon^2), Q_\varepsilon(t)] = 0. \tag{1.43}$$

Now the leading term of this equation, given by

$$[H(t) - i\varepsilon[P'_0(t), P_0(t)], Q_\varepsilon(t)], \tag{1.44}$$

is equal to zero if we choose as a second approximation

$$Q_\varepsilon(t) = P_1(t,\varepsilon) + \varepsilon^2 R_2(t,\varepsilon), \tag{1.45}$$

where $P_1(t,\varepsilon)$ is a spectral projector of the self-adjoint operator

$$H_1(t,\varepsilon) \equiv H(t) - i\varepsilon[P'_0(t), P_0(t)]. \tag{1.46}$$

This definition makes sense since according to perturbation theory, assuming ε to be small, the spectrum of $H_1(t,\varepsilon)$ is still separated in two disjoint pieces, one of which is bounded. We define $P_1(t,\varepsilon)$ as the projector corresponding to the bounded part of the spectrum of $H_1(t,\varepsilon)$ which tends to $P_0(t)$ as $\varepsilon \to 0$. Again we are confident that $R_2(t,\varepsilon)$ is of order 1 in ε. Now we repeat the same procedure and we are led to the equation

$$[H(t) - i\varepsilon[P'_1(t,\varepsilon), P_1(t,\varepsilon)] + \mathcal{O}(\varepsilon^3), Q_\varepsilon(t)] = 0. \tag{1.47}$$

Similarly, the leading order will be set to zero by the choice

$$Q_\varepsilon(t) = P_2(t,\varepsilon) + \varepsilon^2 R_3(t,\varepsilon), \tag{1.48}$$

where $P_2(t,\varepsilon)$ is a well defined spectral projector of

$$H_2(t,\varepsilon) \equiv H(t) - i\varepsilon[P'_1(t,\varepsilon), P_1(t,\varepsilon)] \tag{1.49}$$

when ε is small and $R_3(t,\varepsilon)$ is a rest. We can repeat the whole process as many times as we wish, which provides us with a hierarchy of hamiltonians whose spectral projectors should solve the Heisenberg equation to an increasing accuracy. We define then an iterative scheme starting with $H_0(t) \equiv H(t)$ by the equations

$$H_q(t,\varepsilon) = H(t) - \varepsilon K_{q-1}(t,\varepsilon) \tag{1.50}$$

with

$$K_{q-1}(t,\varepsilon) = i[P'_{q-1}(t,\varepsilon), P_{q-1}(t,\varepsilon)], \tag{1.51}$$

$P_{q-1}(t,\varepsilon)$ being the spectral projector associated with the bounded part of the spectrum of $H_{q-1}(t,\varepsilon)$. As for the iterative schemes mentioned above, $H_q(t,\varepsilon)$ and $H(t)$ coincide at the points $t = t_0$ where the first q derivatives of $H(t)$ vanish.

1.3.1 Higher Order Adiabatic Evolutions

The next step is to build an evolution operator which would follow the decomposition of the Hilbert space $\mathcal{H}$ in $P_q(t,\varepsilon)\mathcal{H} \oplus (\mathbb{I} - P_q(t,\varepsilon))\mathcal{H}$ for any time t, in the spirit of Kato [Kat1] and Krein [Kr], and which would also approximate the evolution operator $U_\varepsilon(t,t_1)$ given by the Schrödinger equation (1.10) when ε is small. We expect such an evolution to approximate the physical evolution up to a correction of order ε^{q+1} since the projectors $P_q(t,\varepsilon)$ seem to approximate $Q_\varepsilon(t)$ up to a term of the same order. Thus, as before, we introduce a parallel transport operator $W_q(t,t_1)$ such that

$$W_q(t,t_1)P_q(t_1,\varepsilon) = P_q(t,\varepsilon)W_q(t,t_1) \quad \forall t \in [t_1,t_2] \tag{1.52}$$

by means of equation (1.12) with $P_q(t,\varepsilon)$ in place of $P(t)$, and a dynamical phase operator $\Phi_q(t,t_1)$ commuting with $P_q(t_1,\varepsilon)$ by the equation

$$i\varepsilon\frac{d}{dt}\Phi_q(t,t_1) = W_q^{-1}(t,t_1)H_q(t,\varepsilon)W_q(t,t_1)\Phi_q(t,t_1), \quad \Phi_q(t_1,t_1) = \mathbb{I} \tag{1.53}$$

Note that here both operators depend on ε. From these very definitions follows the basic estimate

$$\|U_\varepsilon(t,t_1) - W_q(t,t_1)\Phi_q(t,t_1)\| \le \int_{t_1}^{t} \|K_q(t',\varepsilon) - K_{q-1}(t',\varepsilon)\|dt'. \tag{1.54}$$

The simplicity of the above iterative scheme allows the difference $\|K_q - K_{q-1}\|$ to be evaluated by perturbation theory and yields [JP1], [JP2]

$$\|K_q(t',\varepsilon) - K_{q-1}(t',\varepsilon)\| \le \beta_q\varepsilon^q \tag{1.55}$$

where β_q is a constant. Thus, as expected, we obtain a better adiabatic evolution which is of order ε^q instead of ε

$$U_\varepsilon(t,t_1) = W_q(t,t_1)\Phi_q(t,t_1) + \mathcal{O}(\varepsilon^q). \tag{1.56}$$

As a corollary, we get $\mathcal{P}_{21}(\varepsilon) = \mathcal{O}(\varepsilon^{2q})$ if the first q derivatives of $H(t)$ vanish at t_1 and t_2. As we assumed our hamiltonian to be smooth, we can construct adiabatic evolutions of arbitrary order. The price to pay for the simplicity of this construction is that we have to modify the dynamical phase operator and to perform an integration by parts, [JP1], to improve the approximation by a factor ε ([NR]). The expected estimates at the q^{th} step read $U_\varepsilon(t,t_1) = W_q(t,t_1)\overline{\Phi_q(t,t_1)} + \mathcal{O}(\varepsilon^{q+1})$, where $\overline{\Phi_q}$ is the modified dynamical phase operator, and $\mathcal{P}_{21}(\varepsilon) = \mathcal{O}(\varepsilon^{2(q+1)})$.

1.3.2 From Adiabatic to Superadiabatic Evolutions

When the hamiltonian $H(t)$ depends analytically on time, we can get much better bounds on the difference $\|K_q - K_{q-1}\|$. This comes from the fact that, in this case, we can control the dependence on q of the constants β_q appearing in (1.55), for values of q up to $N^*(\varepsilon) = \mathcal{O}(1/\varepsilon)$. We have essentially the factorial behaviour

$$\beta_q \simeq b^q q! \text{ for any } q \le N^*(\varepsilon) \simeq \frac{1}{b\varepsilon}, \tag{1.57}$$

where b is a constant. Thus, for $q = N^*(\varepsilon)$, we get using Stirling formula for $N^*(\varepsilon)!$ [JP3]

$$\|K_q(t',\varepsilon) - K_{q-1}(t',\varepsilon)\| = \mathcal{O}(\exp\{-\tau/\varepsilon\}) \text{ with } \tau \simeq \frac{1}{b}. \tag{1.58}$$

Inserting this result in the approximation of the evolution operator, we obtain a "Nekhoroshev type estimate" which reads [Ne3], [JP3]

$$U_\varepsilon(t,t_1) = W_{N^*(\varepsilon)}(t,t_1)\Phi_{N^*(\varepsilon)}(t,t_1) + \mathcal{O}\left(|t_2 - t_1| \exp\{-\tau/\varepsilon\}\right). \tag{1.59}$$

This means that the approximation $W_{N^*}\Phi_{N^*}$ we have just constructed differs from the physical evolution U_ε by a term which remains small for exponentially long times, i.e. $t_2 - t_1 \sim \mathcal{O}(\exp\{\tau/\varepsilon\})$, in contrast with the usual adiabatic approximation $W\Phi_\varepsilon$ in (1.26) which is valid for $t_2 - t_1 \sim \mathcal{O}(1/\varepsilon)$ only. Because of that property we shall call

$$V_*(t,t_1) \equiv W_{N^*(\varepsilon)}(t,t_1)\Phi_{N^*(\varepsilon)}(t,t_1) \tag{1.60}$$

a *superadiabatic evolution.*

In the setting we consider here, to compute the transition probability $\mathcal{P}_{21}(\varepsilon)$ from the spectral subspace $P(t_1)\mathcal{H}$ of $H(t_1)$ to its complement $(\mathbb{I}-P(t_2))\mathcal{H}$ at time t_2, it is necessary to take first the limits $t_1 \to -\infty$ and $t_2 \to +\infty$. Indeed, the simultaneous requirements for $H(t)$ be analytic in time and to have all its derivatives equal to zero at times t_1 and t_2 are compatible in these limits only, unless H is time-independent. Consequently we further require the existence of limiting hamiltonians H^+ and H^-, which satisfy the gap assumption and towards which $H(t)$ tends sufficiently rapidly as $t \to \pm\infty$. By this we mean in an integrable way.

The construction of the superadiabatic evolution $V_*(t,t_1)$ together with this last remark show that for analytic hamiltonians, a solution of the Schrödinger equation initially in the instantaneous spectral subspace $P(t_1)\mathcal{H}$ of the hamiltonian $H(t_1)$ with t_1 finite, will follow this spectral subspace during the evolution up to an error of order ε only $\forall t \in [t_1,t_2]$, t_2 finite, and not up to an exponentially small error in ε. Nevertheless, there exist time dependent projectors $P_{N^*(\varepsilon)}(t,\varepsilon)$ such that a solution initially in $P_{N^*(\varepsilon)}(t_1,\varepsilon)\mathcal{H}$ will be confined to the subspaces $P_{N^*(\varepsilon)}(t,\varepsilon)\mathcal{H}$ up to exponentially small errors, and this for any time t between t_1 and t_2. These projectors $P_{N^*(\varepsilon)}(t,\varepsilon)$ are a distance of order ε away from the spectral projectors $P(t)$ and coincide with them at times $t_1 = -\infty$ and $t_2 = +\infty$ only. It shows that the transition probability $\mathcal{P}_{21}(\varepsilon)$ from $P(-\infty)\mathcal{H}$ to $(\mathbb{I}-P(+\infty))\mathcal{H}$ between the times $-\infty$ and $+\infty$, satisfies

$$\mathcal{P}_{21}(\varepsilon) = \mathcal{O}\left(\exp\{-2\tau/\varepsilon\}\right). \tag{1.61}$$

It should be noted also that we have the same bound on the transition probability from $(\mathbb{I}-P(-\infty))\mathcal{H}$ to $P(+\infty)\mathcal{H}$, as expected.

The role of such superadiabatic evolutions obtained by optimal truncation of an iterative scheme was emphasized in this context by Berry [B2] and generalized independently by Nenciu [Ne3]. Nenciu's method is inspired by Lenard's one and it applies to analytic hamiltonians as well as more general C^∞ smooth hamiltonians. The main advantage of our approach is that we can control the dependence of the exponential decay rate τ on the width of the gap g isolating the spectral projector $P(t)$ of $H(t)$. The rate τ is directly proportional to the width of the gap g between the components $\sigma_1(t)$ and $\sigma_2(t)$ of the spectrum of the hamiltonian, as expected on physical grounds [JP3]. This property will be crucial for other results to come.

1.4 Complex Time Method

1.4.1 An Asymptotic Formula

Our iterative scheme has allowed us to prove that the transition probability across the gap is bounded by an exponentially decreasing function of ε, thus justifying the folk adiabatic theorem quoted at the beginning of this introduction. But this method cannot give us the leading behaviour of the transition probability in the adiabatic limit. This behaviour will be provided in certain cases by the application of the second main idea used in this work, which we shall now describe. This is the original idea Landau used to compute the transition probability $\mathcal{P}_{21}(\varepsilon)$ for two-level systems [La], which amounts to make the time variable complex and to push the path of integration of the Schrödinger equation from the real axis to the complex plane. This idea was further exploited by Pokrovskii and Khalatnikov [PK] and Dykhne [D] and it was finally made rigorous in some cases by Davis and Pechukas [DP], and Hwang and Pechukas [HP] in two interesting papers. Actually they justified the Dykhne formula (1.7) for two-level systems driven by analytic hamiltonians which are real and symmetric. Let us see in more details what happens when we consider general two-level hamiltonians. Let $H(t)$ be a two-level hamiltonian which is hermitian and possesses an analytic extension $H(z)$ in a strip S_a of width $2a$ surrounding the real axis. We also suppose that it tends rapidly to non degenerate limiting hamiltonians H^+ and H^- as $t \to \pm\infty$. As before, we consider the transition probability $\mathcal{P}_{21}(\varepsilon)$ from the level associated with the eigenvalue $e_1(t_1)$, in the limit $t_1 \to -\infty$, to the level associated with $e_2(t_2)$, in the limit $t_2 \to +\infty$. We also assume that the levels are non degenerate for any real time so that $e_2(t) - e_1(t) \geq g > 0$, $\forall t \in \mathbb{R}$. Let $\varphi_j(t)$ be the normalized instantaneous eigenvectors corresponding to $e_j(t)$, $j = 1, 2$, whose phases are fixed by condition (1.3) or, equivalently, $\varphi_j(t) = W(t, t_0)\varphi_j(t_0)$, with $W(t, t_0)$ the parallel transport operator and $\varphi_j(t_0)$ a normalized eigenvector associated with $e_j(t_0)$. We can expand the solution ψ_ε of the Schrödinger equation on this time dependent basis, introducing unknown coefficients $c_j(t)$ and explicit dynamical phases as

$$\psi_\varepsilon(t) = \sum_{j=1}^{2} c_j(t) \exp\left\{-\frac{i}{\varepsilon}\int_{t_0}^{t} e_j(t')dt'\right\}\varphi_j(t) \quad t_0 \in \mathbb{R}. \tag{1.62}$$

The coefficients c_j are determined by a set of coupled differential equations obtained by inserting the expansion (1.62) in the Schrödinger equation. The situation we consider at $t_1 = -\infty$ is characterized by the condition $c_1(-\infty) = 1$, $c_2(-\infty) = 0$ and the transition probability $\mathcal{P}_{21}(\varepsilon)$ is thus given by the expression $\mathcal{P}_{21}(\varepsilon) = |c_2(+\infty)|^2$. Now, as the hamiltonian $H(t)$ admits an analytic extension $H(z)$ in the strip S_a, the solution $\psi_\varepsilon(t)$ also admits an analytic extension $\psi_\varepsilon(z)$ in S_a, so that we can deform the path of integration of the Schrödinger equation in S_a. The idea is to use the multivaluedness of the analytic continuations $e_j(z)$ and $\varphi_j(z)$ of the instantaneous eigenvalues and eigenvectors. Indeed, these quantities have generically square-root type singularities at complex eigenvalue crossing points, i.e. points z_0 such that $e_1(z_0) = e_2(z_0)$. If we write our two-level hamiltonian under the form $\mathbf{B}(t)\cdot\mathbf{s}$, where s_k, $k = 1, 2, 3$, are the spin-$\frac{1}{2}$ matrices and $\mathbf{B}(t)$ is a magnetic field whose components are analytic in S_a, the eigenvalues have the form

$$e_j(t) = (-1)^j\frac{1}{2}\sqrt{B_1^2(t) + B_2^2(t) + B_3^2(t)} \equiv (-1)^j\frac{1}{2}\sqrt{\rho(t)}, \quad j = 1, 2 \tag{1.63}$$

with $\rho(t) > 0$ $\forall t \in \mathbb{R}$. Thus an eigenvalue crossing point z_0 is a complex zero of the analytic function $\rho(z)$ which is generically simple. Hence the behaviours

$$e_j(z) \simeq (-1)^j\frac{1}{2}\sqrt{\rho'(z_0)(z - z_0)}\; j = 1, 2 \tag{1.64}$$

in the vicinity of z_0. Consider now a loop γ based at $t_0 \in \mathbb{R}$ which encircles the eigenvalue crossing point z_0 (see figure (1.1)). If we analytically continue $e_1(t_0)$ and $\varphi_1(t_0)$ along this loop and denote by $\tilde{e_1}(t_0|\gamma)$ and $\widetilde{\varphi_1}(t_0|\gamma)$ the results of the analytic continuations, it follows from the foregoing that

$$\tilde{e_1}(t_0|\gamma) = e_2(t_0). \tag{1.65}$$

Since $\varphi_1(z)$ is the eigenvector associated with $e_1(z)$, along the whole loop, we must have

$$\widetilde{\varphi_1}(t_0|\gamma) = \exp\{-i\theta_1(t_0|\gamma)\}\,\varphi_2(t_0) \tag{1.66}$$

where $\theta_1(t_0|\gamma)$ is in general a complex phase. Because of the above properties, and the analyticity of $\psi_\varepsilon(z)$, it becomes clear that there must exist a relation between the coefficient $c_2(+\infty)$ obtained by integration of the Schrödinger equation along the real axis and the coefficient $\tilde{c_1}(+\infty)$ obtained by integration of the same equation along a path η off the real axis, but in the analyticity strip S_a, passing above the eigenvalue crossing point z_0 (see figure (1.1)). The relation reads

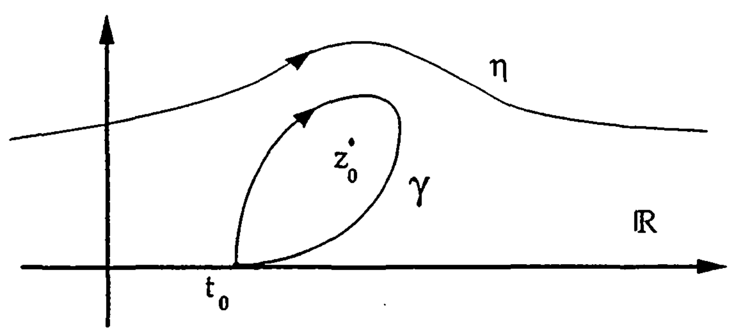

Figure 1.1: The loop γ encircling z_0 and the path of integration η.

$$c_2(+\infty) = \exp\{-i\theta_1(t_0|\gamma)\}\exp\left\{-\frac{i}{\varepsilon}\int_\gamma e_1(z)dz\right\}\tilde{c_1}(+\infty), \tag{1.67}$$

in which we recognize a contribution from the eigenvectors, and a contribution from the dynamical phases (where $\int_\gamma e_1(z)dz$ is the integral of the analytic continuation of $e_1(z)$ along γ). Thus, provided we can control the coefficient $\tilde{c_1}$ along the path η in the complex plane in such a way that

$$\tilde{c_1}(+\infty) = 1 + \mathcal{O}(\varepsilon), \tag{1.68}$$

we have the asymptotic formula for the transition probability [JKP1], [B3], [JKP2]

$$\mathcal{P}_{21}(\varepsilon) = \exp\{2\mathrm{Im}\theta_1(t_0|\gamma)\}\exp\left\{\frac{2}{\varepsilon}\mathrm{Im}\int_\gamma e_1(z)dz\right\}(1+\mathcal{O}(\varepsilon)). \tag{1.69}$$

A few remarks are in order here.

- The first is that the exponential decay rate $2\mathrm{Im}\int_\gamma e_1(z)dz$ is the same as the one appearing in Dykhne formula (1.7) and it is independent of the location of the base point $t_0 \in \mathbb{R}$.
- In the second place, the prefactor $\exp\{2\mathrm{Im}\theta_1(t_0|\gamma)\}$ has a geometrical origin since it is a characteristic of the parallel transport (1.12) as the usual Berry phase [B1] and it is also independent of $t_0 \in \mathbb{R}$. Moreover, we have an explicit formula for this geometrical prefactor in terms of the components of the field $\mathbf{B}(z)$.

- When applied to real symmetric hamiltonians on the real axis, i.e. such that $B_2(t) \equiv 0$, our formula shows at once that the prefactor reduces to one, yielding back the Dykhne formula. This property of the geometrical prefactor explains why its presence had never been noticed up to now. Indeed, the physical situations to which the Dykhne formula giving the transition probability has been applied correspond to real symmetric two-level hamiltonians (see [NU]).
- The presence of the unexpected geometrical prefactor $\exp\{2\text{Im}\theta_1(t_0|\gamma)\}$ in the formula giving the transition probability between two levels in the adiabatic limit has been confirmed experimentally by Zwanziger, Rucker and Chingas [ZRC] who studied the evolution of spin-$\frac{1}{2}$'s in a slowly varying time-dependent magnetic field.
- Last but not least, the validity of the formula (1.69) is subjected to the condition that a fine control of the coefficient $\tilde{c}_1(+\infty)$ of the form (1.68) could be established. Note that proving such an estimate for $\tilde{c}_1(+\infty)$ amounts to extend the usual adiabatic theorem for the coefficient c_1 from the real axis to the path η in the complex plane.

As we shall see, there are cases for which the asymptotic formula (1.69) can be entirely justified analytically and the geometrical prefactor $\exp\{2\text{Im}\theta_1(t_0|\gamma)\}$ is different from one [JKP2].

1.4.2 Dissipative Paths and Stokes Lines

By studying the differential equation satisfied by the coefficients c_j, we can see easily that a sufficient condition for the bound (1.68) to hold can be expressed in terms of the multivalued analytic function

$$\Delta_{12}(z) = \int_{t_0}^{z}(e_1(z') - e_2(z'))dz' \tag{1.70}$$

where the integral is taken along a path going from $t_0 \in \mathbb{R}$ to $z \in S_a$. If the path η going above the eigenvalue crossing point z_0 is parameterized by $\eta(s)$, the condition reads

$$\frac{d}{ds}\text{Im}\Delta_{12}(\eta(s)) \geq 0, \ \ \forall s \in \mathbb{R} \tag{1.71}$$

so that $\text{Im}\Delta_{12}(\eta(s))$ is a non decreasing function of s. A path satisfying this requirement will be called a *dissipative path*. The existence of dissipative paths for a given two-level hamiltonian is a non-trivial matter since the condition they must verify is a global one. Nevertheless, we can handle this situation through the so-called *Stokes lines* of the problem which makes it possible in some cases to conclude to the existence of a dissipative path or, on the contrary, to exclude the existence of such paths in the analyticity strip of the hamiltonian. The Stokes lines here are defined as the level lines

$$\text{Im}\Delta_{12}(z) = \text{Im}\Delta_{12}(z_0) \ \ \forall z \in S_a \tag{1.72}$$

or, by means of the expressions (1.63)

$$\text{Im}\int_{z_0}^{z}\sqrt{\rho(z')}dz' = 0 \ \ \forall z \in S_a. \tag{1.73}$$

As is easily verified by a local analysis around z_0, there are generically three branches of Stokes lines which meet at z_0 and it can be shown also that these branches neither intersect each other or themselves, nor cross the real axis. The relation between Stokes

lines and dissipative paths is essentially the following [JKP2].
There exists a dissipative path passing above z_0 for a given problem if and only if the corresponding Stokes lines are such that one of the branches goes from $-\infty$ to z_0 whereas a second one goes from z_0 to $+\infty$, both these lines being entirely in the analyticity strip S_a.
As a dissipative path cannot cross twice a branch of Stokes lines because of the monotonic-

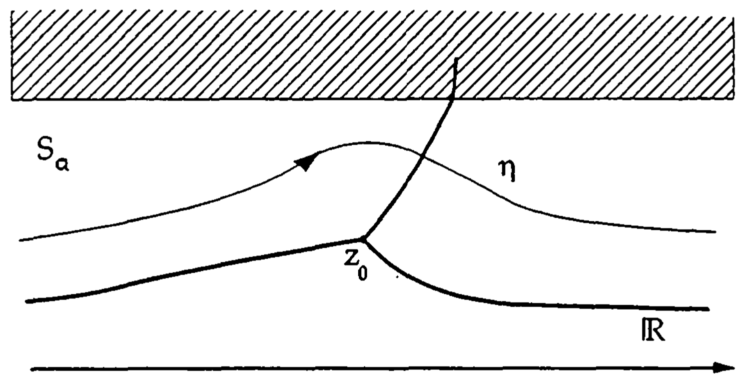

Figure 1.2: The Stokes lines associated with z_0 and the dissipative path η.

ity condition (1.71), it must then find itself above the two branches which are entirely in S_a in order to pass above the eigenvalue crossing point z_0, and cross the third branch of Stokes lines which can be shown to leave S_a, as on figure (1.2). This assertion provides us with an effective tool to decide whether or not the formula (1.69) is valid, since an analytic approach of the Stokes lines is sometimes possible whereas a numerical investigation can be done in more complicated situations.

1.4.3 A Little Geometry

One could think that the existence of dissipative paths we have required and expressed as a condition on the global behaviour of Stokes lines, is a technical limitation with no serious implication on the physics involved. However it should be stressed that this is not the case. Indeed, suppose that instead of having one eigenvalue crossing point only, we are in a situation such that there are N eigenvalue crossing points z_j, $j = 0, \cdots, N-1$, above the real axis. Which one should be selected to compute the asymptotic behaviour of the transition probability given by (1.69) ? This is definitely an important issue since formula (1.69) depends explicitly on that choice. The answer to that question is precisely provided by the global behaviour of the set of Stokes lines of the problem. To each eigenvalue crossing point z_j, $j = 0, \ldots, N-1$, correspond Stokes lines defined as the level lines $\mathrm{Im} \int_{z_j}^{z} \sqrt{\rho(z')}dz' = 0$, which have the general properties given above. Now, if the Stokes lines associated with one eigenvalue crossing point, say z_0, are such that two branches go to plus and minus infinity entirely in S_a, then it can be shown that z_0 is the unique eigenvalue crossing point above which a dissipative path can be constructed and consequently, it is the eigenvalue crossing point to be used in formula (1.69) [JKP2]. Moreover, z_0 is not necessarily the closest complex eigenvalue crossing point to the real axis (in the Euclidian distance), as sometimes erroneously stated. Nevertheless, by considering a different notion of distance in the complex plane, which is more appropriate to our problem, we can recover this intuitive property of z_0. Let us define the distance between two points x, y of the complex plane by

$$d_\rho(x,y) = \inf_\gamma \int_\gamma |\rho(z)|^{1/2}|dz| \tag{1.74}$$

where the infimum is taken on all rectifiable paths linking x and y. It is readily seen that any branch of Stokes line is a geodesic, with respect to that new metric, and that the real axis is also a geodesic. Thus the conditions satisfied by the Stokes lines associated with z_0 imply that there exists an infinite geodesic passing through z_0, which is parallel to the real axis. As a direct consequence, the eigenvalue crossing point z_0 is the closest to the real axis in the metric d_ρ, $d_\rho(z_0, \mathbb{R}) < d_\rho(z_k, \mathbb{R})$, $\forall k \neq j$. The metric d_ρ comes from the theory of quadratic differentials and was used to study Teichmueller spaces (see for example [St] and [Let]). It also allows us to express the transition probability in purely geometrical terms [JKP2]:

$$\mathcal{P}_{21}(\varepsilon) = \exp\left\{-\frac{2}{\varepsilon} d_\rho(z_0, \mathbb{R})\right\} \exp\left\{2\mathrm{Im}\theta_1(t_0|\gamma)\right\}(1 + \mathcal{O}(\varepsilon)). \tag{1.75}$$

1.4.4 Interferences

Up to now, we have considered generic situations with respect to two aspects. We have assumed that the eigenvalue crossing point z_0 was a simple zero of the analytic function $\rho(z)$ and that the Stokes lines associated with it met no other eigenvalue crossing point in S_a. Let us now consider a case with two eigenvalue crossing points, for example z_1 and z_2, such that the sets of Stokes lines associated with z_1 and z_2 possess a common branch which links z_1 and z_2, another which leads from $-\infty$ to z_1 and another one from z_2 to $+\infty$ (see figure (1.3)). We assume that these branches are entirely in the analyticity

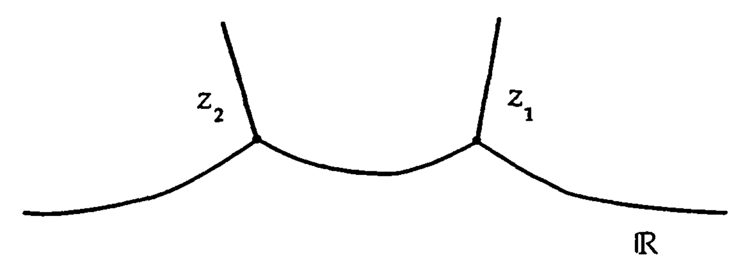

Figure 1.3: The Stokes lines associated with z_1 and z_2.

strip S_a. Such a situation is certainly less generic than the one considered before, but it appears in many examples of time reversal two-level systems. This is due to the symmetry of the Stokes lines with respect to the imaginary axis which this condition induces in the complex plane. A little thoughts shows that it is no possible anymore to find a dissipative path passing either above z_1 or z_2, or both. Hence we have to adopt another strategy to deal with this problem. The approach we shall describe has been designed by Pokrovskii and Khalatnikov [PK] in a semiclassical context and Davis and Pechukas [DP] used it in the simpler case of real symmetric hamiltonians on the real axis. The general idea is to integrate the Schrödinger equation directly on the different branches of Stokes lines which lead from $-\infty$ to $+\infty$, since the Stokes lines are also dissipative paths. But because of the branching points of $e_j(z)$ and $\varphi_j(z)$ at the eigenvalue crossing points, the differential equation satisfied by the coefficients $c_j(z)$ is singular at z_1 and z_2 and we are forced to consider an approximate differential equation for the coefficients in the neighbourhood of these points. The comparison equation retains the most singular terms of the original equation and turns out to be solvable in terms of well known special functions. Then, by using standard stretching and matching techniques of asymptotic solutions, we obtain the leading term of the coefficient $c_2(+\infty)$ as $\varepsilon \to 0$ which yields the transition probability [JMP]

$$\begin{aligned}\mathcal{P}_{21}(\varepsilon) &= \left|\sum_{j=1}^{2} \exp\{-i\theta_j\} \exp\left\{-\frac{i}{\varepsilon}\mathrm{Im}\int_{\gamma_j} e_1(z)dz\right\}\right. \\ &+ \left.\mathcal{O}\left(\exp\left\{\frac{1}{\varepsilon}\mathrm{Im}\int_{\gamma_1} e_1(z)dz\right\}\varepsilon^{1/5}\right)\right|^2 \qquad (1.76)\end{aligned}$$

where γ_j are loops based at the origin which encircle z_j and $\theta_j = \theta_1(0|\gamma_j)$ in the notation used before. As expected we have $\mathrm{Im}\int_{\gamma_1} e_1(z)dz = \mathrm{Im}\int_{\gamma_2} e_1(z)dz$ so that the leading term in the expression (1.76) is given by a decreasing exponential times an oscillatory function of $1/\varepsilon$.

This result shows that the behaviour of the Stokes lines in the complex plane determines the leading order of the transition probability not only quantitatively, as in the generic cases involving several eigenvalue crossings considered before, but also qualitatively through the appearance of oscillations in the current situation. This oscillatory behaviour results from a very general phenomenon in quantum mechanics, namely interferences. In the adiabatic limit, we see that interferences take place between the exponentially small leading contributions of each involved eigenvalue crossing point z_1 and z_2 to the transition probability. It is possible to formulate the transition probability in geometrical terms only in this situation too. By introducing the metric d_ρ, we have a formula which reads, for a case with N eigenvalue crossing points $z_0, z_1, \cdots, z_{N-1}$ on the same Stokes line,

$$\begin{aligned}\mathcal{P}_{21}(\varepsilon) = \exp\left\{-\frac{2\mathrm{d}_\rho(z_1, I\!R)}{\varepsilon}\right\} &\left\{\sum_{j=0}^{N-1} \exp\{2\mathrm{Im}\theta_j\}\right. \\ + 2\sum_{k<j}^{N-1} \exp\{\mathrm{Im}(\theta_j+\theta_k)\}\cos&\left.\left[\frac{1}{\varepsilon}\mathrm{d}_\rho(z_k, z_j) + \mathrm{Re}(\theta_k-\theta_j)\right] + \mathcal{O}(\varepsilon^{1/5})\right\} \qquad (1.77)\end{aligned}$$

displaying explicitly the oscillations due to interferences. Note finally that if the situation we consider here is the result of a time reversal symmetry it will be robust with respect to perturbations which possess the same symmetry.

We shall present in this work a new way of proving these results which leans more on general algebraic properties of two by two matrices than on asymptotic analytic behaviours of special functions, but it also involves integrations along specific paths in the complex plane, around the eigenvalue crossing points. The proof will thus gain in brevity, if not in clarity, and the order of the error bounds in the end results (1.76) and (1.77) will be improved from $\varepsilon^{1/5}$ to ε. The method we shall use to prove this result is adapted from the ones described by Fröman and Fröman [FF] in a simpler context of semiclassical analysis.

In the results we have given here, the system under consideration is in the ground state of the hamiltonian at $t = -\infty$ and we compute the transition probability to the excited state of the hamiltonian at time $t = +\infty$, by considering the Schrödinger equation on a path in the upper half complex plane. When the roles of the excited and ground states are exchanged, we have exactly the same transition probability as can be seen from a symmetry of the Schrödinger equation in the two-level case.

1.4.5 How to Avoid Considering the Stokes Lines ?

As we have just seen, the original idea of considering complex times, first expressed by Landau [La] is a very fruitful one for two-level systems since it gives access to explicit formulae for the leading terms of transition probabilities in the adiabatic limit. Nevertheless, the conditions on the Stokes lines to be verified in order to justify these formulae can be rather difficult to handle analytically and there are examples where these conditions are simply not fulfilled. We can then ask whether this method could be adapted to give results on the transition probability without any information on the Stokes lines. The answer is yes, with a price to pay, which is that we can get only bounds on the transition probability, instead of their leading behaviours. More precisely, when the hamiltonian is a 2×2 hermitian matrix, analytic in a strip enclosing the real axis, which tends sufficiently rapidly to limits as $t \to \pm\infty$ and whose spectrum is separated by a finite gap for any time, we can prove the existence of positive constants τ and M such that

$$\mathcal{P}_{21}(\varepsilon) \leq M \exp(-\tau/\varepsilon) \quad \text{as } \varepsilon \to 0 \tag{1.78}$$

by the following method [JKP1], [JKP2]. We consider the Schrödinger equation on a path η in the complex plane which is above the real axis again but passes under all the eigenvalue crossing points. It can be shown as before that if $\eta(s)$, $s \in I\!R$ is a dissipative path, we can control the analytic continuations of the dynamical phases $\exp\left\{-\frac{i}{\varepsilon}\int_0^z e_j(z')dz'\right\}$ along $\eta(s)$ and moreover, if $\eta(s)$ is at a finite distance κ of the real axis for any $s \in I\!R$ the dynamical phases provide us with an exponentially decreasing factor at the end point of the path, since $\text{Im}\eta(+\infty) \geq \kappa > 0$. In such a case, the exponential decay rate τ is proportional to $\text{Im}\eta(+\infty)$. Again we are led to prove the existence of dissipative paths, but this time, it is the presence of a finite gap between the eigenvalues taken on the real axis which insures the existence of a dissipative path slightly above the real axis. The method can be further adapted to deal with n-level hamiltonians satisfying the same general hypotheses [JKP1], [JKP2] and even with unbounded hamiltonians as well [JP4]. The notion of dissipative path in the latter case is a direct generalization of the two-level case. By dissipative path we mean a path in the complex plane along which it is possible to control the ε-dependent dynamical phase operator $\Phi_\varepsilon(z,0)$ generalizing expressions like $\exp\left\{-\frac{i}{\varepsilon}\int_0^z e_j(z')dz'\right\}$. More precisely, we have to control the numerical range of $\Phi_\varepsilon(z,0)$. Again, the assumed gap in the spectrum of $H(t)$ allows the existence of dissipative paths strictly above the real axis to be proven. It should be noted also that for unbounded hamiltonians it is not possible to consider analytic extensions of the evolution operator in the complex plane, so that we have to prove the result for bounded operators first. Then we approximate the unbounded hamiltonian H by bounded operators H_n, tending to H as $n \to \infty$, and show that the estimate (1.78) holds uniformly in n [JP4]. We shall present this way of obtaining the bound (1.78) in details for bounded hamiltonians only whereas we shall prove the exponential decay of transition probabilities for unbounded hamiltonians by means of our iterative scheme. Yet this method gave the first proof of an exponential estimate on the transition probability across a gap in the adiabatic limit for general unbounded hamiltonians [JP4].

There is a physically relevant situation where formula (1.69) can be used without verifications on the Stokes lines. This occurs when the levels e_1 and e_2 display an avoided crossing at some time $t_0 \in I\!R$ during the evolution. We shall describe this case in details in a forthcoming section.

1.5 Combining the Methods

1.5.1 Asymptotic Formula up to Exponentially Small Errors

Now that we have described our main tools separately as well as the kind of results they lead to, we shall combine the iterative approach with the complex time approach to improve these results by using the merits of both simultaneously. As a first application of this idea, we shall compute higher order corrections to the transition probability for a generic two-level system. Suppose we have a hamiltonian satisfying all the requirements for the transition probability to be computed by the complex time method so that

$$\mathcal{P}_{21}(\varepsilon) = \exp\{2\text{Im}\theta_1(0|\gamma)\}\exp\left\{\frac{2}{\varepsilon}\text{Im}\int_\gamma e_1(z)dz\right\}(1+\mathcal{O}(\varepsilon)) \tag{1.79}$$

where γ is a loop based at the origin, which encircles the relevant eigenvalue crossing point, say z_0 among the set z_j, $j = 0, \cdots, N-1$. We have obtained this result by considering a decomposition of the wave function $\psi_\varepsilon(t)$ of the form

$$\psi_\varepsilon(t) = \sum_{j=1}^{2} c_j(t)\exp\left\{-\frac{i}{\varepsilon}\int_0^t e_j(t')dt'\right\}\varphi_j(t) \quad t \in \mathbb{R} \tag{1.80}$$

with $c_1(-\infty) = 1$, $c_2(-\infty) = 0$ and by making use of the multivaluedness of e_j and φ_j in the analyticity strip S_a together with the formula $\mathcal{P}_{21}(\varepsilon) = |c_2(+\infty)|^2$. Let us consider now our iterative scheme (1.50)

$$H_q(t,\varepsilon) = H(t) - \varepsilon K_{q-1}(t,\varepsilon)\;;\;\; K_q(t,\varepsilon) = i[P_q'(t,\varepsilon), P_q(t,\varepsilon)] \tag{1.81}$$

defined for real values of t. It can be shown [JP2] that if ε is small enough, the 2×2 matrix representing the hamiltonian $H_q(t,\varepsilon)$ has a univalued analytic continuation in the domain $S_a \backslash \cup_{k=0}^{N-1} D_k$ where the D_k's are disks centered at the eigenvalue crossing points z_k, of arbitrarily small radius r. The singularities of $H_q(t,\varepsilon)$ come from the fact that generically the projectors are singular at eigenvalue crossing points. Moreover, the eigenvalues $e_{q,j}(t,\varepsilon)$ of $H_q(t,\varepsilon)$, $j = 1, 2$, have multivalued analytic extensions in $S_a \backslash \cup_{k=0}^{N-1} D_k$, and they experience no eigenvalue crossings in that domain. This means that we can define without ambiguity the normalized eigenvectors $\varphi_{q,j}(t,\varepsilon)$ associated with $e_{q,j}(t,\varepsilon)$, satisfying the usual phase fixing condition (1.3), and that they also have a multivalued analytic extension in $S_a \backslash \cup_{k=0}^{N-1} D_k$. Since the hamiltonians $H_q(t,\varepsilon)$ and $H(t)$ coincide as $t \to \pm\infty$, we can expand our wave function $\psi_\varepsilon(t)$ on the vectors $\varphi_{q,j}(t,\varepsilon)$ as

$$\psi_\varepsilon(t) = \sum_{j=1}^{2} c_{q,j}(t)\exp\left\{-\frac{i}{\varepsilon}\int_0^t e_{q,j}(t',\varepsilon)dt'\right\}\varphi_{q,j}(t,\varepsilon) \quad t \in \mathbb{R} \tag{1.82}$$

with initial conditions $c_{q,1}(-\infty) = 1$ and $c_{q,2}(-\infty) = 0$. Thus the transition probability we are interested in is given by $\mathcal{P}_{21}(\varepsilon) = |c_{q,2}(+\infty)|^2$. The key feature of that construction is that if we analytically continue $e_{q,1}(0,\varepsilon)$ along γ, which we assume to encircle the disk D_0, we obtain when we come back to the origin a value $\widetilde{e_{q,1}}(0,\varepsilon|\gamma)$ such that

$$\widetilde{e_{q,1}}(0,\varepsilon|\gamma) = e_{q,2}(0,\varepsilon). \tag{1.83}$$

Hence, with the same notation,

$$\widetilde{\varphi_{q,1}}(0,\varepsilon|\gamma) = \exp\{-i\theta_{q,1}(0,\varepsilon|\gamma)\}\,\varphi_{q,2}(0,\varepsilon). \tag{1.84}$$

Thus, we have a similar situation to the previous one, so that we can perform the same type of analysis. Indeed, we can prove by perturbation theory the existence of a dissipative path and we get the estimate

$$\mathcal{P}_{21}(\varepsilon) = \exp\{2\text{Im}\theta_{q,1}(0,\varepsilon|\gamma)\}\exp\left\{\frac{2}{\varepsilon}\text{Im}\int_\gamma e_{q,1}(z,\varepsilon)dz\right\}(1+\mathcal{O}(\varepsilon^q)), \tag{1.85}$$

where the correction term $\mathcal{O}(\varepsilon^q)$ comes from the properties of the iterative scheme we have presented in paragraph (1.3.1). It remains to expand the quantities $\theta_{q,1}$ and $e_{q,1}$ in powers of ε to get an asymptotic expansion for the logarithm of the transition probability of the form [JP2]

$$\ln\mathcal{P}_{21}(\varepsilon) = \frac{1}{\varepsilon}2\text{Im}\int_\gamma e_1(z)dz + 2\text{Im}\theta_1(0|\gamma) + \sum_{j=1}^{q-1}\alpha_j\varepsilon^j + \mathcal{O}(\varepsilon^q) \quad \forall q \geq 1. \tag{1.86}$$

Now using our finer knowledge of the asymptotic properties of the iterative scheme, we can actually improve this result by truncating the procedure in an optimal way to obtain by means of our superadiabatic approximation

$$\mathcal{P}_{21}(\varepsilon) = \tag{1.87}$$
$$\exp\left\{2\text{Im}\theta_{N^*(\varepsilon),1}(0,\varepsilon|\gamma)\right\}\exp\left\{\frac{2}{\varepsilon}\text{Im}\int_\gamma e_{N^*(\varepsilon),1}(z,\varepsilon)dz\right\}(1+\mathcal{O}(\exp\{-\tau/\varepsilon\}))$$

where $N^*(\varepsilon) \sim \frac{1}{\varepsilon}$ is the optimal stage and τ is positive. We now have in hand an exponentially decreasing leading order for the transition probability which is accurate up to an exponentially small correction as $\varepsilon \to 0$. But it should be noted that the leading order we have is a discontinuous function of ε, since the index $N^*(\varepsilon)$ is discrete.

1.5.2 Two Levels in a Gap

The most interesting outcome of the combination of the two approaches we have discussed from the point of view of mathematical physics is, in our opinion, the following. Consider an unbounded hamiltonian bounded from below, which is analytic in a strip S_a and possesses limits H^+ and H^- as $t \to \pm\infty$ to which it tends sufficiently rapidly. Assume that its spectrum is such that there exist two non-degenerate eigenvalues $e_1(t)$ and $e_2(t)$ which are bounded away from the rest of the spectrum for any time $t \in \mathbb{R}$. We consider now a solution of the Schrödinger equation which coincides as $t \to -\infty$ with the eigenstate of H^- corresponding to $e_1(-\infty)$. Can we compute the transition probability $\mathcal{P}_{21}(\varepsilon)$ at time $t = +\infty$ to the eigenstate of H^+ corresponding to $e_2(+\infty)$ in the adiabatic limit ? We already know that this transition probability is exponentially small but we would like to have the leading order of its asymptotic form as $\varepsilon \to 0$. On physical grounds we expect that if the two levels e_1 and e_2 are sufficiently isolated in the spectrum, a reduction of the problem to a two-level system should be justified so that the transition probability computed for this sub-system, given by the formula (1.69)

$$\mathcal{P}_{21}(\varepsilon) = \exp\{2\text{Im}\theta_1(0|\gamma)\}\exp\left\{\frac{2}{\varepsilon}\text{Im}\int_\gamma e_1(z)dz\right\}(1+\mathcal{O}(\varepsilon)) \tag{1.88}$$

should be accurate in the adiabatic limit. By using the two approaches we have discussed, we can establish from a mathematical point of view, that this is indeed the correct picture [JP3]. Of course, we have to assume that there exists a complex crossing point z_0

of the analytic continuations in the complex plane of $e_1(t)$ and $e_2(t)$ such that the corresponding Stokes lines behave properly, in the sense described in the previous section. The prefactor $\exp\{2\text{Im}\theta_1(0|\gamma)\}$ is computed by considering the analytic continuation along γ of the eigenvector $\varphi_1(z)$, as in the two-level case. The main steps of the proof are the following. Let us denote by $Q(t)$ the projector on the two dimensional eigenspace of the hamiltonian $H(t)$ associated with $e_1(t)$ and $e_2(t)$. By means of this spectrally isolated projector we can construct a superadiabatic evolution, as in the first section. Then we express the transition probability we are interested in by using this superadiabatic evolution instead of the physical one, thus making an error of order $\exp(-\tau/\varepsilon)$. The error we make here actually represents the transition probability out of the two-dimensional subspace $Q(+\infty)\mathcal{H}$ and its decay rate τ depends on the gap between the set $\{e_1(t), e_2(t)\}$ and the rest of the spectrum of $H(t)$, as noted previously. The expression we get by making that approximation coincides with the transition probability of an effective two-level system living in a time independent subspace. The spectrum of the two-level effective hamiltonian we have to consider is the same as the spectrum of $H_{N^*(\varepsilon)}(t,\varepsilon)$ given by the iterative scheme, restricted to its two-dimensional eigenspace $Q_{N^*(\varepsilon)}(t,\varepsilon)\mathcal{H}$. Thus we can prove by perturbation theory that an asymptotic formula of the type (1.88) is valid for the effective two-level systems. By retaining the lowest order in ε we get formula (1.88), provided the eigenvalues $e_1(t)$ and $e_2(t)$ are sufficiently isolated in the spectrum, so that τ is larger than the exponential decay rate given by (1.88).

1.5.3 Avoided Crossing

This result gives a rigorous mathematical status to the approximation which consists in computing transition probabilities between two isolated levels in the adiabatic limit by using the corresponding formula for two-level systems. It also stresses that one has to consider not only the eigenvalues in the complex plane, but also the eigenvectors in order to compute the leading term of the transition probability. Coming to the hypotheses under which formula (1.88) applies, they are all very general and natural except maybe the condition on the behaviour of the Stokes lines in the complex plane. Now if we look in the huge physical literature on the computation of transition probabilities in the adiabatic limit, we see that in most of the cases considered, the two levels involved display an avoided crossing at some time t_0 during the evolution. We may suspect that in the limiting situation of one avoided crossing between the two levels, the last condition on the Stokes lines should be automatically satisfied. Indeed, we expect in such a case the presence of an eigenvalue crossing point z_0 very close to the real axis in a neighbourhood of $t_0 \in \mathbb{R}$, so that the transition probability should unmistakably be governed by the eigenvalue crossing point z_0. Moreover, when the local structure of the gap between $e_1(t)$ and $e_2(t)$ around t_0 has a form of the type

$$e_2(t) - e_1(t) = \sqrt{a^2(t-t_0)^2 + b^2\delta^2} + \mathcal{O}((t-t_0)^2) \tag{1.89}$$

with δ small, the transition probability in the adiabatic limit should coincide with the Landau-Zener formula (1.6)

$$\mathcal{P}_{21}(\varepsilon) \simeq \exp\left\{-\frac{\delta^2\pi b^2}{\varepsilon 2a}\right\} \quad \text{as } \varepsilon \to 0. \tag{1.90}$$

Let us describe mathematically an avoided crossing situation. We assume now that our hamiltonian $H(t)$ depends on time t and on a small parameter δ. For any fixed value of

δ, $H(t,\delta)$ is analytic in t in a strip S_a and has definite limiting values $H^+(\delta)$ and $H^-(\delta)$ when $t \to +\infty$ to which it tends sufficiently rapidly. We also suppose that $H(t,\delta)$, as a function of the two real variables (t,δ), is smooth enough. As before, we assume that its spectrum contains two eigenvalues $e_1(t,\delta)$ and $e_2(t,\delta)$ which are bounded away from the rest of the spectrum for any $t \in I\!R$ and any $\delta \geq 0$. The avoided crossing between e_1 and e_2 is described as follows. When $\delta = 0$, $e_1(t,0)$ and $e_2(t,0)$ experience a unique genuine crossing at time $t = 0$, i.e.

$$e_1(0,0) = e_2(0,0). \tag{1.91}$$

This means that we have

$$\begin{aligned} e_1(t,0) &< e_2(t,0) \text{ for } t < 0, \\ e_1(t,0) &> e_2(t,0) \text{ for } t > 0. \end{aligned} \tag{1.92}$$

When $\delta > 0$, the degeneracy at $t = 0$ is lifted and we have $e_1(t,\delta) < e_2(t,\delta)$ $\forall t \in I\!R$, δ fixed. We may think of δ as a parameter controlling a perturbation of the hamiltonian $H(t,0)$, which turns the genuine crossing between e_1 and e_1 to an avoided crossing of order δ. Let us go a little further and specify the local structure of the gap between the eigenvalues for t and δ small we shall consider. We assume that

$$e_2(t,\delta) - e_1(t,\delta) = \sqrt{a^2t^2 + 2ct\delta + b^2\delta^2 + R_3(t,\delta)} \tag{1.93}$$

where $R_3(t,\delta)$ is a rest of order 3 in t and δ. The quadratic form under the square root is supposed to be positive definite, i.e. $c^2 < a^2b^2$ and the constants a, b are positive. The problem we want to solve is exactly the same as the previous one, with a supplementary small parameter δ. We assume δ to be small but positive, and we prepare our system at time $t = -\infty$ in an eigenstate of $H^-(\delta)$ associated with the level $e_1(-\infty,\delta)$. We want to compute the probability $\mathcal{P}_{21}(\varepsilon,\delta)$ to find the system at time $t = +\infty$ in an eigenstate of $H^+(\delta)$ associated with $e_2(+\infty,\delta)$ in the adiabatic limit $\varepsilon \to 0$.

For a fixed positive value of δ, this situation coincides with the previously described one, except that we make no hypothesis on the behaviour of the Stokes lines in the complex plane. Thus we are left with hypotheses which correspond to the physics of the problem only, which makes them more natural. Under these natural hypotheses we can turn the heuristic justification of the formula (1.88) in an avoided crossing situation controlled by the parameter δ to a mathematical proof. We have for ε and δ small enough

$$\mathcal{P}_{21}(\varepsilon,\delta) = \exp\{2\text{Im}\theta_1(0,\delta|\gamma)\}\exp\left\{\frac{2}{\varepsilon}\text{Im}\int_\gamma e_1(z,\delta)dz\right\}(1+\mathcal{O}(\varepsilon)) \tag{1.94}$$

where $\text{Im}\theta_1(0,\delta|\gamma)$ and $\text{Im}\int_\gamma e_1(z,\delta)dz$ both tend to zero when $\delta \to 0$ and $\mathcal{O}(\varepsilon)$ is independent of δ. Here the loop γ is based at the origin and encircles one eigenvalue crossing $z_0(\delta)$ which tends to $z = 0$ when $\delta \to 0$. This is the situation we mentioned at the end of the preceding section. Establishing this formula amounts essentially to show the existence of a dissipative path above $z_0(\delta)$. The idea here is to construct such a path above the real axis for $\delta = 0$, a situation where the Stokes lines are known, and then to prove that this path is still dissipative when $\delta > 0$ and small enough so that $z_0(\delta)$ is under the path.

1.5.4 The Landau-Zener Formula

Let us now come to the main point. When the gap between $e_1(t,\delta)$ and $e_2(t,\delta)$ has the generic form specified above for t and δ small, we can indeed compute the transition probability by means of the Landau-Zener formula [JP5]:

$$\mathcal{P}_{21}(\varepsilon,\delta) = \exp\left\{-\frac{\delta^2\pi}{\varepsilon 2}\left(\frac{b^2}{a}-\frac{c^2}{a^3}\right)(1+\mathcal{O}(\delta))\right\}(1+\mathcal{O}(\delta)+\mathcal{O}(\varepsilon)) \tag{1.95}$$

where $\mathcal{O}(\delta)$, respectively $\mathcal{O}(\varepsilon)$, are independent of ε, respectively δ. If $c = 0$, we have the usual Landau-Zener formula. These last results, which we shall prove here in details, have been announced in [JP5]. The Landau-Zener formula is obtained by studying explicit δ-dependent expressions for the decay rate and the geometrical prefactor in (1.94). Expanding these quantities for δ small, we see that $\text{Im}\theta_1(0,\delta|\gamma) = 0 + \mathcal{O}(\delta)$ and that the decay rate reduces to the Landau-Zener decay rate to first order in δ.

We would like to make two remarks about the formula we have here. The first concerns a previous work of Hagedorn [H2] on the Landau-Zener formula. Hagedorn considered a case where the avoided crossing taking place between e_1 and e_2 is not of order δ, with δ held fixed, but of order $\delta = \sqrt{\varepsilon}$, which means that the gap closes as $\varepsilon \to 0$. He showed that in this situation, the transition probability is given by the Landau-Zener formula (1.90) with $\delta^2 = \varepsilon$. We can recover his result by simply putting $\sqrt{\varepsilon}$ in place of δ in (1.95), which yields a transition probability of order one when $\varepsilon \to 0$

$$\mathcal{P}_{21}(\varepsilon,\sqrt{\varepsilon}) = \exp\left\{-\frac{\pi}{2}\left(\frac{b^2}{a}-\frac{c^2}{a^3}\right)\right\}(1+\mathcal{O}(\sqrt{\varepsilon}))\,. \tag{1.96}$$

The second remark is that since the estimates are uniform in δ, we can insert $\delta = 0$ in (1.95) and thus get the result

$$\mathcal{P}_{21}(\varepsilon,0) = (1+\mathcal{O}(\varepsilon)) \tag{1.97}$$

in apparent contradiction with the adiabatic theorem. But it should be recalled that when $\delta = 0$ the eigenvectors undergo a change of label at $t = 0$, in the sense that if $e_1(t,0)$ is the lowest of the two levels for $t < 0$, it is the highest when $t > 0$. So that for $t > 0$, $\varphi_2(t,\delta)$ tends to a vector proportional to $\varphi_1(t,0)$ when $\delta \to 0$ and thus $\mathcal{P}_{21}(\varepsilon,0)$ gives the probability to *stay* on the same instantaneous level when there is a real eigenvalue crossing point at $t = 0$. This probability in consequence must be close to 1 and actually we recover the result of Born and Fock [BF] stating that in such a case, the transition probability is of order ε, instead of ε^2.

1.6 Notes

The results presented in the last three sections cover a period ranging from 1988 up to now and they were obtained in the following chronological order. The iterative method we described in section (1.3) is a tool which was developed in 1988 [JP1] independently of the equivalent construction of Nenciu and Rasche [NR]. The first progresses on the exponential suppression of transition probabilities in the adiabatic limit concerned n-level systems. After Davis and Pechukas [DP] and Hwang and Pechukas [HP] dealt with the real symmetric 2-level case, Berry [B3] and Joye, Kunz and Pfister [JKP1], [JKP2] pointed out independently that the Dykhne formula must be completed by the geometrical prefactor (1.69) for general 2-level hermitian hamiltonians. The detailed analysis of the hypotheses leading to that formula, together with its purely geometrical interpretation was given in [JKP2]. Exponential estimates on the transition probability for n-level analytic hamiltonians satisfying natural conditions only can also be found in [JKP1] and [JKP2].

The extension of this result to general unbounded hamiltonians depending analytically on time was achieved later in [JP4] and gave the first proof of the folk adiabatic theorem mentioned at the beginning of the introduction. Nenciu considered then a more general class of unbounded C^∞ hamiltonians and studied the corresponding Heisenberg equations of motion for a spectral projector, in the spirit of Lenard [Len]. By estimating precisely the coefficients of the resulting asymptotic expansion of the solution, he could truncate the series in an optimal way and obtain "exponentially" small bounds on the error. Then, by a different procedure, he could construct from this truncated series a "superadiabatic" evolution satisfying Nekhoroshev type estimates for the first time in this context [Ne3]. The analytic case becomes then a particular case of his more general results. We have put some words between quotation marks because this is only when the hamiltonian is analytic that they have the meaning we gave in the foregoing. Then came the refinements on the asymptotic expression of the transition probability for two-level systems: higher order corrections in [JP2] and interference phenomena in [JMP]. After discussions with G.Nenciu and correspondence with M.Berry, we adapted the optimal truncation procedure to our iterative scheme in order to obtain superadiabatic evolutions from this scheme. This allowed us to construct effective hamiltonians such that the combination of the results on two-level systems together with Nekhoroshev type estimates for general unbounded hamiltonians was made possible. From this combination result a justification of the use of formulae obtained for two-level systems in more general situations [JP3], and a justification of the well known Landau-Zener formula [JP5].

This work is organized as follows. In the second chapter we state precisely the hypotheses under which we shall work and establish some of their direct consequences. The third chapter is devoted to the achievement of algebraic and exponential estimates on the transition probability by means of our iterative scheme. We turn to two-level systems in the fourth chapter where we compute asymptotic formulae for the transition probability using the method of Landau. The way to obtain exponential estimates on the transition probability by this method is explained in appendix for bounded operators. Then we show in the fifth chapter how to take advantage of both methods, first to improve the results about two-level systems, second to derive an asymptotic formula for the transition probability between two isolated levels in the spectrum of the hamiltonian. Finally, we consider the avoided crossing situation and justify the Landau-Zener formula in the sixth and last chapter. A detailed table of contents can be found at the end of this work.

Chapter 2

Preliminaries

2.1 Hypotheses

Let $H(t)$, $t \in I\!R$, be the hamiltonian of a system described by a separable Hilbert space $\mathcal{H}$. We study the time-dependent Schrödinger equation in the adiabatic limit, i.e

$$i\epsilon \frac{d}{dt}\psi_\epsilon(t) = H(t)\psi_\epsilon(t), \quad t \in I\!R \tag{2.1}$$

when $\epsilon \to 0$. We suppose that the hamiltonian satisfies three conditions. The first one is essentially that $H(t)$ depends analytically on time.

I. Self-adjointness and analyticity

There exists a band S_a in the complex plane, $S_a = \{t + is \ : \ |s| < a\}$, and a dense domain $D \subset \mathcal{H}$ such that for each $z \in S_a$, $H(z)$ is a closed operator defined on D , $H(z)\varphi$ is holomorphic on S_a for each $\varphi \in D$ and $H(z)^* = H(\bar{z})$. Moreover we suppose that $H(t)$ is bounded from below for $t \in I\!R$.

The second hypothesis on the hamiltonian is that it must behave reasonably at infinity.

II. Behaviour at infinity

There exist two self-adjoint operators H^+ and H^-, defined on D and bounded from below, and a positive function $b(t)$ tending to zero as $|t| \to \infty$ in an integrable way such that for all $\varphi \in D$

$$\sup_{|s|<a} \|(H(t+is) - H^+)\varphi\| \leq b(t)(\|\varphi\| + \|H^+\varphi\|), \quad t > 0$$

and

$$\sup_{|s|<a} \|(H(t+is) - H^-)\varphi\| \leq b(t)(\|\varphi\| + \|H^-\varphi\|), \quad t < 0.$$

We shall call such a $b(t)$ an integrable decay function.

The last assumption is the usual gap condition.

III. Separation of the spectrum

There exists a positive constant g such that the spectrum $\sigma(t)$ of $H(t)$ is separated into two parts $\sigma_1(t)$ and $\sigma_2(t)$ with

$$\inf_{t\in I\!R} \mathrm{dist}[\sigma_1(t), \sigma_2(t)] \geq g > 0$$

and the part $\sigma_1(t)$ is bounded.

2.2 Basic Estimates

We review here the main consequences of these three general hypotheses on the hamiltonian. In particular, we establish estimates which will allow us to control the variations of the spectrum of $H(z)$ with z.

2.2.1 Various Norms

Let $z \in S_a$ and $\lambda \in T(z)$, the resolvent set of $H(z)$. We denote by $R(z,\lambda) = (H(z)-\lambda)^{-1}$ the resolvent operator and similarly we set $R(\pm,\lambda) = (H^{\pm}-\lambda)^{-1}$ if $\lambda \in T(\pm)$, $T(\pm)$ being the resolvent set of $H^{\pm}$. Since the operator $H(z)$ is closed, the domain D with the norm

$$\|\varphi\|_z = \|\varphi\| + \|H(z)\varphi\| \tag{2.2}$$

is a Banach space. The same is true for the norms

$$\|\varphi\|_\pm = \|\varphi\| + \|H^\pm\varphi\|. \tag{2.3}$$

Let us denote by X_z, respectively $X_\pm$, the Banach space D equipped with the norm $\|\cdot\|_z$, respectively $\|\cdot\|_\pm$. By the closed graph theorem the function $z \mapsto H(z)$ is an analytic map on S_a taking values in $\mathcal{B}(X_{z'},\mathcal{H})$, respectively $\mathcal{B}(X_\pm,\mathcal{H})$, the set of bounded linear operators from $X_{z'}$, respectively $X_\pm$, to $\mathcal{H}$ for any $z' \in S_a$. The norm in these spaces is denoted by $|||\cdot|||_{z'}$, respectively $|||\cdot|||_\pm$. For any $\varphi \in D$ we define the operator $H^{(n)}(z)$ by

$$H^{(n)}(z)\varphi := \frac{d^n}{dz^n}(H(z)\varphi). \tag{2.4}$$

This operator is symmetric when $z \in \mathbb{R}$ and can be expressed by means of the Cauchy formula

$$H^{(n)}(z) = \frac{n!}{2\pi i}\oint_\gamma \frac{H(z')dz'}{(z'-z)^{n+1}} \tag{2.5}$$

where γ is a simple closed path in S_a around z. The orientation of γ is counterclockwise as will be the orientations of all closed paths in this work, unless otherwise stated. As the operator $H(z) \in \mathcal{B}(X_{z'},\mathcal{H})$, all the norms we have introduced are equivalent

$$\|\varphi\|_z \leq (|||H(z)|||_{z'} + 1)\,\|\varphi\|_{z'}. \tag{2.6}$$

Actually we can bound $|||H(z)|||_{z'}$ uniformly in (z,z') so that these norms can be compared by means of constants only. Moreover, this result together with condition II allows useful bounds on the decrease of $H'(z)$ as $|z| \to \infty$ to be obtained. There will appear many integrable decay functions in the sequel which we shall denote generically by $b(t)$.

Lemma 2.2.1 *If $H(z)$ satisfies conditions I and II and if $0 < r < a$, then there exists a constant M and an integrable decay function $b(t)$ such that*

$$\max\left\{\sup_{z,z'\in S_a}|||H(z)|||_{z'},\ \sup_{z\in S_a}|||H(z)|||_\pm,\ \sup_{z'\in S_a}|||H^\pm|||_{z'}\right\} \leq M$$

and

$$\|H'(t+is)\varphi\| \leq b(t)\|\varphi\|_{z'}$$

for any $t \in \mathbb{R}$, $z' \in S_a$ and $|s| \leq r$.

Remark:
If condition I only is satisfied, we have $\sup_{z,z'\in\Omega}|||H(z)|||_{z'} \leq M$ where Ω is a compact subset of S_a and $b(t)$ must be replaced by a constant B. The proof of this lemma is given in appendix.

2.2.2 Stability of the Spectrum

As a direct consequence of lemma (2.2.1), if $|s| \leq r < a$, we have for any $z \in D(t,\eta)$, where $D(t,\eta)$ is a disc of radius $\eta < r$ centered at $t \in I\!R$

$$\|(H(z) - H(t))\varphi\| \leq |z - t| b(t) \|\varphi\|_t \tag{2.7}$$

with $b(t)$ an integrable decay function. This estimate allows us to compare the spectra of $H(z)$ and $H(t)$ when $|z - t|$ is small enough. Let $\lambda \in T(t)$ so that the operator $H(t)R(t,\lambda) = I\!I + \lambda R(t,\lambda)$ is a bounded operator. From (2.7) we have

$$\|(H(z) - H(t))R(t,\lambda)\| \leq |z - t| b(t) (\|R(t,\lambda)\| + \|H(t)R(t,\lambda)\|) \tag{2.8}$$

and we define $d(t,\lambda) \equiv \|R(t,\lambda)\| + \|H(t)R(t,\lambda)\|$. Then we use the second resolvent identity

$$R(z,\lambda) - R(t,\lambda) = -R(z,\lambda)(H(z) - H(t))R(t,\lambda) \tag{2.9}$$

to write

$$R(z,\lambda) = R(t,\lambda)\left(I\!I + (H(z) - H(t))R(t,\lambda)\right)^{-1} \tag{2.10}$$

provided $|z - t| b(t) d(t,\lambda) < 1$. This means that in this case λ belongs to the resolvent set $T(z)$ and we have the estimates

$$\|R(z,\lambda)\| \leq \|R(t,\lambda)\| \frac{1}{1 - |z - t| b(t) d(t,\lambda)} \tag{2.11}$$

and

$$\|R(z,\lambda) - R(t,\lambda)\| \leq \|R(t,\lambda)\| \frac{|z - t| b(t) d(t,\lambda)}{1 - |z - t| b(t) d(t,\lambda)}. \tag{2.12}$$

Now, if $\lambda \in T(\pm)$, the resolvent set of $H^{\pm}$, it follows from condition II and similar considerations that $\lambda \in T(t + is)$ if $\pm t$ is large enough and

$$\|R(t + is,\lambda) - R(\pm,\lambda)\| \leq \|R(\pm,\lambda)\| \frac{b(t) d(\pm,\lambda)}{1 - b(t) d(\pm,\lambda)} \quad \forall |s| < a \tag{2.13}$$

where $b(t)$ is the integrable decay function of condition II and $d(\pm,\lambda) = \|R(\pm,\lambda)\| + \|H^{\pm}R(\pm,\lambda)\|$.

Let us suppose that $H(t)$ satisfies conditions I, II and III. The spectral projector $P(t)$ corresponding to the bounded part of spectrum $\sigma_1(t)$ is thus given by

$$P(t) = -\frac{1}{2\pi i} \oint_{\Gamma} R(t,\lambda) d\lambda \tag{2.14}$$

where Γ is a simple closed path encircling $\sigma_1(t)$. From the preceding estimates we show the

Lemma 2.2.2 *Let $t \in I\!R$ and Γ be as above. Then we can choose the width of the strip S_a sufficiently small so that the spectrum of $H(z)$ is still separated into two parts $\forall z \in S_a$. Moreover, if $|z - t|$ is small enough, the spectral projector corresponding to $\sigma_1(z)$ is given by*

$$P(z) = -\frac{1}{2\pi i} \oint_{\Gamma} R(z,\lambda) d\lambda$$

where the path Γ in (2.14) encircles the bounded set $\sigma_1(z)$.

Proof: We proceed as follows. From (2.13), there exist $T > 0$ and Γ_- and $\Gamma_+ \in S_a$ such that

$$P(t) = -\frac{1}{2\pi i}\oint_{\Gamma_\pm} R(t,\lambda)d\lambda \tag{2.15}$$

if $t \gtrless \pm T$. Then we see from (2.12) that for any $t \in [-T,T]$, the path Γ used in (2.14) can be chosen locally independently of t. Thus, by compacity of $[-T,T]$ and (2.15) we can define $P(t)$ for any $t \in I\!R$ by choosing Γ in (2.14) among a finite set only of paths $\{\Gamma_j;\ \ j = 1,\cdots,n\}$ with $\Gamma_1 = \Gamma_-$ and $\Gamma_n = \Gamma_+$. The length of these paths is uniformly bounded and they satisfy $\text{dist}[\Gamma_j,\sigma(t)] \geq \eta > 0$. As a consequence, if λ belongs to $\Gamma_j \in T(t)$ for some time t, $d(t,\lambda)$ is uniformly bounded in t and in λ

$$d(t,\lambda) \leq 1 + \frac{|\lambda|+1}{\eta} \leq K < \infty. \tag{2.16}$$

Thus, it follows from (2.11) that if we take the width a of the strip sufficiently small, so that

$$a \sup_{t\in I\!R} b(t)K < 1, \tag{2.17}$$

then $\sigma_1(t+is)$ is encircled by some Γ_j for any time t if $|s| < a$. The formula

$$P(z) = -\frac{1}{2\pi i}\oint_{\Gamma} R(z,\lambda)d\lambda \tag{2.18}$$

also results from (2.11) if $|z-t|$ is small enough.

□

Regarding the regularity of the operators $R(z,\lambda)$ and $P(z)$ for $z \in S_a$ we have the

Lemma 2.2.3 *For any $z \in S_a$, a small enough, and any $\lambda \in T(z)$, $P(z)$ and $R(z,\lambda)$ are holomorphic bounded operators and $P(z)$ has limits $P(\pm)$ as $Rez \to \pm\infty$ to which it tends in an integrable way. Let $r < a$ and $\lambda \in T(\pm)$. We have for any $|s| \leq r$, any $n > 0$ for $|t|$ large enough*

$$\|R^{(n)}(t+is,\lambda)\| \leq b_\lambda(t)$$
$$\|P^{(n)}(t+is)\| \leq b(t)$$

where $b(t)$ and $b_\lambda(t)$ are integrable decay functions.

Proof: That the resolvent is analytic is a standard result obtained by considering identities analogous to (2.9). Using formula (2.18) and the fact that the path Γ can be chosen locally independently of z we conclude that $P(z)$ is analytic as well. The estimates on the derivatives of $R(z,\lambda)$ and $P(z)$ come from the application of Cauchy formula on (2.13) and

$$P(t+is) - P(\pm) = -\frac{1}{2\pi i}\oint_{\Gamma}(R(t+is,\lambda) - R(\pm,\lambda))d\lambda. \tag{2.19}$$

□

Finally, $R(z,\lambda)$ maps $\mathcal{H}$ into D for $\lambda \in T(z)$ by definition and we have that $P(z)$ maps $\mathcal{H}$ into D as well. Moreover, for any $\varphi \in D$,

$$P(z)H(z)\varphi = H(z)P(z)\varphi = -\frac{1}{2\pi i}\oint_{\Gamma}\lambda R(z,\lambda)\varphi d\lambda \tag{2.20}$$

is a bounded operator and when considered on $P(z)\mathcal{H}$ the spectrum of $P(z)H(z)$ coincides with $\sigma_1(z)$. Similar results hold for the unbounded operator $(I\!I - P(z))H(z)$. (see e.g. [Kat2] chapter III, paragraph (6.4)).

2.2.3 Evolution Operators

Under the hypothesis I the solution $\psi_\epsilon(t)$ of the Schrödinger equation

$$i\epsilon\frac{d}{dt}\psi_\epsilon(t) = H(t)\psi_\epsilon(t), \quad \psi_\epsilon(s) = \varphi_0 \in D \quad t \in \mathbb{R} \tag{2.21}$$

can be written by means of the evolution operator $U_\epsilon(t,s)$ as

$$\psi_\epsilon(t) = U_\epsilon(t,s)\varphi_0. \tag{2.22}$$

The evolution $U_\epsilon(t,s)$ is a two-parameter family of unitary operators defined for all real t and s, strongly continuous in t and s, which leaves the domain D invariant. For all t_1, t_2, t_3 we have

$$U_\epsilon(t_1,t_2)U_\epsilon(t_2,t_3) = U_\epsilon(t_1,t_3), \quad U_\epsilon(t_1,t_1) = \mathbb{I} \tag{2.23}$$

and $U_\epsilon(t,s)$ is strongly differentiable in t and s on the domain D:

$$i\epsilon\frac{\partial}{\partial t}U_\epsilon(t,s) = H(t)U_\epsilon(t,s) \tag{2.24}$$

and

$$i\epsilon\frac{\partial}{\partial s}U_\epsilon(t,s) = -U_\epsilon(t,s)H(s). \tag{2.25}$$

For a proof of these properties, see [RS] section X12, for example.

Let us now turn to the solution of

$$\begin{aligned} iW'(t,t_0) &= i[P'(t),P(t)]W(t,t_0) \\ &\equiv K(t)W(t,t_0), \quad W(t_0,t_0) = \mathbb{I} \end{aligned} \tag{2.26}$$

which defines the parallel transport operator. As the generator $K(t)$ is a bounded self-adjoint operator, $W(t,t_0)$ is given by the Dyson series

$$W(t,t_0) = \mathbb{I} + \sum_{j=1}^{\infty}\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{j-1}} dt_j K(t_1)K(t_2)\cdots K(t_j) \tag{2.27}$$

and it is unitary. Moreover, if the projector $P(t)$ admits an analytic extension $P(z)$ in some domain Ω, then $W(t,t_0)$ also admits an analytic extension in the same domain as is readily seen on the series (2.27). The analytic extension $W(z,z_0)$, $z,z_0 \in \Omega$, is a bounded operator satisfying all general properties of an evolution operator except unitarity. The main characteristic of $W(z,z_0)$ is the intertwining relation

$$W(z,z_0)P(z_0) = P(z)W(z,z_0) \quad \forall z,z_0 \in \Omega. \tag{2.28}$$

It can be recovered by considering the derivative with respect to z of the right-hand side and by making use of the identities $P(z)P'(z)P(z) = 0$ and $P'(z) = P'(z)P(z)+P(z)P'(z)$. We get

$$\begin{aligned} (P(z)W(z,z_0))' &= (P'(z) - P(z)P'(z))W(z,z_0) \\ &= P'(z)P(z)W(z,z_0) \\ &= [P'(z),P(z)](P(z)W(z,z_0)) \end{aligned} \tag{2.29}$$

and we conclude by the unicity of the solution (2.26). Another interesting feature of the parallel transport is that it leaves the domain D of the operator H invariant. This property is indeed important since it allows a "bona fide" generator for the dynamical phase operator to be defined (see (1.25)).

Lemma 2.2.4 *Let the $H(z)$ satisfy conditions I, II and III. We assume a to be small enough so that $P(z)$ is analytic in S_a*
i) The operator $W(z, z_0)$ leaves the domain D invariant.
Let $\tilde{H}(z) = W^{-1}(z, t_0)H(z)W(z, t_0)$ be defined on D, $t_0 \in \mathbb{R}$ and let $0 < r < a$. Then
ii) $\tilde{H}(z)$ is a closed operator on D, analytic in S_a, such that $\tilde{H}^*(z) = \tilde{H}(\bar{z})$.
iii) There exists an integrable decay function $\tilde{b}(t)$ such that we have for any $\varphi \in D$

$$\|(\tilde{H}(z) - \tilde{H}(t))\varphi\| \leq |z - t|\tilde{b}(t)(\|\tilde{H}(t)\varphi\| + \|\varphi\|).$$

The proof of this technical lemma can be found in appendix.

We define then $\Phi_\varepsilon(t, t_0)$, $t, t_0 \in \mathbb{R}$ by

$$i\varepsilon\frac{d}{dt}\Phi_\varepsilon(t, t_0) = \tilde{H}(t)\Phi_\varepsilon(t, t_0), \quad \Phi_\varepsilon(t_0, t_0) = \mathbb{I}. \tag{2.30}$$

Because of lemma (2.2.4), point ii), this dynamical phase operator is unitary and satisfies the general properties of evolution operators as well. Since $[\tilde{H}(t), P(t_0)] = 0\ \forall t$, we immediately have $[\Phi_\varepsilon(t, t_0), P(t_0)] = 0\ \forall t$. Let us consider now the operator we called adiabatic evolution which is defined by the product

$$V(t, t_0) = W(t, t_0)\Phi_\varepsilon(t, t_0). \tag{2.31}$$

It follows from the foregoing that V is strongly differentiable on D, maps D into D and satisfies

$$i\varepsilon\frac{d}{dt}V(t, t_0) = (H(t) + \varepsilon K(t))V(t, t_0), \quad V(t_0, t_0) = \mathbb{I}. \tag{2.32}$$

By the properties of W and Φ_ε, the adiabatic evolution is compatible with the decomposition of the Hilbert space $\mathcal{H}$ into $\mathcal{H} = P(t)\mathcal{H} \oplus (\mathbb{I} - P(t))\mathcal{H}$ i.e.

$$V(t, t_0)P(t_0) = P(t)V(t, t_0). \tag{2.33}$$

We shall recover in the sequel the adiabatic theorem of quantum mechanics

$$\|U_\varepsilon(t, t_0) - V(t, t_0)\| = \mathcal{O}(\varepsilon). \tag{2.34}$$

Chapter 3

Iterative Scheme

In this chapter, we study in details the recurrent construction we have introduced and its applications. We first establish the main properties of this construction when the hamiltonian is analytic and in a second part, we use this iterative scheme to construct adiabatic and superadiabatic evolutions. In the latter case, we analyse precisely the dependence of the exponential decay rate on the width of the gap in the spectrum of the hamiltonian.

3.1 Algebraic Estimates

Let us first derive the properties which allow higher order adiabatic evolutions to be constructed. Since we shall prove finer results later, we only sketch the proofs here.

Let $H(z)$ satisfy conditions I and III. We set $H_0(z) \equiv H(z)$ and

$$P_0(z) = P(z) = -\frac{1}{2\pi i}\oint_\Gamma R_0(z,\lambda)d\lambda \tag{3.1}$$

where $R_0(z,\lambda) = (H(z)-\lambda)^{-1}$. The closed path Γ encircles the bounded part $\sigma_1(z)$ of the spectrum $\sigma(z)$ of $H(z)$ and can be chosen a finite distance away from $\sigma(z)$. We drop the ε-dependence in the arguments and define for ε small enough

$$\begin{aligned} H_q(z) &= H(z) - \varepsilon K_{q-1}(z) \\ P_q(z) &= -\frac{1}{2\pi i}\oint_\Gamma R_q(z,\lambda)d\lambda \\ K_q(z) &= i[P_q'(z), P_q(z)] \quad q \geq 1 \end{aligned} \tag{3.2}$$

with $R_q(z,\lambda) = (H_q(z)-\lambda)^{-1}$ for $\lambda \in T_q(z)$, the resolvent set of $H_q(z)$. Remark that since $K_{q-1}(z)$ is bounded for any q, $H_q(z)$ is closed and densely defined on the domain D of $H(z)$ (see theorem (1.1), chapter IV in [Kat2]). Let $D(z,\eta)$ be a disc centered at z of radius η so small that the path $\Gamma \subset T(z')$, for any $z' \in D(z,\eta)$. It is indeed possible to choose η in such a way since by the remark following lemma (2.2.1) we can write

$$\|(H(z')-H(z))R(z,\lambda)\| \leq B|z'-z|(\|R(z,\lambda)\| + \|H(z)R(z,\lambda)\|) \equiv B|z'-z|d(z,\lambda). \tag{3.3}$$

Thus we have

$$R(z',\lambda) = R(z,\lambda)\left(\mathbb{I} + (H(z')-H(z))R(z,\lambda)\right)^{-1} \tag{3.4}$$

if $B|z'-z|d(z,\lambda) < 1$.

Proposition 3.1.1 *Let $H(z)$ satisfy conditions I and III and $D(z,\eta)$ be as above. For any $q \geq 1$, there exists $\varepsilon(q)$ and $\eta(q) < \eta$ such that for all $\varepsilon < \varepsilon(q)$*

$$\|K_q(z') - K_{q-1}(z')\| \leq \beta_q \varepsilon^q \quad \forall z' \in D(z,\eta(q)).$$

Proof: This assertion is proved by induction in the following way: we consider the difference

$$P_q(z') - P_{q-1}(z') \equiv \varepsilon F_q(z') \tag{3.5}$$

and show that the estimate

$$\|F_q^{(n)}(z')\| = \mathcal{O}(\varepsilon^{q-1}) \quad \forall n \geq 0 \tag{3.6}$$

holds for any $z' \in D(z,\eta(q))$ if ε is smaller than some $\varepsilon(q)$. Thus we immediately get

$$\begin{aligned} K_q(z') - K_{q-1}(z') &= i\varepsilon\left([F_q'(z'), P_{q-1}(z')] + [P_{q-1}'(z'), F_q(z')] + \varepsilon[F_q'(z'), F_q(z')]\right) \\ &= \mathcal{O}(\varepsilon^q) \end{aligned} \tag{3.7}$$

for any z' in the same disc. We have used the fact that

$$P_{q-1}(z') = P_0(z') + \sum_{j=1}^{q-1} P_j(z') - P_{j-1}(z') = P_0(z') + \varepsilon \sum_{j=1}^{q-1} F_j(z') = \mathcal{O}(1). \tag{3.8}$$

The step $q = 1$ with $n = 0$ is true by perturbation theory. Indeed, we have $H_1(z') = H_0(z') - \varepsilon K_0(z')$ where $K_0(z')$ is bounded and from the second resolvent identity we get for $\lambda \in T(z')$

$$\begin{aligned} R_1(z',\lambda) - R_0(z',\lambda) &= R_0(z',\lambda)(H_0(z') - H_1(z'))R_1(z',\lambda) \\ &= \varepsilon R_0(z',\lambda)K_0(z')R_1(z',\lambda). \end{aligned} \tag{3.9}$$

Thus if $\varepsilon\|R_0(z',\lambda)K_0(z')\| < 1$, $\lambda \in T_1(z')$ as well and we can write

$$R_1(z',\lambda) = (\mathbb{I} - \varepsilon R_0(z',\lambda)K_0(z'))^{-1} R_0(z',\lambda). \tag{3.10}$$

Now if $\varepsilon \leq \varepsilon(1)$, $\varepsilon(1)$ small enough, $\Gamma \subset T_1(z')$ and we have the bound

$$\|R_1(z',\lambda)\| \leq \frac{\|R_0(z',\lambda)\|}{1 - \varepsilon\|R_0(z',\lambda)\|\|K_0(z')\|} = \mathcal{O}(1) \tag{3.11}$$

for any $\lambda \in \Gamma$ and $z' \in D(z,\eta)$. Hence we can write

$$\begin{aligned} P_1(z') - P_0(z') &= -\frac{1}{2\pi i}\oint_\Gamma \varepsilon R_0(z',\lambda)K_0(z')R_1(z',\lambda)d\lambda \\ &= \varepsilon F_1(z') \end{aligned} \tag{3.12}$$

with $F_1(z') = \mathcal{O}(1) \quad \forall z' \in D(z,\eta)$. Then we use Cauchy formula to obtain the estimate $F_1^{(n)}(z') = \mathcal{O}(1)$ for any $n > 0$ in a disc $D(z,\eta(1))$ slightly smaller i.e. with $\eta(1) < \eta$. We consider now the $q + 1^{st}$ step, assuming the proposition to hold for the q^{th} step. We have by definition

$$\begin{aligned} H_{q+1}(z') &= H_0(z') - \varepsilon K_q(z') \\ &= H_q(z') + \varepsilon(K_{q-1}(z') - K_q(z')). \end{aligned} \tag{3.13}$$

We can use twice the second resolvent identity to obtain for $\lambda \in T(z')$ and ε small enough

$$R_{q+1}(z',\lambda) = (\mathbb{I} - \varepsilon R_0(z',\lambda)K_q(z'))^{-1} R_0(z',\lambda) \tag{3.14}$$

and

$$R_{q+1}(z',\lambda) - R_q(z',\lambda) = \varepsilon R_q(z',\lambda)(K_q(z') - K_{q-1}(z'))R_{q+1}(z',\lambda). \tag{3.15}$$

As by induction hypothesis we have $\|K_q(z')\| = \mathcal{O}(1)$ $\forall z' \in D(z,\eta(q))$, we can choose $\varepsilon(q+1)$ sufficiently small to insure $\Gamma \subset T_{q+1}(z')$ if $\varepsilon < \varepsilon(q+1)$ and

$$\|R_{q+1}(z',\lambda)\| \leq \frac{\|R_0(z',\lambda)\|}{1 - \varepsilon\|R_0(z',\lambda)\|\|K_q(z')\|} = \mathcal{O}(1) \quad \forall z' \in D(z,\eta(q)), \ \forall \lambda \in \Gamma. \tag{3.16}$$

Then we write

$$\begin{aligned} P_{q+1}(z') - P_q(z') &= -\frac{1}{2\pi i}\oint_\Gamma \varepsilon R_q(z',\lambda)(K_q(z') - K_{q-1}(z'))R_{q+1}(z',\lambda)d\lambda \\ &= \varepsilon F_{q+1}(z') \end{aligned} \tag{3.17}$$

so that we get by induction hypothesis

$$F_{q+1}(z') = \mathcal{O}(\varepsilon^q) \quad \forall z' \in D(z,\eta(q)) \tag{3.18}$$

and by Cauchy formula

$$F_{q+1}^{(n)}(z') = \mathcal{O}(\varepsilon^q) \quad \forall z' \in D(z,\eta(q+1)) \tag{3.19}$$

with $\eta(q+1) < \eta(q)$.

□

Remarks:

- If $H(z)$ satisfies hypothesis II as well we can replace the constants β_q by integrable decay functions $\beta_q(t)$ where t is the real part of z, the center of the disc $D(z,\eta(q))$.
- This proposition is true on the real axis for hamiltonians satisfying less restrictive smoothness assumptions.

The proof of proposition (3.1.1) in this setting is very short due to the repeated use of Cauchy formula to compute the derivatives of the analytic quantities $F_q(z)$. The price to pay is that to apply Cauchy formula, we have to shrink the domain $D(z,\eta)$ at each step.

3.1.1 Arbitrary Order Adiabatic Evolutions

We can now construct adiabatic evolutions of arbitrary order by means of our iterative scheme. We assume that $H(t)$ satisfies conditions I and III and consider the proposition for discs $D(t,\eta)$ centered on the real axis. Thus the estimate $\|K_q(t) - K_{q-1}(t)\| \leq \beta_q\varepsilon^q$ holds on any compact subset of $\mathbb{R}$. We introduce the parallel transport $W_q(t,s)$ by

$$iW_q'(t,s) = K_q(t)W_q(t,s), \quad W_q(s,s) = \mathbb{I} \tag{3.20}$$

and the dynamical phase operator $\Phi_q(t,s)$ by

$$\begin{aligned} i\varepsilon\Phi_q'(t,s) &= W_q^{-1}(t,s)H_q(t)W_q(t,s)\Phi_q(t,s) \\ &\equiv \tilde{H}_q(t)\Phi_q(t,s), \quad \Phi_q(s,s) = \mathbb{I}. \end{aligned} \tag{3.21}$$

Since $H_q(t)$ satisfies conditions I and III if ε is small enough, these two evolutions have the same general properties as $W(t,s)$ and $\Phi_\varepsilon(t,s)$. We measure the difference between the physical evolution $U_\varepsilon(t,s)$ given by

$$i\varepsilon U_\varepsilon'(t,s) = H(t)U_\varepsilon(t,s), \quad U_\varepsilon(s,s) = \mathbb{I} \tag{3.22}$$

and the product $W_q(t,s)\Phi_q(t,s) \equiv V_q(t,s)$ by means of the operator $A_q(t,s)$ defined by the relation

$$U_\varepsilon(t,s) = W_q(t,s)\Phi_q(t,s)A_q(t,s) \equiv V_q(t,s)A_q(t,s). \tag{3.23}$$

Proposition 3.1.2 *Let $H(t)$ satisfy conditions I and III and let $U_\varepsilon(t,s)$ be the physical evolution satisfying (3.22). Then the operator $V_q(t,s) = W_q(t,s)\Phi_q(t,s)$ where W_q and Φ_q are defined in (3.20) and (3.21) is an adiabatic evolution of order q, i.e. there exists a constant β_q such that*

$$\|U_\varepsilon(t,s) - V_q(t,s)\| \le \beta_q \varepsilon^q |t-s|.$$

Moreover, if $H(t)$ satisfies condition II as well

$$\sup_{t,s\in\mathbb{R}} \|U_\varepsilon(t,s) - V_q(t,s)\| \le \varepsilon^q \int_{-\infty}^{+\infty} \beta_q(t)dt$$

where $\beta_q(t)$ is an integrable decay function.

Remarks:

- By construction of $V_q = W_q\Phi_q$ we have the intertwining relation

$$P_q(t)V_q(t,s) = V_q(t,s)P_q(s) \tag{3.24}$$

  which shows that an initial condition at time s belonging to the subspace $P_q(s)\mathcal{H}$ will be in $P_q(t)\mathcal{H}$ at time t up to a correction of order $\varepsilon^q|t-s|$.

- If $H(t)$ satisfies condition II, so that the first remark under proposition (3.1.1) applies, the projectors $P_q(t)$ and $P(t)$ coincide at infinity

$$\|P_q(t) - P(\pm)\| \to 0 \text{ as } t \to \pm\infty. \tag{3.25}$$

  This follows from the estimate

$$\|K_q(t)\| \le \|K_0(t)\| + \sum_{j=1}^{q} \|K_j(t) - K_{j-1}(t)\| \le \sum_{j=0}^{q} \beta_j(t)\varepsilon^j \to 0 \quad \text{as} \quad |t| \to \infty, \tag{3.26}$$

  since the $\beta_j(t)$'s are integrable decay functions. Thus the hamiltonians $H_q(t)$ and $H(t)$ coincide at infinity. The last assertion of the proposition together with (3.25) indicate that the transition probability $\mathcal{P}_{21}(\varepsilon)$ from $P(t_1)\mathcal{H}$ to $(\mathbb{I} - P(t_2))\mathcal{H}$ between the times $t_1 \to -\infty$ and $t_2 \to +\infty$ is of order ε^{2q}. But as the evolutions $U_\varepsilon(t,s)$ and $\Phi_q(t,s)$ do not have limits as $t \to \pm\infty$, we first have to express $\mathcal{P}_{21}(\varepsilon)$ in a suitable way to prove this result.

Proof: The operator $A_q(t,s)$ is strongly differentiable on D and satisfies the equation

$$iA_q'(t,s) = V_q^{-1}(t,s)(K_{q-1}(t) - K_q(t))V_q(t,s)A_q(t,s), \quad A_q(s,s) = \mathbb{I}. \tag{3.27}$$

Considering the equivalent Volterra equation and using the fact that A_q and V_q are unitary, we get

$$\|A_q(t,s) - I\!I\| \leq \int_s^t \|K_{q-1}(t') - K_q(t')\|dt' \quad \forall t,s \in I\!R. \tag{3.28}$$

Then, coming back to (3.23) and using proposition (3.1.1) we eventually obtain

$$\|U_\varepsilon(t,s) - V_q(t,s)\| \leq \beta_q \varepsilon^q |t-s| \tag{3.29}$$

if ε is small enough. If condition II is satisfied, we have $\|K_q(t) - K_{q-1}(t)\| \leq \beta_q(t)\varepsilon^q$, with $\beta_q(t)$ a rapidly decreasing function. Thus we immediately obtain from (3.28) the uniform estimate

$$\|A_q(t,s) - I\!I\| \leq \varepsilon^q \int_{-\infty}^{+\infty} \beta_q(t)dt \tag{3.30}$$

and the existence of well-defined unitary limits for $A_q(t,s)$ at infinity

$$\|A_q(t,s) - A_q(\pm\infty, s)\| \to 0 \text{ as } t \to \pm\infty. \tag{3.31}$$

The last assertion follows from (3.23).

□

We now turn to the computation of the transition probability between infinite initial and final times, in the spirit of the second remark following the proposition. Let us set $s = 0$ and

$$A_q(+\infty, -\infty) = A_q(+\infty, 0)A_q^{-1}(-\infty, 0). \tag{3.32}$$

Lemma 3.1.1 *Let $\psi_\varepsilon(t)$ be a normalized solution of the Schrödinger equation with $\psi_\varepsilon(0) = \varphi_0 \in D$ such that*

$$\lim_{t\to-\infty} \|P(t)\psi_\varepsilon(t)\| = 1.$$

Then, there exists a $\psi^* \in P_q(0)\mathcal{H}$ with $\|\psi_*\| = 1$ such that

$$\lim_{t\to+\infty} \|(I\!I - P(t))\psi_\varepsilon(t)\| = \|(I\!I - P_q(0))A_q(+\infty, -\infty)P_q(0)\psi_*\|$$

so that

$$\mathcal{P}_{21}(\varepsilon) = \|(I\!I - P_q(0))A_q(+\infty, -\infty)P_q(0)\|^2.$$

From this lemma and the identity

$$A_q(+\infty, -\infty) = I\!I + i\int_{-\infty}^{+\infty} dt V_q^{-1}(t,0)(K_q(t) - K_{q-1}(t))V_q(t,0)A_q(t,-\infty) \tag{3.33}$$

we immediately get the expected estimate

$$\mathcal{P}_{21}(\varepsilon) = \mathcal{O}(\varepsilon^{2q}). \tag{3.34}$$

Proof: By hypothesis and (3.25) we have

$$\begin{aligned} 1 &= \lim_{t\to-\infty} \|P(t)V_q(t,0)A_q(t,0)\varphi_0\| \\ &= \lim_{t\to-\infty} \|P_q(t)V_q(t,0)A_q(t,0)\varphi_0\| \\ &= \lim_{t\to-\infty} \|V_q(t,0)P_q(0)A_q(t,0)\varphi_0\| \\ &= \|P_q(0)A_q(-\infty,0)\varphi_0\|. \end{aligned} \tag{3.35}$$

Thus the normalized vector $\psi_* = A_q(-\infty, 0)\varphi_0 \in P_q(0)\mathcal{H}$. Similarly

$$\begin{aligned}\lim_{t\to+\infty} \|(\mathbb{I} - P(t))V_q(t,0)A_q(t,0)\varphi_0\| &= \lim_{t\to+\infty} \|(\mathbb{I} - P_q(t))V_q(t,0)A_q(t,0)A_q^{-1}(-\infty,0)\psi_*\| \\ &= \|(\mathbb{I} - P_q(0))A_q(\infty,0)A_q^{-1}(-\infty,0)\psi_*\| \\ &= \|(\mathbb{I} - P_q(0))A_q(\infty,-\infty)\psi_*\|. \end{aligned} \quad (3.36)$$

□

We have been able to construct adiabatic evolutions of arbitrary order in a fairly simple way but we cannot recover the adiabatic theorem yet

$$U_\varepsilon(t,s) = W(t,s)\Phi_\varepsilon(t,s) + \mathcal{O}(\varepsilon). \quad (3.37)$$

To do that, we have to improve our bounds on the difference $\|U_\varepsilon(t,s) - W_q(t,s)\Phi_q(t,s)\|$ by a factor ε. This can be achieved by means of an integration by parts formula as in [ASY]. We give an integration by parts formula in the following lemma whose proof can be found in appendix.

3.1.2 Improvement by a Factor ε

Lemma 3.1.2 (Integration by Parts Formula) *Let $H(t)$ be a strongly C^2 self adjoint operator densely defined on D, which is bounded from below and satisfies condition III. Let $V(t)$ be an operator defined by*

$$i\varepsilon\frac{d}{dt}V(t) = (H(t) + \varepsilon E(t))V(t), \quad V(0) = \mathbb{I}$$

where $E(t)$ is a bounded, strongly C^2, self-adjoint operator. Moreover we assume that the intertwining relation

$$V(t)P(0) = P(t)V(t)$$

holds. Let $B(t)$ be a bounded operator, strongly C^1, and $x(t)$ a strongly C^1 vector of $\mathcal{H}$ which belongs to D for all t. We introduce the operator

$$\mathcal{R}B(t) = \frac{1}{2\pi i}\oint_\Gamma R(t,\lambda)B(t)R(t,\lambda)d\lambda \quad (3.38)$$

where Γ is a path surrounding the bounded part of the spectrum $\sigma_1(t)$. Then we have
1) $\mathcal{R}B(t)$ is strongly C^1 and maps $\mathcal{H}$ into D. Moreover

$$P(t)\mathcal{R}B(t)P(t) = (\mathbb{I} - P(t))\mathcal{R}B(t)(\mathbb{I} - P(t)) \equiv 0, \quad k = 1,2.$$

2)

$$\begin{aligned}&\int_{t'}^t P(0)V(s)^{-1}B(s)V(s)(\mathbb{I} - P(0))x(s)ds = \\ &-i\epsilon P(0)V(s)^{-1}\mathcal{R}B(s)V(s)(\mathbb{I} - P(0))x(s)\Big|_{t'}^t + \\ &i\epsilon\int_{t'}^t P(0)V(s)^{-1}\left(\frac{d}{ds}\mathcal{R}B(s)\right)V(s)(\mathbb{I} - P(0))x(s)ds + \\ &i\epsilon\int_{t'}^t P(0)V(s)^{-1}\mathcal{R}B(s)V(s)(\mathbb{I} - P(0))\frac{d}{ds}x(s)ds - \\ &\epsilon\int_{t'}^t P(0)V(s)^{-1}[E(s),\mathcal{R}B(s)]V(s)(\mathbb{I} - P(0))x(s)ds.\end{aligned}$$

We have an analogous formula for $\int_{t'}^{t}(\mathbb{I}-P(0))V(s)^{-1}B(s)V(s)P(0)x(s)ds$ which is obtained by exchanging $P(0)$ and $(\mathbb{I}-P(0))$ and changing the sign in the right hand side of the above formula.

By a direct application of this lemma at the step $q=0$ we obtain [ASY]

Proposition 3.1.3 (Adiabatic Theorem of Quantum Mechanics) *Let $H(t)$ satisfy conditions I and III. Then*

$$\|U_\varepsilon(t,0)-W(t,0)\Phi_\varepsilon(t,0)\| = \mathcal{O}(\varepsilon|t|).$$

Remarks:

- This result can be extended for any $t \in \mathbb{R}$ with $\mathcal{O}(\varepsilon)$ in place of $\mathcal{O}(\varepsilon|t|)$ if $H(t)$ also satisfies condition II.
- By definition, $W_0(t,0)=W(t,0)$ and $\Phi_0(t,0)=\Phi_\varepsilon(t,0)$ so that $V_0(t,0)=V(t,0)=W(t,0)\Phi_\varepsilon(t,0)$.

Proof: We apply lemma (3.1.2) to the Volterra equation satisfied by $A(t,0)\equiv A_0(t,0)$

$$iA(t,0)=i\mathbb{I}-\int_0^t V^{-1}(s,0)K(s)V(s,0)A(s,0)ds. \tag{3.39}$$

The evolution $V(t,0)$ satisfies the hypothesis of the lemma with $E(t)=K(t)$ (see (2.32)). Moreover, we have the identity

$$K(t)=P(t)K(t)(\mathbb{I}-P(t))+(\mathbb{I}-P(t))K(t)P(t), \tag{3.40}$$

since $P(t)P'(t)P(t)=0$, and the operator $A(t,0)$ maps D into D. Thus we apply (3.39) on a vector $\varphi_0\in D$ and use the integration by parts formula on

$$\begin{aligned}&\int_0^t V^{-1}(s,0)K(s)V(s,0)A(s,0)\varphi_0 ds=\\&\int_0^t P(0)V^{-1}(s,0)K(s)V(s,0)(\mathbb{I}-P(0))A(s,0)\varphi_0 ds\\&+\int_0^t(\mathbb{I}-P(0))V^{-1}(s,0)K(s)V(s,0)P(0)A(s,0)\varphi_0 ds.\end{aligned} \tag{3.41}$$

We obtain for the first term

$$\begin{aligned}&\int_0^t P(0)V^{-1}(s,0)K(s)V(s,0)(\mathbb{I}-P(0))A(s,0)\varphi_0 ds=\\&-i\epsilon P(0)V(s)^{-1}\mathcal{R}K(s)V(s)(\mathbb{I}-P(0))A(s,0)\varphi_0\Big|_0^t+\\&i\epsilon\int_0^t P(0)V(s)^{-1}\left(\frac{d}{ds}\mathcal{R}K(s)\right)V(s)(\mathbb{I}-P(0))A(s,0)\varphi_0 ds-\\&\epsilon\int_0^t P(0)V(s)^{-1}\mathcal{R}K(s)K(s)V(s,0)P(0))A(s,0)\varphi_0 ds\end{aligned} \tag{3.42}$$

making use of (3.39), (3.24), (3.40) and point 1) of the lemma. We have a similar result for the second term so that we conclude

$$\|A(t,0)-\mathbb{I}\|=\mathcal{O}(\varepsilon|t|) \tag{3.43}$$

since $\|\mathcal{R}K(s)\|$ and $\|\frac{d}{ds}\mathcal{R}K(s)\|$ are of order 1 as $\varepsilon \to 0$. This assertion and (3.23) imply in turn the adiabatic theorem $\|U_\varepsilon(t,0) - V(t,0)\| = \mathcal{O}(\varepsilon|t|)$.

□

Now we would like to perform the same type of calculations on the Volterra equation satisfied by A_q

$$iA_q(t,0) - i\mathbb{I} = \int_0^t V_q^{-1}(s,0)(K_{q-1}(s) - K_q(s))V_q(s,0)A_q(s,0)ds \qquad (3.44)$$

when the hamiltonian satisfies conditions I and III. Let us define for an operator $X(t)$ its diagonal part with respect to $P_q(t)$ and $(\mathbb{I} - P_q(t))$ by

$$\mathcal{D}_q X(t) = P_q(t)X(t)P_q(t) + (\mathbb{I} - P_q(t))X(t)(\mathbb{I} - P_q(t)) \qquad (3.45)$$

and similarly, its antidiagonal part is defined by

$$\mathcal{A}_q X(t) = P_q(t)X(t)(\mathbb{I} - P_q(t)) + (\mathbb{I} - P_q(t))X(t)P_q(t). \qquad (3.46)$$

We see that in (3.44) the integrand contains diagonal terms of the type

$$\begin{aligned}
&V_q^{-1}(s,0)P_q(s)(K_{q-1}(s) - K_q(s))P_q(s)V_q(s,0) = \\
&V_q^{-1}(s,0)P_q(s)K_{q-1}(s)P_q(s)V_q(s,0) = \\
&P_q(0)V_q^{-1}(s,0)K_{q-1}(s)V_q(s,0)P_q(0)
\end{aligned} \qquad (3.47)$$

which cannot be integrated by parts. To get rid of the diagonal terms in (3.44) we change our dynamical phase operator $\Phi_q(t,0)$ in $\overline{\Phi}_q(t,0)$ defined by

$$i\varepsilon\overline{\Phi}_q'(t,0) = W_q^{-1}(t,0)\left(H_q(t) + \varepsilon\mathcal{D}_q K_{q-1}(t)\right)W_q(t,0)\overline{\Phi}_q(t,0), \quad \overline{\Phi}_q(0,0) = \mathbb{I} \qquad (3.48)$$

This unitary operator has the same general properties as those of $\Phi_q(t,0)$ and in particular, the identity

$$[\overline{\Phi}_q(t,0), P_q(0)] \equiv 0 \qquad (3.49)$$

still holds. We introduce similarly the unitary operators $\overline{V_q}(t,0)$ and $\overline{A}_q(t,0)$ by the relations

$$U_\varepsilon(t,0) = W_q(t,0)\overline{\Phi}_q(t,0)\overline{A}_q(t,0) = \overline{V_q}(t,0)\overline{A}_q(t,0). \qquad (3.50)$$

Theorem 3.1.1 *Let $H(t)$ satisfy conditions I and III and let $U_\varepsilon(t,0)$ be the physical evolution satisfying (3.22). Then, if ε is small enough, the operator $\overline{V}_q(t,0) = W_q(t,0)\overline{\Phi}_q(t,0)$, where W_q is defined by (3.20) and $\overline{\Phi}_q$ by (3.48), is an adiabatic evolution of order ε^{q+1} i.e.*

$$\|U_\varepsilon(t,0) - \overline{V}_q(t,0)\| = \mathcal{O}(\varepsilon^{q+1}|t|)$$

and

$$\overline{V}_q(t,0)P_q(0) = P_q(t)\overline{V}_q(t,0).$$

Moreover, if condition II is satisfied, the above estimate is valid for any $t \in \mathbb{R}$ with $\mathcal{O}(\varepsilon^{q+1})$ in place of $\mathcal{O}(\varepsilon^{q+1}|t|)$ and the transition probability $\mathcal{P}_{21}(\varepsilon)$ defined in lemma (3.1.1) is such that

$$\mathcal{P}_{21}(\varepsilon) = \mathcal{O}(\varepsilon^{2(q+1)}).$$

Proof: By construction, the operator $\overline{A_q}(t,0)$ satisfies the equation

$$\begin{aligned} i\overline{A_q}'(t,0) &= \overline{V_q}^{-1}(t,0)\left(\mathcal{A}_q K_{q-1}(t) - K_q(t)\right)\overline{V_q}(t,0)\overline{A_q}(t,0) \\ &= \overline{V_q}^{-1}(t,0)\mathcal{A}_q(K_{q-1}(t) - K_q(t))\overline{V_q}(t,0)\overline{A_q}(t,0). \end{aligned} \tag{3.51}$$

We are thus led to consider the integrals

$$\begin{aligned} & i\overline{A_q}(t,0)\varphi_0 - i\varphi_0 = \\ & \int_0^t P_q(0)\overline{V_q}^{-1}(s,0)(K_{q-1}(s) - K_q(s))\overline{V_q}(s,0)(\mathbb{I} - P_q(0))\overline{A_q}(s,0)\varphi_0 ds + \\ & \int_0^t (\mathbb{I} - P_q(0))\overline{V_q}^{-1}(s,0)(K_{q-1}(s) - K_q(s))\overline{V_q}(s,0)P_q(0)\overline{A_q}(s,0)\varphi_0 ds \end{aligned} \tag{3.52}$$

where $\overline{V_q}$ also satisfies the intertwining relation (3.24). Thus we can apply lemma (3.1.2) to both integrals with $H(t)$ replaced by $H_q(t)$, $P(t)$ by $P_q(t)$ and $V(t) = \overline{V_q}(t,0)$ so that

$$E(t) = K_q(t) + \mathcal{D}_q K_{q-1}(t) \tag{3.53}$$

and $B(t) = K_{q-1}(t) - K_q(t)$. By using (3.24) and point 1) of the lemma, we obtain for the first integral

$$\begin{aligned} & \int_0^t P_q(0)\overline{V_q}^{-1}(s,0)(K_{q-1}(s) - K_q(s))\overline{V_q}(s,0)(\mathbb{I} - P_q(0))\overline{A_q}(s,0)\varphi_0 ds = \\ & -i\varepsilon P_q(0)\overline{V_q}^{-1}(s,0)\mathcal{R}(K_{q-1}(s) - K_q(s))\overline{V_q}(s,0)(\mathbb{I} - P_q(0))\overline{A_q}(s,0)\varphi_0\Big|_0^t \\ & +i\varepsilon\int_0^t P_q(0)\overline{V_q}^{-1}(s,0)\left(\frac{d}{ds}\mathcal{R}(K_{q-1}(s) - K_q(s))\right)\overline{V_q}(s,0)(\mathbb{I} - P_q(0))\overline{A_q}(s,0)\varphi_0 ds \\ & +\varepsilon\int_0^t P_q(0)\overline{V_q}^{-1}(s,0)\mathcal{R}(K_{q-1}(s) - K_q(s))(K_{q-1}(s) - K_q(s))\overline{V_q}(s,0)P_q(0)\overline{A_q}(s,0)\varphi_0 ds \\ & -\varepsilon\int_0^t P_q(0)\overline{V_q}^{-1}(s,0)[K_{q-1}(s),\mathcal{R}(K_{q-1}(s) - K_q(s))]\overline{V_q}(s,0)(\mathbb{I} - P_q(0))\overline{A_q}(s,0)\varphi_0 ds. \end{aligned} \tag{3.54}$$

As the resolvents R_q are of order 1 in ε (see (3.16))

$$R_q(t,\lambda) = \mathcal{O}(1), \tag{3.55}$$

$$\|\mathcal{R}(K_{q-1}(s) - K_q(s))\| = \mathcal{O}\left(\|K_{q-1}(s) - K_q(s)\|\right) = \mathcal{O}(\varepsilon^q) \tag{3.56}$$

by proposition (3.1.1) so that the above integral is of order ε^{q+1}. The same is true for the second term of (3.52). Thus we have obtained the estimate

$$\|\overline{A_q}(t,0) - \mathbb{I}\| = \mathcal{O}(\varepsilon^{q+1}|t|) \tag{3.57}$$

from which the theorem follows. Finally, if condition II is satisfied as well, all integrals are finite in the limit $t \to \pm\infty$ and they are still of order ε^{q+1}. We conclude by lemma (3.1.1).

□

This theorem can be improved significantly by exploiting the analyticity of $H(z)$ in a more efficient way than what was done in proposition (3.1.1). Indeed it is possible to obtain useful bounds on the behaviour in q of the constants β_q appearing in the estimate

$$\|K_q - K_{q-1}\| \leq \beta_q \varepsilon^q. \tag{3.58}$$

3.2 Exponential Estimates

We prove here a proposition and show later that its hypotheses are fulfilled in our setting. Let $H(z)$ satisfy conditions I, II and III and let $z \in S_a$. The spectral projector of $H(z) = H_0(z)$ is given by (3.1)

$$P_0(z) = -\frac{1}{2\pi i}\oint_\Gamma R_0(z,\lambda)d\lambda \tag{3.59}$$

where Γ is a finite distance away from $\sigma(z)$. We choose η so small that $\forall z' \in D(z,\eta)$, $\Gamma \subset T(z')$ and

$$P_0(z') = -\frac{1}{2\pi i}\oint_\Gamma R_0(z',\lambda)d\lambda. \tag{3.60}$$

Proposition 3.2.1 *Let z, Γ and η be given as above. Let us assume that there exist constants a, b, and c such that for all integers p, all $z' \in D(z,\eta)$ and all $\lambda \in \Gamma$*

$$i) \qquad \|R_0^{(p)}(z',\lambda)\| = \|\frac{d^p}{dz'^p}R_0(z',\lambda)\| \le ac^p\frac{p!}{(1+p)^2}$$

$$ii) \qquad \|K_0^{(p)}(z')\| \le bc^p\frac{p!}{(1+p)^2}.$$

If ε is small enough, $\varepsilon < \varepsilon^*$ with ε^* given by (3.63), then there exists a constant d, given by (3.80), such that

$$\|K_q^{(p)}(z') - K_{q-1}^{(p)}(z')\| \le b\varepsilon^q d^q c^{p+q}\frac{(p+q)!}{(1+p)^2}$$

for all $z' \in D(z,\eta)$ and all integers p and q such that

$$p+q \le \left[\frac{1}{\mathrm{e}cd\varepsilon}\right] \equiv N^*.$$

Here $[x]$ is the integer part of x and e is the basis of the neperian logarithm. Moreover for $p+q \le N^*$

$$\|K_q^{(p)}(z')\| \le b\frac{\mathrm{e}}{\mathrm{e}-1}c^p\frac{p!}{(1+p)^2}.$$

Proof: Let α be the best constant such that for all integers n

$$\sum_{\substack{n_1\ge 0,\, n_2\ge 0\\ n_1+n_2=n}}\frac{1}{(1+n_1)^2}\frac{1}{(1+n_2)^2} \le \frac{\alpha}{(1+n)^2} \tag{3.61}$$

$(1 < \alpha \le 16\pi^2/3)$. We assume that ε is small enough so that $\varepsilon ab\frac{\mathrm{e}}{\mathrm{e}-1} < 1$ and we define

$$\delta(\varepsilon) := \frac{1}{1-\varepsilon ab\frac{\mathrm{e}}{\mathrm{e}-1}} < \infty. \tag{3.62}$$

Let ε^* be the largest ε so that

$$\sum_{k\ge 1}\left(\delta(\varepsilon)\varepsilon\alpha^2 ab\frac{\mathrm{e}}{\mathrm{e}-1}\right)^k \le \alpha \tag{3.63}$$

where α is the constant of (3.61). From now on $0 < \varepsilon < \varepsilon^*$ and $\delta = \delta(\varepsilon^*)$ is independent of ε.

i) Let us do the first iteration. Since $ab\varepsilon < 1$ we can define, for all $z' \in D(z,\eta)$ and all $\lambda \in \Gamma$,

$$(I\!I - \varepsilon R_0 K_0)^{-1} = \sum_{k\geq 0} (\varepsilon R_0 K_0)^k \tag{3.64}$$

and

$$\|(I\!I - \varepsilon R_0 K_0)^{-1}\| \leq \frac{1}{1 - ab\varepsilon} \leq \delta. \tag{3.65}$$

Since R_0 and K_0 are bounded holomorphic operators on $D(z,\eta)$, the same is true for $(I\!I - \varepsilon R_0 K_0)^{-1}$.

Lemma 3.2.1 *For all $p \in I\!N$ and $z' \in D(z,\eta)$*

$$\|\frac{d^p}{dz'^p}(I\!I - \varepsilon R_0(z',\lambda)K_0(z'))^{-1}\| \leq \delta \frac{p!c^p}{(1+p)^2}.$$

Proof: We first estimate using (3.61)

$$\begin{aligned}\|(R_0K_0)^{(p)}\| &\leq ab\sum_{k=0}^{p}\binom{p}{k}c^p \frac{k!}{(1+k)^2}\frac{(p-k)!}{(1+(p-k))^2} \\ &\leq \alpha ab c^p \frac{p!}{(1+p)^2}.\end{aligned} \tag{3.66}$$

Then we use the formula

$$\begin{aligned}&\frac{d^p}{dz^p}(I\!I - A(z))^{-1} = \\ &\sum_{k=1}^{p}\sum_{\substack{n_1\geq 1,\dots,n_k\geq 1\\ n_1+\dots+n_k=p}}\binom{p}{n_1\dots n_k}(I\!I - A(z))^{-1}A(z)^{(n_1)}(I\!I - A(z))^{-1}A(z)^{(n_2)}\dots \\ &\cdots A(z)^{(n_k)}(I\!I - A(z))^{-1}.\end{aligned} \tag{3.67}$$

Therefore we get

$$\begin{aligned}&\|\frac{d^p}{dz^p}(I\!I - \varepsilon R_0K_0)^{-1}\| \leq \\ &p!c^p\delta\sum_{k=1}^{p}(\varepsilon\delta\alpha ab)^k \sum_{\substack{n_1\geq 1,\dots,n_k\geq 1\\ n_1+\dots+n_k=p}} \frac{1}{(1+n_1)^2}\frac{1}{(1+n_2)^2}\cdots\frac{1}{(1+n_k)^2} \leq \\ &p!c^p\delta\sum_{k=1}^{p}(\varepsilon\delta\alpha ab)^k\alpha^{k-1}\frac{1}{(1+p)^2}.\end{aligned} \tag{3.68}$$

The factor α^{k-1} comes from the summation over $n_1, \dots, n_k$, which is done iteratively as follows

$$\begin{aligned}&\sum_{\substack{n_1\geq 1,\dots,n_k\geq 1\\ n_1+\dots+n_k=p}} \frac{1}{(1+n_1)^2}\frac{1}{(1+n_2)^2}\cdots\frac{1}{(1+n_k)^2} = \\ &\sum_{\substack{n_1\geq 1,\dots,n_{k-2}\geq 1, m\geq 2\\ n_1+\dots+n_{k-2}+m=p}} \frac{1}{(1+n_1)^2}\cdots\frac{1}{(1+n_{k-2})^2}\sum_{\substack{n_{k-1}\geq 1, n_k\geq 1\\ n_{k-1}+n_k=m}}\frac{1}{(1+n_{k-1})^2}\frac{1}{(1+n_k)^2} \leq \\ &\alpha\sum_{\substack{n_1\geq 1, n_2\geq 1\dots, n_{k-1}\geq 1\\ n_1+n_2\dots+n_{k-1}=p}} \frac{1}{(1+n_1)^2}\frac{1}{(1+n_2)^2}\cdots\frac{1}{(1+n_{k-1})^2}\end{aligned} \tag{3.69}$$

using (3.61). Since $\varepsilon < \varepsilon*$ we get

$$\|\frac{d^p}{dz^p}(\mathbb{I} - \varepsilon R_0 K_0)^{-1}\| \leq \delta \frac{p! c^p}{(1+p)^2}. \tag{3.70}$$

□

We can define

$$R_1(z,\lambda) = (\mathbb{I} - \varepsilon R_0(z,\lambda) K_0(z))^{-1} R_0(z,\lambda) \tag{3.71}$$

which is the resolvent of $H_0(z) - \varepsilon K_0(z)$ at λ. Using lemma (3.2.1), Leibniz formula and (3.61) we get

$$\|\frac{d^p}{dz^p} R_1(z,\lambda)\| \leq \alpha\delta a c^p \frac{p!}{(1+p)^2}. \tag{3.72}$$

The next step is to estimate $\|K_1^{(p)}(z) - K_0^{(p)}(z)\|$. We have

$$\begin{aligned} &\|K_1^{(p)} - K_0^{(p)}\| \leq \\ &\|((P_1' - P_0')P_1)^{(p)}\| + \|(P_0'(P_1 - P_0))^{(p)}\| + \\ &\|(P_1(P_1' - P_0'))^{(p)}\| + \|((P_1 - P_0)P_0')^{(p)}\|. \end{aligned} \tag{3.73}$$

Since all $\lambda \in \Gamma$ are in the resolvent set of H_1 we can write

$$\begin{aligned} P_1(z) - P_0(z) &= -\frac{1}{2\pi i}\oint_\Gamma (R_1(z,\lambda) - R_0(z,\lambda) d\lambda \\ &= -\frac{\varepsilon}{2\pi i}\oint_\Gamma R_0(z,\lambda) K_0(z) R_1(z,\lambda) d\lambda. \end{aligned} \tag{3.74}$$

Using Leibniz formula we have

$$\|(R_0 K_0 R_1)^{(p)}\| \leq \alpha^3 \delta a^2 b c^p \frac{p!}{(1+p)^2} \tag{3.75}$$

and therefore

$$\|(P_1 - P_0)^{(p)}\| \leq \frac{L}{2\pi}\varepsilon \alpha^3 \delta a^2 b c^p \frac{p!}{(1+p)^2} \tag{3.76}$$

where L is the length of the path Γ. Using again a Riesz formula for the projectors P_0 and P_1 and the estimates for R_0 and R_1, we get

$$\|P_0^{(p)}\| \leq \frac{L}{2\pi} a c^p \frac{p!}{(1+p)^2} \tag{3.77}$$

and

$$\|P_1^{(p)}\| \leq \frac{L}{2\pi}\alpha\delta a c^p \frac{p!}{(1+p)^2}. \tag{3.78}$$

Lemma 3.2.2 ([Ne3]) *Let A and B be two analytic bounded operators such that*

$$\|A^{(p)}\| \leq a c^{k+p} \frac{(k+p)!}{(1+p)^2}$$

and

$$\|B^{(p)}\| \leq b c^{l+p} \frac{(l+p)!}{(1+p)^2}.$$

Then

$$\|(AB)^{(p)}\| \leq \alpha a b c^{k+l+p} \frac{(k+l+p)!}{(1+p)^2}.$$

Using this lemma and the above results we finally have

$$\|K_1^{(p)} - K_0^{(p)}\| \leq \varepsilon b\tilde{d}c^{p+1}\frac{(p+1)!}{(1+p)^2} \tag{3.79}$$

with

$$\begin{aligned}\tilde{d} &= 2\left(\frac{L}{2\pi}\right)^2 (a^3\delta\alpha^4 + a^3\delta^2\alpha^5)\\ &\leq 4\left(\frac{L}{2\pi}\right)^2 a^3\delta^3\alpha^6 \equiv d\end{aligned} \tag{3.80}$$

(since $\alpha > 1$, $\delta > 1$). We can now estimate

$$\begin{aligned}\|K_1^{(p)}\| &\leq \|K_1^{(p)} - K_0^{(p)}\| + \|K_0^{(p)}\|\\ &\leq \varepsilon bdc^{p+1}\frac{(p+1)!}{(1+p)^2} + bc^p\frac{p!}{(1+p)^2}\\ &= bc^p\frac{p!}{(1+p)^2}(1+\varepsilon dc(p+1))\\ &\leq bc^p\frac{p!}{(1+p)^2}\sum_{k\geq 0}(\varepsilon cdN^*)^k\\ &\leq bc^p\frac{p!}{(1+p)^2}\sum_{k\geq 0}\mathrm{e}^{-k}\\ &= b\frac{\mathrm{e}}{\mathrm{e}-1}c^p\frac{p!}{(1+p)^2}\end{aligned} \tag{3.81}$$

if $p+1 \leq N^*$. With this last estimate we have finished the first step.

ii) By our hypothesis on ε (see (3.62) and (3.63)), we can define for all $\lambda \in \Gamma$ and all $z' \in D(z,\eta)$

$$(\mathbb{I} - \varepsilon R_0K_1)^{-1} = \sum_{k\geq 0}(\varepsilon R_0K_1)^k \tag{3.82}$$

with $\|(\mathbb{I} - \varepsilon R_0K_1)^{-1}\| \leq \delta$ and lemma (3.2.1) holds for the operator (3.82). Therefore the resolvent of $H_2(z) = H(z) - \varepsilon K_1(z)$ is given at $\lambda \in \Gamma$ by

$$R_2(z,\lambda) = (\mathbb{I} - \varepsilon R_0(z)K_1(z))^{-1}R_0(z) \tag{3.83}$$

and thus

$$\|\frac{d^p}{dz^p}R_2(z,\lambda)\| \leq \alpha\delta ac^p\frac{p!}{(1+p)^2} \tag{3.84}$$

provided $1+p \leq N^*$. Then we estimate $\|(K_2 - K_1)^{(p)}\|$ as above by writing

$$\begin{aligned}P_2(z) - P_1(z) &= -\frac{1}{2\pi i}\oint_\Gamma (R_2(z,\lambda) - R_1(z,\lambda))d\lambda\\ &= -\frac{\varepsilon}{2\pi i}\oint_\Gamma R_1(z,\lambda)(K_1(z) - K_0(z))R_2(z,\lambda))d\lambda.\end{aligned} \tag{3.85}$$

We get, instead of (3.76)

$$\|(P_2 - P_1)^{(p)}\| \leq \frac{L}{2\pi}\varepsilon^2 bd\alpha^4\delta^2a^2c^{p+1}\frac{(p+1)!}{(1+p)^2} \tag{3.86}$$

for $p+1 \leq N^*$ and by lemma (3.2.2)

$$\begin{aligned} &\|K_2^{(p)} - K_1^{(p)}\| \\ &\leq \varepsilon^2 db4 \left(\frac{L}{2\pi}\right)^2 \alpha^6 \delta^3 a^3 c^{p+2} \frac{(p+2)!}{(1+p)^2} = b\varepsilon^2 d^2 c^{p+2} \frac{(p+2)!}{(1+p)^2} \end{aligned} \quad (3.87)$$

and therefore for all $2+p \leq N^*$

$$\begin{aligned} \|K_2^{(p)}\| &\leq \|K_2^{(p)} - K_1^{(p)}\| + \|K_1^{(p)} - K_0^{(p)}\| + \|K_0^{(p)}\| \\ &\leq b\frac{\mathrm{e}}{\mathrm{e}-1} c^p \frac{p!}{(1+p)^2}. \end{aligned} \quad (3.88)$$

We can iterate this procedure since all estimates are reproduced as long as

$$p+q \leq N^* \quad (3.89)$$

is satisfied.

□

Remark:
The constant d defined by (3.80) is independent of ε.

3.2.1 Superadiabatic Evolution

We give a first application of proposition (3.2.1) by proving the existence of a superadiabatic evolution. Let t be some point of the real axis. Since $H(t)$ is self-adjoint we have for all λ in the resolvent set of $H(t)$

$$\|R_0(t,\lambda)\| = \frac{1}{\mathrm{dist}(\lambda, \sigma(t))} \quad (3.90)$$

where $\sigma(t)$ is the spectrum of $H(t)$. For each t we choose Γ_t as in figure (3.1), so that for each $\lambda \in \Gamma_t$

$$\mathrm{dist}(\lambda, \sigma(t)) \geq \frac{1}{2}\mathrm{dist}(\sigma_1(t), \sigma_2(t)) \geq \frac{g}{2}. \quad (3.91)$$

From the estimates of section (2.2) and formula (2.11) it follows that there exists $0 < r < a$

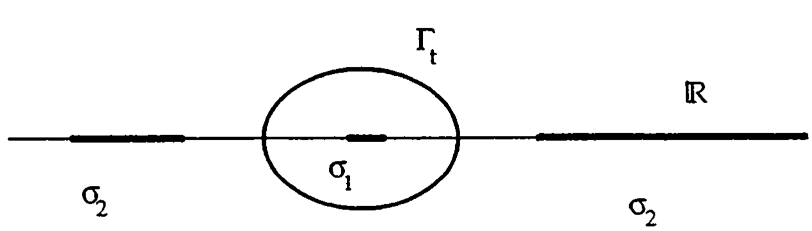

Figure 3.1: The contour Γ_t for $t \in I\!R$.

such that for each $z \in D(t,r)$, and each $\lambda \in \Gamma_t$

$$\begin{aligned} \|R_0(z,\lambda)\| &\leq 2\|R_0(t,\lambda)\| \\ &\leq \frac{4}{\mathrm{dist}(\sigma_1(t), \sigma_2(t))} \leq \frac{4}{g} \end{aligned} \quad (3.92)$$

and that there exists a constant C such that for all $z \in D(t,r)$ and all $t \in I\!R$

$$||K_0(z)|| \leq Cb(t) \tag{3.93}$$

with $b(t)$ the integrable decay function of condition II. Using Cauchy formula we get for all $z \in D(t,\eta)$, η some small number $< r$,

$$||R_0^{(p)}(z,\lambda)|| \leq \frac{4}{g} p! \left(\frac{1}{r-\eta}\right)^p \tag{3.94}$$

and

$$||K_0^{(p)}(z)|| \leq C'b(t)p! \left(\frac{1}{r-\eta}\right)^p. \tag{3.95}$$

Therefore we can apply proposition (3.2.1) with $a = \frac{4}{g}$, $b = C'b(t)$, C' some constant and $c = \frac{8}{r}$ provided that η is small enough. Indeed, to get the estimate

$$\tilde{c}^p \leq \frac{c^p}{(1+p)^2} \quad \forall p \tag{3.96}$$

with $\tilde{c} = \frac{1}{r-\eta}$ and $c = \tau\tilde{c}$, for some $\tau > 1$, we must choose τ in such a way that

$$\tau \geq (1+p)^{2/p} \quad \forall p \tag{3.97}$$

which is satisfied for $\tau = 4$. Hence, with $\eta < r/2$, we obtain $c = 8/r$. From the proposition there exists ε^* independent of t such that for all $\varepsilon < \varepsilon^*$ the iteration scheme is well-defined up to order $N^* = [(ecd\varepsilon)^{-1}]$ with

$$d = \frac{\delta^3\alpha^6}{\pi^2} L^2 a^3 = \mathcal{O}(L^2 a^3) = \mathcal{O}\left(\frac{L^2}{g^3}\right) \tag{3.98}$$

where L is the supremum of the length of the paths Γ_t. We set

$$H_*(t) := H_{N^*}(t) = H(t) - \varepsilon K_{N^*-1}(t) \tag{3.99}$$

and

$$P_*(t) := P_{N^*}(t) = -\frac{1}{2\pi i}\oint_\Gamma R_{N^*}(t,\lambda)d\lambda. \tag{3.100}$$

Since $||K_{N^*-1}(t)|| \leq O(b(t))$, we have

$$\lim_{t\to\pm\infty} ||P_*(t) - P(t)|| = 0. \tag{3.101}$$

The superadiabatic evolution V_* is defined by

$$V_*(t,s) := V_{N^*}(t,s) = W_{N^*}(t,s)\Phi_{N^*}(t,s), \tag{3.102}$$

where W_{N^*} and Φ_{N^*} are the parallel transport and dynamical phase operators (3.20) and (3.21).

Theorem 3.2.1 (Nekhoroshev Type Estimates) *Let $H(t)$ satisfy conditions I, II and III. There exists $\varepsilon^* > 0$ such that for $\varepsilon < \varepsilon^*$ we can construct a superadiabatic evolution $V_*(t,s)$ and projectors $P_*(t)$ satisfying*

$$\|U_\varepsilon(t,s) - V_*(t,s)\| \leq M \exp\{-\tau/\varepsilon\} \quad \forall t,s \in \mathbb{R}$$

where τ and M are two positive constants and

$$P_*(t)V_*(t,s) = V_*(t,s)P_*(s).$$

Moreover the transition probability $\mathcal{P}_{21}(\varepsilon)$ from $P(-)\mathcal{H}$ to $(\mathbb{I} - P(+))\mathcal{H}$ between the times $t_1 = -\infty$ and $t_2 = +\infty$ satisfies

$$\mathcal{P}_{21}(\varepsilon) = \mathcal{O}\left(\exp\{-2\tau/\varepsilon\}\right).$$

Proof: Consider the estimate (3.28) for $A_{N^*}(t,s) = \Phi_{N^*}^{-1}(t,s)W_{N^*}^{-1}(t,s)U_\varepsilon(t,s)$, which reads

$$\|A_{N^*}(t,s) - \mathbb{I}\| \leq \int_s^t \|K_{N^*-1}(t') - K_{N^*}(t')\| dt'. \tag{3.103}$$

From proposition (3.2.1) we have

$$\begin{aligned} \|K_{N^*-1}(t) - K_{N^*}(t)\| &\leq C'b(t)\varepsilon^{N^*}d^{N^*}c^{N^*}N^*! \\ &\leq C'b(t)(\varepsilon dcN^*)^{N^*} \\ &\leq C'b(t)e^{-N^*} \\ &\leq C'eb(t)e^{-\frac{1}{ecd\varepsilon}} \\ &= \mathcal{O}(b(t))\exp\{-\tau/\varepsilon\} \end{aligned} \tag{3.104}$$

with $\tau = \frac{1}{ecd} = \mathcal{O}\left(\frac{1}{cd}\right) = \mathcal{O}\left(\frac{g^3}{L^2}r\right)$. Since $b(t)$ is integrable it follows that

$$\|V_*^{-1}(t,s)U(t,s) - \mathbb{I}\| \leq M \exp\{-\tau/\varepsilon\} \tag{3.105}$$

for some constant M. The intertwining property is true by construction and considering lemma (3.1.1) together with (3.33) we immediately get the estimate on $\mathcal{P}_{21}(\varepsilon)$.

□

Remark:
If $H(t)$ satisfies conditions I and III only, the first two conclusions of the theorem are true for s and t in any compact subset of $\mathbb{R}$, whereas the last conclusion does not make sense.

We expect on physical grounds that the larger the gap g between $\sigma_1(t)$ and $\sigma_2(t)$, the larger the exponential decay rate τ. We show in the next section that this is indeed the case.

3.2.2 Dependence in the Gap

Let us consider the family of hamiltonians $H_\gamma(t)$ obtained from $H(t)$ by shifting the part of the spectrum $\sigma_2(t)$ away from $\sigma_1(t)$ by a distance $\gamma \geq 0$. We proceed as follows. The part $\sigma_2(t)$ of the spectrum of $H(t)$ is generally given by

$$\sigma_2(t) = \sigma_-(t) \cup \sigma_+(t), \quad \text{where } \sigma_-(t) \cap \sigma_+(t) = \emptyset \tag{3.106}$$

and $\sigma_1(t)$ is in between $\sigma_-(t)$ and $\sigma_+(t)$ (the part $\sigma_-(t)$ being possibly absent). The corresponding spectral projectors are $P_-(t)$ and $P_+(t)$ such that $[P_\pm(t), H(t)] = 0$ and $P_+(t) + P_-(t) = \mathbb{I} - P(t)$. We define

$$H_\gamma(t) \equiv H(t)P_-(t) + (H(t) + \gamma)P(t) + (H(t) + 2\gamma)P_+(t). \tag{3.107}$$

It is easily checked that

$$(H_\gamma(t)-\lambda)^{-1} \equiv R_\gamma(t,\lambda) = \\ R(t,\lambda)P_-(t) + R(t,\lambda-\gamma)P(t) + R(t,\lambda-2\gamma)P_+(t) \tag{3.108}$$

and that the spectrum of $H_\gamma(t)$, denoted by $\sigma_\gamma(t)$, is given by

$$\sigma_\gamma(t) = \sigma_-(t) \cup (\sigma_1(t)+\gamma) \cup (\sigma_+(t)+2\gamma). \tag{3.109}$$

Thus if $\mathrm{dist}(\sigma_1(t),\sigma_2(t)) \geq g \ \forall t \in \mathbb{R}$ then

$$\mathrm{dist}(\sigma_{1\gamma}(t),\sigma_{2\gamma}(t)) \geq g+\gamma \equiv g(\gamma) \tag{3.110}$$

where $\sigma_{1\gamma}(t) \equiv \sigma_1(t)+\gamma$ and $\sigma_{2\gamma}(t) \equiv \sigma_\gamma(t) \setminus \sigma_{1\gamma}(t)$. (See figure (3.2).)

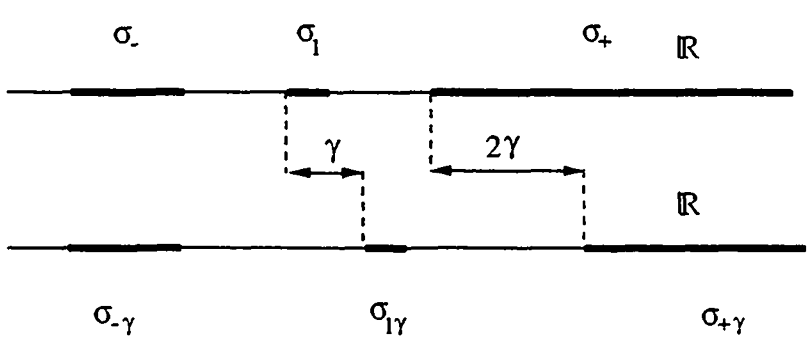

Figure 3.2: The spectrum of $H_\gamma(t)$.

We consider now proposition (3.2.1) with H_γ in place of H, using the identity (3.107) and paying attention to the dependence in γ of the different quantities encountered. We show that there exist constants $a(\gamma)$, $b(\gamma)$ and $c(\gamma)$ such that the following proposition hold:

Proposition 3.2.2 *If $H(t)$ is replaced by $H_\gamma(t)$ then the exponential decay rate τ is replaced by $\tau(\gamma)$ such that*

$$\tau(\gamma) \geq Cg(\gamma), \quad \forall\gamma \geq 0.$$

for some constant C.

This proposition shows that the larger the gap between σ_1 and σ_2, the better the agreement between U_ϵ and V_*. This property will be important for other results to come and does not follow from the estimates of lemma (3) and (4) in [Ne3].

Proof: The proof consists in finding a constant r independent of γ, possibly smaller than the one of paragraph (3.2.1), such that the estimates corresponding to (3.92) and (3.93) hold with the same b and with $a(\gamma) = \mathcal{O}(g(\gamma)^{-1})$. The constant c will thus be independent of γ.

As the spectral projectors of H and H_γ are identical, we can use the estimate (3.93) which holds for any $r > 0$, yielding the same constant b as before. The hamiltonian $H_\gamma(z)$ is reduced by $P_-(z)$, $P(z)$ and $P_+(z)$. Let $W(z,t)$ be the solution of the equation

$$iW'(z,t) = i(P_-'(z)P_-(z) + P'(z)P(z) + P_+'(z)P_+(z))W(z,t) \\ W(t,t) = \mathbb{I} \tag{3.111}$$

This equation generalizes the definition (2.26) in the sense that the intertwining property is true for all three projectors

$$W(z,t)P_{\pm}(t) = P_{\pm}(z)W(z,t), \quad W(z,t)P(t) = P(z)W(z,t). \tag{3.112}$$

Note that

$$\sup_{z,t\in S_a} \|W(z,t)\| < \infty, \quad \sup_{z,t\in S_a} \|W^{-1}(z,t)\| < \infty \tag{3.113}$$

as a consequence of condition II. Indeed this is true for $z \in I\!R$ by unitarity and for z complex we use the decomposition $W(z,t) = W(z, \mathrm{Re}z)W(\mathrm{Re}z, t)$. Then by lemma (2.2.3) we can bound uniformly the corresponding Dyson series (2.27) for $W(z, \mathrm{Re}z)$. We introduce $\tilde{H}(z) \equiv W^{-1}(z,t)H(z)W(z,t)$, which is a closed holomorphic operator in S_a, and which is reduced by $P_{\pm}(t)$ and $P(t)$ by lemma (2.2.4). Instead of the path Γ_t we now consider the path $\Gamma_t(\gamma)$ defined similarly (see figure (3.3)).

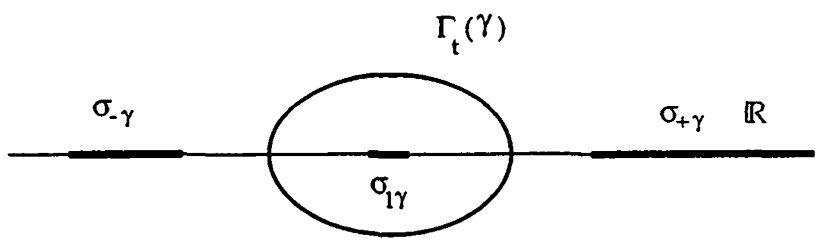

Figure 3.3: The path $\Gamma_t(\gamma)$.

For a bounded operator B leaving $P(t)\mathcal{H}$ invariant we set

$$\|B\|_P = \sup_{\varphi\in P(t)\mathcal{H}} \frac{\|B\varphi\|}{\|\varphi\|} \tag{3.114}$$

and we define $\|B\|_{P_\pm}$ similarly. By definition of H_γ we have

$$R_\gamma(z,\lambda) = W(z,t)\tilde{R}_\gamma(z,\lambda)W^{-1}(z,t) \tag{3.115}$$

with

$$\tilde{R}_\gamma(z,\lambda) = \tilde{R}(z,\lambda)P_-(t) + \tilde{R}(z,\lambda-\gamma)P(t) + \tilde{R}(z,\lambda-2\gamma)P_+(t). \tag{3.116}$$

and $\tilde{R}(z,\lambda) = (\tilde{H}(z) - \lambda)^{-1}$. Since $P_{\pm}(t)$ and $P(t)$ are orthogonal projections

$$\begin{aligned}
&\|R_\gamma(z,\lambda)\varphi\| \le \|W(z,t)\|\|\tilde{R}_\gamma(z,\lambda)W^{-1}(z,t)\varphi\| \\
&\le \|W(z,t)\|\|\tilde{R}_\gamma(z,\lambda)(P_-(t) + P(t) + P_+(t))W^{-1}(z,t)\varphi\| \\
&\le \|W(z,t)\| \max\left\{\|\tilde{R}(z,\lambda)\|_{P_-}, \|\tilde{R}(z,\lambda-\gamma)\|_P, \|\tilde{R}(z,\lambda-2\gamma)\|_{P_+}\right\} \times \\
&\|W^{-1}(z,t)\|\|\varphi\|.
\end{aligned} \tag{3.117}$$

Since $P_{\pm}(t)$ and $P(t)$ commute with $\tilde{H}(z)$ and $\tilde{R}(z,\lambda)$ there exists, as above (see (3.92) and lemma (2.2.4)), a constant r, independent of γ, such that

$$\|\tilde{R}(z,\lambda)\|_{P_\pm} \le 2\|\tilde{R}(t,\lambda)\|_{P_\pm} = 2\|R(t,\lambda)\|_{P_\pm} \tag{3.118}$$

and

$$\|\tilde{R}(z,\lambda)\|_P \leq 2\|R(t,\lambda)\|_P \tag{3.119}$$

provided $z \in D(t,r)$. By taking $\lambda \in \Gamma_t(\gamma)$ we have

$$\|\tilde{R}(z,\lambda)\|_{P_-} \leq \frac{2}{\gamma+g}, \quad \|\tilde{R}(z,\lambda-\gamma)\|_P \leq \frac{2}{\gamma+g} \tag{3.120}$$

and

$$\|\tilde{R}(z,\lambda-2\gamma)\|_{P_+} \leq \frac{2}{\gamma+g} \tag{3.121}$$

(see the end of paragraph (2.2.2)). Then, using Cauchy formula, we get

$$\begin{aligned} \|R_\gamma(z,\lambda)\| &\leq a(\gamma)c^p\frac{p!}{(1+p)^2} \\ \|K_0(z)\| &\leq bc^p\frac{p!}{(1+p)^2} \end{aligned} \tag{3.122}$$

with $a(\gamma) = \mathcal{O}\left(\frac{1}{g(\gamma)}\right)$, $c = \mathcal{O}\left(\frac{1}{r}\right)$ and $b = \mathcal{O}\left(b(t)\right)$ independent of γ. Thus we get

$$\tau(\gamma) = \mathcal{O}\left(\frac{g(\gamma)^3}{L(\gamma)^2}\right) = \mathcal{O}\left(g(\gamma)\right) \tag{3.123}$$

since $\frac{L(\gamma)}{g(\gamma)} \to 1$ as $\gamma \to \infty$ by construction of $\Gamma_t(\gamma)$.

□

Chapter 4

Complex Time Method

Up to now we have dealt with very general systems for which we showed that the transition probability $\mathcal{P}_{21}(\varepsilon)$ across a gap was exponentially small in the adiabatic limit $\varepsilon \to 0$. We have thus proved the folk adiabatic theorem quoted in the introduction. We want to turn now to the study of the simplest interesting systems in this context, namely two-level systems. Their relative simplicity will allow us to describe the transition probability $\mathcal{P}_{21}(\varepsilon)$ in the asymptotic regime $\varepsilon \ll 1$ in great details for such systems. Indeed, we shall derive asymptotic formulae for $\mathcal{P}_{21}(\varepsilon)$, instead of mere bounds.

4.1 Spin-1/2 in a Time-Dependent Magnetic Field

4.1.1 Coordinate-Dependent Formulation of the Problem

Let $H(t)$ be a 2×2 matrix which satisfies conditions I, II and III. Without restricting the generality we suppose that the trace of $H(t)$ is identically zero, so that we can write

$$\begin{aligned} H(t) &= \mathbf{B}(t) \cdot \mathbf{s} \\ &\equiv B_1(t)\frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + B_2(t)\frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + B_3(t)\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned} \tag{4.1}$$

The hamiltonian (4.1) is interpreted as the hamiltonian of a spin-1/2 in a time-dependent magnetic field $\mathbf{B}(t)$. By conditions I and II, the functions $B_k(t)$ have analytic extensions $B_k(z)$ in S_a satisfying $B_k(\bar{z}) = \overline{B_k(z)}$ and there exist real limits $B_k(\pm)$ and an integrable decay function $b(t)$ such that

$$\sup_{|s|<a} |B_k(t+is) - B_k(\pm)| < b(t) \quad \text{if } t \gtrless 0 \tag{4.2}$$

for $k = 1, 2, 3$. Let $\rho(z) = B_1^2(z) + B_2^2(z) + B_3^2(z)$. The spectrum of $H(z)$ consists of the two values $\pm\frac{1}{2}\sqrt{\rho(z)}$ where $\sqrt{\cdot}$ is the branch of the square-root which takes the value 1 at $z = 1$. Condition III implies that $\rho(t) > 0$ for $t \in \mathbb{R}$. We define

$$\begin{aligned} \sigma_1(t) &= \{e_1(t)\} = \{-\frac{1}{2}\sqrt{\rho(t)}\} \\ \sigma_2(t) &= \{e_2(t)\} = \{\frac{1}{2}\sqrt{\rho(t)}\} \end{aligned} \tag{4.3}$$

so that the corresponding spectral projectors are

$$P(t) \equiv P_1(t) = \frac{1}{2}\left(\mathbb{I} - \frac{\mathbf{B}(t) \cdot \mathbf{s}}{\frac{1}{2}\sqrt{\rho(t)}}\right)$$

$$(\mathbb{I} - P(t)) \equiv P_2(t) = \frac{1}{2}\left(\mathbb{I} + \frac{\mathbf{B}(t)\cdot \mathbf{s}}{\frac{1}{2}\sqrt{\rho(t)}}\right). \tag{4.4}$$

We shall keep this notation in the sequel. Let us consider the solution $\psi_\varepsilon(t)$ of the Schrödinger equation

$$i\varepsilon\psi_\varepsilon'(t) = H(t)\psi_\varepsilon(t), \quad \psi_\varepsilon(0) = \varphi_0. \tag{4.5}$$

As in the preceding chapter, we select a normalized solution having the property

$$\lim_{t\to-\infty} \|P_1(t)\psi_\varepsilon(t)\| = 1 \tag{4.6}$$

and we are interested in the transition probability

$$\mathcal{P}_{21}(\varepsilon) = \lim_{t\to\infty} \|P_2(t)\psi_\varepsilon(t)\|^2. \tag{4.7}$$

Since the hamiltonian is analytic in S_a, the solution $\psi_\varepsilon(t)$ possesses a univalued analytic extension $\psi_\varepsilon(z)$ in S_a satisfying

$$i\varepsilon\psi_\varepsilon'(z) = H(z)\psi_\varepsilon(z). \tag{4.8}$$

In the previous chapter, we had chosen the width $2a$ of the analyticity strip S_a in such a way that $\sigma_1(z)\cap\sigma_2(z) = \emptyset$ for all $z \in S_a$. Here, on the contrary, we want to make use of the multivaluedness of the analytic extensions $e_k(z)$ and $P_k(z)$ of the eigenvalues and spectral projectors when S_a contains eigenvalue crossing points to compute $\mathcal{P}_{21}(\varepsilon)$. The eigenvalue crossing points z_j such that $e_1(z_j) = e_2(z_j)$ coincide with the zeros of the analytic function $\rho(z)$ so that they are necessarily complex and come by complex conjugated pairs $\{z_j, \bar{z}_j\}$. Moreover, there is a finite number of them since $\rho(t+is)$ tends to positive limits $\rho(\pm)$ when $t \to \pm\infty$, uniformly in $|s| \leq a$, as can be seen from the identity

$$\rho(z) - \rho(\pm) = \sum_{j=1}^{3}(B_j(z) - B_j(\pm))(B_j(z) + B_j(\pm)). \tag{4.9}$$

Let X denote the set of eigenvalue crossing points $\{z_j, \bar{z}_j\}_{j=0}^{N-1}$. The expressions (4.3) and (4.4) can be continued analytically from the real axis to the punctured strip $S_a\backslash X$, where they give rise to multivalued analytic functions. Let us construct analytic eigenvectors $\varphi_k(t)$ of the hamiltonian $H(t)$ by means of the parallel transport $W(t,0)$, solution of

$$iW'(t,0) = K(t)W(t,0), \quad W(0,0) = \mathbb{I}. \tag{4.10}$$

Its generator is given by

$$K(t) = i[P_1'(t), P_1(t)] = \frac{\mathbf{B}'(t)\wedge \mathbf{B}(t)}{\rho(t)}\cdot \mathbf{s} \tag{4.11}$$

where $\mathbf{B}'\wedge\mathbf{B}$ is the vector product of $\mathbf{B}'$ and $\mathbf{B}$ and thus possesses a univalued analytic extension $K(z)$ in $S_a\backslash X$. But since $S_a\backslash X$ is not simply connected, the analytic extension $W(z,0)$ of the parallel transport is multivalued in $S_a\backslash X$. In order to deal with univalued functions only we define a simply connected domain $\Omega \subset S_a$ by removing vertical lines issued at z_j and $\bar{z}_j$ and joining the boundary of S_a (see figure (4.1)). Thus the real axis is included in Ω and all analytic extensions encountered so far are univalued in Ω. Let $\varphi_1(0)$ and $\varphi_2(0)$ be two normalized eigenvectors of $H(0)$,

$$H(0)\varphi_k(0) = e_k(0)\varphi_k(0), \quad k = 1, 2. \tag{4.12}$$

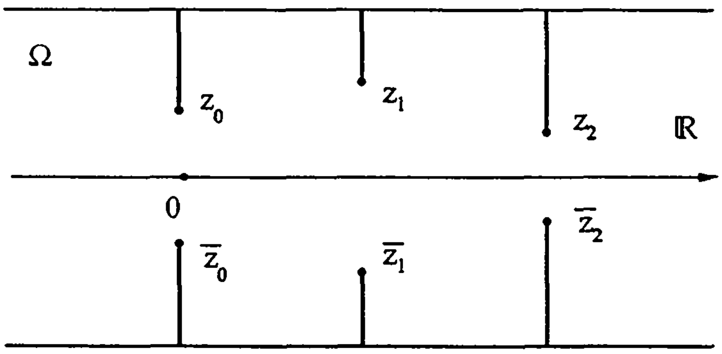

Figure 4.1: The domain Ω.

Using the parallel transport $W(z,0)$, (we drop from now on the second argument of W), we define

$$\varphi_k(z) = W(z)\varphi_k(0), \quad k = 1,2. \tag{4.13}$$

This construction gives a choice of analytic eigenvectors of $H(z)$ since

$$P_k(z)\varphi_k(z) = P_k(z)W(z)\varphi_k(0) = W(z)P_k(0)\varphi_k(0) = \varphi_k(z). \tag{4.14}$$

Moreover the φ_k's have the property

$$P_k(z)\varphi_k'(z) = 0, \quad k = 1,2 \tag{4.15}$$

which reduces to the phase fixing condition (1.3) on the real axis. Indeed for any $z \in \Omega$ we can write

$$P_k(z)\varphi_k'(z) = -iP_k(z)K(z)\varphi_k(z) = -iP_k(z)K(z)P_k(z)\varphi_k(z) = 0 \tag{4.16}$$

since $K(z)$ is antidiagonal and on the real axis we have

$$\langle\varphi_k(t)|\varphi_k'(t)\rangle = \langle P_k(t)\varphi_k(t)|\varphi_k'(t)\rangle = \langle\varphi_k(t)|P_k(t)\varphi_k'(t)\rangle \equiv 0. \tag{4.17}$$

Note also that $W(z)$ has well-defined unitary limits $W(\pm\infty)$ as $\mathrm{Re}z \to \pm\infty$ and $|\mathrm{Im}z| < a$. It follows from lemma (2.2.3) that we can write $\|K(t+is)\| \leq b(t)$ where $b(t)$ is an integrable decay function and by considering the Dyson series (2.27) for $W(z)$ we easily get

$$\lim_{t\to\pm\infty} \sup_{|s|<a} \|W(t+is) - W(\pm\infty)\| = 0. \tag{4.18}$$

Hence, the eigenvectors $\varphi_k(t+is)$ have limits $\varphi_k(\pm\infty)$ as $t \to \pm\infty$ which are independent of s. Let

$$\lambda_k(z) = \int_0^z e_k(z')dz'\,,\ k = 1,2 \tag{4.19}$$

and

$$\Delta_{ij}(z) = \lambda_i(z) - \lambda_j(z), \quad i \neq j \tag{4.20}$$

where in (4.19) the integral is over any path in Ω starting at 0 and ending at z. We write for $z \in \Omega$

$$\psi_\epsilon(z) = \sum_{j=1}^{2} c_j(z)e^{-\frac{i}{\epsilon}\lambda_j(z)}\varphi_j(z) \tag{4.21}$$

thus defining unknown coefficients c_j. These coefficients are the counterparts of the operator A of the previous chapter whereas the phases $e^{-\frac{i}{\varepsilon}\lambda_j}$ correspond to Φ_ε, as already noted. These coefficients satisfy

$$\sum_{j=1}^{2}\left(c_j'(z)e^{-\frac{i}{\varepsilon}\lambda_j(z)}\varphi_j(z)+c_j(z)e^{-\frac{i}{\varepsilon}\lambda_j(z)}\varphi_j'(z)\right)=0 \tag{4.22}$$

as a consequence of (4.8). Taking the scalar product of the expression (4.22) with the vector $(W(z)^{-1})^*\varphi_k(0)$ we obtain, using (4.14) and (4.15)

$$c_k'(z)=\sum_{j=1}^{2}a_{kj}(z)e^{\frac{i}{\varepsilon}\Delta_{kj}(z)}c_j(z)\ ,\ j\neq k \tag{4.23}$$

with

$$\begin{aligned} a_{kj}(z) &= -\langle\varphi_k(0)|W(z)^{-1}\varphi_j'(z)\rangle \\ &= i\langle\varphi_k(0)|W(z)^{-1}K(z)W(z)\varphi_j(0)\rangle. \end{aligned} \tag{4.24}$$

Since $\|W(z)\|$ is uniformly bounded, we have

$$|a_{kj}(z)|\leq Cb(t)\ \ ,\ \ z=t+is \tag{4.25}$$

for $|\mathrm{Im}z|<a$ and $|\mathrm{Re}z|$ large enough, where C is a constant. Although $\psi_\varepsilon(z)$ does not have a limit as $\mathrm{Re}z\to\pm\infty$, due to the presence of the phases $\lambda_k(z)$, the vectors $\varphi_k(z)$ and the coefficients $c_k(z)$ have well-defined limits, as we are about to see. In particular the boundary condition (4.6) for normalized $\psi_\varepsilon(z)$ reads

$$\begin{aligned} \lim_{t\to-\infty}|c_1(t)| &= |c_1(-\infty)|=1 \\ \lim_{t\to-\infty}|c_2(t)| &= |c_2(-\infty)|=0. \end{aligned} \tag{4.26}$$

Our problem becomes equivalent to the determination of the coefficient $c_2(+\infty)$ since we have

$$\mathcal{P}_{21}(\varepsilon)=|c_2(+\infty)|^2. \tag{4.27}$$

The coefficients $c_k(z)$ are analytic functions on Ω. They satisfy equation (4.23) or the equivalent Volterra equations

$$c_1(z)=c_1(z_0)+\int_{z_0}^{z}a_{12}(z')e^{\frac{i}{\varepsilon}\Delta_{12}(z')}c_2(z')dz' \tag{4.28}$$

and

$$c_2(z)=c_2(z_0)+\int_{z_0}^{z}a_{21}(z')e^{\frac{i}{\varepsilon}\Delta_{21}(z')}c_1(z')dz' \tag{4.29}$$

where the integration is over any path in Ω starting at z_0 and ending at z. Explicitly, if $u\mapsto\gamma(u)$ is a path with $\gamma(u_0)=z_0$ and $\gamma(u)=z$, then

$$c_1(z)=c_1(z_0)+\int_{u_0}^{u}du'\dot\gamma(u')a_{12}(\gamma(u'))e^{\frac{i}{\varepsilon}\Delta_{12}(\gamma(u'))}c_2(\gamma(u')) \tag{4.30}$$

and a similar expression holds for (4.29). From these equations and (4.25), we get

$$\lim_{t\to\pm\infty}c_k(t+is)=c_k(\pm\infty),\quad k=1,2;\quad |s|<a \tag{4.31}$$

with $c_k(\pm\infty)$ independent of s.

4.1.2 Analytic Continuation of $W(z)$

We consider here different analytic continuations of $W(z)$ into the punctured strip $S_a\backslash X$ which will allow us to construct new families of analytic eigenvectors of $H(z)$. As noticed above, $K(z)$ is meromorphic in $S_a\backslash X$ so that the equation

$$iW'(z) = K(z)W(z) \tag{4.32}$$

is well defined and has singular points at X. We want to consider solutions of (4.32) which are analytic extensions of the solution $W(z)$ defined on Ω previously. They are determined by the initial value at $z = 0$, $W(0) = \mathbb{I}$. Let γ_1 and γ_2 be two closed paths in $S_a\backslash X$ based at 0. We perform the analytic continuation of W along the paths γ_1 and γ_2. Coming back at 0 the values of these analytic continuations are $W(0|\gamma_1)$ and $W(0|\gamma_2)$. They depend only on the *homotopy class* of γ_1 and γ_2. If $\gamma_2 \cdot \gamma_1$ represents the closed path at 0 by first following γ_1 and then γ_2, we have

$$W(0|\gamma_2 \cdot \gamma_1) = W(0|\gamma_2)W(0|\gamma_1). \tag{4.33}$$

Thus $W(0|\gamma)$ gives a representation of the fundamental group $\Pi_1(S_a\backslash X; 0)$ of $S_a\backslash X$ at 0. Note that if γ is parameterized by $u \in [0,1]$, then

$$W(0|\gamma) = \mathbb{I}+ \sum_{n\geq 1}(-i)^n \int_0^1 du_n \int_0^{u_n} du_{n-1} \cdots \int_0^{u_2} du_1 K(\gamma(u_n))\dot{\gamma}(u_n) \cdots K(\gamma(u_1))\dot{\gamma}(u_1). \tag{4.34}$$

Let now γ_1 and γ_2 be two paths starting at $z = 0$ and ending at z. The values of the analytic continuations of W along γ_1, respectively γ_2, at the point z are $W(z|\gamma_1)$, respectively $W(z|\gamma_2)$. They are related as follows :

$$\begin{aligned} W(z|\gamma_2) &= W(z|\gamma_1)W(z|\gamma_1)^{-1}W(z|\gamma_2) \\ &= W(z|\gamma_1)W(0|\gamma_1^{-1} \cdot \gamma_2) \end{aligned} \tag{4.35}$$

where $\gamma_1^{-1} \cdot \gamma_2$ is a closed path at 0. Let z_0 be a point of X, which we shall assume to be a *simple zero* of the function $\rho(z)$, and let γ be a simple closed loop based at 0 around the branching point z_0. Let $\{\varphi_1(0), \varphi_2(0)\}$ be the basis of orthonormal eigenvectors of $H(0)$ chosen previously. We can transport the basis $\{\varphi_1(0), \varphi_2(0)\}$ along γ by means of $W(z)$. Coming back to the origin we have a new basis

$$\{W(0|\gamma)\varphi_1(0), W(0|\gamma)\varphi_2(0)\}. \tag{4.36}$$

Both basis vectors in (4.36) are eigenvectors of $H(0)$. Since γ is a simple closed loop and z_0 is a simple zero of $\rho(z)$, the square root in (4.3) changes sign so that the eigenvalues exchange their labels at the end of γ. Thus we have

$$H(0)\left(W(0|\gamma)\varphi_1(0)\right) = e_2(0)\left(W(0|\gamma)\varphi_1(0)\right) \tag{4.37}$$

and

$$H(0)\left(W(0|\gamma)\varphi_2(0)\right) = e_1(0)\left(W(0|\gamma)\varphi_2(0)\right). \tag{4.38}$$

We express the resulting proportionality between $W(0|\gamma)\varphi_j(0)$ and $\varphi_k(0)$, $k \neq j$, by phases $\theta_j(0|\gamma)$ defined as follows

$$W(0|\gamma)\varphi_j(0) = e^{-i\theta_j(0|\gamma)}\varphi_k(0). \tag{4.39}$$

Since $W(0|\gamma)$ is not necessarily unitary, the new basis vectors are not normalized anymore and the phases θ_j are in general complex. There exists a simple relation between θ_1 and θ_2 which can be obtained as follows. For the system of differential equation (4.32) we have the general relation

$$\det W(t) = \det W(0) \exp\left\{\frac{1}{i}\int_0^t \mathrm{Tr}K(s)ds\right\} \quad t \in \mathbb{R}. \tag{4.40}$$

On the real axis, the trace of $K(t)$ can be computed by means of the normalized vectors $\varphi_k(t)$ defined in Ω. We obtain

$$\mathrm{Tr}K(t) = \sum_{k=1}^{2} \langle \varphi_k(t)|K(t)\varphi_k(t)\rangle \equiv 0 \tag{4.41}$$

and with the initial condition $W(0) = \mathbb{I}$, we get $\det W(t) = 1$ $\forall t \in \mathbb{R}$. By analyticity we conclude

$$\det W(z) = 1 \quad \forall z \in S_a. \tag{4.42}$$

This is true in particular for $W(0|\gamma)$ which is represented in the basis $\{\varphi_1(0), \varphi_2(0)\}$ by the matrix

$$W(0|\gamma) = \begin{pmatrix} 0 & \exp\{-i\theta_2(0|\gamma)\} \\ \exp\{-i\theta_1(0|\gamma)\} & 0 \end{pmatrix}. \tag{4.43}$$

Hence the relation

$$\exp\{-i\theta_1(0|\gamma)\}\exp\{-i\theta_2(0|\gamma)\} = -1. \tag{4.44}$$

4.1.3 Circuit Matrix

We can replace these considerations in the framework of the theory of systems of differential equations (see e.g. Wasow [Wa]). We have a system

$$iW(z)' = K(z)W(z) \tag{4.45}$$

considered in $S_a \backslash X$, with generator $K(z)$ meromorphic in S_a. Let us denote by $W^+(z)$ the analytic continuation of the solution $W(z)$ of (4.45) such that $W(0) = \mathbb{I}$ obtained after a revolution around a point of X, say z_0. The matrix $W^+(z)$ is still a solution of (4.45) so that we can write

$$W^+(z) = W(z)C^+ \tag{4.46}$$

where C^+ is the corresponding circuit matrix. Thus we have $W(0|\gamma) = C^+$. If $V(z)$ is another fundamental solution of (4.45), i.e. $V(z) = W(z)Y$ with Y a 2×2 matrix such $\det Y \neq 0$, the circuit matrix D^+ obtained similarly for V is related to C^+ by

$$D^+ = Y^{-1}C^+Y. \tag{4.47}$$

Now, from the general theory [Wa], we know that for a regular singularity at z_0, i.e. a simple pole of $K(z)$ at z_0, there exists a fundamental solution of (4.45) of the type

$$V(z) = Q(z)\exp\{\ln(z - z_0)\kappa(z_0)\} \tag{4.48}$$

where $Q(z)$ is holomorphic at z_0, $\det Q(z_0) \neq 0$, and

$$\kappa(z_0) = \lim_{z \to z_0} K(z)(z - z_0) = \frac{\mathbf{B}'(z_0) \wedge \mathbf{B}(z_0)}{\rho'(z_0)} \cdot \mathrm{s}. \tag{4.49}$$

For this solution the circuit matrix is given by

$$D^{+} = \exp\{\pm 2\pi i\kappa(z_0)\}, \tag{4.50}$$

the sign being determined by the sense of rotation around z_0. However, this knowledge does not provide supplementary information about $\theta_j(0|\gamma)$ since the link between D^+ and $W(0|\gamma)$ is given by the matrix Y which is an unknown at that point.

4.1.4 Formula for $\theta_j(0|\gamma)$

Nevertheless, we can obtain an explicit expression of $\theta_j(0|\gamma)$ in a way which emphasizes its relationship with the geometrical phase obtained on the real axis for cyclic evolutions [B1]. Consider the set of analytic eigenvectors of $H(z)$

$$\psi_j(z) = \Big(B_3(z) + (-1)^j\sqrt{\rho(z)}\,,\ B_1(z) + iB_2(z)\Big), \quad j = 1,2 \tag{4.51}$$

associated with the eigenvalues

$$e_j(z) = (-1)^j \frac{1}{2}\sqrt{\rho(z)}, \quad j = 1,2. \tag{4.52}$$

Denoting by $\psi_j(0|\gamma)$ the analytic continuations of $\psi_j(z)$ along γ at the origin, we have

$$\psi_j(0|\gamma) = \psi_k(0) \ \text{ with } \ j \neq k. \tag{4.53}$$

We define new analytic phases $\delta_j(z)$ in a neighbourhood of the origin by the relation

$$\psi_j(z) = \mathrm{e}^{i\delta_j(z)}\varphi_j(z) \tag{4.54}$$

with initial condition

$$\mathrm{e}^{i\delta_j(0)} = \|\psi_j(0)\|. \tag{4.55}$$

Applying the projector $P_j(z)$ to the identity

$$\psi_j'(z) = i\delta_j'(z)\psi_j(z) + \mathrm{e}^{i\delta_j(z)}\varphi_j'(z), \tag{4.56}$$

we obtain by using property (4.15)

$$P_j(z)\psi_j'(z) = i\delta_j'(z)\psi_j(z). \tag{4.57}$$

Then, taking the scalar product of this expression with $\psi_j(z)$, we get the identity

$$i\delta_j'(z) = \frac{\langle\psi_j(z)|P_j(z)\psi_j'(z)\rangle}{\|\psi_j(z)\|^2}. \tag{4.58}$$

Now, using property (4.53) and the definitions (4.54) and (4.55), we eventually obtain

$$\begin{aligned}
\varphi_j(0|\gamma) &= \mathrm{e}^{-i\theta_j(0|\gamma)}\varphi_k(0) \\
&= \mathrm{e}^{-i\delta_j(0|\gamma)}\psi_j(0|\gamma) \\
&= \exp\left\{-i\int_\gamma \delta_j'(z)dz - i\delta_j(0) + i\delta_k(0)\right\}\varphi_k(0) \\
&= \frac{\|\psi_k(0)\|}{\|\psi_j(0)\|}\exp\left\{-i\int_\gamma \frac{\langle\psi_j(z)|P_j(z)\psi_j'(z)\rangle}{\|\psi_j(z)\|^2}\right\}\varphi_k(0)
\end{aligned} \tag{4.59}$$

so that

$$e^{-i\theta_j(0|\gamma)} = \frac{\|\psi_k(0)\|}{\|\psi_j(0)\|} \exp\left\{-i\int_\gamma \frac{\langle\psi_j(z)|P_j(z)\psi_j'(z)\rangle}{\|\psi_j(z)\|^2}\right\}. \tag{4.60}$$

It remains to insert the explicit formulae (4.51) in the above expression to obtain the phases θ_j as functions of the field **B**. The details can be found in appendix and the result of this analysis is given in the following

Proposition 4.1.1 *The phase $\theta_1(0|\gamma)$ defined by (4.39) for the vectors $\varphi_j(0)$ defined by (4.54) and (4.55) is given by the formula*

$$\exp\{-i\theta_1(0|\gamma)\} =$$
$$\exp\left\{in\pi - i\int_\gamma \frac{B_3(z)\left(B_1(z)B_2'(z) - B_2(z)B_1'(z)\right)}{2\sqrt{\rho(z)}\left(B_1^2(z) + B_2^2(z)\right)}dz\right\}$$

where n is an integer and γ is chosen in such a way that it contains no zero of $B_1^2(z) + B_2^2(z)$.

4.1.5 Asymptotic Formula for $\mathcal{P}_{21}(\varepsilon)$

Let us denote by

$$\varphi_k(z|\gamma) = W(z|\gamma)\varphi_k(0) \tag{4.61}$$

the vector which is obtained by transporting $\varphi_k(0)$ along γ where γ is a path from 0 to z. Using (4.39) and (4.35) we have the following relation if γ_1 and γ_2 are two paths from 0 to z and such that $\gamma_1^{-1}\cdot\gamma_2$ is a simple closed path based at 0 around z_0 (see figure (4.2))

$$\varphi_k(z|\gamma_2) = e^{-i\theta_k(0|\gamma_1^{-1}\cdot\gamma_2)}\varphi_j(z|\gamma_1), \quad k \neq j. \tag{4.62}$$

Now we can determine the coefficient $c_2(+\infty) = \lim_{t\to\infty} c_2(t)$ of the solution $\psi_\varepsilon(t)$ of the

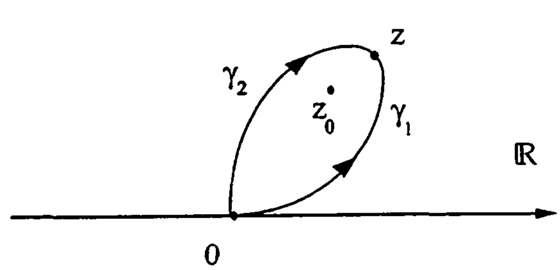

Figure 4.2: The paths γ_1 and γ_2.

Schrödinger equation (4.5) subject to the boundary condition (4.6). The method consists in controlling the solution ψ_ε along a path $t \mapsto \tilde{\gamma}(t) \in S_a$ parameterized by $t \in \mathbb{R}$ which has the following properties:

- $\lim_{t\to\pm\infty} \mathrm{Re}\tilde{\gamma}(t) = \pm\infty$, $\lim_{t\to\pm\infty} \mathrm{Im}\tilde{\gamma}(t) = s_\pm$, $|s_\pm| < a$
- $\tilde{\gamma}$ passes over the branching point z_0 in the upper half plane.

Since $\tilde{\gamma}$ is not in Ω we cannot use the decomposition (4.21)

$$\psi_\varepsilon(z) = \sum_{j=1}^{2} c_j(z) e^{-\frac{i}{\varepsilon}\lambda_j(z)} \varphi_j(z) \tag{4.63}$$

along the whole path $\tilde{\gamma}$. But we can use it for $t \ll -1$. Then we make an analytic continuation of (4.63) along $\tilde{\gamma}$. The resulting decomposition is written

$$\psi_\varepsilon(z) = \sum_{j=1}^{2} \tilde{c_j}(z) e^{-\frac{i}{\varepsilon}\tilde{\lambda_j}(z)} \tilde{\varphi_j}(z) \tag{4.64}$$

where $\tilde{f}$ means that we have made an analytic continuation of f along $\tilde{\gamma}$. The coefficients $\tilde{c_k}(z)$ satisfy now the analytic continuation of the equations (4.28) and (4.29) along $\tilde{\gamma}$. Let z be some point of $\tilde{\gamma}$ with $t \gg 1$ (see figure (4.3)). Using (4.62), we see that

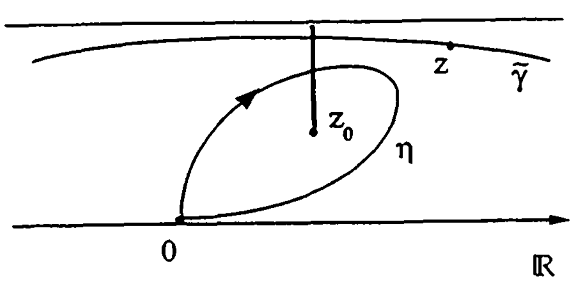

Figure 4.3: The paths $\tilde{\gamma}$, η and the point $z \in \tilde{\gamma}$.

$$\tilde{\varphi_1}(z) = e^{-i\theta_1(0|\eta)} \varphi_2(z) \tag{4.65}$$

and

$$\tilde{\varphi_2}(z) = e^{-i\theta_2(0|\eta)} \varphi_1(z) \tag{4.66}$$

where η is the simple closed path at 0 of figure (4.3), which is homotopic to the path $\gamma_1^{-1} \cdot \gamma_2$ of (4.62). Comparing (4.63) and (4.64), we obtain

$$\begin{aligned} \psi_\varepsilon(z) &= c_1(z) e^{-\frac{i}{\varepsilon}\lambda_1(z)} \varphi_1(z) + c_2(z) e^{-\frac{i}{\varepsilon}\lambda_2(z)} \varphi_2(z) \\ &= \tilde{c_2}(z) e^{-\frac{i}{\varepsilon}\tilde{\lambda_2}(z)} e^{-i\theta_2(0|\eta)} \varphi_1(z) + \tilde{c_1}(z) e^{-\frac{i}{\varepsilon}\tilde{\lambda_1}(z)} e^{-i\theta_1(0|\eta)} \varphi_2(z) \end{aligned} \tag{4.67}$$

and therefore we have the relation

$$\begin{aligned} c_2(z) &= e^{-i\theta_1(0|\eta)} e^{-\frac{i}{\varepsilon}\tilde{\lambda_1}(z) + \frac{i}{\varepsilon}\lambda_2(z)} \tilde{c_1}(z) \\ &= \exp\{-i\theta_1(0|\eta)\} \exp\left\{-\frac{i}{\varepsilon}\int_\eta e_1(z)dz\right\} \tilde{c_1}(z) \end{aligned} \tag{4.68}$$

where $\int_\eta e_1(z)dz$ is the integral over η of the analytic continuation of e_1 along η. Similarly we have

$$c_1(z) = \exp\{-i\theta_2(0|\eta)\} \exp\left\{-\frac{i}{\varepsilon}\int_\eta e_2(z)dz\right\} \tilde{c_2}(z). \tag{4.69}$$

If we can control $\tilde{c_1}$, then we gain information on c_2 and on the transition probability.

The equation for $\widetilde{c_1}$ is given in (4.30) where we must replace γ by $\tilde{\gamma}$ and all quantities appearing in (4.30) are defined by analytic continuation along $\tilde{\gamma}$. We introduce the notations $\widetilde{c_k}(t)$ for $\widetilde{c_k}(\tilde{\gamma}(t))$, $\widetilde{\Delta_{ij}}(t)$ for $\widetilde{\Delta_{ij}}(\tilde{\gamma}(t))$ and $\widetilde{a_{ij}}(t)$ for $\widetilde{a_{ij}}(\tilde{\gamma}(t))$. The boundary condition (4.6) is equivalent to $\lim_{t\to-\infty}\widetilde{c_1}(t) = c_1(-\infty)$, $|c_1(-\infty)| = 1$ and $\lim_{t\to-\infty}\widetilde{c_2}(t) = 0$. With these notations the equations for $\widetilde{c_1}$ and $\widetilde{c_2}$ read

$$\widetilde{c_1}(t) = c_1(-\infty) + \int_{-\infty}^{t} du\dot{\tilde{\gamma}}(u)\widetilde{a_{12}}(u)e^{\frac{i}{\varepsilon}\widetilde{\Delta_{12}}(u)}\widetilde{c_2}(u) \tag{4.70}$$

and

$$\widetilde{c_2}(t) = \int_{-\infty}^{t} du\dot{\tilde{\gamma}}(u)\widetilde{a_{21}}(u)e^{\frac{i}{\varepsilon}\widetilde{\Delta_{21}}(u)}\widetilde{c_1}(u). \tag{4.71}$$

We perform an integration by parts in equation (4.70) in order to use the fact that ε is a small parameter.

$$\begin{aligned}\widetilde{c_1}(t) &= c_1(-\infty) + \frac{\varepsilon}{i}\frac{\widetilde{a_{12}}(t)}{\widetilde{\Delta'_{12}}(t)}e^{\frac{i}{\varepsilon}\widetilde{\Delta_{12}}(t)}\widetilde{c_2}(t)\\ &- \frac{\varepsilon}{i}\int_{-\infty}^{t} du\dot{\tilde{\gamma}}(u)\left(\frac{\widetilde{a_{12}}}{\widetilde{\Delta'_{12}}}\right)'(u)e^{\frac{i}{\varepsilon}\widetilde{\Delta_{12}}(u)}\widetilde{c_2}(u)\\ &- \frac{\varepsilon}{i}\int_{-\infty}^{t} du\dot{\tilde{\gamma}}(u)\frac{\widetilde{a_{12}}\widetilde{a_{21}}}{\widetilde{\Delta'_{12}}}(u)\widetilde{c_1}(u).\end{aligned} \tag{4.72}$$

We recall that $'$ means $\frac{d}{dz}$ so that

$$\widetilde{\Delta'_{12}}(u) = \frac{d}{dz}\,\widetilde{\Delta'_{12}}(z)\Big|_{z=\tilde{\gamma}(u)} = \widetilde{e_1}(z) - \widetilde{e_2}(z)\big|_{z=\tilde{\gamma}(u)}. \tag{4.73}$$

Up to this point, we have only used the property that $\tilde{\gamma}$ must go over the branching point z_0, in order to get the essential relation (4.68). To treat the second and third terms in (4.72), we suppose that $\tilde{\gamma}$ satisfies the new condition IV.

IV. Dissipative path

The path $\tilde{\gamma}(t)$ is such that $\mathrm{Im}\widetilde{\Delta_{12}}(\tilde{\gamma}(t))$ is a non-decreasing function of t for all $t \in \mathbb{R}$.

Condition IV is a strong condition since it is a global condition on $\tilde{\gamma}$. This requirement is typical in the WKB method and we shall investigate it in details later on. Using it and the identity $\Delta_{12} = -\Delta_{21}$, we can estimate $\widetilde{c_2}$. Indeed, from (4.71), we have

$$\begin{aligned}|\widetilde{c_2}(t)| &\leq \int_{-\infty}^{t} du|\dot{\tilde{\gamma}}(u)||\widetilde{a_{21}}(u)|e^{\frac{1}{\varepsilon}\mathrm{Im}\widetilde{\Delta_{12}}(u)}|\widetilde{c_1}(u)|\\ &\leq e^{\frac{1}{\varepsilon}\mathrm{Im}\widetilde{\Delta_{12}}(t)}\int_{-\infty}^{t} du|\dot{\tilde{\gamma}}(u)||\widetilde{a_{21}}(u)|e^{\frac{1}{\varepsilon}\mathrm{Im}\widetilde{\Delta_{12}}(u)-\mathrm{Im}\widetilde{\Delta_{12}}(t)}|\widetilde{c_1}(u)|\\ &\leq e^{\frac{1}{\varepsilon}\mathrm{Im}\widetilde{\Delta_{12}}(t)}\|\widetilde{c_1}\|\int_{-\infty}^{+\infty}|\dot{\tilde{\gamma}}(u)||\widetilde{a_{21}}(u)|du\end{aligned} \tag{4.74}$$

where $\|f\| \equiv \sup_{t\in\mathbb{R}}|f(\tilde{\gamma}(t))|$. Condition II implies that $\int|\widetilde{a_{21}}(t)|dt < \infty$ (the proof is the same as for (4.25)). Similarly $\int|\widetilde{a_{21}}/\widetilde{\Delta'_{12}}(t)|dt < \infty$. Since $\widetilde{a_{21}}/\widetilde{\Delta'_{12}}$ is an analytic function of z, we also conclude by the Cauchy formula that $\int|\left(\widetilde{a_{21}}/\widetilde{\Delta'_{12}}\right)'(t)|dt < \infty$. Inserting (4.74) in (4.72) we have

$$|\widetilde{c_1}(t)| \leq 1 + \varepsilon k\|\widetilde{c_1}\| \tag{4.75}$$

where k is a constant, hence, taking the supremum over $t \in \mathbb{R}$,

$$\|\widetilde{c_1}\| \leq \frac{1}{1-\varepsilon k} \leq k' \tag{4.76}$$

for another constant k'. Coming back to (4.72) we conclude

$$\tilde{c_1}(t) = c_1(-\infty) + \mathcal{O}(\varepsilon), \quad \forall t \in \mathbb{R} \tag{4.77}$$

which is nothing but the extension of the adiabatic theorem of Born and Fock to the path $\tilde{\gamma}$ in the complex plane for the coefficient c_1. From (4.77) and (4.68), we obtain the asymptotic formula

$$\begin{aligned}\lim_{t\to+\infty} \|P_2(t)\psi_\varepsilon(t)\|^2 &= \lim_{t\to+\infty} |c_2(t)|^2 \\ &= \exp\{2\mathrm{Im}\theta_1(0|\eta)\}\exp\left\{\frac{2}{\varepsilon}\mathrm{Im}\int_\eta e_1(z)dz\right\}(1+\mathcal{O}(\varepsilon)).\end{aligned} \tag{4.78}$$

This equation, which is the basic result of this section, is a generalization of the Dykhne formula. Indeed, the exponential decay rate can be rewritten as

$$\mathrm{Im}\int_\eta e_1(z)dz = \mathrm{Im}\int_0^{z_0} e_1(z) - e_2(z)dz \tag{4.79}$$

where the integration path follows η. Moreover, if the hamiltonian is real and symmetric on the real axis, i.e. $B_2(z) \equiv 0$, the geometrical prefactor $\exp\{2\mathrm{Im}\theta_1(0|\eta)\}$ reduces to 1, see proposition (4.1.1), and we recover the usual Dykhne formula. However, in general

$$\exp\{2\mathrm{Im}\theta_1(0|\eta)\} \neq 1 \tag{4.80}$$

and the presence of this geometrical prefactor in (4.78) has been verified experimentally by Zwanziger et. al. [ZRC].

Remarks:

- Formula (4.78) has been obtained under the boundary conditions $c_2(-\infty) = 0$ and $|c_1(-\infty)| = 1$. Nevertheless, if we consider a solution $\psi_\varepsilon(t)$ such that

$$\lim_{t\to-\infty} \|P_2(t)\psi_\varepsilon(t)\| = 1, \tag{4.81}$$

  corresponding to $|c_2(-\infty)| = 1$ and $|c_1(-\infty)| = 0$, the transition probability

$$\mathcal{P}_{12}(\varepsilon) = \lim_{t\to+\infty} \|P_1(t)\psi_\varepsilon(t)\|^2 \tag{4.82}$$

  is still given by formula (4.78). Indeed, if $(c_1(t), c_2(t))$ are solutions of (4.23) for $t \in \mathbb{R}$ with $c_1(-\infty) = 1$ and $c_2(-\infty) = 0$, then $(-\overline{c_2}(t), \overline{c_1}(t))$ satisfy the same equation with reversed boundary conditions as a consequence of the identity $\overline{a_{kj}(t)} = -a_{jk}(t)$ $\forall t \in \mathbb{R}$.

- In the derivation of formula (4.78) we have chosen the origin as base point for γ. Of course this choice has no influence on the transition probability. If γ_0 is a loop based at $t_0 \in \mathbb{R}$ which encircles z_0, we have the relation

$$W(t_0|\gamma_0) = W(t_0)W(0|\gamma)W(t_0)^{-1} \tag{4.83}$$

  since we can deform the paths, and $W(t_0)$ is unitary. Consequently

$$\mathrm{Im}\theta_j(t_0|\gamma_0) = \mathrm{Im}\theta_j(0|\gamma). \tag{4.84}$$

- We have assumed that z_0 was a simple zero of $\rho(z)$, which is generically the case. But the important point in these considerations is the exchange of labels of the eigenvectors along the loop γ which leads to formula (4.68). Any zero of odd order implies a similar relation but, as we are about to see, the requirement for $\tilde{\gamma}$ to be dissipative (condition IV) can be fulfilled for simple zeros of $\rho(z)$ only.

4.1.6 Quadratic Differential

We have just seen that an asymptotic formula for the transition probability could be obtained provided there exists a dissipative path above the eigenvalue crossing point z_0. This requirement may seem to be merely technical but it is an essential condition for the proof of (4.78) to hold. We study this global condition in this paragraph from a geometrical point of view by means of the concept of quadratic differential. This analysis allows us to express the formula giving the transition probability in purely geometrical terms.

The monotonicity condition IV involves the multivalued function $\Delta(z) \equiv \int_0^z \sqrt{\rho(u)}du$ on $S_a \backslash X$, where the integration is performed along any path in $S_a \backslash X$ leading from 0 to z. In particular, the level lines $\text{Im}\Delta(z) = \text{cst}$ will play an important role. Let us recall the definition of quadratic differential and precise the link between this notion and the function $\Delta(z)$. We follow closely Strebel's monograph [St]. The function $\rho(z) = B_1^2(z) + B_2^2(z) + B_3^2(z)$ is holomorphic in the simply connected domain S_a and it defines a quadratic differential $\rho(z)d^2z$ on S_a. A point $z \in S_a$ is called *regular* if $\rho(z) \neq 0$ and it is called *critical* if $\rho(z) = 0$. A *θ-straight arc* is a smooth curve $t \mapsto \gamma(t)$ in S_a such that for all t

$$\arg\left(\rho(\gamma(t))\dot{\gamma}^2(t)\right) = \theta = \text{cst}. \tag{4.85}$$

This implies in particular that $\rho(\gamma(t)) \neq 0$ and therefore a straight arc contains only regular points. If $\theta = 0$ the straight arc is *horizontal* and if $\theta = \pi$ it is *vertical*. A maximal horizontal arc is called a *trajectory* of the quadratic differential ρ, and on a trajectory we have

$$\rho(\gamma(t))\dot{\gamma}^2(t) > 0. \tag{4.86}$$

By a reparameterization of the trajectory we see that it is a maximal solution of the differential equation

$$\rho(z)\left(\frac{dz}{du}\right)^2 = 1. \tag{4.87}$$

The trajectories of the quadratic differential $\rho(z)dz^2$ coincide with the level lines $\text{Im}\Delta(z) = \text{cst}$ as is seen from the following property. Let $z^* \in S_a \backslash X$. A *ρ-disc* of center z^* and radius r is a region $U \subset S_a \backslash X$ containing z^* which is mapped homeomorphically onto a disc of radius r by a branch of $\Delta(z)$, z^* being mapped on the center of the disc. In the ρ-disc U we can solve the differential equation (4.87) with initial condition $z^* \in U$ at u_0. The solution $u \mapsto \gamma(u)$ satisfies the equation

$$u - u_0 = \pm \int_{z^*}^{\gamma(u)} \sqrt{\rho(z)}dz \tag{4.88}$$

which can be rewritten as

$$u - u_0 = \Delta(\gamma(u)) - \Delta(z^*). \tag{4.89}$$

Note that if $\gamma(t)$ is a θ straight-arc such that $\gamma(t_0) = z^*$, we have

$$\Delta(\gamma(t)) = \Delta(z^*) \pm \exp\{i\theta/2\} \int_{t_0}^{t} |\dot{\gamma}(t)\sqrt{\rho(\gamma(t))}|dt, \tag{4.90}$$

the sign depending on the chosen branch. Hence, for a ρ-disc of radius r centered at a regular point z^*, the set of trajectories is homeomorphic to a set of horizontal lines in a disc of radius r. In particular two different trajectories cannot cross. We can parameterize globally the trajectory α passing through z^* as follows. Let us choose a parameterization $u \mapsto \alpha(u)$ in such a way that $\alpha(0) = z^*$. With $|u| < r$, we get by (4.89)

$$\alpha(u) = \Delta^{-1}(\Delta(z^*) + u). \tag{4.91}$$

Then we continue analytically the suitable branch of $\Delta(z)$ along α. By construction, we obtain a function $\Delta_\alpha(z)$ whose restriction on α is injective (see (4.89)). The image of α by Δ_α is the set

$$\{w = \Delta(z^*) + u, \quad u \in (u_-, u_+) \subset I\!R\} \tag{4.92}$$

where the interval (u_-, u_+) is maximal and we have

$$\alpha(u) = \Delta_\alpha^{-1}(\Delta(z^*) + u) \tag{4.93}$$

for all $u \in (u_-, u_+)$. This parameterization is called a natural parameterization of α. By definition a trajectory is called *critical* if $\lim_{u \to u_-} \alpha(u)$ or $\lim_{u \to u_+} \alpha(u)$ is a critical point of ρ, i.e. in our setting, a point of X. Let us review the different type of trajectories we can have close to a critical point. Let $\hat{z}$ be a zero of order $n \geq 1$ of the analytic function $\rho(z)$. In a neighbourhood of $\hat{z}$ we can write

$$\rho(z) = a_n(z - \hat{z})^n (1 + a_{n+1}(z - \hat{z}) + \ldots) \tag{4.94}$$

so that

$$\int_{\hat{z}}^{z} \sqrt{\rho(u)}du = b_n(z - \hat{z})^{\frac{n+2}{2}} (1 + b_{n+1}(z - \hat{z}) + \ldots) \tag{4.95}$$

with $b_n = \frac{2\sqrt{a_n}}{n+2} \neq 0$. Thus the level lines $\mathrm{Im}\Delta(z) = \mathrm{Im}\Delta(\hat{z})$ for z in a neighbourhood of $\hat{z}$ are homeomorphic to the set of level lines $\mathrm{Im}\xi^{\frac{n+2}{2}} = 0$, for ξ close to the origin. Thus there are $n + 2$ critical trajectories which meet at $z = \hat{z}$. The tangents at $\hat{z}$ of two consecutive critical trajectories form an angle of value $\frac{2\pi}{n+2}$. When restricted to a neighbourhood of $\hat{z}$, the interior of the domain enclosed by consecutive critical trajectories is mapped homeomorphically by $\Delta(z) - \Delta(\hat{z})$ on a neighbourhood of the origin, in the upper or lower half plane (see figure (4.4)). The critical trajectories are also called *Stokes lines*. These

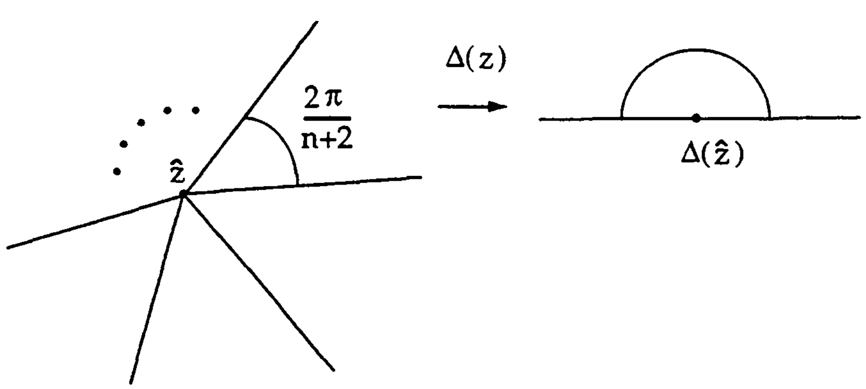

Figure 4.4: The critical trajectories close to a zero of order n.

lines play an essential role in the analysis of the WKB method.

Let us introduce the metric associated with the quadratic differential $\rho(z)dz^2$, which will turn out to be adequate for our problem. Let γ be some rectifiable curve. Its *ρ-length* is defined by

$$|\gamma|_\rho = \int_\gamma |\rho(z)|^{1/2}|dz|. \tag{4.96}$$

If x and $y \in S_a$ then the *ρ-distance* $\mathrm{d}_\rho(x, y)$ between x and y is given by the infimum of $|\gamma|_\rho$ where γ is a rectifiable curve from x to y in S_a. If γ is contained in a ρ-disc U of radius r then its ρ-length $|\gamma|_\rho$ is equal to the euclidean length of the image of γ by a branch of

Δ defined on U. In particular a ρ-disc of radius r is a disc of radius r in the ρ-metric. A natural parameterization of α is essentially the parameterization of the arc-length for the ρ-metric (see (4.90)). Finally we call a curve $t \mapsto \gamma(t)$, $a < t < b$ a *geodesic* if it is locally shortest. This means that for every t there is an interval $[t_1, t_2]$ such that $t \in [t_1, t_2]$ and the arc $\gamma([t_1, t_2])$ is the shortest connection of the two points $\gamma(t_1)$ and $\gamma(t_2)$. In a neighborhood of any regular point a geodesic is a θ-straight arc.

Teichmueller's lemma will be our main tool to describe the global behaviour of the critical trajectories (or Stokes lines). Before stating this lemma we need a last definition. A *geodesic* polygon is a curve γ composed of open straight arcs and their end points which can be critical points of ρ. We quote Teichmueller's lemma from [Let]. A more general version for meromorphic quadratic differential is given in [St].

Lemma 4.1.1 (Teichmueller's lemma) *Let ρ be holomorphic in the closure of a domain A in the complex plane which is bounded by a simple closed geodesic polygon in the ρ-metric, whose sides γ_j form interior angles θ_j at the vertices, $0 < \theta_j \leq 2\pi$. If m_i and n_j denote the orders of the zeros of ρ in A and on ∂A, respectively, then*

$$\sum_j \left(1 - (n_j + 2)\frac{\theta_j}{2\pi}\right) = 2 + \sum_i m_i.$$

This lemma is a consequence of the argument principle. The precise relation between critical trajectories or Stokes lines and dissipative paths is provided by the following

Proposition 4.1.2 *Let $z_0 \in X$ be a zero of ρ and $\tilde{\gamma}$ be a dissipative path above z_0. Then*
1) $\tilde{\gamma}$ is a simple curve.
2) The open region Σ in S_a between the path $\tilde{\gamma}$ and the real axis contains exactly one eigenvalue crossing point, z_0, which is a simple zero of ρ.
3) There are three distinct critical trajectories α_1, α_2, α_3 having z_0 as unique critical point.
4) The trajectory α_1 is entirely inside Σ and has a natural parameterization with $u \in (-\infty, 0)$ so that $\lim_{u\to 0} \alpha_1(u) = z_0$, $\lim_{u\to -\infty} \mathrm{Re}\alpha_1(u) = -\infty$.
The trajectory α_2 is entirely inside Σ and has a natural parameterization with $u \in (0,\infty)$ so that $\lim_{u\to 0} \alpha_2(u) = z_0$, $\lim_{u\to\infty} \mathrm{Re}\alpha_2(u) = \infty$.
The trajectory α_3 has a natural parameterization with $u \in (0, u_+)$ so that $\lim_{u\to 0} \alpha_3(u) = z_0$. The set of $u \in (0, u_+)$ such that $\alpha_3(u)$ is a point of $\tilde{\gamma}$ is a non-empty connected set.

Conversely, if there is a simple zero z_0 of ρ such that there exists two critical trajectories $\alpha_1(t)$ and $\alpha_2(t)$ in S_a, having z_0 as unique critical point, satisfying

$$\lim_{t\to\pm\infty} \mathrm{Re}\alpha_j(t) = \pm\infty, \quad \alpha_1(0) = \alpha_2(0) = z_0$$

and

$$|\mathrm{Im}\alpha_j(t)| < a, \quad j = 1, 2,$$

then there exists a dissipative path $\tilde{\gamma} \subset S_a \backslash X$ passing above z_0.

Remarks:

- This proposition allows the problem of the existence of a dissipative path above an eigenvalue crossing point to be expressed in terms of Stokes lines or critical trajectories. This is an important step since in concrete problems the properties of these lines can sometimes be discussed analytically or at least numerically.

- The line $\alpha_1 \cup \alpha_2$ forms an infinite horizontal geodesic through the critical point z_0 in the metric d_ρ.
- Let us define an open simply connected domain $\Omega \subset S_a$ whose boundary is given by

$$\partial\Omega \equiv \alpha_1 \cup \alpha_2 \cup \overline{\alpha_1} \cup \overline{\alpha_2}. \tag{4.97}$$

  This set is then mapped homeomorphically to the strip $|\mathrm{Im}w| < |\mathrm{Im}\Delta_{12}(z_0)|$ by the function $\Delta_{12}(z)$ defined by (4.20).

We postpone the proof of this proposition to give the main theorem of this section and to see through concrete examples how it applies. The proposition (4.1.2), together with the last remark and formula (4.68) yield the following theorem, which we formulate in a purely geometrical form.

Theorem 4.1.1 *Let $H(z) = (B_1(z)\cdot s_1 + B_2(z)\cdot s_2 + B_3(z)\cdot s_3)$ be a 2×2 matrix which satisfies conditions I, II and III on S_a. Let ψ_ε be a normalized solution of the Schrödinger equation $i\varepsilon\psi_\varepsilon' = H\psi_\varepsilon$ such that $\lim_{t\to-\infty}\|P_1(t)\psi_\varepsilon(t)\| = 1$. If there exists a horizontal geodesic in S_a (in the ρ-geometry, $\rho = B_1^2 + B_2^2 + B_3^2$), $t \mapsto g(t)$, $t \in I\!R$ containing exactly one eigenvalue crossing point of H which is a simple zero of ρ, say z_0, such that*

$$\lim_{t\to\pm\infty} \mathrm{Re}g(t) = \pm\infty$$

and

$$|\mathrm{Im}g(t)| < a\ , \quad |t| \text{ large enough}$$

then

$$\lim_{t\to\infty} \|P_2(t)\psi_\varepsilon(t)\|^2 = \exp\{2\mathrm{Im}\theta_1(0|\gamma)\}\exp\left\{-\frac{2}{\varepsilon}\mathrm{d}_\rho(z_0, I\!R)\right\}(1 + \mathcal{O}(\varepsilon))$$

and for all eigenvalue-crossings z_k, $k > 0$, $\mathrm{d}_\rho(z_k, I\!R) > \mathrm{d}_\rho(z_0, I\!R)$. The geometrical factor $\exp\{2\mathrm{Im}\theta_1(0|\gamma)\}$ is given in proposition (4.1.1) and $\mathrm{d}_\rho(z_0, I\!R) = \mathrm{Im}\int_\gamma e_1(z)dz$.

Remark:
The adequacy of the metric d_ρ for this problem is reflected by the expression giving the exponential decay rate and by the fact that the relevant eigenvalue crossing point z_0 is the closest to the real axis in this metric, whereas this may be wrong in the euclidian metric. Note also that the formula giving $\mathrm{d}_\rho(z_0, I\!R)$ holds because $\Delta(z)$ is univalued on Ω. In general $\Delta(z)$ is multivalued and we cannot expect a simple formula in terms of $\Delta(z)$ for $\mathrm{d}_\rho(z_k, I\!R)$, $k > 0$.

4.1.7 Examples

Competition between eigenvalue crossing points

This example illustrates the problem of selecting the relevant eigenvalue-crossing for the generalized Dykhne formula. In this example the relevant eigenvalue-crossing *is not* the closest one to the real axis in the euclidean metric. This has the following consequence. We could choose the width of the analyticity strip too small so that the strip contains only the (irrelevant) closest eigenvalue-crossing to the real axis and its complex conjugate. A local analysis of the problem as in [HP] is still valid but it leads to an incorrect result. Let

$H(z) = \mathbf{B}(z) \cdot \mathrm{s}$ be defined by

$$B_1(z) = 2\frac{(z-c)^2 + b^2 \tanh(z)}{(z-c)^2 + a^2} \tag{4.98}$$

$$B_2(z) = 2\frac{(z-c)^2 \tanh(z) - b^2}{(z-c)^2 + a^2} \tag{4.99}$$

$$B_3(z) \equiv 0 \tag{4.100}$$

with $a > 3/2$, $b > 0$ and $c \in I\!R$.
The singularities of $H(z)$ are located at the points $c \pm ia$ and $i\pi/2 + ki\pi$, $k = \pm 1, \pm 2, \cdots$. Hence $H(z)$ satisfies condition I in $S_{3/2} = \{z = t + is \mid |s| < 3/2\}$. One verifies that $\mathbf{B}(t + is)$ tends to $(2, 2, 0)$ as $1/t^2$ when $|t| \to \infty$ in $S_{3/2}$, so that condition II is satisfied. The function

$$\rho(z) = 4\frac{(z-c)^4 + b^4}{((z-c)^2 + a^2)^2}(1 + \tanh(z)^2) \tag{4.101}$$

is strictly positive on the real axis and its zeros in $S_{3/2}$,

$$z_1 = i\frac{\pi}{4}\ ,\ z_2 = c + \frac{b}{\sqrt{2}}(-1 + i)\ ,\ z_3 = c + \frac{b}{\sqrt{2}}(1 + i)$$

and $\bar{z}_1$, $\bar{z}_2$, $\bar{z}_3$ are all simple. We define Ω as the simply connected domain obtained from the intersection of the upper half plane and $S_{3/2}$, by removing three vertical cuts starting at z_1, z_2, z_3. In order to determine the relevant zero, we must study the Stokes lines $\mathrm{Im}\Delta_{12}(z) = \mathrm{Im}\Delta_{12}(z_j)$, $j = 1, 2, 3$ in Ω. We have computed these lines numerically for certain values of the parameters a, b and c. For the choice $a = 4$, $b = 1.2$, $c = 2$ we have the situation of figure (4.5) which shows that z_2 is the relevant eigenvalue-crossing and that theorem (4.1.1) holds. Note that $\mathrm{Im}z_1 = \pi/4 < 1.2/\sqrt{2} = \mathrm{Im}z_2$.

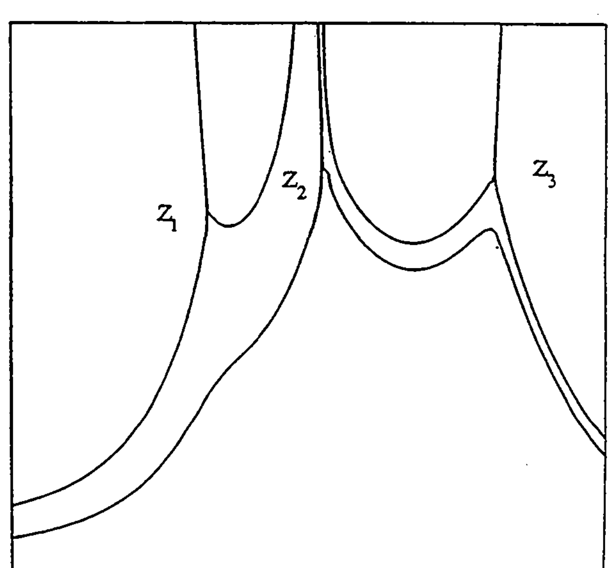

Figure 4.5: The Stokes lines of the first example.

Remarks:

- Condition II allows us to consider the Stokes lines in a compact subset of Ω.

- For the different values of the parameters we have considered, theorem (4.1.1) was always true for some zero z_k.
- In this example $\text{Im}\theta_1 = 0$ since $B_3 \equiv 0$ (see lemma (4.1.1)).

Competition between eigenvalue crossing point and singularity

In this example we can control the position of a singularity of H in a fixed strip. Thus the analyticity strip of the hamiltonian depends on its location. As before it is not the fact that the singularity is closer or not to the real axis (in the euclidean distance) than the eigenvalue-crossing which matters, but whether this is the case in the metric d_ρ as we shall see. Let $\mathbf{B}(z)$ be defined by

$$\mathbf{B}(z) = 2(\cos(\alpha(z)), \sin(\alpha(z)), \tanh(z)) \text{ with } \alpha(z) = \frac{\pi}{4}\tanh\left(\frac{z-c}{\omega}\right) \tag{4.102}$$

where $0 < \omega < 1$; $c \in \mathbb{R}$. The hamiltonian $\mathbf{B}(t+is)\cdot\mathbf{s}$ is singular at the points

$$z(\omega, c) = c + i\frac{\pi\omega}{2} + ik\pi\omega \quad k = \pm1, \pm2, \cdots \tag{4.103}$$

in the fixed strip $S_{3/2}$ defined as above and tends exponentially fast to its limiting values as $|t| \to \infty$ with $|s| < 3\omega/2$. Hence $H(z)$ is analytic in the strip $S_{\frac{3\omega}{2}}$. Moreover the function

$$\rho(z) = 4(1 + \tanh^2(z)) \tag{4.104}$$

is strictly positive for $z \in \mathbb{R}$ so that conditions II and III are verified. There is one pair of eigenvalue crossing points given by $z_1 = i\pi/4$ and $\overline{z_1}$. An important feature of this example is that ρ is independent of c and ω. This implies that the ρ-geometry is also independent of the location of the singularity $z(\omega, c)$.

We first prove that any horizontal path $\gamma(t)$ over $z_1 = i\frac{\pi}{4}$ is a dissipative path. Let $\gamma(t)$ be parameterized by

$$\gamma(t) = t + is\ ,\ -\infty \le t \le \infty\ ,\ \frac{\pi}{4} < s < \frac{\pi}{2} \tag{4.105}$$

Such a path is dissipative if and only if

$$\frac{d}{dt}\text{Im}\Delta_{12}(\gamma(t)) = -\text{Im}\sqrt{\rho(\gamma(t))} \ge 0 \quad \forall t. \tag{4.106}$$

To see that this is true in our case, we consider the image of $\gamma(t)$ by $\rho(z)$. We compute

$$\rho(t+is) = 4 + 4\frac{\sinh^2(2t) - \sin^2(2s)}{(\cosh(2t) + \cos(2s))^2} + i\frac{8\sinh(2t)\sin(2s)}{(\cosh(2t) + \cos(2s))^2} \tag{4.107}$$

thus $\forall\ s \in (\pi/4, \pi/2)$, the image of γ by ρ looks like figure (4.6). By taking the square root, the image of $\rho(\gamma(t))$ is entirely in the lower half plane and condition IV is satisfied.
Remark:
The only property of the path $\rho(\gamma(t))$ which is used is that this path does not cross the positive real axis.
Since there exists a dissipative path we know from proposition (4.1.2) that there exists a horizontal geodesic (in the ρ-geometry) passing through z_1 as in theorem (4.1.1). Moreover, a qualitative study of the differential equation satisfied by the geodesic $t \mapsto g(t) = g_1(t) + ig_2(t)$

$$\dot{g}_1(t)\text{Im}\sqrt{\rho(g(t))} + \dot{g}_2(t)\text{Re}\sqrt{\rho(g(t))} = 0 \tag{4.108}$$

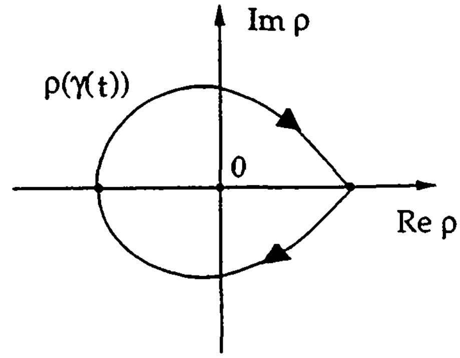

Figure 4.6: The image of γ by ρ.

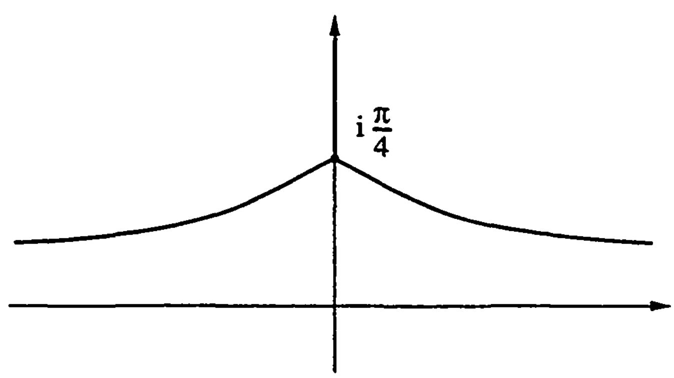

Figure 4.7: The Stokes lines of the second example.

shows that the Stokes lines must behave as on figure (4.7). As

$$\mathrm{Im}\Delta_{12}(i\pi/4) = -2\int_0^{\pi/4}\sqrt{1-\tan^2(s)}ds = -\pi(\sqrt{2}-1) \qquad (4.109)$$

$d_\rho(z_1, \mathbb{R}) = \pi(\sqrt{2}-1)$. We have several cases:

- $\omega > 1/2$.

  In this case we can choose as dissipative path any horizontal path over the eigenvalue-crossing z_1 and below the singularity $z(\omega, c)$ of H. Therefore theorem (4.1.1) can be applied.

- $\omega \leq 1/2$.

  Here the above choice of γ does not work because the singularity of H is always below γ, since γ must go over z_1. However, the Stokes lines are independent of ω and c.

  - Hence, as long as $z(\omega, c)$ is above the Stokes lines, there exists an infinite geodesic passing through z_1 which is entirely in the analyticity domain of $H(z)$ and therefore theorem (4.1.1) is valid. We obtain

$$\lim_{t\to\infty}\|P_2(t)\psi_\varepsilon(t)\|^2 = \exp\left\{-\frac{2}{\varepsilon}\pi(\sqrt{2}-1)\exp(2\mathrm{Im}\theta_1)\right\}(1+\mathcal{O}(\varepsilon)). \qquad (4.110)$$

In this example it can be shown that we have a non trivial geometrical factor, $\mathrm{Im}\theta_1 < 1$, if ω is not too small. Note that in the above two case

$$\mathrm{d}_\rho(z_1, I\!R) < \mathrm{d}_\rho(z(\omega, c), I\!R). \tag{4.111}$$

– Finally, if the singularity is below the Stokes lines, we cannot prove the generalized Dykhne formula with the method described above, since the hypotheses of theorem (4.1.1) are not fulfilled. Nevertheless, we can prove upper bounds for the transition probability, using the complex time method as shown in appendix (A).

Proof of proposition (4.1.2):
1) We assume that $\tilde{\gamma}$ is parameterized by $t \in I\!R$. Let us consider the branch of Δ such that $\mathrm{Im}\Delta(\tilde{\gamma}(t))$ is non-decreasing in t. The image of this part of $\tilde{\gamma}$ by Δ is a simple path from $w_1 = \Delta(\tilde{\gamma}(t_1))$ to $w_2 = \Delta(\tilde{\gamma}(t_2))$. Indeed, if $\mathrm{Im}\Delta(\tilde{\gamma}(t))$ is constant on some interval then $\mathrm{Re}\Delta(\tilde{\gamma}(t))$ is strictly increasing or decreasing on that interval. Elsewhere $\mathrm{Im}\Delta(\tilde{\gamma}(t))$ is increasing. We choose t_1 and $t_2 > t_1$ and consider only the part of $\tilde{\gamma}$ for $t \in [t_1, t_2]$. We can approximate this path from w_1 to w_2 by a polygonal line $t \mapsto p(t)$ made of horizontal and vertical euclidean segments such that $\mathrm{Im}p(t)$ is non decreasing, see figure (4.8). Taking

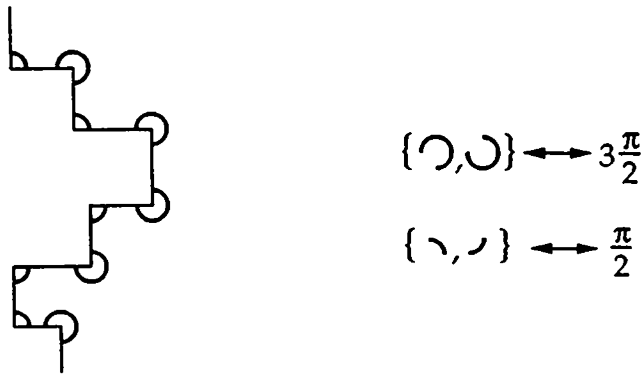

Figure 4.8: The image of $p(t)$ by $\Delta(z)$.

the image by Δ^{-1} of this line we get a geodesic polygonal line in the ρ-geometry which approximates the path $\tilde{\gamma}$ for $t \in [t_1, t_2]$ (The inverse map Δ^{-1} is well-defined locally). Let us suppose that $\tilde{\gamma}$ is not simple. Then there exist t_1 and $t_2 > t_1$ so that $\tilde{\gamma}(t_1) = \tilde{\gamma}(t_2)$. We can assume that $t \in [t_1, t_2] \mapsto \tilde{\gamma}(t)$ is a simple closed path. This path can be approximated by a simple closed geodesic polygon. The interior angles of this polygon are equal to $\pi/2$ or $3\pi/2$ by conformal invariance. Since $\mathrm{Im}p(t)$ is non decreasing the number of interior angles with $\theta_i = \pi/2$, $N(\pi/2)$, and the number of interior angles $\theta_j = 3\pi/2$, $N(3\pi/2)$, satisfy the inequality

$$|N(3\pi/2) - N(\pi/2)| \leq 2. \tag{4.112}$$

Indeed, between two successive vertical segments of the image of $p(t)$ by Δ, $N(\pi/2) = N(3\pi/2)$. Then by considering the different possible configurations at the extremities of $\Delta(p(t))$ we obtain the above inequality (see figure (4.9)). The application of Teichmueller's lemma with $n_j = 0$ and $m_j = 0$ yields

$$1 \geq \sum_j \left(1 - 2\frac{\theta_j}{2\pi}\right) = 2 \tag{4.113}$$

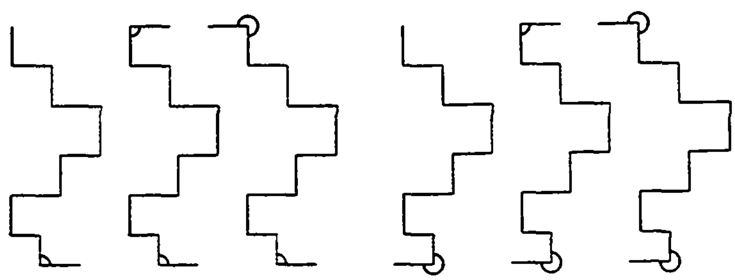

Figure 4.9: The different configurations at the extremities of $\Delta(p(t))$.

so that we get a contradiction which proves 1).

2) The geometry of the trajectories is well-understood in the regions $|\text{Im}z| < a$ and $|\text{Re}z|$ large enough. Indeed, in these regions ρ is essentially constant and tends to positive values as $|\text{Re}z| \to \infty$. Therefore, the ρ-geometry is essentially the euclidean geometry. The trajectories are essentially horizontal in the euclidean sense and the vertical straight arcs are essentially vertical lines in the euclidean sense. Thus we can find a pair of points x_1, on the negative real axis, and $z_1 = \tilde{\gamma}(t_1)$ which can be joined by a vertical straight arc γ_1 in Σ. Similarly there exists a pair of points x_2, on the positive real axis, and $z_2 = \tilde{\gamma}(t_2)$ which can be joined by a vertical straight arc γ_2 in Σ. Moreover the curve Γ which is composed of γ_1, γ_2, $[x_1, x_2]$ and the part of $\tilde{\gamma}$ for $t \in [t_1, t_2]$ can be assumed to be simple and closed (see figure(4.10)). For later purposes we denote by Σ' the bounded region with boundary Γ. As above we approximate the curve by a geodesic simple closed polygon. In

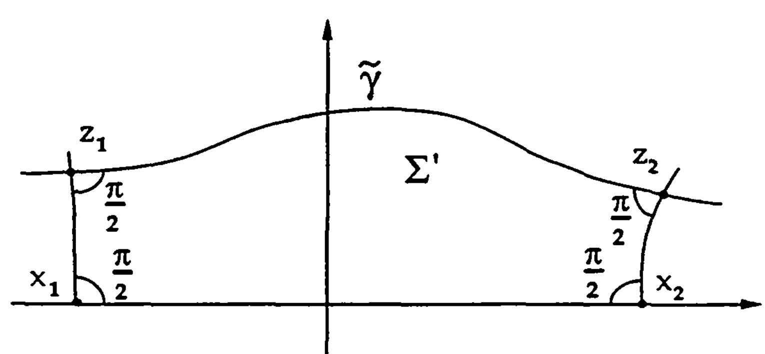

Figure 4.10: The domain Σ'.

this case, by adding the interior angles $\theta_j = \pi/2$ at x_1,z_1, x_2 and z_2, we have (see figure (4.10))

$$|N(3\pi/2) - N(\pi/2)| \leq 6. \tag{4.114}$$

Hence by Teichmueller's lemma

$$\sum_i m_i + 2 = \sum_j \left(1 - 2\frac{\theta_j}{2\pi}\right) \leq 3 \tag{4.115}$$

so that there is at most one critical point in Σ. There is in fact exactly one critical point otherwise (4.65) and (4.66) could not be true.

3) If α_1 and α_2 are not distinct, then they coincide. Let us suppose that this is the case. Then α_1 and z_0, the critical point in Σ, form a simple closed geodesic polygon. Applying Teichmueller's lemma with one interior angle of value $\theta_0 = 2\pi/3$ at z_0 with $n_0 = 1$, we get a contradiction.
4) Let us consider the set Σ' with boundary Γ defined in 2). Let $\Delta(z)$ be the analytic continuation in $\Sigma'\backslash\{z_0\}$ of the function

$$2\int_{z_0}^{z} e_1(z')dz' \tag{4.116}$$

defined in a neighborhood U of z_0 (the integration path being in U). This function is 2-valued since z_0 is the only critical point and there exists $C < \infty$ such that

$$|\mathrm{Re}\Delta(z)| \leq C \tag{4.117}$$

for any $z \in \Sigma'\backslash\{z_0\}$ and any value $\Delta(z)$ over z. If we follow a branch of $\Delta(z)$ along α_i then $\mathrm{Re}\Delta$ is strictly increasing or strictly decreasing. More precisely, since

$$\begin{aligned}\frac{d}{dt}\mathrm{Im}\Delta(\alpha_i(t)) &= -\mathrm{Re}\dot{\alpha}_i(t)\mathrm{Im}\sqrt{\rho(\alpha_i(t))} - \mathrm{Im}\dot{\alpha}_i(t)\mathrm{Re}\sqrt{\rho(\alpha_i(t))} \\ &\equiv 0 \end{aligned} \tag{4.118}$$

we can choose the parameterization

$$\begin{aligned}\mathrm{Re}\dot{\alpha}_i(t) &= \mathrm{Re}\sqrt{\rho(\alpha_i(t))} \\ \mathrm{Im}\dot{\alpha}_i(t) &= -\mathrm{Im}\sqrt{\rho(\alpha_i(t))}.\end{aligned} \tag{4.119}$$

In this case

$$\left|\frac{d}{dt}\mathrm{Re}\Delta(\alpha_i(t))\right| = |\Delta'(\alpha_i(t))| > d > 0. \tag{4.120}$$

Thus inequality (4.117) implies that α_i must intersect Γ. However, each vertical straight arc γ_i of Γ can be intersected by at most one α_j and only once. This follows again from Teichmueller's lemma. Since the real interval $[x_1, x_2]$ is an horizontal straight arc it cannot be intersected by α_1, α_2 or α_3. Thus one of the α_j's, say α_3, has to intersect $\tilde{\gamma}$.
Let us suppose that α_3 intersects $\tilde{\gamma}$ at $\tilde{\gamma}(t_3)$ and α_1 intersects at $\tilde{\gamma}(t_1)$. We may suppose that $t_1 < t_3$. Let α' be the part of α_1 between z_0 and $\tilde{\gamma}(t_1)$ and α'' be the part of α_3 between $\tilde{\gamma}(t_3)$ and z_0, see figure (4.11). Then the path α' followed by the part of $\tilde{\gamma}$ with $t \in [t_1, t_3]$ and then followed by α'' is a path along which $\mathrm{Im}\Delta$ is non decreasing for the analytic continuation of Δ along this path. By point 1) this path is simple and if we add to it z_0 we get a simple closed path which can be approximated by a simple closed geodesic polygon. The angle at z_0, the critical point, is $2\pi/3$ or $4\pi/3$ and for the other angles (4.112) holds. Again, we obtain a contradiction from Teichmueller's lemma. Note that the same argument shows that the set of intersection points of any α_i with $\tilde{\gamma}$ is connected. From this fact the first part of the proposition is completed. We consider now the converse statement. Let us first note that the hypothesis imply that there is no critical point in the open set between the real axis and the geodesic $g \equiv \alpha_1 \cup \alpha_2$ (this follows again from Teichmueller's lemma). We know from the remark following the proposition that Δ is univalued in this region and also that $\mathrm{d}_\rho(z_k, I\!R) > \mathrm{d}_\rho(z_0, I\!R)$ if $k > 1$. The result is proven if we can find a path $\tilde{\gamma}$ satisfying condition IV. We assume that the parameterization of the geodesics α_j are natural for $j = 1, 2$. By hypothesis α_1 and α_2 are critical trajectories. Let α_3 be the third critical trajectory having z_0 as accumulation point. Let U be a small

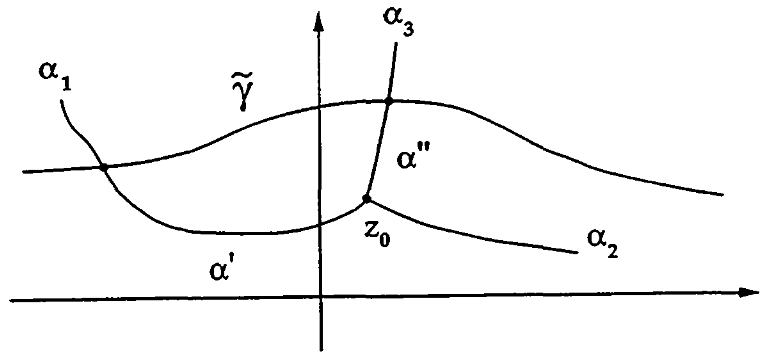

Figure 4.11: The segments α' and α''.

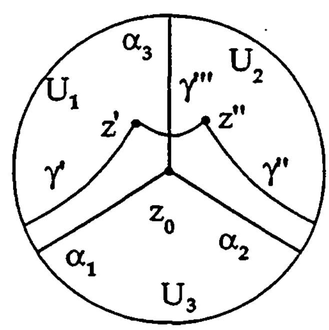

Figure 4.12: The critical trajectories in U.

disc of center z_0. The three trajectories α_1, α_2 and α_3 divide U into three sectors as in figure (4.12).

Let $z' \in U_1$ and let $u \mapsto \gamma'(u)$, $u \in (u'_-, u'_+)$ be the trajectory passing through z'. We assume that the parameterization is natural and is chosen in such a way that $\gamma'(0) = z'$. Since condition II holds, we have that $u'_- = -\infty$ if z' is sufficiently close to z_0 and that $\gamma'(u) \to \alpha_1(u)$ for all $u < 0$ if z' tends to z_0. Similarly if $z'' \in U_2$, then the trajectory γ'' through z'' can be parameterized by $u \in (u''_-, \infty)$ in such a way that $\gamma''(0) = z''$ and $\gamma''(u)$ tends to $\alpha_2(u)$, $u > 0$ provided z'' is near z_0. Let γ''' be the vertical straight arc through z' and let us choose z'' on γ'''. We can do this so that the trajectories γ' and γ'' have the above properties. The path $\tilde{\gamma}$ is defined as the composition of the path γ' ,the part of γ''' between z' and z'', and γ''. Let $\widetilde{\Delta_{12}}$ be the analytic continuation of Δ_{12} along $\tilde{\gamma}$, starting from some disc V containing $\gamma'(u)$, $u < 0$. If u tends to $-\infty$, then we have

$$\text{Im}\Delta(\gamma'(-\infty)) = \text{Im}\Delta_{12}(\gamma'(-\infty)) < \text{Im}\Delta_{12}(\alpha_1(-\infty)) \tag{4.121}$$

This implies that

$$\text{Im}\Delta(z') < \text{Im}\Delta_{12}(z_0) \tag{4.122}$$

and

$$\text{Im}\Delta(z'') > \text{Im}\Delta_{12}(z_0). \tag{4.123}$$

Therefore the path $\tilde{\gamma}$ has all required properties.

□

Now that we have dealt with the generic case, we turn to the study of situations where several eigenvalue crossing points lie on the same Stokes line.

4.2 Interferences

Suppose we have at hand a time reversal hamiltonian, $H(t) = H(-t)$, driving a two-level system which satisfies conditions I to III. The function ρ thus satisfies $\rho(z) = \rho(-z)$, and consequently the pattern of Stokes lines in the complex plane is symmetric with respect to the real and the imaginary axis. Suppose there exist two zeros of $\rho(z)$ in the upper half plane, which are not on the imaginary axis. Then, either the Stokes lines do not cut the imaginary axis, and thus will not meet, or they will cut the imaginary axis and connect both zeros. The preceding argument shows that this situation is worth being studied since realistic models are often time reversal (see [NU]), and it can occur for more general systems as well.

Let $H(z)$ be a two-level hamiltonian satisfying conditions I to III and the new condition

V. Infinite Stokes line through N zeros

There exist N eigenvalue crossing points $z_0, \cdots, z_{N-1}$ which are simple zeros of ρ in the upper half plane and a Stokes line $t \mapsto \gamma(t)$, $t \in \mathbb{R}$ in S_a passing through $z_0, \cdots, z_{N-1}$ such that

$$\lim_{t\to\pm\infty} \mathrm{Re}\gamma(t) = \pm\infty \quad \textit{and} \quad |\mathrm{Im}\gamma(t)| < a.$$

Proposition (4.1.2) shows that it is not possible anymore to find a dissipative path above any of the zeros z_j. Let us consider the domain Ω whose boundary is given by $\partial\Omega = \gamma \cup \overline{\gamma}$. The interior of Ω contains no eigenvalue crossing point as is readily seen from Teichmueller's lemma. Indeed if $|T|$ is large enough, we can find two vertical straight arcs v_+ and v_- leading from $\gamma(\pm T)$ to $\overline{\gamma(\pm T)}$ and any zero z_j of $\rho(z)$, $j = 0, \cdots, N-1$, is such that $|\mathrm{Re}z_j| < \max|\mathrm{Re}\gamma(\pm T)|$. Thus the boundary of the subset of Ω we have just constructed is a geodesic polygon with interior angles $\pi/2$ at $\gamma(\pm T)$ and $\overline{\gamma(\pm T)}$ and $2\pi/3$ at the zeros $\{z_j, \overline{z_j}\}$, $j = 0, \dots, N-1$. Applying Teichmueller lemma, we see that Ω contain no eigenvalue crossing point. Thus, in this simply connected domain Ω containing the real axis, the analytic functions with have encountered so far will be univalued.

The idea is to integrate the differential equation (4.23) for the coefficients in Ω directly along the Stokes line leading from $-\infty$ to $+\infty$. The main problem is that since equation (4.23) is not defined at points of X, we have to leave the Stokes line in neighbourhoods of z_j, $j = 0, \dots, N-1$, to avoid these singularities. Hence, in these neighbourhoods, the paths we use to connect in Ω two consecutive branches of Stokes lines which meet at z_j, cannot be dissipative. Nevertheless, we can express the solution of (4.23) on the second branch of Stokes line as a function of the solution on the first branch and of the circuit matrix $W(0|\gamma)$.

Let us consider the eigenvalue crossing z_0. By condition V, in a neighbourhood of z_0 we have the structure of Stokes lines depicted in the figure (4.13). The dashed lines represent the level lines

$$\mathrm{Re}\Delta(z) = \mathrm{Re}\Delta(z_0) = \mathrm{cst} \tag{4.124}$$

of a branch of $\Delta(z) = \int_0^z \sqrt{\rho(u)}du$ and are also called anti-Stokes lines. Let us fix a branch of $\Delta(z)$ by requiring

$$\Delta(z) = \Delta_{12}(z) = \int_0^z -\sqrt{\rho(u)}du \quad \forall z \in \Omega, \tag{4.125}$$

where $\sqrt{\rho(u)}$ is the analytic continuation for $u \in \Omega$ of $\sqrt{\rho(t)}$, $t \in \mathbb{R}$. Now, we can continue this branch of Δ around z_0 up to a cut which we introduce in order to deal with univalued functions only. Thus we consider the situation represented in figure (4.14). The equation

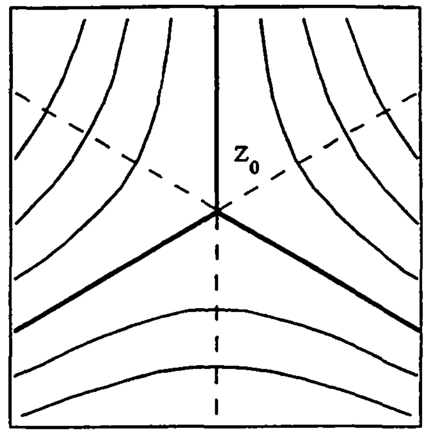

Figure 4.13: Local structure of the Stokes lines near z_0.

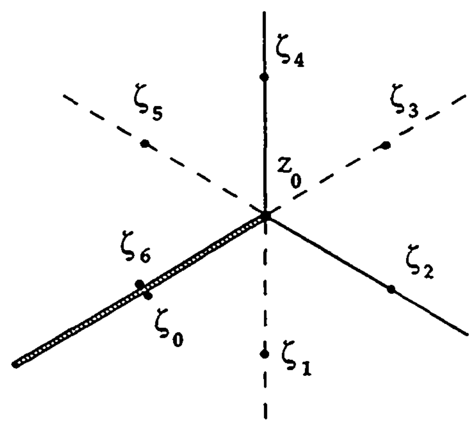

Figure 4.14: The cut neighbourhood of z_0.

we are interested in reads

$$\begin{aligned} c_1'(z) &= a_{12}(z)\exp\left\{\frac{i}{\varepsilon}\Delta(z)\right\}c_2(z) \\ c_2'(z) &= a_{21}(z)\exp\left\{-\frac{i}{\varepsilon}\Delta(z)\right\}c_1(z) \end{aligned} \tag{4.126}$$

where a_{kj} are given in (4.24). Since we are close to z_0, we "normalize" the solution by explicitly putting the value $\exp\left\{\frac{i}{\varepsilon}\Delta(z_0)\right\} \equiv \exp\left\{\frac{i}{\varepsilon}\Delta_0\right\}$ into the game, i.e. we consider

$$\begin{aligned} \widehat{c_1}(z) &\equiv c_1(z) \\ \widehat{c_2}(z) &\equiv c_2(z)\exp\left\{\frac{i}{\varepsilon}\Delta_0\right\}. \end{aligned} \tag{4.127}$$

satisfying

$$\begin{aligned} \widehat{c_1}'(z) &= a_{12}(z)\exp\left\{\frac{i}{\varepsilon}(\Delta(z)-\Delta_0)\right\}\widehat{c_2}(z) \\ \widehat{c_2}'(z) &= a_{21}(z)\exp\left\{-\frac{i}{\varepsilon}(\Delta(z)-\Delta_0)\right\}\widehat{c_1}(z). \end{aligned} \tag{4.128}$$

Let us denote by $V(z,z')$ a fundamental solution of the system

$$\frac{d}{dz}V(z,z') = \begin{pmatrix} 0 & a_{12}(z)\exp\left\{\frac{i}{\varepsilon}(\Delta(z)-\Delta_0)\right\} \\ a_{21}(z)\exp\left\{-\frac{i}{\varepsilon}(\Delta(z)-\Delta_0)\right\} & 0 \end{pmatrix} V(z,z') \tag{4.129}$$

with initial condition $V(z',z') = I\!I$. Our problem amounts to compute $V(\zeta_2,\zeta_0)$ to the leading order in ε (see figure (4.14)).

4.2.1 Adaptation of Frõman Frõman's Method

Let us perform an integration by parts in the Volterra equation corresponding to (4.128)

$$\begin{aligned}
\hat{c}_1(z) &= \hat{c}_1(z') + \frac{\varepsilon}{i}\frac{a_{12}}{\Delta'}(u)\exp\left\{\frac{i}{\varepsilon}(\Delta(u)-\Delta_0)\right\}\hat{c}_2(u)\Big|_{z'}^{z} \\
&- \frac{\varepsilon}{i}\int_{z'}^{z} du\left(\frac{a_{12}}{\Delta'}\right)'(u)\exp\left\{\frac{i}{\varepsilon}(\Delta(u)-\Delta_0)\right\}\hat{c}_2(u) - \frac{\varepsilon}{i}\int_{z'}^{z} du\frac{a_{12}a_{21}}{\Delta'}(u)\hat{c}_1(u) \\
\hat{c}_2(z) &= \hat{c}_2(z') - \frac{\varepsilon}{i}\frac{a_{21}}{\Delta'}(u)\exp\left\{-\frac{i}{\varepsilon}(\Delta(u)-\Delta_0)\right\}\hat{c}_1(u)\Big|_{z'}^{z} \\
&+ \frac{\varepsilon}{i}\int_{z'}^{z} du\left(\frac{a_{21}}{\Delta'}\right)'(u)\exp\left\{-\frac{i}{\varepsilon}(\Delta(u)-\Delta_0)\right\}\hat{c}_1(u) \\
&+ \frac{\varepsilon}{i}\int_{z'}^{z} du\frac{a_{21}a_{12}}{\Delta'}(u)\hat{c}_2(u). \qquad (4.130)
\end{aligned}$$

Supposing there exists a dissipative path γ from z' to z, we can get information on the leading term of $V(z,z')$ by the following method. Consider the solution of (4.128) with initial condition

$$\begin{pmatrix} \hat{c}_1(z') \\ \hat{c}_2(z') \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad (4.131)$$

at $z = z'$. From (4.130) and the fact that $\mathrm{Im}\Delta(z)$ is non decreasing along γ we obtain with the notation $\|f\| = \sup_{u\in\gamma}|f(u)|$

$$|\hat{c}_1(z)| \leq 1 + \varepsilon k\left(\|\hat{c}_1\| + \left\|\exp\left\{\frac{i}{\varepsilon}(\Delta-\Delta_0)\right\}\hat{c}_2\right\|\right) \quad \forall z\in\gamma, \qquad (4.132)$$

and

$$\left|\exp\left\{\frac{i}{\varepsilon}(\Delta(z)-\Delta_0)\right\}\hat{c}_2(z)\right| \leq \varepsilon k\left(\|\hat{c}_1\| + \left\|\exp\left\{\frac{i}{\varepsilon}(\Delta-\Delta_0)\right\}\hat{c}_2\right\|\right) \qquad (4.133)$$

where k is some ε-independent constant. Taking the supremum over $z\in\gamma$ and summing the resulting inequalities we have

$$\|\hat{c}_1\| + \left\|\exp\left\{\frac{i}{\varepsilon}(\Delta-\Delta_0)\right\}\hat{c}_2\right\| \leq \frac{1}{1-2\varepsilon k} \leq k' \qquad (4.134)$$

for ε small enough so that we can write

$$\begin{aligned}
&\hat{c}_1(z) = 1 + \mathcal{O}(\varepsilon) && \hat{c}_1(z') = 1 \\
&\hat{c}_2(z) = \mathcal{O}\left(\varepsilon\exp\left\{\tfrac{1}{\varepsilon}\,\mathrm{Im}(\Delta(z)-\Delta_0)\right\}\right) && \hat{c}_2(z') = 0
\end{aligned} \qquad (4.135)$$

for any $z\in\gamma$. These relations give the leading order of the matrix elements $v_{ij}(z,z')$ of the first column of $V(z,z')$. Now consider (4.130) along a path γ' leading from z' to z which is *antidissipative*, i.e. such that $\mathrm{Im}\Delta$ is non increasing along γ'.

By similar computations, we can get information in this case on the solution with reversed initial conditions, i.e. $\hat{c}_1(z') = 0$ and $\hat{c}_2(z') = 1$. We have

$$\left|\exp\left\{-\frac{i}{\varepsilon}(\Delta(z)-\Delta_0)\right\}\hat{c}_1(z)\right| \leq \varepsilon k\left(\|\hat{c}_2\| + \left\|\exp\left\{-\frac{i}{\varepsilon}(\Delta-\Delta_0)\right\}\hat{c}_1\right\|\right) \qquad (4.136)$$

and

$$|\hat{c}_2(z)| \le 1 + \varepsilon k \left(\|\hat{c}_2\| + \|\exp\left\{-\frac{i}{\varepsilon}(\Delta - \Delta_0)\right\} \hat{c}_1\| \right) \quad \forall z \in \gamma', \tag{4.137}$$

which implies, after taking the supremum over $z \in \gamma'$

$$\|\hat{c}_2\| + \|\exp\left\{-\frac{i}{\varepsilon}(\Delta - \Delta_0)\right\} \hat{c}_1\| \le k' \tag{4.138}$$

if ε is small enough. Hence the estimates

$$\begin{array}{ll} \hat{c}_1(z) = \mathcal{O}\left(\varepsilon \exp\left\{-\frac{1}{\varepsilon}\,\mathrm{Im}(\Delta(z) - \Delta_0)\right\}\right) & \hat{c}_1(z') = 0 \\ \hat{c}_2(z) = 1 + \mathcal{O}(\varepsilon) & \hat{c}_2(z') = 1 \end{array} \tag{4.139}$$

for any $z \in \gamma'$. From (4.135) we have along a dissipative path

$$V(z,z') = \begin{pmatrix} 1 + \mathcal{O}(\varepsilon) & v_{12}(z,z') \\ \mathcal{O}\left(\varepsilon \exp\left\{\frac{1}{\varepsilon}\,\mathrm{Im}(\Delta(z) - \Delta_0)\right\}\right) & v_{22}(z,z') \end{pmatrix}. \tag{4.140}$$

Then we make use of the identity $\det V(z,z') \equiv 1$ to write

$$V(z',z) = V^{-1}(z,z') = \begin{pmatrix} v_{22}(z,z') & -v_{12}(z,z') \\ -v_{21}(z,z') & v_{11}(z,z') \end{pmatrix}. \tag{4.141}$$

Remarking that as γ is a dissipative path leading from z' to z, the reversed path $\gamma' = \gamma^{-1}$ from z to z' is antidissipative so that we can use (4.139) to obtain the leading order of the second column of (4.141). Thus we can write

$$-v_{12}(z,z') = \mathcal{O}\left(\varepsilon \exp\left\{-\frac{1}{\varepsilon}\,\mathrm{Im}(\Delta(z') - \Delta_0)\right\}\right) \tag{4.142}$$

recalling that the roles of z and z' are reversed here. Finally, if there exists a dissipative path leading from z' to z, the solution of (4.129) has the form

$$V(z,z') = \tag{4.143}$$

$$\begin{pmatrix} 1 + \mathcal{O}(\varepsilon) & \mathcal{O}\left(\varepsilon \exp\left\{-\frac{1}{\varepsilon}\mathrm{Im}(\Delta(z') - \Delta_0)\right\}\right) \\ \mathcal{O}\left(\varepsilon \exp\left\{\frac{1}{\varepsilon}\mathrm{Im}(\Delta(z) - \Delta_0)\right\}\right) & 1 + \mathcal{O}(\varepsilon) + \mathcal{O}\left(\varepsilon^2 \exp\left\{\frac{1}{\varepsilon}\,\mathrm{Im}(\Delta(z) - \Delta(z'))\right\}\right) \end{pmatrix}$$

where we have used $\det V = 1$ to estimate $v_{22}(z,z')$. Moreover, we can compute exactly the circuit matrix $V(\zeta_0,\zeta_6)$ by means of the relations (4.68) and (4.69) obtained in paragraph (4.1.5)

$$\begin{aligned} c_1(z) &= \exp\{-i\theta_2(0|\eta_0)\} \exp\left\{-\frac{i}{\varepsilon}\int_{\eta_0} e_2(z)dz\right\} \tilde{c}_2(z) \\ c_2(z) &= \exp\{-i\theta_1(0|\eta_0)\} \exp\left\{-\frac{i}{\varepsilon}\int_{\eta_0} e_1(z)dz\right\} \tilde{c}_1(z) \quad \forall z \in S_a \backslash X. \end{aligned} \tag{4.144}$$

Let us recall that here η_0 is a clockwise oriented loop around z_0, which is based at the origin, and $\tilde{c}_j(z)$ the analytic continuation of $c_j(z)$ obtained after a revolution around z_0 in the negative sense (see figure (4.3)). Passing to the variables $\hat{c}_j$ we can write thanks to (4.144)

$$\begin{aligned} \begin{pmatrix} \hat{c}_1(\zeta_0) \\ \hat{c}_2(\zeta_0) \end{pmatrix} &= V(\zeta_0,\zeta_6) \begin{pmatrix} \hat{c}_1(\zeta_6) \\ \hat{c}_2(\zeta_6) \end{pmatrix} \\ &= \begin{pmatrix} \exp\{i\theta_1(0|\eta_0)\} \exp\left\{\frac{i}{\varepsilon}\int_{\eta_0} e_1(z)dz\right\} \exp\left\{-\frac{i}{\varepsilon}\Delta_0\right\} \hat{c}_2(\zeta_0) \\ \exp\{i\theta_2(0|\eta_0)\} \exp\left\{\frac{i}{\varepsilon}\int_{\eta_0} e_2(z)dz\right\} \exp\left\{\frac{i}{\varepsilon}\Delta_0\right\} \hat{c}_1(\zeta_0) \end{pmatrix} \end{aligned} \tag{4.145}$$

Now we use the fact that

$$\Delta_0 = \Delta_{12}(z_0) = \int_{\eta_0} e_1(z)dz = -\int_{\eta_0} e_2(z)dz \tag{4.146}$$

to get

$$V(\zeta_0, \zeta_6) = \begin{pmatrix} 0 & \exp\{i\theta_{1,0}\} \\ \exp\{i\theta_{2,0}\} & 0 \end{pmatrix} \tag{4.147}$$

with the notation $\theta_{j,0} = \theta_j(0|\eta_0)$.

Lemma 4.2.1 *Let $V(z,z')$ satisfying (4.129) and ζ_j, $j = 1, \cdots, 6$, be defined in figure (4.21). Then we have the asymptotic behaviours*

$$\begin{aligned} V(\zeta_2, \zeta_0) &= \begin{pmatrix} 1 & 0 \\ \exp\{-i\theta_{1,0}\} & 1 \end{pmatrix} + \mathcal{O}(\varepsilon) \\ V(\zeta_6, \zeta_4) &= \begin{pmatrix} 1 & 0 \\ \exp\{-i\theta_{1,0}\} & 1 \end{pmatrix} + \mathcal{O}(\varepsilon) \\ V(\zeta_4, \zeta_2) &= \begin{pmatrix} 1 & -\exp\{i\theta_{1,0}\} \\ 0 & 1 \end{pmatrix} + \mathcal{O}(\varepsilon). \end{aligned}$$

with $\theta_{1,0}$ appearing in (4.147).

This lemma tells us how the solutions of (4.128) change when we pass from one branch of Stokes line to another. We go on with the consequences of this lemma and we prove it at the end of the section. It remains to estimate these solutions along Stokes lines with *any* initial conditions of order 1 in ε. Considering (4.143) along a Stokes lines γ containing no eigenvalue crossing, we obtain at once

$$\begin{pmatrix} \hat{c}_1(z) \\ \hat{c}_2(z) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \hat{c}_1(z') \\ \hat{c}_2(z') \end{pmatrix} + \mathcal{O}(\varepsilon) \tag{4.148}$$

for all $z \in \gamma$, since $\mathrm{Im}\Delta(z) = \mathrm{Im}\Delta(z') = \mathrm{Im}\Delta_0$ on γ, provided

$$|\hat{c}_1(z')| + |\hat{c}_2(z')| = \mathcal{O}(1). \tag{4.149}$$

Thus we can write

$$\begin{aligned} \begin{pmatrix} \hat{c}_1(\zeta_2) \\ \hat{c}_2(\zeta_2) \end{pmatrix} &= V(\zeta_2, \zeta_0) V(\zeta_0, -\infty) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} 1 \\ \exp\{-i\theta_{1,0}\} \end{pmatrix} + \mathcal{O}(\varepsilon) \end{aligned} \tag{4.150}$$

and by (4.127)

$$\begin{pmatrix} c_1(\zeta_2) \\ c_2(\zeta_2) \end{pmatrix} = \begin{pmatrix} 1 + \mathcal{O}(\varepsilon) \\ \exp\left\{-\frac{i}{\varepsilon}\Delta(z_0)\right\} \exp\{-i\theta_{1,0}\}(1 + \mathcal{O}(\varepsilon)) \end{pmatrix}. \tag{4.151}$$

Now, we repeat the whole procedure along the branch of Stokes lines leading from ζ_2 to a neighbourhood of z_1, defining a new $\hat{c}_2(z)$ by $\exp\left\{\frac{i}{\varepsilon}\Delta(z_1)\right\} c_2(z)$. The local analysis around z_1 is the same and it suffices to replace $\theta_{1,0}$ by $\theta_{1,1} \equiv \theta_1(0|\eta_1)$ where η_1 is a loop based at the origin encircling z_1 with negative orientation. Note that the new initial condition at ζ_2 for the new $\hat{c}_j$'s are

$$\begin{pmatrix} \hat{c}_1(\zeta_2) \\ \hat{c}_2(\zeta_2) \end{pmatrix} = \begin{pmatrix} 1+\mathcal{O}(\varepsilon) \\ \exp\left\{\frac{i}{\varepsilon}(\Delta(z_1)-\Delta(z_0))\right\}\exp\{-i\theta_{1,0}\}(1+\mathcal{O}(\varepsilon)) \end{pmatrix} = \mathcal{O}(1) \qquad (4.152)$$

so that we are exactly in the same situation we were in at $-\infty$ on the Stokes line. We can thus summarize this analysis in the

Proposition 4.2.1 *Let H be a two-level hamiltonian satisfying conditions I, II, III and V. Then, the coefficients c_j's defined by (4.21) with initial condition $c_1(-\infty)=1$, $c_2(-\infty)=0$ have the asymptotic behaviours*

$$\begin{aligned} c_1(+\infty) &= 1+\mathcal{O}(\varepsilon) \\ c_2(+\infty) &= \sum_{j=0}^{N-1}\exp\left\{-\frac{i}{\varepsilon}\Delta(z_j)\right\}\exp\{-i\theta_{1,j}\}+\mathcal{O}\left(\varepsilon\exp\left\{\frac{1}{\varepsilon}\text{Im}\Delta(z_0)\right\}\right) \end{aligned}$$

where $\theta_{1,j}=\theta_1(0|\eta_j)$ are given in proposition (4.1.1), η_j being a closed loop based at the origin, encircling z_j in the negative sens.

Note that in this formula $\text{Im}\Delta(z_0)=\text{Im}\Delta(z_j)<0$, $j=0,\cdots,N-1$. This proposition, which is actually the main result of this section can be rephrased in geometrical terms only by using the metric d_ρ.

Theorem 4.2.1 *Let $H(t)$ be a two-level hamiltonian satisfying conditions I, II, III and V and let $\psi_\varepsilon(t)$ be a normalized solution of the Schrödinger equation $i\varepsilon\psi'_\varepsilon=H\psi_\varepsilon$ such that $\lim_{t\to-\infty}\|P_1(t)\psi_\varepsilon(t)\|=1$. Then the transition probability $\mathcal{P}_{21}(\varepsilon)=\lim_{t\to+\infty}\|P_2(t)\psi_\varepsilon(t)\|^2$ in the adiabatic limit is given by*

$$\begin{aligned} \mathcal{P}_{21}(\varepsilon) &= \left|\sum_{j=0}^{N-1}\exp\left\{-\frac{i}{\varepsilon}\int_{\eta_j}e_1(z)dz\right\}\exp\{-i\theta_1(0|\eta_j)\}\right|^2+\mathcal{O}\left(\varepsilon\exp\left\{\frac{2}{\varepsilon}\text{Im}\Delta(z_0)\right\}\right) \\ &= \exp\left\{-\frac{2}{\varepsilon}d_\rho(z_0,\mathbb{R})\right\}\left[\sum_{j=0}^{N-1}\exp\{2\text{Im}\theta_1(0,\eta_j)\}+2\sum_{j>k}^{N-1}\exp\{\text{Im}(\theta_1(0,\eta_j)+\theta_1(0,\eta_k))\}\right. \\ &\quad\left.\times\cos\left\{\frac{1}{\varepsilon}d_\rho(z_j,z_k)+\text{Re}(\theta_1(0,\eta_k)-\theta_1(0,\eta_j))\right\}+\mathcal{O}(\varepsilon)\right]. \end{aligned}$$

Remarks:

- When there is only one eigenvalue crossing point on the infinite Stokes line, we recover theorem (4.1.1) without loss on the correction terms. This is not the case when we use the standard stretching and matching techniques of asymptotics analysis (see [JMP]).
- In this formula, the eigenvalue crossing points z_j must be ordered according to their index on the infinite Stokes line, z_0 being the closest to $-\infty$ and z_{N-1} the closest to $+\infty$.
- The loops η_j by means of which we compute the analytical continuations of the dynamical phases and the geometrical phase factors are all based at the origin.

Proof: The second formula is obtained by expanding the modulus. Then we use

$$\Delta(z_j) = -\int_0^{z_j} \sqrt{\rho(z)}dz = \int_{\eta_j} e_1(z)dz \tag{4.153}$$

and the fact that the z_j's are located on a horizontal geodesic in the metric d_ρ. Thus we have $d_\rho(z_j, \mathbb{R}) = d_\rho(z_0, \mathbb{R})$ and

$$d_\rho(z_0, \mathbb{R}) = |\mathrm{Im}\Delta(z_0)| \tag{4.154}$$

(see paragraph (4.1.6)). Moreover, we have

$$\mathrm{Re}\Delta(z_j) - \mathrm{Re}\Delta(z_k) = \mathrm{Re}\int_{z_j}^{z_k} \sqrt{\rho(z)}dz \tag{4.155}$$

where the path of integration is in Ω. Choosing the geodesic as integration path we obtain the formula

$$\mathrm{Re}\Delta(z_j) - \mathrm{Re}\Delta(z_k) = \pm d_\rho(z_j, z_k) \quad \text{if} \quad j \lessgtr k. \tag{4.156}$$

Indeed, the geodesic $\gamma(t)$ is applied by $\Delta(z)$ on the straight line $\mathrm{Im}w = \mathrm{Im}\Delta(z_0) < 0$ and we have $\lim_{t\to\pm\infty} \mathrm{Re}\Delta(\gamma(t)) = \mp\infty$. As the z_j's are met along γ from $-\infty$ to $+\infty$ in sequence, the formula follows.

4.2.2 Example of Interferences

Let us now turn to a family of examples which will provide a wide variety of behaviours in the leading term of the asymptotic transition probability, as well as emphasize the global character of condition V. Let $H(t) = \mathbf{B}(t) \cdot \mathbf{s}$ be defined by

$$\mathbf{B}(t) = \left(\frac{t^3 + \alpha' t}{\sqrt{t^6 + d^6}}, \frac{\beta' t}{\sqrt{t^6 + d^6}}, \frac{\gamma' t}{\sqrt{t^6 + d^6}}\right) \tag{4.157}$$

where α', β' and γ' are constants to be determined later and d is a large constant. Again, hypotheses I to III are easily verified. The function $\rho(z)$ is

$$\rho(z) = \frac{z^6 + 2\alpha' z^4 + (\alpha'^2 + \beta'^2)z^2 + \gamma'^2}{z^6 + d^6} \equiv \frac{z^6 + \alpha z^4 + \beta z^2 + \gamma}{z^6 + d^6} \tag{4.158}$$

and we choose the constants appearing in (4.158) in such a way that the simple zeros of $\rho(z)$ are $z_1 = b + ic$, $z_2 = ia$, $z_3 = -b + ic$ and their complex conjugates. Thus we must have

$$\rho(z) = \frac{(z - z_1)(z - \overline{z_1})(z - z_2)(z - \overline{z_2})(z - z_3)(z - \overline{z_3})}{z^6 + d^6} \tag{4.159}$$

and by expanding and comparing the coefficients of the powers of z we obtain

$$\begin{aligned} \alpha &= 2\alpha' = a^2 + 2(c^2 - b^2) \\ \beta &= \alpha'^2 + \beta'^2 = (b^2 + c^2)^2 + 2a^2(c^2 - b^2) \\ \gamma &= \gamma'^2 = a^2(b^2 + c^2)^2. \end{aligned} \tag{4.160}$$

Then the magnetic field $\mathbf{B}(t)$ is completely determined with

$$\alpha' = \frac{\alpha}{2}\, ; \beta' = \pm\sqrt{\beta - \frac{\alpha^2}{4}}\, ; \gamma' = \pm\sqrt{\gamma}. \tag{4.161}$$

In order to have a real magnetic field for real values of z, we have to impose

$$\beta - \frac{\alpha^2}{4} \geq 0 \qquad (4.162)$$

which in terms of a, b and c reads $2c \geq a$. We choose the values $a = 1/2$, $c = 1$ and $d = 2$ and keep b as a parameter of the model. By analyzing the model we can see that there are two different regimes characterized by $b \ll 1$ and $b \gg 1$ separated by a limiting case. By a numerical investigation we have obtained for three values of b, $b_1 = 3$, $b_0 \simeq 3.88$, $b_2 = 5$, the Stokes lines displayed in figures (4.15), (4.16) and (4.17). These figures lead

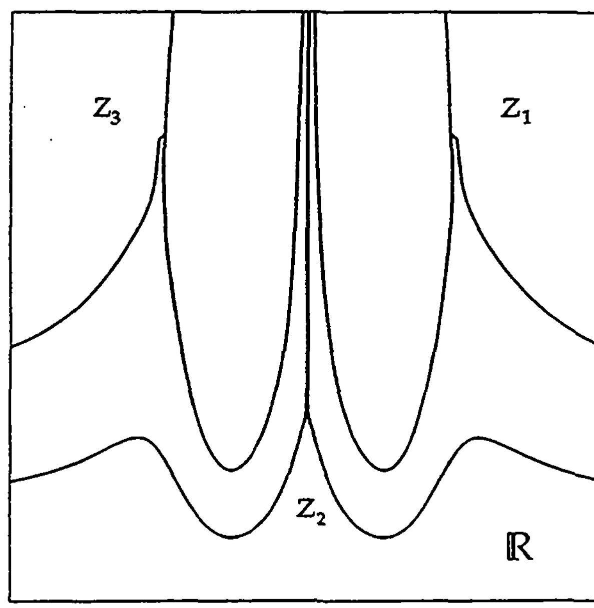

Figure 4.15: The Stokes lines for $b = b_1 = 3$.

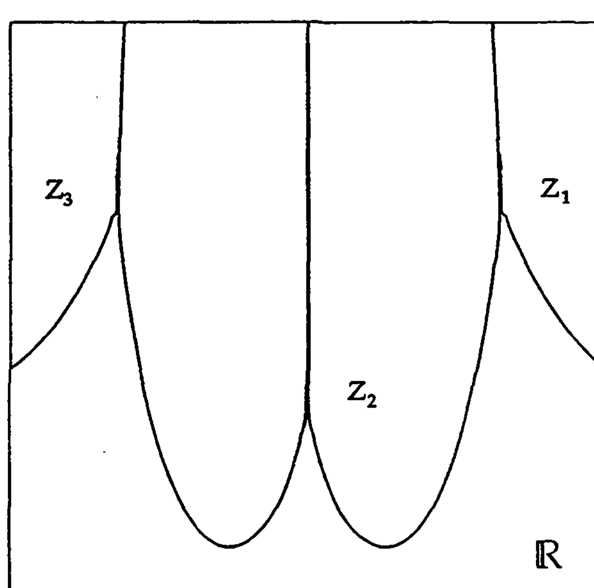

Figure 4.16: The Stokes lines for $b = b_0 \simeq 3.88$.

to the following conclusions about the leading term of the transition probability:

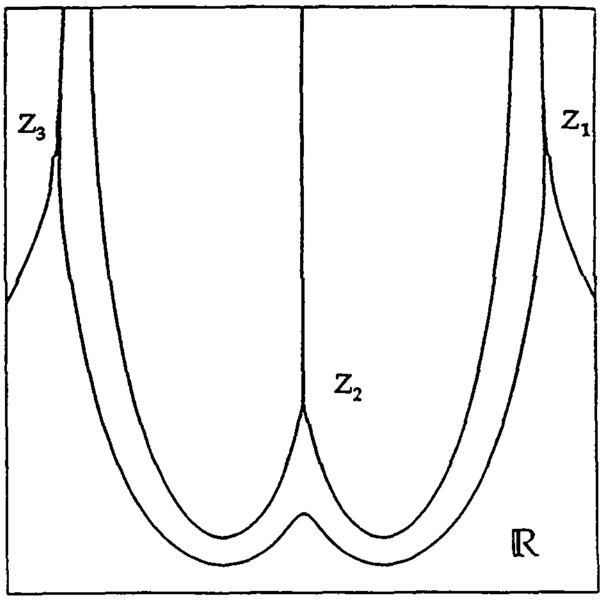

Figure 4.17: The Stokes lines for $b = b_2 = 5$.

- In the case $b = b_1$, there is an infinite Stokes line passing through z_2 only, the closest eigenvalue crossing to the real axis in the euclidean and the ρ-metric(see paragraph (4.1.6)). Thus the leading term of the transition probability can be computed by means of the analysis given in section (4.1).
- In the case $b = b_0$, there is an infinite Stokes line passing through z_1, z_2 and z_3, and the analysis developed in this section is necessary. Thus the leading term of the transition probability will display the interference phenomenon described above. Note that the euclidean distance between the real axis and z_1 (or z_3) is greater than between z_2 and the real axis, although we have in the ρ- distance: $d_\rho(z_1, \mathbb{R}) = d_\rho(z_2, \mathbb{R}) = d_\rho(z_3, \mathbb{R})$.
- In the case $b = b_2$, there is an infinite Stokes line passing through z_1 and z_3 only, showing that: $d_\rho(z_1, \mathbb{R}) = d_\rho(z_3, \mathbb{R}) < d_\rho(z_2, \mathbb{R})$ although the contrary is true in the euclidean metric. In this case too, an interference phenomenon, governed by z_1 and z_3, will take place in the leading term of the transition probability.

We have also computed the values of $\exp\{-i\theta_{1,j}\}$ numerically and plotted the leading terms of the transition probability in the different cases considered. See figures (4.18),(4.19) and (4.20).

$$\mathcal{P}_{21}(\varepsilon) \sim \exp\left\{\frac{2}{\varepsilon}\mathrm{Im}\Delta_{12}(z_2)\right\} \quad \text{if } b = b_1 = 3 \tag{4.163}$$

$$\begin{aligned}\mathcal{P}_{21}(\varepsilon) \sim\ & \exp\left\{\frac{2}{\varepsilon}\mathrm{Im}\Delta_{12}(z_1)\right\}\{\exp\{2\mathrm{Im}\theta_{1,1}\} + \exp\{-2\mathrm{Im}\theta_{1,1}\} + 1 \\ +\ & 2\exp\{2\mathrm{Im}\theta_{1,1}\}\cos\left[\frac{1}{\varepsilon}\mathrm{Re}(\Delta_{12}(z_2) - \Delta_{12}(z_1)) + \mathrm{Re}(\theta_{1,2} - \theta_{1,1})\right] \\ +\ & 2\exp\{-2\mathrm{Im}\theta_{1,1}\}\cos\left[\frac{1}{\varepsilon}\mathrm{Re}(\Delta_{12}(z_1) + \Delta_{12}(z_2)) + \mathrm{Re}(\theta_{1,1} + \theta_{1,2})\right]\end{aligned}$$

$$+ \quad 2\cos\left[\frac{2}{\varepsilon}\mathrm{Re}\Delta_{12}(z_1)\right]\Bigg\}$$
$$\text{if } b = b_0 \simeq 3.88 \tag{4.164}$$

and

$$\mathcal{P}_{21}(\varepsilon) \sim \exp\left\{\frac{2}{\varepsilon}\mathrm{Im}\Delta_{12}(z_1)\right\}\left\{\exp\{2\mathrm{Im}\theta_{1,1}\} + \exp\{-2\mathrm{Im}\theta_{1,1}\} + 2\cos\left[\frac{2}{\varepsilon}\mathrm{Re}\Delta_{12}(z_1)\right]\right\}$$
$$\text{if } b = b_2 = 5. \tag{4.165}$$

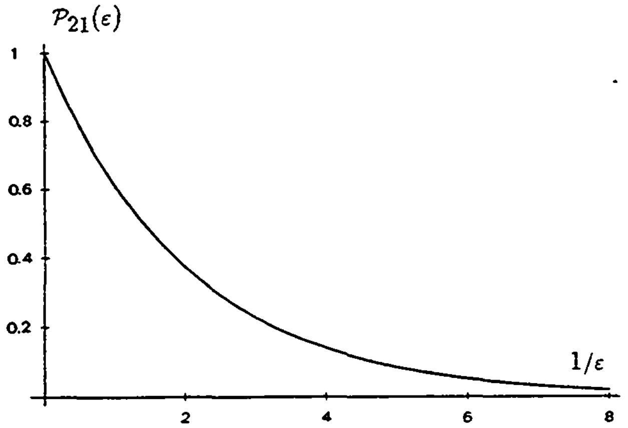

Figure 4.18: $\mathcal{P}_{21}(\varepsilon)$ for $b = b_1 = 3$.

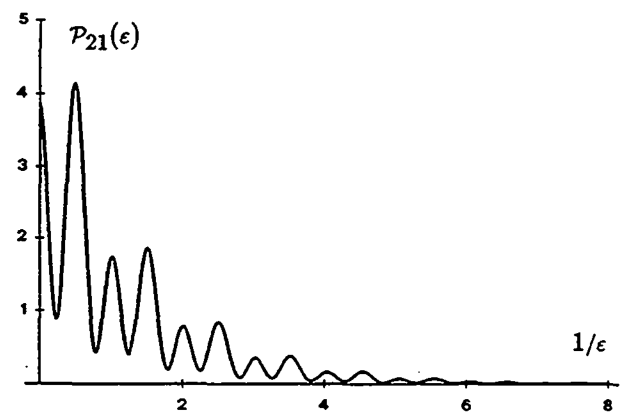

Figure 4.19: $\mathcal{P}_{21}(\varepsilon)$ for $b = b_0 \simeq 3.88$.

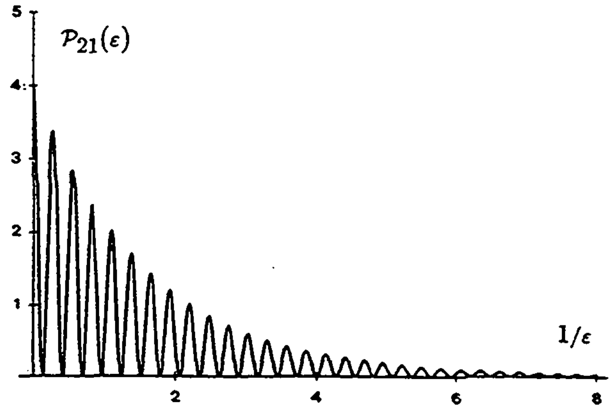

Figure 4.20: $\mathcal{P}_{21}(\varepsilon)$ for $b = b_2 = 5$.

Proof of lemma (4.2.1:)
Let us consider the existence of dissipative paths around z_0, passing through the different points ζ_j, $j = 0, \cdots, 6$. As the points ζ_j are in a neighbourhood of z_0, we can easily construct a ring of dissipative paths around z_0, as shown on figure (4.21), where the arrows give their direction. Before starting the computations, let us describe the strategy

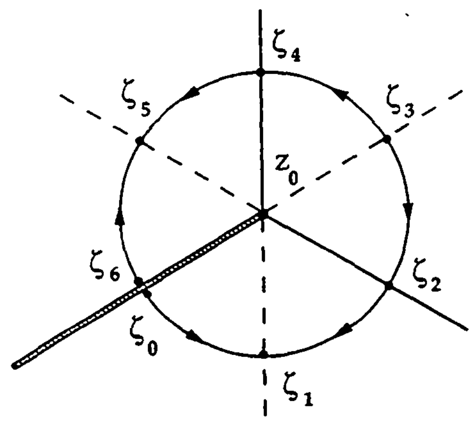

Figure 4.21: Ring of dissipative paths around z_0.

we shall follow. We consider the identity

$$V(\zeta_1, \zeta_0) = V(\zeta_1, \zeta_2)V(\zeta_2, \zeta_0) \tag{4.166}$$

and we express three matrix elements of $V(\zeta_2, \zeta_0)$ as a function of the fourth one and of the matrix elements of $V(\zeta_1, \zeta_2)$ and $V(\zeta_1, \zeta_0)$. For these matrices the estimates (4.143) hold. Then we eliminate in these expressions the elements $v_{22}(\zeta_\mu, \zeta_\nu)$, for which we have no useful estimation here, by means of the identity

$$\det V(\zeta_\mu, \zeta_\nu) = 1. \tag{4.167}$$

Finally we determine the fourth matrix element of $V(\zeta_2, \zeta_0)$, which will be $v_{21}(\zeta_2, \zeta_0)$, by using algebraic identities on the matrices $V(\zeta_\mu, \zeta_\nu)$ and the explicit form (4.147) of $V(\zeta_0, \zeta_6)$.

Let us introduce the short hand

$$v_{ij}(\mu, \nu) = v_{ij}(\zeta_\mu, \zeta_\nu). \tag{4.168}$$

We consider the general relation

$$V(\zeta_{\nu+1}, \zeta_\nu) = V(\zeta_{\nu+1}, \zeta_{\nu+2})V(\zeta_{\nu+2}, \zeta_\nu) \quad \nu \leq 4 \tag{4.169}$$

and

$$\det V(\zeta_\mu, \zeta_\nu) = 1 \quad \forall \nu, \mu. \tag{4.170}$$

These equations lead after simple algebraic manipulations to the expressions

$$\begin{aligned}
v_{11}(\nu+2,\nu) &= \frac{v_{11}(\nu+1,\nu)}{v_{11}(\nu+1,\nu+2)} - \frac{v_{12}(\nu+1,\nu+2)}{v_{11}(\nu+1,\nu+2)}v_{21}(\nu+2,\nu) \\
v_{22}(\nu+2,\nu) &= \frac{v_{11}(\nu+1,\nu+2)}{v_{11}(\nu+1,\nu)} + \frac{v_{12}(\nu+1,\nu)}{v_{11}(\nu+1,\nu)}v_{21}(\nu+2,\nu) \\
v_{12}(\nu+2,\nu) &= \frac{v_{12}(\nu+1,\nu)}{v_{11}(\nu+1,\nu+2)} - \frac{v_{12}(\nu+1,\nu+2)}{v_{11}(\nu+1,\nu)} \\
&\quad - \frac{v_{12}(\nu+1,\nu)v_{12}(\nu+1,\nu+2)}{v_{11}(\nu+1,\nu)v_{11}(\nu+1,\nu+2)}v_{21}(\nu+2,\nu).
\end{aligned} \tag{4.171}$$

When $\nu = 0$ or $\nu = 4$ we have the estimate (4.143) for $V(\zeta_{\nu+1}, \zeta_\nu)$ and $V(\zeta_{\nu+1}, \zeta_{\nu+2})$, and by definition

$$\mathrm{Im}\Delta(\zeta_\nu) = \mathrm{Im}\Delta(\zeta_{\nu+2}) = \mathrm{Im}\Delta_0. \tag{4.172}$$

For example the element $v_{12}(\nu+1, \nu+2)$ satisfies

$$v_{12}(\nu+1,\nu+2) = \mathcal{O}\left(\varepsilon \exp\left\{-\frac{1}{\varepsilon}\mathrm{Im}\left(\Delta(\zeta(\nu+2)) - \Delta_0\right)\right\}\right) = \mathcal{O}(\varepsilon). \tag{4.173}$$

Thus we obtain the following asymptotic relations from similar computations on (4.171)

$$\begin{aligned} v_{11}(\nu+2,\nu) &= 1 + \mathcal{O}(\varepsilon) + \mathcal{O}(\varepsilon)v_{21}(\nu+2,\nu) \\ v_{22}(\nu+2,\nu) &= 1 + \mathcal{O}(\varepsilon) + \mathcal{O}(\varepsilon)v_{21}(\nu+2,\nu) \\ v_{12}(\nu+2,\nu) &= \mathcal{O}(\varepsilon) + \mathcal{O}(\varepsilon^2)v_{21}(\nu+2,\nu) \end{aligned} \tag{4.174}$$

when ε is small enough. At that point, we consider the formula

$$V(\zeta_3,\zeta_2)V(\zeta_2,\zeta_0)V(\zeta_0,\zeta_6) = V(\zeta_3,\zeta_4)V(\zeta_4,\zeta_6) \tag{4.175}$$

and in particular the equation giving the 22- and 21-coefficients

$$\begin{aligned} &v_{21}(3,2)v_{11}(2,0)\exp\{i\theta_{1,0}\} + v_{22}(3,2)v_{21}(2,0)\exp\{i\theta_{1,0}\} = \\ &v_{21}(3,4)v_{12}(4,6) + v_{22}(3,4)v_{22}(4,6) \\ &v_{21}(3,2)v_{12}(2,0)\exp\{i\theta_{2,0}\} + v_{22}(3,2)v_{22}(2,0)\exp\{i\theta_{2,0}\} = \\ &v_{21}(3,4)v_{11}(4,6) + v_{22}(3,4)v_{21}(4,6). \end{aligned} \tag{4.176}$$

The matrix elements of $V(\zeta_3, \zeta_4)$ and $V(\zeta_3, \zeta_2)$ can be estimated by means of (4.141) and (4.143) and we get in particular

$$\begin{aligned} v_{21}(3,2) = \mathcal{O}(\varepsilon) \quad &, \quad v_{21}(3,4) = \mathcal{O}(\varepsilon), \\ v_{22}(3,4) = 1 + \mathcal{O}(\varepsilon) \quad &, \quad v_{22}(3,2) = 1 + \mathcal{O}(\varepsilon). \end{aligned} \tag{4.177}$$

Inserting these estimations together with (4.174) in the above two relations yield

$$\begin{aligned} v_{21}(2,0) &= \exp\{-i\theta_{1,0}\} + \mathcal{O}(\varepsilon) + \mathcal{O}(\varepsilon)v_{21}(6,4) + \mathcal{O}(\varepsilon^2)v_{21}(2,0) \\ v_{21}(6,4) &= -\exp\{i\theta_{2,0}\} + \mathcal{O}(\varepsilon) + \mathcal{O}(\varepsilon)v_{21}(2,0) + \mathcal{O}(\varepsilon^2)v_{21}(6,4). \end{aligned} \tag{4.178}$$

We have also used the identity $V(\zeta_4, \zeta_6) = V^{-1}(\zeta_6, \zeta_4)$ and and the fact that $\exp\{i\theta_{j,0}\}$ is independent of ε. These expressions imply

$$\begin{aligned} |v_{21}(2,0)| &\leq k(1 + \varepsilon|v_{21}(6,4)| + \varepsilon^2|v_{21}(2,0)|) \\ |v_{21}(6,4)| &\leq k(1 + \varepsilon|v_{21}(2,0)| + \varepsilon^2|v_{21}(6,4)|) \end{aligned} \tag{4.179}$$

where k is some constant independent of ε and it remains to sum these inequalities to get for ε small enough

$$|v_{21}(2,0)| + |v_{21}(6,4)| \leq k', \tag{4.180}$$

for k' another constant. Coming back to (4.178) we have

$$\begin{aligned} v_{21}(2,0) &= \exp\{-i\theta_{1,0}\} + \mathcal{O}(\varepsilon) \\ v_{21}(6,4) &= -\exp\{i\theta_{2,0}\} + \mathcal{O}(\varepsilon). \end{aligned} \tag{4.181}$$

Thus, using these formulae in (4.174), the relation (4.44) and the identity

$$V(\zeta_4,\zeta_2) = V(\zeta_4,\zeta_6)V(\zeta_6,\zeta_0)V(\zeta_0,\zeta_2), \tag{4.182}$$

we eventually obtain the results of the lemma.

□

Chapter 5

Combination of Both Methods

5.1 Full Asymptotic Expansion of $\mathcal{P}_{21}(\varepsilon)$

We come back in this section to generic two-level systems for which an asymptotic formula for $\mathcal{P}_{21}(\varepsilon)$ can be obtained, using the complex time method of paragraph (4.1.5). We show here that by combining the iterative scheme of chapter (3) and this complex time method it is possible to obtain a more accurate asymptotic formula for $\mathcal{P}_{21}(\varepsilon)$. We first improve the relative correction between the leading term and $\mathcal{P}_{21}(\varepsilon)$, given by the ratio between $\mathcal{P}_{21}(\varepsilon)$ and this leading term, from ε to ε^q, for any integer q. As a consequence we shall see that the logarithm of $\mathcal{P}_{21}(\varepsilon)$ possesses an asymptotic expansion in powers of ε, up to any order. The second result, which is based on the optimal truncation of the iterative scheme, yields a relative error term of order $\exp\{-\tau/\varepsilon\}$, for some $\tau > 0$.

5.1.1 Iterated Two-Level Systems

Let $H(t)$ be a two-level hamiltonian satisfying conditions I to III. Using the same notations as in chapter (4) we recall that the eigenvalues and spectral projectors of $H(t) = \mathbf{B}(t)\cdot \mathbf{s}$ are given by

$$\begin{aligned} e_j(t) &= (-1)^j\frac{1}{2}\sqrt{\rho(t)}, \quad \rho(t) = B_1^2(t)+B_2^2(t)+B_3^2(t), \\ P_j(t) &= \frac{1}{2}\left(\mathbb{I} + (-1)^j\frac{\mathbf{B}(t)\cdot\mathbf{s}}{\frac{1}{2}\sqrt{\rho(t)}}\right). \end{aligned} \tag{5.1}$$

An analytic choice of corresponding eigenvectors $\varphi_j(t)$ is provided by

$$\varphi_j(t) = W(t,0)\varphi_j(0) \tag{5.2}$$

with

$$iW'(t,0) = K(t)W(t,0) = \frac{\mathbf{B}'(t)\wedge\mathbf{B}(t)}{\rho(t)}\cdot \mathbf{s}, \quad W(0,0) = \mathbb{I}. \tag{5.3}$$

In chapter (4) we expanded the solution $\psi_\varepsilon(t)$ of the Schrödinger equation on the eigenvectors, and we made use of the multivaluedness of these quantities in an essential way to obtain an asymptotic formula for $\mathcal{P}_{21}(\varepsilon)$. The idea now is to construct a more suitable set of basis vectors by means of the iterative scheme of chapter (3) on which we shall expand the solution $\psi_\varepsilon(t)$. Then we shall follow essentially the same strategy as above to obtain an asymptotic formula for the transition probability $\mathcal{P}_{21}(\varepsilon)$. But the use of the iterative scheme will allow us to obtain a better approximation of $\mathcal{P}_{21}(\varepsilon)$.

Let $X = \{z_k, \overline{z_k}\}_{k=0}^{N-1}$ be the set of zeros of $\rho(z)$ in S_a. We assume that condition IV holds for $z_0 \in X$, i.e. that there exists a dissipative path γ passing above z_0. Let z be in the complement of X. We consider now the iterative scheme (3.2) with

$$H_0(z) = H(z), \quad P_0(z) = P_{0,1}(z) = \frac{1}{2}\left(\mathbb{I} - \frac{\mathbf{B}(z)\cdot \mathbf{s}}{\frac{1}{2}\sqrt{\rho(z)}}\right). \tag{5.4}$$

At the first step we have

$$\begin{aligned} H_1(z,\varepsilon) &= H(z) - \varepsilon K_0(z) \\ &= \left(\mathbf{B}(z) + \varepsilon\frac{\mathbf{B}(z)\wedge \mathbf{B}'(z)}{\rho(z)}\right)\cdot \mathbf{s} \\ &\equiv \mathbf{B}_1(z,\varepsilon)\cdot \mathbf{s}. \end{aligned} \tag{5.5}$$

The 2×2 matrix H_1 is meromorphic in S_a, and all its poles, if any, coincide with the points of X. We thus see that the iterated hamiltonians are not necessarily holomorphic in S_a. Let

$$\rho_1(z,\varepsilon) \equiv B_{1,1}^2(z,\varepsilon) + B_{1,2}^2(z,\varepsilon) + B_{1,3}^2(z,\varepsilon). \tag{5.6}$$

The eigenvalues of $H_1(z,\varepsilon)$ are given by

$$e_{1,j}(z,\varepsilon) = (-1)^j\frac{1}{2}\sqrt{\rho_1(z,\varepsilon)}, \quad j = 1,2 \tag{5.7}$$

where the branch of the square root is chosen so that

$$\lim_{\varepsilon\to 0} e_{1,j}(z,\varepsilon) = e_j(z). \tag{5.8}$$

Then we define $P_{1,j}(z,\varepsilon)$, $j = 1,2$ by

$$P_{1,j}(z,\varepsilon) = \left(\mathbb{I} + (-1)^j\frac{\mathbf{B}_1(z,\varepsilon)\cdot \mathbf{s}}{\frac{1}{2}\sqrt{\rho_1(z,\varepsilon)}}\right) \tag{5.9}$$

and we compute (see (5.3))

$$K_1(z,\varepsilon) = \frac{\mathbf{B}_1'(z,\varepsilon)\wedge \mathbf{B}_1(z,\varepsilon)}{\rho_1(z,\varepsilon)}\cdot \mathbf{s}. \tag{5.10}$$

Thus by iterating the procedure we obtain at the q^{th} step

$$\begin{aligned} H_q(z,\varepsilon) &= \mathbf{B}_q(z,\varepsilon)\cdot \mathbf{s} \\ \mathbf{B}_q(z,\varepsilon) &= \mathbf{B}_{q-1}(z,\varepsilon) + \varepsilon\frac{\mathbf{B}_{q-1}(z,\varepsilon)\wedge \mathbf{B}_{q-1}'(z,\varepsilon)}{\rho_{q-1}(z,\varepsilon)} \\ \rho_q(z,\varepsilon) &= B_{q,1}^2(z,\varepsilon) + B_{q,2}^2(z,\varepsilon) + B_{q,2}^2(z,\varepsilon) \end{aligned} \tag{5.11}$$

as long as z is not a zero of $\rho_j(z,\varepsilon)$, $j = 0,\cdots,q-1$. The eigenvalues of $H_q(z,\varepsilon)$ are given by

$$e_{q,j}(z,\varepsilon) = (-1)^j\frac{1}{2}\sqrt{\rho_q(z,\varepsilon)}. \tag{5.12}$$

and the branch is fixed as above by imposing $e_{q,j}(z,\varepsilon) \to e_j(z)$ when $\varepsilon \to 0$. Let r be some fixed small positive number and let

$$D(z_k, r) = \{z : |z - z_k| < r\} \tag{5.13}$$

be the disc of center $z_k \in X$. We define the set Ω

$$\Omega = S_a \backslash \bigcup_{z_k \in X} D(z_k, r) \tag{5.14}$$

and we choose r so small that

$$\begin{aligned}
\overline{D(z_k, r)} &\subset S_a && (5.15)\\
\overline{D(z_k, r)} &\cap \overline{D(z_l, r)} = \emptyset \quad \forall k \neq l && (5.16)\\
\overline{D(z_k, r)} &\cap I\!R = \emptyset && (5.17)\\
\overline{D(z_k, r)} &\cap \gamma = \emptyset, \quad \forall k = 0, \cdots, N-1. && (5.18)
\end{aligned}$$

where γ is the dissipative path of condition IV going above z_0. The next proposition describes the general features of the iterated hamiltonians defined on Ω.

Proposition 5.1.1 *There exist constants a, c and d, an integrable decay function $b(t)$ and a positive ε^* such that for any $\varepsilon < \varepsilon^*$ and for all $q \leq N^*(\varepsilon) \equiv \left[\frac{1}{\varepsilon c d e}\right]$*
i) The hamiltonian $H_q(z,\varepsilon) = \mathbf{B}_q(z,\varepsilon) \cdot \mathrm{s}$ defined by (3.2) and (5.11) is analytic in Ω.
ii) There are no eigenvalue crossing points of $H_q(z,\varepsilon)$ in Ω.
iii) The variation (in the positive sense) of the argument of

$$\rho_q(z,\varepsilon) = B_{q,1}^2(z,\varepsilon) + B_{q,2}^2(z,\varepsilon) + B_{q,3}^2(z,\varepsilon)$$

around the boundary of $D(z_0, r)$ is 2π.
iv)

$$\|K_q(z,\varepsilon) - K_{q-1}(z,\varepsilon)\| \leq b(t)\varepsilon^q d^q c^q q! \quad \forall z = t + is \in \Omega.$$

v)

$$\|K_q(z,\varepsilon)\| \leq b(t)\frac{\mathrm{e}}{\mathrm{e}-1} \quad \forall z = t + is \in \Omega.$$

Proof: We shall use proposition (3.2.1) to prove these results. Let $z \in \Omega$. By construction of Ω and by analyticity there exists $\eta(z) > 0$ such that the hypotheses of proposition (3.2.1) are verified for all $z' \in D(z, \eta(z))$ (see paragraph (3.2.1)). Note that the constants a, b and c in this case depend on $\eta(z)$. Moreover, it follows from condition II and lemma (2.2.3) that there exists $T > 0$ and $r > 0$ such that proposition (3.2.1) holds in the sets $D_\pm(T) = \left\{z = t + is | t \gtrless \pm T, |s| < r\right\}$ with b replaced by an integrable decay function $b(t)$. Now, as the set $\Omega \backslash (D_+ \cup D_-)$ is compact, we can cover it by a finite number of open discs $D(z, \eta(z))$. Thus adding D_+ and D_- we obtain a finite covering of Ω by open sets in which proposition (3.2.1) holds. Hence we can find constants a and c, which are independent of z, and an integrable decay function $b(t)$ such that proposition (3.2.1) holds for any $z = t + is \in \Omega$. From this follow the existence of d and the definition of $N^*(\varepsilon)$ such that point i), iv) and v) hold if ε is smaller than some finite ε_1, provided $q \leq N^*(\varepsilon)$. As a consequence of v), we can write

$$H_q(z,\varepsilon) = H(z) - \varepsilon K_{q-1}(z,\varepsilon) \tag{5.19}$$

with $K_{q-1}(z,\varepsilon)$ uniformly bounded in z, ε and q, if $\varepsilon < \varepsilon_1$. Thus we can apply perturbation theory to show that point ii) holds provided $\varepsilon < \varepsilon_2$, where ε_2 is uniform in z and q. Indeed, by construction of Ω, there exists $R > 0$ such that $\rho(z)$ given by (5.1) satisfies

$$|\rho(z)| > R \quad \forall z \in \Omega, \tag{5.20}$$

so that

$$|e_j(z)| = \frac{1}{2}|\sqrt{\rho(z)}| > \frac{1}{2}\sqrt{R} \quad j = 1,2. \tag{5.21}$$

Since $H_q(z,\varepsilon)$ is traceless, the eigenvalue crossing points are characterized by $e_{q,j}(z) = 0$. Then by perturbation theory and uniformity of $\|K_{q-1}\|$

$$|e_{q,j}(z,\varepsilon) - e_j(z)| \leq k\varepsilon \tag{5.22}$$

where k is a constant uniform in z and q so that if $\varepsilon < \varepsilon_2$, $|e_{q,j}(z,\varepsilon)| > \frac{1}{4}\sqrt{R} > 0$ for any $z \in \Omega$, and $q \leq N^*(\varepsilon)$. To establish iii) we use the argument principle. From (5.11) and v) again, we can write for $\varepsilon < \varepsilon_1$

$$\mathbf{B}_q(z,\varepsilon) = \mathbf{B}(z) + \varepsilon\mathbf{R}_q(z,\varepsilon) \tag{5.23}$$

where $\mathbf{R}_q(z,\varepsilon)$ is an analytic vector such that $\max_{j=1,2,3}|R_{q,j}(z,\varepsilon)| < R'$ where R' is a constant uniform in $z \in \Omega$ and $q \leq N^*(\varepsilon)$. As a consequence

$$\rho_q(z,\varepsilon) = \rho(z) + \varepsilon r_q(z,\varepsilon) \tag{5.24}$$

with $|r_q(z,\varepsilon)| < r'$, r' another uniform constant. Then, there exists $\varepsilon_3 > 0$ such that if $\varepsilon < \varepsilon_3$, we have using (5.20)

$$\left|\frac{\rho_q(z,\varepsilon)}{\rho(z)} - 1\right| < 1 \quad \forall z \in \Omega. \tag{5.25}$$

Let η be the boundary of a disc $D(z_k, r)$, $k = 0,\cdots,N-1$, oriented in the positive sense, and let $G(z,\varepsilon) = \rho_q(z,\varepsilon)/\rho(z)$. By (5.20) and point i), this is a well defined function on η. The index of the image of η by $G(z,\varepsilon)$ with respect to $z = 0$ is zero since the image curve is contained in a disc of center $z = 1$ and radius smaller than 1. Thus

$$\frac{1}{2\pi i}\int_\eta \frac{G'(z,\varepsilon)}{G(z,\varepsilon)}dz = \frac{1}{2\pi i}\int_\eta \frac{\rho_q'(z,\varepsilon)}{\rho_q(z,\varepsilon)}dz - \frac{1}{2\pi i}\int_\eta \frac{\rho'(z)}{\rho(z)}dz = 0. \tag{5.26}$$

If η encircle $D(z_0, r)$, z_0 being a simple zero of $\rho(z)$ (this follows from proposition (4.1.2)), we obtain $\int_\eta \frac{\rho'(z)}{\rho(z)}dz = 2\pi$ which proves iii). The proposition holds if we take $\varepsilon^* = \min_{j=1,2,3}\varepsilon_j$.

□

5.1.2 Superadiabatic Basis

Let $\varepsilon < \varepsilon^*$ and $q \leq N^*(\varepsilon)$. We introduce for $t \in I\!R \subset \Omega$ the operator $W_q(t,\varepsilon)$ by

$$iW_q'(t,\varepsilon) = K_q(t,\varepsilon)W_q(t,\varepsilon), \quad W_q(0,\varepsilon) = I\!I \tag{5.27}$$

It follows from proposition (5.1.1), point v), that $W_q(t,\varepsilon)$ has unitary, ε-dependent limits $W_q(\pm\infty,\varepsilon)$ when $t \to \pm\infty$. Let $\{\varphi_{q,1}(0,\varepsilon), \varphi_{q,2}(0,\varepsilon)\}$ be an orthonormal basis of eigenvectors of $H_q(0,\varepsilon)$. We set

$$\varphi_{q,j}(t,\varepsilon) = W_q(t,\varepsilon)\varphi_{q,j}(0,\varepsilon). \tag{5.28}$$

By the general properties of $W_q(t,\varepsilon)$ (see (3.20)), $\varphi_{q,j}(t,\varepsilon)$ are eigenvectors of $H_q(t,\varepsilon)$ associated with $e_{q,j}(t,\varepsilon) = (-1)^j\frac{1}{2}\sqrt{\rho_q(t,\varepsilon)}$. Moreover, since $\|K_q(z,\varepsilon)\| \to 0$ as $\text{Re}z \to \pm\infty$ the hamiltonians $H_q(t,\varepsilon)$ and $H(t)$ coincide at $t = \pm\infty$ so that

$$\varphi_{q,j}(\pm\infty,\varepsilon) = W_q(\pm\infty,\varepsilon)\varphi_{q,j}(0,\varepsilon) \tag{5.29}$$

are normalized eigenvectors of $H^{\pm}$ associated with $e_j(\pm\infty) = (-1)^j \frac{1}{2}\sqrt{\rho(\pm\infty)}$. We also define generalized dynamical phases

$$\lambda_{q,j}(t,\varepsilon) = \int_0^t e_{q,j}(t',\varepsilon)dt' \quad j = 1,2 \tag{5.30}$$

and we consider a normalized vector $\psi_\varepsilon(t)$ satisfying

$$\begin{aligned} i\varepsilon\psi_\varepsilon'(t) &= H(t)\psi_\varepsilon(t) \\ \lim_{t\to-\infty} \|P_1(t)\psi_\varepsilon(t)\| &= 1. \end{aligned} \tag{5.31}$$

We expand the solution $\psi_\varepsilon(t)$ on the vectors we have just introduced as

$$\psi_\varepsilon(t) = \sum_{j=1}^{2} c_{q,j}(t) \exp\left\{-\frac{i}{\varepsilon}\lambda_{q,j}(t,\varepsilon)\right\} \varphi_{q,j}(t,\varepsilon) \tag{5.32}$$

with the suitable generalized dynamical phases and unknown coefficients $c_{q,j}$ depending on ε. Rewriting (5.31) under the form

$$i\varepsilon\psi_\varepsilon'(t) = (H_q(t,\varepsilon) + \varepsilon K_{q-1}(t,\varepsilon))\psi_\varepsilon(t) \tag{5.33}$$

and exploiting the fact that $\varphi_{q,j}$ are eigenvectors of H_q, we obtain the equation

$$\sum_{j=1}^{2} \left(c_{q,j}' \exp\left\{-\frac{i}{\varepsilon}\lambda_{q,j}\right\} \varphi_{q,j} + c_{q,j} \exp\left\{-\frac{i}{\varepsilon}\lambda_{q,j}\right\} \varphi_{q,j}' + i c_{q,j} \exp\left\{-\frac{i}{\varepsilon}\lambda_{q,j}\right\} K_{q-1}\varphi_{q,j} \right) = 0. \tag{5.34}$$

Taking the scalar product of this expression with $\left(W_q^{-1}(t,\varepsilon)\right)^* \varphi_j(0,\varepsilon)$ and using (5.27) for $\varphi_{q,j}'$ we get the differential equation for the $c_{q,j}$'s

$$c_{q,j}'(t) = \sum_{j=1}^{2} a_q^{jk}(t,\varepsilon) \exp\left\{\frac{i}{\varepsilon}\Delta_q^{jk}(t,\varepsilon)\right\} c_{q,k}(t) \tag{5.35}$$

where

$$a_q^{jk}(t,\varepsilon) = i\langle \varphi_{q,j}(0,\varepsilon) | W_q^{-1}(t,\varepsilon) \left(K_q(t,\varepsilon) - K_{q-1}(t,\varepsilon)\right) W_q(t,\varepsilon) \varphi_{q,j}(0,\varepsilon)\rangle \tag{5.36}$$

and

$$\Delta_q^{jk}(t,\varepsilon) = \lambda_{q,j}(t,\varepsilon) - \lambda_{q,k}(t,\varepsilon). \tag{5.37}$$

By proposition (5.1.1) there exist limits for $c_{q,j}(t)$ at infinity and the boundary conditions (5.31) are equivalent to

$$|c_{q,1}(-\infty)| = 1, \quad c_{q,2}(-\infty) = 0 \tag{5.38}$$

whereas the transition probability is given by

$$\mathcal{P}_{21}(\varepsilon) = |c_{q,2}(\infty)|^2. \tag{5.39}$$

Let us consider the analytic continuation of these quantities in the complex plane. Let η be a loop based at the origin which encircles the disc $D(z_0, r)$ in the negative sense. By proposition (5.1.1), point iii), the analytic continuation of the eigenvalue $e_{q,j}(0,\varepsilon)$ along η back to the origin coincides with $e_{q,k}(0,\varepsilon)$, $k \neq j$, so that we have the same situation as in paragraph (4.1). Thus, we define $\theta_{q,j}(0,\varepsilon|\eta)$ by

$$\widetilde{\varphi_{q,j}}(0,\varepsilon|\eta) = \exp\{-i\theta_{q,j}(0,\varepsilon|\eta)\} \varphi_{q,k}(0,\varepsilon) \tag{5.40}$$

where $\widetilde{\varphi_{q,j}}(0,\varepsilon|\eta)$ is the result of the analytic continuation of $\varphi_{q,j}(0,\varepsilon)$ along η, when we come back to the origin. Then, as a consequence of the analyticity of the solution of the Schrödinger equation (5.31), we can compare the coefficients $c_{q,j}(+\infty)$ defined on the real axis with $\widetilde{c_{q,k}}(+\infty)$, $k \neq j$ obtained by integration of the analytic continuation of (5.35) along the path γ passing above $D(z_0,r)$. The analytic continuation $W_q(z,\varepsilon)$ of $W_q(t,\varepsilon)$ defined by (5.27) along the path γ of condition IV can be expressed by means of a Dyson series. Applying point v) of proposition (5.1.1) to each term shows that

$$\sup_{z\in\gamma} \|W_q(z,\varepsilon)\| \leq w < \infty, \quad \sup_{z\in\gamma} \|W_q^{-1}(z,\varepsilon)\| \leq w < \infty \tag{5.41}$$

where w is independent of ε. Thus the analytic continuations along γ of the coefficients a_q^{jk} defined by (5.36) satisfy the inequality

$$|a_q^{jk}(z,\varepsilon)| \leq w^2 b(t)\varepsilon^q d^q c^q q!, \quad z = t + is \in \gamma \tag{5.42}$$

where we have used point iv) of proposition (5.1.1). The integrability of $b(t)$ at infinity insures the existence of $\widetilde{c_{q,j}}(\pm\infty)$. We have

$$\begin{aligned} c_{q,2}(+\infty) &= \exp\left\{-\frac{i}{\varepsilon}\int_\eta e_{q,1}(z,\varepsilon)dz\right\}\exp\left\{-i\theta_{q,1}(0,\varepsilon|\eta)\right\}\widetilde{c_{q,1}}(+\infty) \\ c_{q,1}(+\infty) &= \exp\left\{-\frac{i}{\varepsilon}\int_\eta e_{q,2}(z,\varepsilon)dz\right\}\exp\left\{-i\theta_{q,2}(0,\varepsilon|\eta)\right\}\widetilde{c_{q,2}}(+\infty) \end{aligned} \tag{5.43}$$

where $\int_\eta e_{q,j}(z,\varepsilon)dz$ is the integral of the analytic continuation of $e_{q,j}$ along the loop η encircling $D(z_0,r)$ considered above. It should be noted that $\theta_{q,1}(0,\varepsilon|\eta)$ can be computed by means of the formula given by proposition (4.1.1) with $B_{q,j}(z,\varepsilon)$ in place of $B_j(z)$. The proof is the same. It remains to control $\widetilde{c_{q,1}}$ along γ to obtain an estimation of $\mathcal{P}_{21}(\varepsilon)$ (see (5.39)). But this will be an easy task now since we can apply the estimate (5.42) for $z \in \gamma$, and γ is by hypothesis a dissipative path for $\Delta_{12}(z) \equiv \Delta_0^{12}(z,\varepsilon)$.

Theorem 5.1.1 *Let $H(t)$ satisfy the hypotheses of theorem (4.1.1). Then*
i) For any integer q, there exists $\varepsilon^*(q)$ such that for all $\varepsilon < \varepsilon^*(q)$ we have

$$\mathcal{P}_{21}(\varepsilon) = \exp\left\{\frac{2}{\varepsilon}\mathrm{Im}\int_\eta e_{q,1}(z,\varepsilon)dz\right\}\exp\left\{2\mathrm{Im}\theta_{q,1}(0,\varepsilon|\eta)\right\}(1+\mathcal{O}(\varepsilon^q))$$

where $e_{q,1}(z,\varepsilon)$ is defined by (5.12), $\theta_{q,1}(0,\varepsilon|\eta)$ is given in (5.40) and η is a loop encircling $D(z_0,r)$. These expressions can be expanded to obtain

$$\mathcal{P}_{21}(\varepsilon) = \exp\left\{\sum_{j=-1}^{q-1}\alpha_j\varepsilon^j\right\}(1+\mathcal{O}(\varepsilon^q))$$

where

$$\alpha_{-1} = 2\mathrm{Im}\int_\eta e_j(z)dz < 0 \quad, \alpha_0 = 2\mathrm{Im}\theta_1(0|\eta).$$

ii) Moreover, there exist $\varepsilon^* > 0$ and $\tau > 0$ such that for all $\varepsilon < \varepsilon^*$

$$\mathcal{P}_{21}(\varepsilon) = \exp\left\{\frac{2}{\varepsilon}\mathrm{Im}\int_\eta e_{N^*(\varepsilon),1}(z,\varepsilon)dz\right\}\exp\left\{2\mathrm{Im}\theta_{N^*(\varepsilon),1}(0,\varepsilon|\eta)\right\}(1+\mathcal{O}(\exp\{-\tau/\varepsilon\})).$$

Remarks:

- Assertion i) results from a rough application of proposition (5.1.1) and shows that the logarithm of $\mathcal{P}_{21}(\varepsilon)$ possesses an asymptotic power series in ε, up to any order. This assertion is, in a sense, the direct generalization of theorem (4.1.1) in which we had computed the first two terms of the expansion, and it provides a constructive method to compute the coefficients α_j.
- The second assertion, giving an asymptotic formula for $\mathcal{P}_{21}(\varepsilon)$ accurate up to exponentially small corrections, comes from an optimal truncation of the iterative procedure. It should be noticed that the leading term is in general a discontinuous function of ε since the optimal integer index $N^*(\varepsilon)$ depends on ε.
- As shown by proposition (4.1.2), the hypotheses of theorem (4.1.1) imply the existence of a dissipative path above z_0 satisfying condition IV.

Proof: Let $\gamma(t)$ be the parameterization of the path of condition IV. We introduce again the notation $f(t) \equiv f(\gamma(t))$ for an analytic function $f(z)$. We consider $N^*(\varepsilon) = \left[\frac{1}{ecd\varepsilon}\right]$ defined in proposition (5.1.1) and we choose a $q \leq N^*(\varepsilon)$. The Volterra equation for the coefficients reads (see (5.35))

$$\begin{aligned} c_{q,j}(t) &= c_{q,j}(-\infty) + \int_{-\infty}^{t} ds\dot{\gamma}(s) a_q^{jj}(s,\varepsilon) c_{q,j}(s) \\ &+ \int_{-\infty}^{t} ds\dot{\gamma}(s) a_q^{jk}(s,\varepsilon) \exp\left\{\frac{i}{\varepsilon}\Delta_q^{jk}(s,\varepsilon)\right\} c_{q,k}(s). \end{aligned} \tag{5.44}$$

Let $\mathbf{X}_q$ be defined by its components

$$\begin{aligned} X_{q,1}(t) &= c_{q,1}(t) \\ X_{q,2}(t) &= \exp\left\{\frac{i}{\varepsilon}\Delta_q^{12}(t,\varepsilon)\right\} c_{q,2}(t). \end{aligned} \tag{5.45}$$

Inserting (5.45) in (5.44) we can write

$$\mathbf{X}_q(t) = \mathbf{X}_q(-\infty) + \int_{-\infty}^{t} ds\dot{\gamma}(s) A_q(t,s,\varepsilon) \mathbf{X}_q(s) \tag{5.46}$$

where the matrix $A_q(t,s,\varepsilon)$ is given by

$$\begin{pmatrix} a_q^{11}(s,\varepsilon) & a_q^{12}(s,\varepsilon) \\ a_q^{21}(s,\varepsilon)\exp\left\{\frac{i}{\varepsilon}\left(\Delta_q^{12}(t,\varepsilon) - \Delta_q^{12}(s,\varepsilon)\right)\right\} & a_q^{22}(s,\varepsilon)\exp\left\{\frac{i}{\varepsilon}\left(\Delta_q^{12}(t,\varepsilon) - \Delta_q^{12}(s,\varepsilon)\right)\right\} \end{pmatrix}. \tag{5.47}$$

Now we can apply perturbation theory and proposition (5.1.1) to

$$H_q(z,\varepsilon) = H(z) - \varepsilon K_{q-1}(z,\varepsilon) \tag{5.48}$$

to obtain

$$e_{q,j}(z,\varepsilon) = e_j(z) + \mathcal{O}(\varepsilon b(t)) \quad z = t = is \in \Omega \tag{5.49}$$

where the correction term is uniformly bounded in q. Thus, for any $z \in \gamma$, we have $\Delta_q^{12}(z,\varepsilon) = \Delta_{12}(z) + \mathcal{O}(\varepsilon)$ with $\Delta_{12}(z) = \int_0^z e_1(z') - e_2(z')dz'$, where the analytic continuations are performed along γ. By hypothesis, the path $\gamma(t)$ is dissipative for Δ_{12}, i.e. $\text{Im}\Delta_{12}(\gamma(t))$ is non decreasing along $\gamma(t)$, so that

$$\left|\exp\left\{\frac{i}{\varepsilon}\left(\Delta_q^{12}(t,\varepsilon) - \Delta_q^{12}(s,\varepsilon)\right)\right\}\right| \leq k \tag{5.50}$$

if $t \geq s$, where k is some constant uniform in q, t, s and ε. It follows from these considerations and (5.42), that there exists a constant α uniform in q such that

$$\int_{-\infty}^{t} |\dot{\gamma(s)}| \|A_q(t,s,\varepsilon)\| ds \leq \alpha \varepsilon^q d^q c^q q!. \tag{5.51}$$

From here the proofs of the two assertions differ. We finish the proof of assertion i). Considering the initial conditions (5.38) and (5.51) we can write from (5.46)

$$\|\mathbf{X}_q(t)\| \leq 1 + \alpha_q \varepsilon^q \sup_{t\in I\!R} \|\mathbf{X}_q\| \tag{5.52}$$

where α_q is a q-dependent constant. Thus, taking the supremum over $t \in I\!R$ in (5.52) we obtain the estimate

$$\sup_{t\in I\!R} \|\mathbf{X}_q(t)\| \leq \frac{1}{1-\alpha_q\varepsilon^q} \leq k_q \tag{5.53}$$

if ε is small enough. Then, coming back to (5.46) we finally get with (5.51)

$$\|\mathbf{X}_q(+\infty) - \mathbf{X}_q(-\infty)\| \leq k'_q \varepsilon^q \tag{5.54}$$

for some constant k'_q independent of ε. With the definition (5.45) we obtain from this last estimate

$$|\widetilde{c_{q,1}}(+\infty) - \widetilde{c_{q,1}}(-\infty)| = \mathcal{O}(\varepsilon^q) \tag{5.55}$$

which, together with (5.39), (5.43) and the initial condition $|\widetilde{c_{q,1}}(-\infty)| = 1$ yield the first assertion of the theorem. To obtain the asymptotic expansion in powers of ε of the logarithm of $\mathcal{P}_{21}(\varepsilon)$, it remains to write such an expansion for the quantities $e_{q,1}(z,\varepsilon)$ and $\theta_{q,1}(0,\varepsilon|\eta)$. This creates no difficulty since all quantities to be expanded are analytic in z and ε for $z \in \Omega$, and $|\varepsilon|$ small enough, and uniformly bounded in $z \in \Omega$. To obtain the first two coefficients α_{-1} and α_0 of the expansion, it suffices to note that

$$H_q = H - \varepsilon K_0 + \varepsilon(K_0 - K_{q-1}) \tag{5.56}$$

so that there is no term proportional to ε in $e_{q,1}$. Indeed, by perturbation theory and proposition (5.1.1), the term of order ε in $e_{q,j}$ is given by

$$\begin{aligned} &\varepsilon\langle\varphi_{0,j}(0)|W_0(z)^{-1}K_0(z)W_0(z)\varphi_{0,j}(0)\rangle = \\ &\varepsilon\langle\varphi_{0,j}(0)|W_0(z)^{-1}P_{0,j}(z)K_0(z)P_{0,j}(z)W_0(z)\varphi_{0,j}(0)\rangle \equiv 0. \end{aligned} \tag{5.57}$$

Note that for a fixed value of q, ε has to be smaller than some $\varepsilon^*(q)$ in order to have $N^*(\varepsilon) \geq q$ and for the estimate (5.53) to hold. We now turn to the end of the proof of the second assertion. Considering (5.51) with $q = N^*(\varepsilon) = \left[\frac{1}{ecd\varepsilon}\right]$ yields

$$\begin{aligned} &\int_{-\infty}^{t} |\dot{\gamma(t)}| \|A_{N^*(\varepsilon)}(t,s,\varepsilon)\| ds \leq \alpha\left(\varepsilon dc N^*(\varepsilon)\right)^{N^*(\varepsilon)} \\ &\leq \alpha \exp\{-N^*(\varepsilon)\} \leq \alpha e \exp\left\{-\frac{1}{ecd\varepsilon}\right\} \equiv \alpha' \exp\{-\tau/\varepsilon\} \end{aligned} \tag{5.58}$$

where $\tau = \frac{1}{ecd} > 0$. With this estimate, we can bound $\|\mathbf{X}_{N^*(\varepsilon)}(t)\|$ as before, to obtain

$$\sup_{t\in I\!R} \|\mathbf{X}_{N^*(\varepsilon)}(t)\| \leq \frac{1}{1-\alpha'\exp\{-\tau/\varepsilon\}} \leq k \tag{5.59}$$

which together with (5.46) and (5.58) yield the exponential estimate

$$\left|X_{N^*(\varepsilon),1}(+\infty) - X_{N^*(\varepsilon),1}(-\infty)\right| \leq k' \exp\{-\tau/\varepsilon\}. \tag{5.60}$$

Considering the initial condition (5.38) and the definition (5.45), we eventually obtain the desired estimate

$$|c_{\widetilde{N^*(\varepsilon)},1}(+\infty) - c_{\widetilde{N^*(\varepsilon)},1}(-\infty)| = \mathcal{O}(\exp\{-\tau/\varepsilon\}) \tag{5.61}$$

which ends the proof of the theorem.

□

5.2 Transition Probability Between Two Isolated Levels

5.2.1 Definition of the Problem

In this section we consider again general unbounded hamiltonians $H(t)$ satisfying the hypotheses I and II. But now we assume that the spectrum of $H(t)$ contains two non degenerate eigenvalues $e_1(t)$ and $e_2(t)$ which are bounded away from the rest of the spectrum for any time $t \in \mathbb{R}$. More precisely we suppose that condition VI below holds.

VI. Two levels in a gap

There exists a constant g such that for any $z \in S_a$, the spectrum $\sigma(z)$ of $H(z)$ consists in two parts $\sigma_1(z)$ and $\sigma_2(z)$ with

$$\inf_{z\in S_a} \text{dist}[\sigma_1(z), \sigma_2(z)] \geq g.$$

Moreover, on the real axis, the part $\sigma_1(t)$ consists of two non degenerate eigenvalues $e_1(t)$, $e_2(t)$ such that

$$\inf_{t\in\mathbb{R}}(e_2(t) - e_1(t)) \geq \delta > 0.$$

We denote by $P_j(t)$, $j = 1, 2$, the one-dimensional projectors associated with $e_j(t)$. It results from condition VI that the analytic continuation $Q(z)$ of the two dimensional projector $Q(t) = P_1(t) + P_2(t)$, is well defined everywhere in S_a. We consider a normalized solution $\psi_\varepsilon(t)$ of the Schrödinger equation

$$i\varepsilon\psi_\varepsilon'(t) = H(t)\psi_\varepsilon(t), \quad \psi_\varepsilon(0) = \varphi_0 \in D \tag{5.62}$$

such that

$$\lim_{t\to-\infty} \|P_1(t)\psi_\varepsilon(t)\| = 1. \tag{5.63}$$

The transition probability $\mathcal{P}_{21}(\varepsilon)$ between the two levels is given by

$$\mathcal{P}_{21}(\varepsilon) = \lim_{t\to+\infty} \|P_2(t)\psi_\varepsilon(t)\|^2. \tag{5.64}$$

We already know from section (3.2) that $\mathcal{P}_{21}(\varepsilon)$ decays exponentially fast to zero when $\varepsilon \to 0$ but we want to obtain here an asymptotic formula for $\mathcal{P}_{21}(\varepsilon)$, as for two level systems, and not only bounds.

The strategy is the following. We introduce a superadiabatic approximation of the physical evolution by means of which we can isolate in a certain sense the transitions between the two levels from the transitions out of the two dimensional subspace they live in. Actually, we can express the transition probability (5.64) as the transition probability of an effective two level hamiltonian plus a contribution of order $\exp\{-\tau/\varepsilon\}$, $\tau > 0$. We study the effective two level hamiltonian by the methods of chapter (4) which gives an asymptotic formula for the corresponding transition probability. Finally we show that provided τ is sufficiently large, this procedure yields an asymptotic formula for the transition probability of the initial problem. We shall also see that if the two levels are sufficiently isolated in the spectrum, then τ becomes large and the asymptotic formula holds. Moreover, the leading term coincides with the formula we would have written down if the two levels e_1 and e_2 were alone in the spectrum. From the analysis of two level systems performed in chapter (4) it is clear that we have to impose conditions on the behaviour of the analytic continuations $e_j(z)$ of the eigenvalues $e_j(t)$ in the complex plane. It follows from the analyticity of the hamiltonian and condition VI that such multivalued analytic continuations exist, with branching points $\{z_j, \overline{z_j}\}$, $j = 0, 1, \cdots, N-1$ at the eigenvalue crossing point z_j such that $e_1(z_j) = e_2(z_j)$. We define $\Delta_{12}(z)$ as in chapter (4) by

$$\Delta_{12}(z) = \int_0^z e_1(z') - e_2(z')dz'. \tag{5.65}$$

This function is multivalued in S_a with branching points at the eigenvalue crossing points z_j. The set of Stokes lines of the problem are given by the level lines

$$\text{Im}\Delta_{12}(z) = \text{Im}\Delta_{12}(z_j), \quad j = 0, \cdots, N-1 \tag{5.66}$$

for some branch of $\Delta_{12}(z)$.

VII. Behaviour of the Stokes lines

There exists an eigenvalue crossing point $z_0 \in S_a$ with $\text{Im}z_0 > 0$ which is a square root type singularity for the functions $e_j(z)$. Moreover the Stokes lines associated with z_0 have two branches α_1 and α_2 such that $\alpha_1 \subset S_a$ goes from $-\infty$ to z_0 and $\alpha_2 \subset S_a$ goes from z_0 to $+\infty$, without meeting any other eigenvalue crossing point.

Let $\varphi_j(t)$, $j = 1, 2$, be the normalized analytic eigenvectors of $H(t)$

$$H(t)\varphi_j(t) = e_j(t)\varphi_j(t) \tag{5.67}$$

whose phases are fixed by the condition

$$\langle\varphi_j(t)|\varphi_j'(t)\rangle \equiv 0 \quad \forall t \in \mathbb{R}. \tag{5.68}$$

We introduce a loop η based at the origin which encircles the eigenvalue crossing z_0 in the negative sense. By using the same notations as in chapter (4) for the analytic continuations of $e_j(0)$ and $\varphi_j(0)$ along η, we have as a consequence of VII,

$$\begin{aligned} \widetilde{e_1}(0|\eta) &= e_2(0) \\ \widetilde{\varphi_1}(0|\eta) &= \exp\{-i\theta_1(0|\eta)\}\varphi_2(0). \end{aligned} \tag{5.69}$$

Theorem 5.2.1 *Let $H(t)$ satisfy conditions I, II, VI and VII, and let $\psi_\varepsilon(t)$ be a normalized solution of the Schrödinger equation*

$$i\varepsilon\psi_\varepsilon'(t) = H(t)\psi_\varepsilon(t), \quad \psi_\varepsilon(t) = \varphi_0 \in D$$

such that

$$\lim_{t\to-\infty} \|P_1(t)\psi_\varepsilon(t)\| = 1.$$

Then,

$$\begin{aligned}\mathcal{P}_{21}(\varepsilon) &= \lim_{t\to+\infty} \|P_2(t)\psi_\varepsilon(t)\|^2 \\ &= \exp\{2\mathrm{Im}\theta_1(0|\eta)\}\exp\left\{\frac{2}{\varepsilon}\mathrm{Im}\int_\eta e_1(z)dz\right\}(1+\mathcal{O}(\varepsilon))\end{aligned}$$

provided the two levels are sufficiently isolated in the spectrum of $H(t)$.

Remarks:

- The condition on the spectrum, which is natural from a physical point of view, is made explicit in the course of the proof (see (5.113)).
- This theorem is the direct generalization of theorem (4.1.1) dealing with two level systems. A purely geometrical version of it, along the same lines as theorem (4.1.1) can also be stated.
- The above result gives a full mathematical justification of the heuristic procedure which consists in neglecting the rest of the spectrum when computing the transition probability between two isolated levels in a gap, in the adiabatic limit.
- The geometrical prefactor $\exp\{2\mathrm{Im}\theta_1(0|\eta)\}$ can be explicitly computed by means of a formula analogous the expression of proposition (4.1.1). This formula is derived in a separate proposition given in the next chapter, proposition (6.2.6).

5.2.2 Reduction to an Effective Two-Level System

Proof: The first part of the proof consists in reducing the complete problem to a two level effective system, by means of a superadiabatic evolution.

Let $K(t) = i[Q'(t), Q(t)]$ where $Q(t) = P_1(t) + P_2(t)$. Then, as in section (3.2) and with the same notations, we can construct a superadiabatic evolution $V_* = W_{N^*}\Phi_{N^*}$, with $Q(t)$ in place of $P(t)$. We recall the definitions of these evolutions

$$\begin{aligned} iW'_{N^*}(t) &= K_{N^*}(t)W_{N^*}(t), \quad W_{N^*}(0) = \mathbb{I} \\ i\varepsilon\Phi'_{N^*}(t) &= W_{N^*}^{-1}(t)H_{N^*}(t)W_{N^*}(t)\Phi_{N^*}(t), \quad \Phi_{N^*}(0) = \mathbb{I} \end{aligned} \tag{5.70}$$

where the derivatives are considered in the strong sense and on the dense domain D. The operators $K_q(t)$ and $H_q(t)$ are defined by the iterative scheme (3.2) and $N^*(\varepsilon) = \left[\frac{1}{\varepsilon c d e}\right]$ is given in proposition (3.2.1). For notational convenience, we have dropped the ε-dependence and the second argument of the evolutions, here 0. Both evolutions leave the domain D invariant. We recall also the existence of the spectral projector $Q_{N^*}(t)$ of $H_{N^*}(t)$ such that

$$\lim_{t\to\pm\infty} \|Q_{N^*}(t) - Q(t)\| = 0 \tag{5.71}$$

(see (3.101)) satisfying by construction

$$W_{N^*}(t)Q_{N^*}(0) = Q_{N^*}(t)W_{N^*}(t) \tag{5.72}$$

and

$$[\Phi_{N^*}(t), Q_{N^*}(0)] = 0, \quad \forall t \in \mathbb{R}. \tag{5.73}$$

If ε is small enough, we can define $P_j^{N^*}(t), j = 1, 2$, the one-dimensional spectral projectors of $H_{N^*}(t)$ such that $Q_{N^*}(t) = P_1^{N^*}(t) + P_2^{N^*}(t)$ and

$$\lim_{t \to \pm\infty} \|P_j^{N^*}(t) - P_j(t)\| = 0. \tag{5.74}$$

By definition the operator $A_{N^*}(t)$ is given by

$$U_\varepsilon(t, 0) = W_{N^*}(t)\Phi_{N^*}(t)A_{N^*}(t) \tag{5.75}$$

where $U_\varepsilon(t, 0)$ satisfies

$$i\varepsilon U_\varepsilon'(t, 0) = H(t)U_\varepsilon(t, 0), \quad U_\varepsilon(0, 0) = \mathbb{I}. \tag{5.76}$$

We have the essential estimate (see (3.103) and (3.104))

$$A_{N^*}(t) = \mathbb{I} + \mathcal{O}(\exp\{-\tau/\varepsilon\}), \quad \tau > 0. \tag{5.77}$$

Let us denote by $\widehat{H}_*(t)$ the self adjoint operator defined on D by

$$\widehat{H}_*(t) = W_{N^*}^{-1}(t)H_{N^*}(t)W_{N^*}(t). \tag{5.78}$$

This operator commutes with $Q_{N^*}(0)$ and if ε is small enough, $Q_{N^*}(0) = \widehat{P_1^*}(t) + \widehat{P_2^*}(t)$, with

$$\widehat{P_j^*}(t) = W_{N^*}^{-1}(t)P_j^{N^*}(t)W_{N^*}(t) \tag{5.79}$$

denoting the spectral projectors of $\widehat{H}_*(t)$. As the equation (5.70) is a Schrödinger like equation with $\widehat{H}_*$ in place of H, we can decompose $\Phi_{N^*}(t)$ as we did for $U_\varepsilon(t, 0)$. We introduce the evolution $\widehat{V}_*(t)$

$$i\varepsilon \widehat{V}_*'(t) = \left(\widehat{H}_*(t) + i\varepsilon \sum_{j=1}^{2} \widehat{P_j^*}'(t)\widehat{P_j^*}(t)\right)\widehat{V}_*(t), \quad \widehat{V}_*(0) = \mathbb{I} \tag{5.80}$$

and we set

$$\Phi_{N^*}(t) := \widehat{V}_*(t)\widehat{A}_*(t). \tag{5.81}$$

By construction $\widehat{V}_*(t)$ is compatible with the decomposition of $Q_*(0)\mathcal{H}$ into

$$Q_*(0)\mathcal{H} = \widehat{P_1^*}(t)\mathcal{H} \oplus \widehat{P_2^*}(t)\mathcal{H} \tag{5.82}$$

since

$$\widehat{P_j^*}(t)\widehat{V}_*(t) = \widehat{V}_*(t)\widehat{P_j^*}(0), \quad j = 1, 2. \tag{5.83}$$

The operator $\widehat{A}_*(t)$ is the solution of the equation

$$i\widehat{A}_*'(t) = -\left(\widehat{V}_*^{-1}(t)i\left(\sum_{j=1}^{2} \widehat{P_j^*}'(t)\widehat{P_j^*}(t)\right)\widehat{V}_*(t)\right)\widehat{A}_*(t), \quad \widehat{A}_*(0) = \mathbb{I}. \tag{5.84}$$

Since $\|\sum_{j=1}^2 \widehat{P_j^*}'(t)\widehat{P_j^*}(t)\|$ is integrable as $t \to \pm\infty$ the operator $\widehat{A}_*(t)$ has well-defined limits when $t \to \pm\infty$. We define $\widehat{A}_*(+\infty, -\infty) = \widehat{A}_*(+\infty)\widehat{A}_*^{-1}(-\infty)$.

Proposition 5.2.1 *The transition probability $\mathcal{P}_{21}(\varepsilon)$ defined by (5.64) is given by*

$$\mathcal{P}_{21}(\varepsilon) = \|\widehat{P_2^*}(0)\widehat{A}_*(+\infty, -\infty)\widehat{P_1^*}(0)\|^2 + \mathcal{O}(\exp\{-\tau/\varepsilon\}).$$

Proof: Let $\psi_\varepsilon(t)$ with $\psi_\varepsilon(0) = \varphi_0 \in D$ be given. We have (using (5.74), (5.79), (5.81), and (5.83))

$$\begin{aligned} 1 &= \lim_{t\to-\infty} \|P_1(t)\psi_\varepsilon(t)\| \\ &= \lim_{t\to-\infty} \|P_1^{N^*}(t)W_{N^*}(t)\Phi_{N^*}(t)A_*(t)\varphi_0\| \\ &= \lim_{t\to-\infty} \|W_{N^*}(t)\widehat{P_1^*}(t)\Phi_{N^*}(t)A_*(t)\varphi_0\| \\ &= \lim_{t\to-\infty} \|\widehat{P_1^*}(t)\widehat{V_*}(t)\widehat{A_*}(t)A_*(t)\varphi_0\| \\ &= \lim_{t\to-\infty} \|\widehat{V_*}(t)\widehat{P_1^*}(0)\widehat{A_*}(t)A_*(t)\varphi_0\| \\ &= \|\widehat{P_1^*}(0)\widehat{A_*}(-\infty)A_*(-\infty)\varphi_0\|. \end{aligned} \tag{5.85}$$

Therefore we can write

$$\varphi_0 = A_*^{-1}(-\infty)\widehat{A_*}^{-1}(-\infty)\varphi_* \tag{5.86}$$

where $\varphi_* \in \widehat{P_1^*}(0)\mathcal{H}$ and $\|\varphi_*\| = 1$. By a computation similar to (5.85) we have

$$\begin{aligned} &\lim_{t\to\infty} \|P_2(t)\psi_\varepsilon(t)\| = \\ &\|\widehat{P_2^*}(0)\widehat{A_*}(+\infty)A_*(+\infty)\varphi_0\| = \\ &\|\widehat{P_2^*}(0)\widehat{A_*}(+\infty)A_*(+\infty)A_*^{-1}(-\infty)\widehat{A_*}^{-1}(-\infty)\widehat{P_1^*}(0)\|. \end{aligned} \tag{5.87}$$

The assertion follows from (5.77).

□

But as $[\Phi_{N^*}(t), Q_{N^*}(0)] = 0$, the expression $\|\widehat{P_2^*}(0)\widehat{A_*}(+\infty,-\infty)\widehat{P_1^*}(0)\|^2$ is the transition probability of the following two-dimensional problem in $Q_*(0)\mathcal{H}$ (see lemma (3.1.1) and (5.78)).

Let $\varphi(t)$ be a normalized solution of the equation

$$i\varepsilon\frac{\partial}{\partial t}\varphi(t) = \widehat{H_*}(t)\varphi(t) \tag{5.88}$$

such that

$$\lim_{t\to-\infty} \|\widehat{P_1^*}(t)\varphi(t)\| = 1. \tag{5.89}$$

Then

$$\begin{aligned} \widehat{\mathcal{P}_{21}}(\varepsilon) &\equiv \lim_{t\to-\infty} \|\widehat{P_2^*}(t)\varphi(t)\|^2 \\ &= \|\widehat{P_2^*}(0)\widehat{A_*}(+\infty,-\infty)\widehat{P_1^*}(0)\|^2 \end{aligned} \tag{5.90}$$

is the transition probability from $\widehat{P}_1^*(-\infty)$ to $\widehat{P}_2^*(+\infty)$. Therefore, if τ is large enough, we have reduced the initial problem to an effective two-dimensional problem.

5.2.3 Asymptotic Formula for $\widehat{\mathcal{P}_{21}}(\varepsilon)$

In this paragraph we consider the operator $\widehat{H_*}(t)$ on the two-dimensional subspace $Q_*(0)\mathcal{H}$ only and we study the effective two-level system (5.90). If ε is small enough, then $\widehat{H_*}(t)$ has two separated eigenvalues $e_1^*(t)$ and $e_2^*(t)$ which coincide with the eigenvalues of $H_{N^*}(t)$. As in the preceding section, we can apply perturbation theory and proposition (3.2.1) to obtain

$$\begin{aligned} e_j^*(t) &= e_j(t) + \mathcal{O}\left(\varepsilon\|K_{N^*-1}(t)\|\right) \\ &= e_j(t) + \mathcal{O}(\varepsilon b(t)), \ j = 1,2 \end{aligned} \tag{5.91}$$

with $b(t)$ an integrable decay function. We first have to show that the effective two level problem we have arrived to can be studied in the strip S_a, provided ε is small enough.

Lemma 5.2.1 *Let $0 < \alpha < a$ be given. Then, there exists $\varepsilon(\alpha) > 0$ such that for all $\varepsilon < \varepsilon(\alpha)$, $\widehat{H_*}(t)$ has an analytic continuation in a neighbourhood of $\{z = t + is : |s| \leq \alpha\}$.*

Proof: It is sufficient to show that K_{N^*-1} and K_{N^*} have analytic continuations in a neighbourhood of $\{z = t + is : |s| \leq \alpha\}$, since this implies that H_{N^*} and W_{N^*} have analytic continuations in the same neighbourhood. For large values of $|t|$ the analytic continuation follows from proposition (3.2.1), since we can apply it with $D(z, \eta)$ replaced by $\{z = t + is : |s| \leq \alpha, t > T\}$ or $\{z = t + is : |s| \leq \alpha, t < -T\}$, by choosing T large enough. Indeed we can verify the hypothesis of this proposition using condition II. Let us consider the compact set $\omega = \{z = t + is : |s| \leq \alpha, |t| \leq T\}$. For each $z \in \omega$ we can find a $\eta(z)$ so that proposition (3.2.1) applies. Therefore the union of the open discs $D(z, \eta(z))$ is a covering of the compact set ω and consequently we can cover ω by a finite number of discs $D(z, \eta(z))$. Thus there exists a nonzero $\varepsilon(\alpha)$ so that, for all $\varepsilon < \varepsilon(\alpha)$, K_{N^*-1} and K_{N^*} have analytic continuation in a neighbourhood of $\{z = t + is : |s| \leq \alpha\}$.

□

In the strip S_a there is an eigenvalue-crossing point for $e_1(z)$ and $e_2(z)$ at z_0 with $\text{Im} z_0 > 0$. Let $0 < r < \alpha$ be given with $\text{Im} z_0 < r$ and $\rho(z) = (e_1(z) - e_2(z))^2$. By condition VII, this function is analytic in a neighbourhood of z_0 and it is equal to zero at z_0 only in this neighbourhood. Similarly we set $\rho_*(z) = (e_1^*(z) - e_2^*(z))^2$. From (5.91) we have

$$\rho_*(z) = \rho(z) + r_*(z, \varepsilon) \tag{5.92}$$

where $|r_*(t+is, \varepsilon)| = \mathcal{O}(\varepsilon b(t))$. Hence, an application of Rouché's theorem states that there is exactly one simple zero of $\rho_*(z)$ close to z_0, which means that there is one eigenvalue crossing point $\hat{z}_0$ for $e_1^*(z)$ and $e_2^*(z)$ in the strip $\{z = t + is \,|\, 0 \leq s \leq r\}$, which is close to z_0, provided ε is small enough. Moreover the singularity of $e_j^*(z)$ at $\hat{z}_0$ is of the same type as the one of $e_j(z)$ at z_0. Let η be the closed path in figure (5.1) and $\varphi_j(0)$, $j = 1, 2$, be two normalized eigenvectors of $H(0)$ with eigenvalues $e_j(0)$. Let $\widehat{\varphi_j^*}(0)$, respectively $\varphi_j^*(0)$,

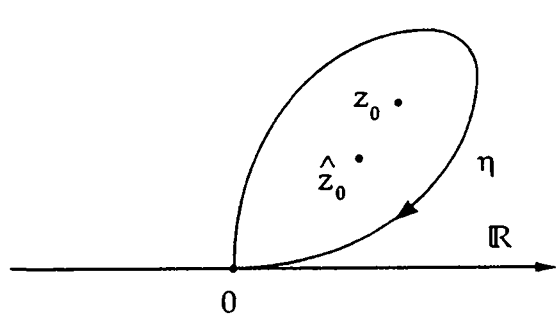

Figure 5.1: The path η encircling z_0 and $\hat{z}_0$.

$j = 1, 2$, be two normalized eigenvectors of $\widehat{H_*}(0)$, respectively $H_{N^*}(0)$ with eigenvalues $e_j^*(0)$. The phases of $\widehat{\varphi_j^*}(t)$ are fixed as in (5.68). We make an analytic continuation of all these objects along the path η and we denote with a $\tilde{}$ the result of the analytic continuation when we come back to the origin. We know that

$$\tilde{e_1}(0) = e_2(0) \tag{5.93}$$

and

$$\widetilde{\varphi_1}(0) = \exp\{-i\theta_1(0|\eta)\}\varphi_2(0). \tag{5.94}$$

For ε small enough we also have

$$\widetilde{e_1^*}(0) = e_2^*(0) \tag{5.95}$$

and therefore

$$\widetilde{\varphi_1}^*(0) = \exp\{-i\theta_1^*(0|\eta)\}\varphi_2^*(0) \tag{5.96}$$

and

$$\widetilde{\widehat{\varphi_1}}^*(0) = \exp\left\{-i\widehat{\theta_1^*}(0|\eta)\right\}\widehat{\varphi_2^*}(0) \tag{5.97}$$

where $\widehat{\varphi_j}^* = W_{N^*}^{-1}\varphi_j^*$. Since $W_{N^*}(t)$ is analytic in the strip we conclude that

$$\theta_1^*(0|\eta) = \widehat{\theta_1^*}(0|\eta). \tag{5.98}$$

We can write, using perturbation theory,

$$\varphi_j^*(0) = \varphi_j(0) + \chi_j(0), \quad j = 1,2 \tag{5.99}$$

with

$$\|\chi_j(0)\| = \mathcal{O}(\varepsilon). \tag{5.100}$$

Therefore we have

$$\begin{aligned} \widetilde{\varphi_1}^*(0) &= \widetilde{\varphi_1}(0) + \widetilde{\chi_1}(0) \\ &= \exp\{-i\theta_1(0|\eta)\}\varphi_2(0) + \widetilde{\chi_1}(0) \\ &= \exp\{-i\theta_1^*(0|\eta)\}\varphi_2^*(0) \\ &= \exp\{-i\theta_1^*(0|\eta)\}(\varphi_2(0) + \chi_2(0)). \end{aligned} \tag{5.101}$$

After analytic continuation we still have $\|\widetilde{\chi_1}(0)\| = \mathcal{O}(\varepsilon)$, thus we conclude that

$$\exp\{i\theta_1^*(0|\eta) - i\theta_1(0|\eta)\} = 1 + \mathcal{O}(\varepsilon) \tag{5.102}$$

so that

$$\theta_1^*(0|\eta) = \theta_1(0|\eta) + \mathcal{O}(\varepsilon). \tag{5.103}$$

It remains to show that the generalized Dykhne formula is valid for our effective problem. According to proposition (4.1.2), condition VII insures the existence of a dissipative path γ for the function Δ_{12} defined by (5.65). But here we need a dissipative path for the function $\Delta_{12}^*(z)$ which is defined as the analytic continuation of the function

$$\int_0^z (e_1^*(z') - e_2^*(z'))\,dz'. \tag{5.104}$$

Nevertheless, even if $\gamma(t)$ is not dissipative for $\Delta_{12}^*(z)$, we can still control the phase factors along $\gamma(t)$, as in the preceding section, (see (5.50)) so that we have

$$\left|\exp\left\{\frac{i}{\varepsilon}\Delta_{12}^*(\gamma(t)) - \Delta_{12}^*(\gamma(s))\right\}\right| \leq k \quad \forall t > s \tag{5.105}$$

where k is independent of ε. It is then straightforward to check that the integration by parts procedure used in paragraph (4.1.5) can be carried over without changes and gives uniform bounds in ε when performed with $\widehat{H}_*$. Therefore, there exists some ε^*, such that for all $\varepsilon < \varepsilon^*$

$$\widehat{\mathcal{P}_{21}}(\varepsilon) = \exp\left\{2\mathrm{Im}\widehat{\theta_1^*}(0|\eta)\right\}\exp\left\{\frac{2}{\varepsilon}\mathrm{Im}\int_\eta e_1^*(z)dz\right\}(1+O(\varepsilon)). \tag{5.106}$$

Note that $e_1^*(t)$ is the eigenvalue of the operator $H_{N^*}(t)$ which can be written as

$$\begin{aligned} H_{N^*}(t) &= H(t) - \varepsilon K_0(t) + \varepsilon(K_0(t) - K_{N^*-1}(t)) \\ &= H(t) - \varepsilon K_0(t) + \mathcal{O}(\varepsilon^2). \end{aligned} \tag{5.107}$$

Let $\varphi_1(t)$ be the eigenvector of $H(t)$ for the eigenvalue $e_1(t)$. Then

$$e_1^*(t) = e_1(t) - \varepsilon\langle\varphi_1(t)|K_0(t)\varphi_1(t)\rangle + \mathcal{O}(\varepsilon^2). \tag{5.108}$$

The term of first order in ε vanishes because

$$P_1(t)[Q'(t), Q(t)]P_1(t) = 0 \tag{5.109}$$

since

$$Q(t)Q'(t)Q(t) = 0. \tag{5.110}$$

Therefore we have

$$\widehat{\mathcal{P}_{21}}(\varepsilon) = \exp\{2\mathrm{Im}\theta_1\}\exp\left\{\frac{2}{\varepsilon}\mathrm{Im}\int_\eta e_1(z)dz\right\}(1+\mathcal{O}(\varepsilon)) \tag{5.111}$$

provided ε is small enough.

5.2.4 Condition on the Gap

The above analysis yields the asymptotic formula

$$\mathcal{P}_{21}(\varepsilon) = \exp\{2\mathrm{Im}\theta_1(0|\eta)\}\exp\left\{\frac{2}{\varepsilon}\mathrm{Im}\int_\eta e_1(z)dz\right\}(1+\mathcal{O}(\varepsilon)) + \mathcal{O}(\exp\{-\tau/\varepsilon\}) \tag{5.112}$$

which gives a definite leading term only if

$$\tau > \left|2\mathrm{Im}\int_\eta e_1\right| \tag{5.113}$$

where τ is given in paragraph (3.2.1). This is the meaning of the last condition on the spectrum of $H(t)$ in the hypotheses of theorem (5.2.1). We show in the next example how it is possible to fulfill this condition by isolating the two levels e_1 and e_2 in the spectrum of the hamiltonian. This remark ends the proof of this theorem.

□

Example:
Suppose we have at hand a family of hamiltonians $H_\gamma(t)$ constructed from $H(t)$ as in paragraph (3.2.2), where $H(t)$ satisfies all hypotheses of theorem (5.2.1) but (5.113). The hamiltonians $H_\gamma(t)$ are obtained by shifting the part of spectrum $\sigma_2(t)$ away from the two levels $\sigma_1(t) = \{e_1(t), e_2(t)\}$ without touching the spectral projectors. They are defined by

$$H_\gamma(t) = H(t)Q_-(t) + (H(t)+\gamma)Q(t) + (H(t)+2\gamma)Q_+(t). \tag{5.114}$$

Thus the gap g between the isolated levels and the rest of the spectrum is replaced by $g(\gamma) = g + \gamma$ and τ is replaced by $\tau(\gamma)$. But now, it follows from proposition (3.2.2) that

$$\tau(\gamma) \geq Cg(\gamma) > \left| 2\mathrm{Im} \int_\eta e_1(z)dz \right| \tag{5.115}$$

for γ large enough. It remains to check that if we replace $H(t)$ by $H_\gamma(t)$, in the spirit of paragraph (3.2.2), the asymptotic formula (5.111) is still valid. But this is true because this formula depends on the analytic continuations of the eigenvector $\varphi_1(t)$ and eigenvalue $e_1(t)$ of $H(t)$ only. Indeed, $\varphi_1(t)$ is also an eigenvector of $H_\gamma(t)$ associated with the eigenvalue $e_1(t) + \gamma$ so that the γ-dependent two-dimensional effective hamiltonian will yield the same asymptotic formula for the transition probability.

Chapter 6

Landau-Zener Formula

We consider here again the transition probability $\mathcal{P}_{21}(\varepsilon)$ between two non-degenerate levels $e_1(t)$ and $e_2(t)$ isolated in the spectrum of the hamiltonian under the same basic assumptions as in the preceding section. But we shall assume, as is often the case in physical applications, that the two levels display an avoided crossing during the evolution. This means that at time $t = 0$, for example, the gap between $e_1(0)$ and $e_2(0)$ is extremely small, but finite, with respect to the typical energies of the system. Such situations occur for example when a reference system displaying a real crossing of eigenvalues at $t = 0$ is slightly perturbed so that the degeneracy is lifted and a small gap between $e_1(0)$ and $e_2(0)$ appears. In such circumstances, the transition probability from one level to the other is still exponentially small but the exponential decay rate is related to the local structure only of the energy levels close to the avoided crossing. This transition probability is given by the well known Landau-Zener formula. Moreover we will show that the avoided crossing assumption suffices to insure a good behaviour of the Stokes lines of interest. As a consequence, the hypotheses under which the Landau-Zener formula can be rigorously justified, are very general assumptions on the analyticity and regularity of the hamiltonian and the physically relevant condition on the existence of one avoided crossing between the considered levels.

6.1 Formalisation of the Problem

6.1.1 Hypotheses

We consider a family of hamiltonians $H(t,\delta)$, $t \in I\!R$ and $\delta \geq 0$ a small parameter, defined on the same separable Hilbert space $\mathcal{H}$. We suppose that the hamiltonians $H(t,\delta)$ satisfy the following two conditions which are generalizations of conditions I and II.

The first condition is that the hamiltonian is analytic in time and sufficiently smooth in t and δ:

VIII. Self-adjointness, analyticity and smoothness

There exist a strip $S_a = \{t + is : |s| \leq a\}$, an interval $I_\Delta = [0, \Delta]$ and a dense domain D in $\mathcal{H}$ such that for each $z \in S_a$ and $\delta \in I_\Delta$

i) $H(z,\delta)$ is a closed operator defined on D

ii) $H(z,\delta)\varphi$ is holomorphic on S_a, for each $\varphi \in D$ and for each fixed $\delta \in I_\Delta$

iii) $H^*(z,\delta) = H(\bar{z},\delta)$; $H(t,\delta)$ is bounded from below if $t \in I\!R$

iv) $H(z,\delta)\varphi$ is C^1 as a function of $(z,\delta) \in S_a \times I_\Delta$ for each $\varphi \in D$.

The next condition states that $H(t,\delta)$ tends sufficiently rapidly to two limiting hamiltonians as $t \to \pm\infty$. These limiting hamiltonians also have to be smooth in δ.

IX. Behaviour at infinity
There exist two families of self adjoint operators $H^{\pm}(\delta)$, defined on D, strongly C^1 in δ and bounded from below and an integrable decay function $b(t)$ independent of δ such that

$$\sup_{|s|<a} \|(H(t+is,\delta) - H^+(\delta))\varphi\| \leq b(t)(\|\varphi\| + \|H^+(\delta)\varphi\|)\ ,\ t>0$$

and

$$\sup_{|s|<a} \|(H(t+is,\delta) - H^-(\delta))\varphi\| \leq b(t)(\|\varphi\| + \|H^-(\delta)\varphi\|)\ ,\ t<0$$

for all $\varphi \in D$ and $\delta \in I_\Delta$. Moreover, for each $\varphi \in D$,

$$\|\frac{\partial}{\partial\delta}H(z,\delta)\varphi\| \leq N\ ,\ \forall(z,\delta) \in S_a \times I_\Delta.$$

When $\delta = 0$, the derivatives with respect to δ are to be considered as right derivatives. Finally, the last condition expresses the fact that when the parameter $\delta = 0$, the levels e_1 and e_2 display a real crossing at $t = 0$ and when $\delta > 0$, this crossing becomes an avoided crossing.

X. Separation of the spectrum and avoided crossing
There exists a constant g independent of t and δ such that the spectrum $\sigma(t,\delta)$ of $H(t,\delta)$, $t \in I\!R$, $\delta \in I_\Delta$, is given by

$$\sigma(t,\delta) = \sigma_1(t,\delta) \cup \sigma_2(t,\delta)\ ,\ \sigma_1(t,\delta) = \{e_1(t,\delta), e_2(t,\delta)\},$$

and satisfies

$$dist[\sigma_1(t,\delta),\sigma_2(t,\delta)] \geq g > 0\ \ \forall t \in I\!R, \delta \in I_\Delta.$$

Moreover,

$$e_2(t,\delta) - e_1(t,\delta) > 0\ ,\ \forall t \in I\!R \text{ and } \delta > 0$$

and if $\delta = 0$,

$$\begin{aligned} &e_2(t,0) - e_1(t,0) > 0\ ,\ \forall t<0 \\ &e_2(t,0) - e_1(t,0) < 0\ ,\ \forall t>0 \\ &e_2(0,0) = e_1(0,0) \end{aligned}$$

where $t = 0$ is a simple zero of the function $e_2(t,0) - e_1(t,0)$ (see figure 6.1).

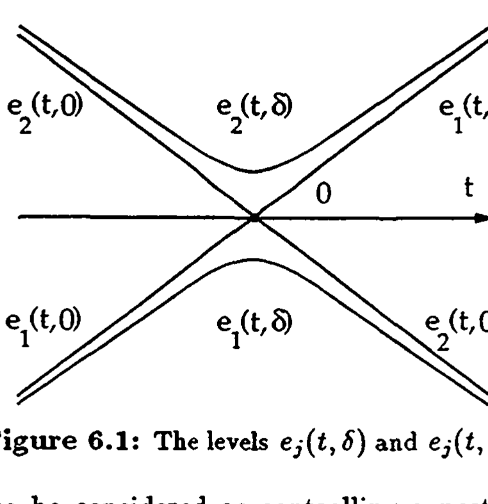

Figure 6.1: The levels $e_j(t,\delta)$ and $e_j(t,0)$.

The parameter δ is to be considered as controlling a perturbation which turns the genuine crossing between $e_1(t,0)$ and $e_2(t,0)$ at $t = 0$ into an avoided crossing of minimum gap of order δ. The corresponding one-dimensional projectors are denoted by $P_1(t,\delta)$ and $P_2(t,\delta)$. By condition VIII, the functions $e_j(z,\delta)$ and operators $P_j(z,\delta)$ are analytic and multivalued in S_a with branch points at the complex eigenvalue crossing points. If the eigenvalue crossing point is real, $e_j(z,\delta=0)$ and $P_j(z,\delta=0)$ are analytic at this point as a consequence of a theorem by Rellich [R], so that the last condition makes sense. It also implies, as we shall see, that there is a complex eigenvalue crossing point $z_0(\delta)$ together with its complex conjugate in a neighbourhood of $z=0$ if δ is small enough and that $z_0(\delta)$ is a square root type branch point for the eigenvalues. We also define $Q(t,\delta)=P_1(t,\delta)+P_2(t,\delta)$ which is analytic everywhere in S_a.

To investigate the local structure of the hamiltonian close to the avoided crossing, we need only consider the restriction of $H(t,\delta)$ to the two dimensional subspace $Q(t,\delta)\mathcal{H}$. We specify in a fourth condition the generic form of avoided crossings to which the Landau-Zener formula applies. The assumption is that the quadratic form giving the square of the gap between the levels close to $(t,\delta)=(0,0)$ must be positive definite.

XI. Behaviour at the avoided crossing

i) There exist constants $a>0$, $b>0$ and c with $c^2<a^2b^2$, such that

$$e_2(t,\delta)-e_1(t,\delta)=\sqrt{a^2t^2+2ct\delta+b^2\delta^2+R_3(t,\delta)}.$$

where $R_3(t,\delta)$ is a rest of order 3 in (t,δ).

ii) Let φ_1 and φ_2 form a basis of $Q(0,0)\mathcal{H}$. The matrix elements $\langle\varphi_j|Q(t,\delta)\varphi_k\rangle$ and $\langle\varphi_j|H(t,\delta)Q(t,\delta)\varphi_k\rangle$, $k,j=1,2$, are C^2 as functions of the two real variables (t,δ).

Remark:

The point ii) of this condition is automatically satisfied if the hamiltonian $H(t,\delta)$ is strongly C^2 as an operator-valued function depending on the two real variables (t,δ).

The avoided crossing considered can be rewritten as

$$e_2(t,\delta)-e_1(t,\delta)=\sqrt{a^2t^2+2ct\delta+b^2\delta^2}\,(1+R_1(t,\delta)) \tag{6.1}$$

if $t=\mathcal{O}(\delta)$, with closest approach at $t_0(\delta)=-\frac{c\delta}{a^2}+\mathcal{O}\left(\delta^2\right)$ given by

$$e_2(t_0(\delta),\delta)-e_1(t_0(\delta),\delta)=\delta\sqrt{b^2-\frac{c^2}{a^2}}\,(1+\mathcal{O}(\delta)). \tag{6.2}$$

6.1.2 Main Results

We are interested in the normalized solutions in the limit $t\to+\infty$ of the Schrödinger equation

$$i\varepsilon\frac{\partial}{\partial t}\psi_\varepsilon(t)=H(t,\delta)\psi_\varepsilon(t)\ ,\ \ \psi_\varepsilon(0)=\varphi_0\in D \tag{6.3}$$

subject to the boundary condition

$$\lim_{t\to-\infty}\|P_1(t,\delta)\psi_\varepsilon(t)\|=1. \tag{6.4}$$

More precisely we want to compute the transition probability to the level e_2 at time $t=\infty$ given by

$$\mathcal{P}_{21}(\varepsilon,\delta)=\lim_{t\to+\infty}\|P_2(t,\delta)\psi_\varepsilon(t)\|^2 \tag{6.5}$$

in the limit of small ε and δ. Let δ be fixed and let η be a closed loop based at the origin which encloses the complex eigenvalue $z_0(\delta)$ ($\text{Im}z_0(\delta)>0$) as in figure (6.2). We fix

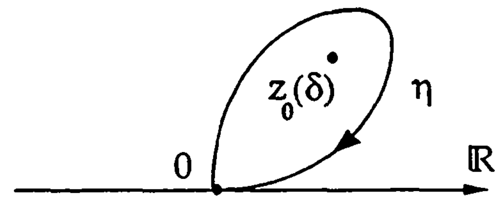

Figure 6.2: The loop η and the eigenvalue crossing $z_0(\delta)$.

the phases of the normalized eigenvectors $\varphi_1(t,\delta)$ and $\varphi_2(t,\delta)$ of $H(t,\delta)$ associated with $e_1(t,\delta)$ and $e_2(t,\delta)$ by the condition

$$\langle\varphi_j(t,\delta)|\frac{\partial}{\partial t}\varphi_j(t,\delta)\rangle \equiv 0\,,\quad \forall t \in \mathbb{R}. \tag{6.6}$$

Consider $e_1(0,\delta)$ and $\varphi_1(0,\delta)$ and their analytic continuations along η. If we denote by $\tilde{e_1}(0,\delta)$ and $\widetilde{\varphi_1}(0,\delta)$ the results of these analytic continuations at the end of the loop η, we have

$$\begin{aligned} \tilde{e_1}(0,\delta) &= e_2(0,\delta) \\ \widetilde{\varphi_1}(0,\delta) &= \exp\{-i\theta_1(\delta)\}\,\varphi_2(0,\delta) \end{aligned} \tag{6.7}$$

because $z_0(\delta)$ is a square root branch point for the energies. The phase θ_1 is now δ-dependent and we have used the notation $\theta_1(\delta)$ for $\theta_1(0,\delta|\eta)$.

Theorem 6.1.1 (Landau-Zener Formula) *Let $H(t,\delta)$ be a self-adjoint operator analytic in t satisfying conditions VIII to X. Let $\psi_\varepsilon(t)$ be a normalized solution of the Schrödinger equation*

$$i\varepsilon\frac{\partial}{\partial t}\psi_\varepsilon(t) = H(t,\delta)\psi_\varepsilon(t)\,,\quad \psi_\varepsilon(0) = \varphi_0 \in D$$

such that

$$\lim_{t\to-\infty}\|P_1(t,\delta)\psi_\varepsilon(t)\| = 1.$$

If ε and δ are small enough,

$$\begin{aligned} \mathcal{P}_{21}(\varepsilon,\delta) &= \lim_{t\to+\infty}\|P_2(t,\delta)\psi_\varepsilon(t)\|^2 \\ &= \exp\{2\mathrm{Im}\theta_1(\delta)\}\exp\left\{\frac{2}{\varepsilon}\mathrm{Im}\int_\eta e_1(z,\delta)dz\right\}(1+\mathcal{O}(\varepsilon)) \end{aligned}$$

where $\mathcal{O}(\varepsilon)$ is independent of δ and

$$\lim_{\delta\to 0}\mathrm{Im}\int_\eta e_1(z,\delta)dz = 0$$
$$\lim_{\delta\to 0}\mathrm{Im}\theta_1(\delta) = 0.$$

Moreover, if condition XI is satisfied, we have

$$\mathcal{P}_{21}(\varepsilon,\delta) = \exp\left\{-\frac{\delta^2\pi}{\varepsilon 2}\left(\frac{b^2}{a}-\frac{c^2}{a^3}\right)(1+\mathcal{O}(\delta))\right\}(1+\mathcal{O}(\delta)+\mathcal{O}(\varepsilon))$$

where $\mathcal{O}(\varepsilon)$, respectively $\mathcal{O}(\delta)$, are independent of δ, respectively ε.

We can recover the results obtained by Hagedorn [H2] specialized to our setting as a direct corollary:

Proposition 6.1.1 *If the width δ of the avoided crossing is rescaled according to $\delta = \sqrt{\varepsilon}$, then*

$$\mathcal{P}_{21}(\varepsilon, \sqrt{\varepsilon}) = \exp\left\{-\frac{\pi}{2}\left(\frac{b^2}{a} - \frac{c^2}{a^3}\right)\right\}(1 + \mathcal{O}(\sqrt{\varepsilon})).$$

Remark:
As already noticed in the introduction, if we set $\delta = 0$ in the above results, we get $\mathcal{P}_{21}(\varepsilon, 0) = (1 + \mathcal{O}(\varepsilon))$. This behaviour is explained by figure (6.1), which shows that $\varphi_1(t, \delta)$ tends to an eigenvector associated with $e_2(t, 0)$ as δ tends to 0. Thus $\mathcal{P}_{21}(\varepsilon, 0)$ is the probability to stay on the eigenstate associated with $e_1(t, 0)$, which must be close to 1, according to the adiabatic theorem. The transition probability is therefore of order ε, as should be the case in presence of a real crossing [BF].

6.2 Proof of the Landau-Zener Formula

The rest of the chapter is devoted to the proof of theorem (6.1.1). Although the general idea of the proof is quite clear, we want to apply theorem (5.2.1) and expand the result to the lowest order in δ, we have to go through the whole proof of that theorem again, to check that it is valid uniformly in δ, under our hypotheses VIII, IX, X. The structure of the proof is the following. We first derive a generalization of lemma (2.2.1) from which the variations of the spectrum of $H(z, \delta)$ with δ and z can be controlled and we investigate the smoothness properties of the resolvent and of the spectral projectors. The second stage consists in checking that proposition (5.2.1) holds for $H(z, \delta)$, uniformly in δ, so that the reduction process to a two level effective system can be achieved up to errors of order $\exp\{-\tau/\varepsilon\}$ with $\tau > 0$ independent of δ. Next, we show perturbatively that the Stokes lines associated with the effective two level problem allow the complex time method to be applied and that the error terms are uniform in δ. We eventually obtain the Landau-Zener formula by inserting the local expressions given in condition XI in the result and by expanding the formula to the lowest order in δ.

6.2.1 Basic Estimates

This paragraph is devoted to the generalization of the results of section (2.2) when the hamiltonian H depends on the supplementary parameter δ. The techniques being similar to the ones already used, we state the main results and give their proofs in appendix.

We introduce different norms, as in paragraph (2.2.1). Let $\varphi \in D$. We define for $z \in S_a$ and $\delta \in I_\Delta$

$$\begin{aligned} \|\varphi\|_{z,\delta} &= \|\varphi\| + \|H(z,\delta)\varphi\| \\ \|\varphi\|_{\pm,\delta} &= \|\varphi\| + \|H^{\pm}(\delta)\varphi\|. \end{aligned} \tag{6.8}$$

The domain D equipped with any of these norms is a Banach space we shall denote by $X_{z,\delta}$, respectively $X_{\pm,\delta}$. By the closed graph theorem again we have for any $z, z' \in S_a$ and $\delta, \delta' \in I_\Delta$

$$H(z,\delta) \in \mathcal{B}(X_{z',\delta'}, \mathcal{H}). \tag{6.9}$$

Similarly

$$\begin{aligned} H(z,\delta) &\in \mathcal{B}(X_{\pm,\delta'},\mathcal{H}) \\ H^{\pm}(\delta) &\in \mathcal{B}(X_{z',\delta'},\mathcal{H}) \\ H^{\pm}(\delta) &\in \mathcal{B}(X_{\pm,\delta'},\mathcal{H}). \end{aligned} \tag{6.10}$$

We denote the norms in these spaces of bounded operators by

$$|||\cdot|||_{z',\delta'} \quad \text{and} \quad |||\cdot|||_{\pm,\delta'}. \tag{6.11}$$

The norms in $X_{z,\delta}$ are related by

$$\|\varphi\|_{z,\delta} \leq (1 + |||H(z,\delta)|||_{z',\delta'})\, \|\varphi\|_{z',\delta'} \tag{6.12}$$

where z or z' can also be replaced by $+$ or $-$. We prove in appendix the following

Lemma 6.2.1 *Under the assumptions VIII and IX, there exists a constant M, independent of $z, z' \in S_a$ and $\delta, \delta' \in I_\Delta$ such that*

$$\max\left(|||H(z,\delta)|||_{z',\delta'}, |||H(z,\delta)|||_{\pm,\delta'}, |||H^{\pm}(\delta)|||_{z',\delta'}, |||H^{\pm}(\delta)|||_{\pm,\delta'}\right) < M$$

and there exists an integrable decay function $b(t)$ and a positive constant B, both uniform in δ, such that for all $\varphi \in D$

$$\begin{aligned} \|\frac{\partial}{\partial z}H(z,\delta)\varphi\| &\equiv \|H'(z,\delta)\varphi\| \leq b(t)\|\varphi\|_{z',\delta'} \\ \|\frac{\partial}{\partial \delta}H(z,\delta)\varphi\| &\leq B\|\varphi\|_{z',\delta'} \\ \|\frac{\partial}{\partial \delta}H^{\pm}(\delta)\varphi\| &\leq B\|\varphi\|_{z',\delta'} \end{aligned}$$

for any $z = t + is$, $z' \in S_a$ and $\delta, \delta' \in I_\Delta$.

We use the notation

$$R(z,\delta,\lambda) = (H(z,\delta) - \lambda)^{-1} \tag{6.13}$$

for $\lambda \in T(z,\delta)$, the resolvent set of $H(z,\delta)$. It follows from the above lemma that

$$\begin{aligned} \|(H(z,\delta) - H(t,0))\varphi\| &\leq \\ \|(H(z,\delta) - H(t,\delta))\varphi\| &+ \|(H(t,\delta) - H(t,0))\varphi\| \\ &\leq (|z-t|b(t) + \delta B)\, \|\varphi\|_{t,0} \end{aligned} \tag{6.14}$$

so that, for $\lambda \in T(t,0)$ we can write

$$\begin{aligned} \|(H(z,\delta) - H(t,0))R(t,0,\lambda)\| &\leq \\ (|z-t|b(t) + \delta B)\,(\|R(t,0,\lambda)\| &+ \|H(t,0)R(t,0,\lambda)\|) \\ &\equiv (|z-t|b(t) + \delta B)\, d(t,\lambda). \end{aligned} \tag{6.15}$$

Now, if $(|z-t|b(t) + \delta B)\, d(t,\lambda) < 1$ we have the identity

$$R(z,\delta,\lambda) - R(t,0,\lambda) = -R(z,\delta,\lambda)(H(z,\delta) - H(t,0))R(t,0,\lambda) \tag{6.16}$$

showing that $\lambda \in T(z,\delta)$ as well and

$$\|R(z,\delta,\lambda)\| \leq \frac{\|R(t,0,\lambda)\|}{1-(|z-t|b(t)+\delta B)\,d(t,\lambda)} \tag{6.17}$$

$$\|R(z,\delta,\lambda)-R(t,0,\lambda)\| \leq \|R(t,0,\lambda)\|\frac{(|z-t|b(t)+\delta B)\,d(t,\lambda)}{1-(|z-t|b(t)+\delta B)\,d(t,\lambda)}. \tag{6.18}$$

Similarly, if $|\mathrm{Re}z| \gg 1$, we use condition IX, lemma (6.2.1) and (6.12) to write

$$\begin{aligned} \|(H(z,\delta)-H^{\pm}(0))\varphi\| &\leq \|(H(z,\delta)-H^{\pm}(\delta))\varphi\| + \\ \|(H^{\pm}(\delta)-H^{\pm}(0))\varphi\| &\leq b(t)\|\varphi\|_{\pm,\delta} + \delta B\|\varphi\|_{0,0} \\ &\leq (1+M)(b(t)+\delta B)\|\varphi\|_{\pm,0} \end{aligned} \tag{6.19}$$

where $z = t+is$. Thus if $\lambda \in T(\pm,0)$ and $(1+M)(b(t)+\delta B)d(\pm,\lambda) < 1$ where

$$d(\pm,\lambda) = \|R(\pm,0,\lambda)\| + \|H^{\pm}(0)R(\pm,0,\lambda)\|, \tag{6.20}$$

then $\lambda \in T(z,\delta)$ as well and we have the estimates

$$\|R(z,\delta,\lambda)\| \leq \frac{\|R(\pm,0,\lambda)\|}{1-(1+M)\,(b(t)+\delta B)\,d(\pm,\lambda)} \tag{6.21}$$

$$\|R(z,\delta,\lambda)-R(\pm,0,\lambda)\| \leq \|R(\pm,0,\lambda)\|\frac{(1+M)\,(b(t)+\delta B)\,d(\pm,\lambda)}{1-(1+M)\,(b(t)+\delta B)\,d(\pm,\lambda)}. \tag{6.22}$$

For $t \in \mathbb{R}$ and $\delta = 0$, we define the two-dimensional projector $Q(t,0)$ by

$$Q(t,0) = -\frac{1}{2\pi i}\oint_{\Gamma} R(t,0,\lambda)d\lambda \tag{6.23}$$

where Γ encircles $\sigma_1(t)$.

Lemma 6.2.2 *Let $t \in \mathbb{R}$ and Γ be as above. We can choose the width a of the strip S_a and the length Δ of the interval I_Δ sufficiently small so that the spectrum of $H(z,\delta)$ is separated in two parts $\sigma_1(z,\delta)$ and $\sigma_2(z,\delta)$ for any $z \in S_a$, $\delta \in I_\Delta$. Moreover, if $|z-t|$ and δ are small enough, the spectral projector $Q(z,\delta)$ corresponding to $\sigma_1(z,\delta)$ is given by*

$$Q(z,\delta) = -\frac{1}{2\pi i}\oint_{\Gamma} R(z,\delta,\lambda)d\lambda \tag{6.24}$$

where Γ encircles $\sigma_1(z,\delta)$.

Proof:
The proof of this lemma is made along the same lines as the proof of lemma (2.2.2) from which we know that for $t \in \mathbb{R}$ the paths Γ can be chosen among the finite set

$$\{\Gamma_j;\ j = 1,\cdots,n\} \tag{6.25}$$

where $\Gamma_- = \Gamma_1$ and $\Gamma_+ = \Gamma_n$. Moreover, if $\lambda \in \Gamma \subset T(t,0)$, respectively $\lambda \in \Gamma_\pm$ if $|t| > T$, we have the uniform estimate (2.16)

$$d(t,\lambda) \leq K < \infty. \tag{6.26}$$

Then by choosing a and Δ so small that

$$\left(a \sup_{t\in\mathbb{R}} b(t) + \Delta B\right) K < 1 \tag{6.27}$$

and

$$(1+M)\,(b(T)+\Delta B)\,K<1 \tag{6.28}$$

for T large, we have that $\Gamma_j \subset T(t+is,\delta)$, respectively $\Gamma_\pm \subset T(t+is,\delta)$, as well so that the spectrum is still separated in two pieces.

□

For later purposes we define

$$d(t,\delta,\lambda)=\|R(t,\delta,\lambda)\|+\|H(t,\delta)R(t,\delta,\lambda)\|. \tag{6.29}$$

It follows from the foregoing that for any $\lambda \in \Gamma_j \subset T(t,\delta)$

$$d(t,\delta,\lambda)\le \overline{K}<\infty, \tag{6.30}$$

where $\overline{K}$ is independent of δ, λ and t. We shall assume from now on that a and Δ are so small that the preceding lemma holds. We define limiting projectors by

$$Q(\pm,\delta)=-\frac{1}{2\pi i}\oint_\Gamma R(\pm,\delta,\lambda)d\lambda. \tag{6.31}$$

The smoothness and regularity conditions on the hamiltonian imply the following behaviours for the resolvent and projector.

Lemma 6.2.3 *For any $z\in S_a$, $\delta\in I_\Delta$ and $\lambda\in T(z,\delta)$, $R(z,\delta,\lambda)$ and $Q(z,\delta)$ are strongly C^1 as functions of $(z,\delta)\in S_a\times I_\Delta$, and $R(\pm,\delta,\lambda)$ and $Q(\pm,\delta)$ are strongly C^1 in $\delta\in I_\Delta$. Moreover, for a fixed δ, $R(z,\delta,\lambda)$ and $Q(z,\delta)$ are holomorphic bounded operators and there exist integrable decay functions $b_{\lambda,\delta}(t)$ and $b(t)$ independent of δ such that if $\lambda\in T(\pm,\delta)$*

$$\begin{aligned}
\|R(t+is,\delta,\lambda)-R(\pm,\delta,\lambda)\| &\le b_{\lambda,\delta}(t)\\
\|R^{(n)}(t+is,\delta,\lambda)\| &\le b_{\lambda,\delta}(t)\\
\|Q(t+is,\delta)-Q(\pm,\delta)\| &\le b(t)\\
\|Q^{(n)}(t+is,\delta)\| &\le b(t)\quad t\gtrless 0,\quad |t|\gg 1,
\end{aligned}$$

for any $|s|<r<a$ and for any integer n.

The proof of this lemma is given in appendix.

6.2.2 Uniform Reduction Process

Let $t\in I\!R$ and let $\Gamma_t\in\{\Gamma_j;\ j=1,\cdots,n\}$ such that $\Gamma_t\in T(t,0)$. By the choice (6.27) of a and Δ, we have that $\Gamma_t\in T(z,\delta)$ $\forall\delta\in I_\Delta$ and $\forall z\in D(t,r)$, provided $r<a$. Thus it follows from (6.17) and (6.21) that there exists a constant N such that

$$\sup_{t\in I\!R}\ \sup_{\substack{z\in D(t,r)\\ \delta\in I_\Delta}}\ \sup_{\lambda\in\Gamma_t}\|R(z,\delta,\lambda)\|\le N. \tag{6.32}$$

We define

$$K(z,\delta)=i[Q'(z,\delta),Q(z,\delta)] \tag{6.33}$$

and by lemma (6.2.3) and the foregoing, there exists an integrable decay function $b(t)$ such that

$$\sup_{\substack{z\in D(t,r)\\ \delta\in I_\Delta}}\|K(z,\delta)\|\le b(t). \tag{6.34}$$

Hence, using Cauchy formula in discs $D(t,\eta)$ with $\eta < r$, we have the estimates

$$\begin{aligned} \|R^{(p)}(z,\delta,\lambda)\| &\leq Nc^p \frac{p!}{(1+p)^2} \\ \|K^{(p)}(z,\delta)\| &\leq b(t)c^p \frac{p!}{(1+p)^2} \quad \forall z \in D(t,\eta), \quad \lambda \in \Gamma_t, \end{aligned} \tag{6.35}$$

for any $t \in \mathbb{R}$, uniformly in $\delta \in I_\Delta$, with $c = 8/r$, provided η is small enough. We can again diminish the width of the strip S_a, so that the above estimates hold uniformly in $z \in S_a$, $\delta \in I_\Delta$. As a consequence proposition (3.2.1) holds uniformly in δ for $\varepsilon < \varepsilon^*$ where ε^* is independent of δ. Then we introduce with the same notations as in the preceding section, the operators W_{N^*}, Φ_{N^*}

$$\begin{aligned} iW'_{N^*}(t,\delta) &= K_{N^*}(t,\delta)W_{N^*}(t,\delta), \quad W_{N^*}(0,\delta) = \mathbb{I}, \\ i\varepsilon\Phi'_{N^*}(t,\delta) &= W_{N^*}^{-1}(t,\delta)H_{N^*}(t,\delta)W_{N^*}(t,\delta)\Phi_{N^*}(t,\delta), \quad \Phi_{N^*}(0,\delta) = \mathbb{I} \end{aligned} \tag{6.36}$$

where $N^*(\varepsilon)$ is δ-independent and is defined in proposition (3.2.1). The operators $K_q(t,\delta)$ and $H_q(t,\delta)$ are defined by the iterative scheme (3.2). All these operators depend on ε and have the same general properties as in section (3.2). In particular, $K_{N^*}(t,\delta)$ is analytic in $z \in S_a$ for any $\delta \in I_\Delta$ and $\varepsilon < \varepsilon^*$ so that the same is true for $H_{N^*}(z,\delta)$ and for $W_{N^*}(z,\delta)$. Moreover,

$$\begin{aligned} W_{N^*}(z,\delta)Q_{N^*}(0,\delta) &= Q_{N^*}(z,\delta)W_{N^*}(z,\delta) \\ [\Phi_{N^*}(z,\delta), Q_{N^*}(0,\delta)] &= 0 \quad \forall z \in S_a. \end{aligned} \tag{6.37}$$

The key point is that due to the uniform estimates (6.35) we have by proposition (3.2.1)

$$\begin{aligned} \|K_{N^*}(z,\delta) - K_{N^*-1}(z,\delta)\| &\leq e b(t) \exp\{-\tau/\varepsilon\} \\ \|K_q(z,\delta)\| &\leq \frac{e}{e-1} b(t) \quad \forall q \leq N^* \end{aligned} \tag{6.38}$$

where τ is independent of δ and $z = t + is$. Thus the operator A_{N^*} defined by

$$U_\varepsilon(t,0) = W_{N^*}(t,\delta)\Phi_{N^*}(t,\delta)A_{N^*}(t,\delta) \tag{6.39}$$

satisfies

$$A_{N^*}(t,\delta) = \mathbb{I} + \mathcal{O}(\exp\{-\tau/\varepsilon\}) \tag{6.40}$$

uniformly in δ. Note that (6.38) also implies

$$\|W_{N^*}(z,\delta)\| \leq w; \quad \|W_{N^*}^{-1}(z,\delta)\| \leq w \tag{6.41}$$

where w is a constant uniform in ε, δ and $z \in S_a$. Let

$$\widehat{H}_*(t,\delta) = W_{N^*}^{-1}(t,\delta)H_{N^*}(t,\delta)W_{N^*}(t,\delta) \tag{6.42}$$

and

$$\widehat{P}_j^*(t,\delta) = W_{N^*}^{-1}(t,\delta)P_j^{N^*}(t,\delta)W_{N^*}(t,\delta) \tag{6.43}$$

where $P_j^{N^*}(t,\delta)$ are the spectral projectors of $H_{N^*}(t,\delta)$. Thus $Q_{N^*}(0,\delta) = \widehat{P}_1^*(t,\delta) + \widehat{P}_2^*(t,\delta)$. Moreover, since by (6.38)

$$\begin{aligned} H_{N^*}(t,\delta) &= H(t,\delta) - \varepsilon K_{N^*-1}(t,\delta) \\ &= H(t,\delta) + \mathcal{O}(\varepsilon b(t)) \end{aligned} \tag{6.44}$$

where the correction term is uniformly bounded in δ, we have

$$\lim_{t\to\pm\infty} \|P_j^{N^*}(t,\delta) - P_j(t,\delta)\| = 0. \tag{6.45}$$

Note also that if δ is very small, then close to $t = 0$, real eigenvalue crossing points of the eigenvalues $e_j^*(t,\delta)$ of $H_{N^*}(t,\delta)$ could exist due to the correction term $-\varepsilon K_{N^*-1}(t,\delta)$ since $e_j^*(t,\delta) - e_j(t,\delta)$ is of the same order as the perturbation. But we shall see later that there are no real eigenvalue crossing points when $\delta > 0$ (see proposition (6.2.3)). We introduce $\widehat{V_*}(t,\delta)$ such that

$$\widehat{V_*}(t,\delta)\widehat{P_j^*}(0,\delta) = \widehat{P_j^*}(t,\delta)\widehat{V_*}(t,\delta) \tag{6.46}$$

by

$$i\varepsilon\widehat{V_*}'(t,\delta) = \left(\widehat{H_*}(t,\delta) + i\varepsilon\sum_{j=1}^{2}\widehat{P_j^*}'(t,\delta)\widehat{P_j^*}(t,\delta)\right)\widehat{V_*}(t,\delta), \quad \widehat{V_*}(0,\delta) = \mathbb{I} \tag{6.47}$$

and we decompose $\Phi_{N^*}(t,\delta)$ as follows

$$\Phi_{N^*}(t,\delta) = \widehat{V_*}(t,\delta)\widehat{A_*}(t,\delta). \tag{6.48}$$

This defines an operator $\widehat{A_*}(t,\delta)$ satisfying

$$i\widehat{A_*}'(t,\delta) = -\widehat{V_*}^{-1}(t,\delta)i\sum_{j=1}^{2}\widehat{P_j^*}'(t,\delta)\widehat{P_j^*}(t,\delta)\widehat{V_*}(t,\delta)\widehat{A_*}(t,\delta), \quad \widehat{A_*}(0,\delta) = \mathbb{I} \tag{6.49}$$

and possessing well defined unitary limits at infinity. We set

$$\widehat{A_*}(+\infty,-\infty;\delta) \equiv \widehat{A_*}(+\infty,\delta)\widehat{A_*}^{-1}(-\infty,\delta). \tag{6.50}$$

Proposition 6.2.1

$$\mathcal{P}_{21}(\varepsilon,\delta) = \|\widehat{P_2^*}(0,\delta)\widehat{A_*}(+\infty,-\infty;\delta)\widehat{P_1^*}(0,\delta)\|^2 + \mathcal{O}(\exp\{-\tau/\varepsilon\})$$

where $\mathcal{O}(\exp\{-\tau/\varepsilon\})$ *is independent of* δ.

The proof is identical to the one of proposition (5.2.1) and the uniformity in δ is a consequence of (6.40). We are thus led to the computation of the transition probability $\widehat{\mathcal{P}_{21}}(\varepsilon,\delta)$ of the effective two-level problem in $Q_{N^*}(0,\delta)\mathcal{H}$

$$\begin{aligned} & i\varepsilon\frac{\partial}{\partial t}\psi(t) = \widehat{H_*}(t,\delta)\psi(t), \quad \|\psi(t)\| = 1, \\ & \lim_{t\to-\infty} \|\widehat{P_1^*}(t,\delta)\psi(t)\| = 1, \\ & \widehat{\mathcal{P}_{21}}(\varepsilon,\delta) = \lim_{t\to+\infty} \|\widehat{P_2^*}(t,\delta)\psi(t)\|^2 \\ = \ & \|\widehat{P_2^*}(0,\delta)\widehat{A_*}(+\infty,-\infty,\delta)\widehat{P_1^*}(0,\delta)\|^2. \end{aligned} \tag{6.51}$$

6.2.3 Study of the Effective Problem

From now on we consider $\widehat{H_*}(t,\delta)$ restricted to the two dimensional subspace $Q_{N^*}(0,\delta)\mathcal{H}$ and we recall that $\widehat{H_*}(z,\delta)$ is analytic in $z \in S_a$ for any $\delta \in I_\Delta$ and $\varepsilon < \varepsilon^*$. As

$$\widehat{H_*}(z,\delta) = W_{N^*}^{-1}(z,\delta)H_{N^*}(z,\delta)W_{N^*}(z,\delta) \tag{6.52}$$

its eigenvalues coincide with the ones of $H_{N^*}(z,\delta)$ and are given by perturbation theory by (see (6.44))

$$e_j^*(z,\delta) = e_j(z,\delta) + \mathcal{O}(\varepsilon b(t)) \tag{6.53}$$

where the correction term is uniformly bounded in δ. We first deal with the eigenvalues $e_j(t,\delta)$ of $H(t,\delta)$. Let φ_1 and φ_2 belong to the range of $Q(0,0)$. We define for $t \in \mathbb{R}$

$$\begin{aligned} \psi_1(t,\delta) &= \frac{Q(t,\delta)\varphi_1}{\sqrt{\langle\varphi_1|Q(t,\delta)\varphi_1\rangle}} \\ \psi_2(t,\delta) &= \frac{Q(t,\delta)\left(\varphi_2 - \frac{\langle\varphi_1|Q(t,\delta)\varphi_2\rangle}{\langle\varphi_1|Q(t,\delta)\varphi_1\rangle}\varphi_1\right)}{\sqrt{\left\langle\varphi_2|Q(t,\delta)(\varphi_2 - \frac{\langle\varphi_1|Q(t,\delta)\varphi_2\rangle}{\langle\varphi_1|Q(t,\delta)\varphi_1\rangle}\varphi_1)\right\rangle}}. \end{aligned} \tag{6.54}$$

These vectors form an orthonormal basis of $Q(t,\delta)\mathcal{H}$ for (t,δ) close to $(0,0)$. Moreover, they are continuously differentiable in (t,δ) and they are analytic in t for δ fixed, by assumptions VIII and IX. Without loss of generality we suppose that $e_1(t,\delta)+e_2(t,\delta)=0$, so that we can write

$$H(t,\delta)|_{Q(t,\delta)\mathcal{H}} = \mathbf{B}(t,\delta)\cdot \mathbf{s} \tag{6.55}$$

in the basis $\{\psi_1(t,\delta),\psi_2(t,\delta)\}$ with s_j, $j=1,2,3$, the spin-1/2 matrices and with the definitions

$$\begin{aligned} B_1(t,\delta) &= 2\mathrm{Re}\langle\psi_1(t,\delta)|H(t,\delta)\psi_2(t,\delta)\rangle \\ B_2(t,\delta) &= -2\mathrm{Im}\langle\psi_1(t,\delta)|H(t,\delta)\psi_2(t,\delta)\rangle \\ B_3(t,\delta) &= 2\langle\psi_1(t,\delta)|H(t,\delta)\psi_1(t,\delta)\rangle. \end{aligned} \tag{6.56}$$

The expressions

$$\frac{\langle\varphi_1|H(t,\delta)Q(t,\delta)\varphi_1\rangle}{\langle\varphi_1|Q(t,\delta)\varphi_1\rangle} \tag{6.57}$$

and

$$\langle\psi_1(t,\delta)|H(t,\delta)\psi_2(t,\delta)\rangle = \frac{\langle\varphi_1|H(t,\delta)Q(t,\delta)\psi_2(t,\delta)\rangle}{\sqrt{\langle\varphi_1|Q(t,\delta)\varphi_1\rangle}} \tag{6.58}$$

have analytic extensions in the complex plane, so that the same is true for their real or imaginary parts considered as real analytic functions on the real axis. Thus the magnetic field $\mathbf{B}(z,\delta)$ is analytic in $z \in S_a$ for all $\delta \in I_\Delta$ and it is continuously differentiable in z and δ. Moreover, as a consequence of condition IX there exist real limits $B_j(\pm\infty,\delta)$, $j=1,2,3$, which are C^1 in δ and an integrable decay function $b(t)$ independent of δ such that

$$\sup_{|s|<a} |B_j(t+is,\delta) - B_j(\pm\infty,\delta)| \le b(t). \tag{6.59}$$

This is easily seen from the identity

$$H(z,\delta)Q(z,\delta) = -\frac{1}{2\pi i}\oint_\Gamma \lambda R(z,\delta,\lambda)d\lambda \tag{6.60}$$

and lemma (6.2.3), for example. Hence the eigenvalues of $H(t,\delta)Q(t,\delta)$ are given by the relation

$$e_j(t,\delta) = (-1)^j \frac{1}{2}\sqrt{\rho(t,\delta)} \tag{6.61}$$

where

$$\rho(t,\delta) = \sum_{j=1}^{3} B_j^2(t,\delta) \tag{6.62}$$

is analytic in $z \in S_a$ for any $\delta \in I_\Delta$ and is C^1 in $(z, \delta) \in S_a \times I_\Delta$. Let us define the function $\Delta_{12}(t, \delta)$ by

$$\Delta_{12}(t,\delta) = -\int_0^t \sqrt{\rho(u,\delta)}du. \tag{6.63}$$

Lemma 6.2.4 *For any positive δ small enough there exists a unique eigenvalue crossing point $z_0(\delta)$ such that* $\mathrm{Im} z_0(\delta) > 0$ *and $z_0(\delta)$ is a simple zero of $\rho(z,\delta)$. As a function of δ, $z_0(\delta)$ is continuous and*

$$\lim_{\delta \to 0} z_0(\delta) = 0.$$

Proof: By assumption, $\rho(z, 0)$ has a double zero at $z = 0$. Let $D(0, r)$ be a circle of radius $r > 0$ centered at $z = 0$ and let us consider

$$\rho(z,\delta) = \rho(z,0) + (\rho(z,\delta) - \rho(z,0)). \tag{6.64}$$

For any r sufficiently small,

$$|\rho(z,0)| > R > 0, \quad \forall z \in \partial D(0,r) \tag{6.65}$$

and there exists δ small enough such that

$$|\rho(z,\delta) - \rho(z,0)| < \frac{R}{3} \quad \forall z \in \partial D(0,r), \tag{6.66}$$

by continuity of $\rho(z, \delta)$ in z and δ and compactness of $\partial D(0, r)$. Applying Rouché' s theorem we see that $\rho(z, \delta)$ has as many zeros as $\rho(z, 0)$ in $D(0, r)$, counted with their multiplicity. As $\rho(t, \delta) > 0$ $\forall t \in \mathbb{R}$ if $\delta > 0$ and $\rho(\bar{z}, \delta) = \bar{\rho}(z, \delta)$ by Schwarz's principle, we conclude that there exists in $D(0, r)$ a unique simple zero $z_0(\delta)$ of $\rho(z, \delta)$ with $\mathrm{Im} z_0(\delta) > 0$. The continuity in δ of $z_0(\delta)$ is proven in a similar way.

□

We come to the main proposition of this section.

Proposition 6.2.2 *There exists a dissipative path $\gamma_\delta(t)$, $t \in \mathbb{R}$ for a branch of $\Delta_{12}(z, \delta)$, passing above $z_0(\delta)$, such that*

$$\lim_{t\to\pm\infty} \mathrm{Re}\gamma_\delta(t) = \pm\infty$$
$$\inf_{t\in\mathbb{R}} \mathrm{Im}\gamma_\delta(t) \geq h > 0$$
$$\sup_{t\in\mathbb{R}} |\dot{\gamma}_\delta(t)| \leq k$$

where h and k are independent of δ.

We postpone the proof of this proposition to the end of the chapter and we use it to compute the transition probability $\widehat{\mathcal{P}_{21}}(\varepsilon, \delta)$ of the effective problem. The existence of a dissipative path above $z_0(\delta)$ is sufficient to apply theorem (5.2.1) for a fixed value of δ, with $\varepsilon < \varepsilon(\delta)$, for $\varepsilon(\delta)$ small enough. But here we want uniformity in δ and ε so that we have to investigate the situation a little further. Consider the hamiltonian $\widehat{H}_*(z, \delta)$ given by (6.52) restricted to $Q_{N^*}(0, \delta)\mathcal{H}$. Its eigenvalues coincide with the eigenvalues $e_j^*(z, \delta)$ of $H_{N^*}(z, \delta)$ which can be expressed by means of an analytic function $\rho_*(z, \delta)$, depending on ε as

$$e_j^*(z,\delta) = (-1)^j \frac{1}{2}\sqrt{\rho_*(z,\delta)} \quad j = 1, 2. \tag{6.67}$$

The function $\rho_*(z,\delta)$ is constructed in the same way as $\rho(z,\delta)$, by replacing $Q(t,\delta)$ and $H(t,\delta)$ by $Q_{N^*}(t,\delta)$ and $H_{N^*}(t,\delta)$ in (6.56). Because of the relation (6.53), obtained by perturbation theory, we can write

$$\rho_*(z,\delta) = \rho(z,\delta) + R_*(z,\delta,\varepsilon) \tag{6.68}$$

where $R_*(z,\delta,\varepsilon)$ is a rest satisfying

$$|R_*(z,\delta,\varepsilon)| \leq \varepsilon b(t) \quad \forall z = t + is \in S_a, \tag{6.69}$$

where $b(t)$ is an integrable decay function independent of δ.

Proposition 6.2.3 *There exists ε^* and δ^*, independent of δ and ε respectively, such that for all $\varepsilon < \varepsilon^*$, $\delta < \delta^*$*
i) if $\delta > 0$, there exists a unique complex eigenvalue crossing point $z_0^*(\delta)$ of $e_j^*(z,\delta)$ with $\text{Im}z_0^*(\delta) > 0$ *in S_a,*
ii) if $\delta = 0$, there exists a unique real eigenvalue crossing point $z_0^*(0)$ of $e_j^*(z,0)$.
In any case $|z_0^*(\delta)| < r$.

Proof: We assume that $\delta > 0$ and we choose ε, independently of δ, in such a way that

$$|\rho_*(z,\delta) - \rho(z,\delta)| \leq \frac{R}{3} \quad \forall z \in S_a \backslash D(0,r), \quad \forall \delta \in I_\Delta. \tag{6.70}$$

As

$$\lim_{\varepsilon \to 0} e_j^*(t,\delta) = e_j(t,\delta), \tag{6.71}$$

the real eigenvalue crossing points, if any, must appear by pairs in order to to have $e_1^*(-\infty,\delta) < 0$ and $e_1^*(+\infty,\delta) < 0$. Recall that $H_{N^*}(t,\delta)$ and $H(t,\delta)$ coincide at infinity. To show that actually there is no real eigenvalue crossing point we use the fact that ((6.66), (6.70))

$$|\rho_*(z,\delta) - \rho(z,0)| \leq \frac{2R}{3} < |\rho(z,0)| \tag{6.72}$$

if $z \in \partial D(0,r)$ and we apply Rouché's theorem to

$$\rho_*(z,\delta) = \rho(z,\delta) + (\rho_*(z,\delta) - \rho(z,0)). \tag{6.73}$$

As there is one double zero of $\rho(z,0)$ in $D(0,r)$, at $z = 0$, there are either two simple conjugate zeros $z_0^*(\delta)$ and $\overline{z_0^*(\delta)}$ or only one real double zero of $\rho_*(z,\delta)$ in $D(0,r)$. But the latter case must be excluded because this corresponds to one crossing only. Recall that a real crossing corresponds to a double zero of $\rho^*(z,\delta)$ because of the analyticity of the eigenvalues at that point. If $\delta = 0$, the same type of argument shows that there is one real double zero $z_0^*(0)$ of $\rho_*(z,0)$, in order to insure $e_1^*(-\infty,0) < 0$ and $e_1^*(+\infty,0) > 0$, which corresponds to one real crossing of eigenvalue.

□

Let us define $\Delta_{12}^*(z,\delta)$ by

$$\Delta_{12}^*(z,\delta) = -\int_0^z \sqrt{\rho_*(u,\delta)}du \tag{6.74}$$

which yields an analytic function in $S_a^+ \backslash D(0,r)$. The path of integration is the same as the one defining $\Delta_{12}(z,\delta)$. A direct consequence of propositions (6.2.2) and (6.2.3) is that for any $0 < \delta < \delta^*$ and $\varepsilon < \varepsilon^*$ we can apply the complex time method to the effective two-level problem (6.51). Indeed, the main points to apply this technique are to have a complex eigenvalue crossing point $z_0^*(\delta)$ and to control the quantity

$$\exp\left\{\frac{1}{\varepsilon}\mathrm{Im}\left(\Delta_{12}^*(\gamma_\delta(s),\delta)-\Delta_{12}^*(\gamma_\delta(t),\delta)\right)\right\} \tag{6.75}$$

where $s \leq t$ (see (4.74)). We can do this uniformly in δ and ε since it follows from (6.53) that

$$\mathrm{Im}\Delta_{12}^*(z,\delta) = \mathrm{Im}\Delta_{12}(z,\delta) + \mathcal{O}(\varepsilon) \tag{6.76}$$

and by construction $\mathrm{Im}\Delta_{12}(z,\delta)$ is non decreasing along γ_δ. Hence (6.75) is uniformly bounded in $s \leq t$, ε and δ. We define a loop β based at the origin by the path going from 0 to $-r$ along the real axis, from $-r$ to r along $\partial D(0,r)$ and from r back to the origin along the real axis again. By proposition (6.2.3), $z_0^*(\delta)$ does not belong to β, for any $\delta > 0$. To obtain the asymptotic formula for $\widehat{\mathcal{P}_{21}}(\varepsilon,\delta)$ (see (4.78))

$$\widehat{\mathcal{P}_{21}}(\varepsilon,\delta) = \exp\left\{\frac{2}{\varepsilon}\mathrm{Im}\int_\beta e_1^*(z,\delta)dz\right\}\exp\left\{2\mathrm{Im}\theta_1^*(\delta)\right\}(1+\mathcal{O}(\varepsilon)) \tag{6.77}$$

where $\theta_1^*(\delta)$ is defined in (6.81) with a correction term $\mathcal{O}(\varepsilon)$ independent of δ, it remains to check that along the dissipative path $\gamma_\delta(t)$, we can bound the corresponding coefficients $a_{kj}^*(z,\delta)$ uniformly in δ (see (4.74)). In our case, these coefficients are defined as (see (4.24))

$$a_{kj}^*(z,\delta) = i\langle\varphi_k^*(0,\delta)|\widehat{W_*}^{-1}(z,\delta)\widehat{K_*}(z,\delta)\widehat{W_*}(z,\delta)\varphi_j^*(0,\delta)\rangle \tag{6.78}$$

where $\varphi_k^*(0,\delta)$, $k=1,2$, is a pair of normalized eigenvectors of $\widehat{H_*}(0,\delta)Q_{N^*}(0,\delta)$,

$$\widehat{K_*}(z,\delta) = Q_{N^*}(0,\delta)i[\widehat{P_1^*}'(z,\delta),\widehat{P_1^*}(z,\delta)]Q_{N^*}(0,\delta) \tag{6.79}$$

and

$$i\widehat{W_*}'(z,\delta) = \widehat{K_*}(z,\delta)\widehat{W_*}(z,\delta), \quad \widehat{W_*}(0,\delta) = \mathbb{I}_{Q_{N^*}(0,\delta)\mathcal{H}}. \tag{6.80}$$

Lemma 6.2.5 *There exists an integrable decay function $b(t)$ independent of δ and ε such that*

$$|a_{kj}^*(z,\delta)| \leq b(t) \quad \forall z = t+is \in S_a^+\backslash D(0,r).$$

This lemma shows that formula (6.77) is indeed true for the effective two-level problem (6.51) with a correction term independent of δ. The proof is given in appendix.

Let us denote the intersection of $\partial D(0,r)$ with the upper half plane by C_r^+. We can replace β in the integral of (6.77) by C_r^+ without altering the formula, so that we have to evaluate $e_1^*(z,\delta)$, on C_r^+, far from the eigenvalue crossing point $z_0(\delta)$. Moreover, $\theta_1^*(\delta)$ is given by (see (5.98))

$$\widetilde{\varphi_1^*}(0,\delta) = \exp\left\{-i\theta_1^*(\delta)\right\}\varphi_2^*(0,\delta) \tag{6.81}$$

where $\varphi_j^*(z,\delta)$ are the eigenvectors of $H_{N^*}(z,\delta)$ associated with $e_j^*(z,\delta)$, whose phases are fixed by $\langle\varphi_j^*(t,\delta)|\varphi_j^{*\prime}(t,\delta)\rangle \equiv 0$, $\forall t \in \mathbb{R}$. Since these vectors are normalized on the real axis, $\exp\left\{\mathrm{Im}\theta_1^*(\delta)\right\}$ represents the change of norm of the analytic continuation of $\varphi_1^*(z,\delta)$ from $-r$ to r along C_r^+. For any $z \in C_r^+$ we can use perturbation theory to obtain as in the previous section

$$\begin{aligned}\mathrm{Im}\int_\beta e_1^*(z,\delta)dz &= \mathrm{Im}\int_\beta e_1(z,\delta)dz + \mathcal{O}(\varepsilon)\\ \mathrm{Im}\theta_1^*(\delta) &= \mathrm{Im}\theta_1(\delta) + \mathcal{O}(\varepsilon)\end{aligned} \tag{6.82}$$

where $\theta_1(\delta)$ is defined by (6.81) with $\varphi_1(z,\delta)$, the eigenvector of $H(z,\delta)$ associated with $e_1(z,\delta)$, in place of $\varphi_1^*(z,\delta)$. Due to (6.38), the term $\mathcal{O}(\varepsilon)$ is uniformly bounded in δ.

Proposition 6.2.4 *Assume that conditions VIII to X hold and consider Im* $\int_\beta e_1(z,\delta)dz$ *and* $Im\theta_1(\delta)$ *defined above. Then*

$$\lim_{\delta\to 0}\mathrm{Im}\int_\beta e_1(z,\delta)dz = 0$$
$$\lim_{\delta\to 0}\mathrm{Im}\theta_1(\delta) = 0.$$

Remark:
This last proposition implies that for δ small enough

$$\left|2\mathrm{Im}\int_\beta e_1(z,\delta)dz\right| < \tau, \tag{6.83}$$

τ being the exponential decay rate of the correction term in proposition (6.2.1). Thus we have

$$\mathcal{P}_{21}(\varepsilon,\delta) = \exp\left\{\frac{2}{\varepsilon}\mathrm{Im}\int_\beta e_1(z,\delta)dz\right\}\exp\left\{2\mathrm{Im}\theta_1(\delta)\right\}(1+\mathcal{O}(\varepsilon)) \tag{6.84}$$

for ε and δ small enough. This proves the first assertion of theorem (6.1.1).
Proof: The geometrical interpretation of (6.84) given in theorem (4.1.1) yields

$$\left|\mathrm{Im}\int_\beta e_1(z,\delta)dz\right| = |\mathrm{Im}\Delta_{12}(z_0(\delta),\delta)| = \mathrm{d}_\rho(z_0(\delta),\mathbb{R}). \tag{6.85}$$

As $\rho(z,\delta)\to\rho(z,0)$ and $z_0(\delta)\to 0$ when $\delta\to 0$ (proposition (6.2.2)), we get

$$\lim_{\delta\to 0}\mathrm{d}_\rho(z_0(\delta),\mathbb{R}) = 0. \tag{6.86}$$

Let us introduce $\widehat{W}(z,t;\delta)$, $z\neq z_0(\delta)$, $t\in\mathbb{R}$, by

$$\begin{aligned} i\widehat{W}'(z,t;\delta) &= i\left(P_1'(z,\delta)P_1(z,\delta)+P_2'(z,\delta)P_2(z,\delta)-Q'(z,\delta)(\mathbb{I}-Q(z,\delta))\right)\widehat{W}(z,t;\delta) \\ &\equiv \widehat{K}(z,\delta)\widehat{W}(z,t;\delta),\quad \widehat{W}(t,t;\delta)=\mathbb{I}. \end{aligned} \tag{6.87}$$

We have

$$\varphi_1(z,\delta) = \widehat{W}(z,0;\delta)\varphi_1(0,\delta), \tag{6.88}$$

where $\varphi_1(0,\delta)$ satisfies

$$H(0,\delta)\varphi_1(0,\delta) = e_1(0,\delta)\varphi_1(0,\delta),\quad \|\varphi_1(0,\delta)\| = 1. \tag{6.89}$$

Moreover, as noted previously

$$\|\widehat{W}(r,-r;\delta)\varphi_1(-r,\delta)\| = \exp\left\{\mathrm{Im}\theta_1(\delta)\right\} \tag{6.90}$$

where the path of integration of $\widehat{W}(r,-r,\delta)$ from $-r$ to r is along C_r^+. Let us show that

$$\widehat{W}(r,-r;\delta)\to\widehat{W}(r,-r;0) \tag{6.91}$$

strongly as $\delta\to 0$. Consider the identity

$$\begin{aligned} &\left(\widehat{W}^{-1}(z,-r;\delta)\widehat{W}(z,-r;0)-\mathbb{I}\right)\varphi = \\ &i\int_{-r}^{z}\widehat{W}^{-1}(z',-r;\delta)\left(\widehat{K}(z',0)-\widehat{K}(z',\delta)\right)\widehat{W}(z',-r;0)\varphi dz' \end{aligned} \tag{6.92}$$

where z and the path of integration are along C_r^+. It follows from condition VIII (see lemma (6.2.3)), that $\widehat{K}(z,\delta)$ is strongly continuous in z and δ, $\forall z \in S_a^+ \backslash D(0,r)$ so that, by compactness of C_r^+, $\widehat{K}(z,\delta)\varphi$ tends to $\widehat{K}(z,0)\varphi$ uniformly in $z \in C_r^+$ when $\delta \to 0$ and

$$\sup_{\substack{z\in C_r^+\\ \delta\in I_\Delta}} \|\widehat{W}(z,-r;\delta)\| \leq w', \quad \sup_{\substack{z\in C_r^+\\ \delta\in I_\Delta}} \|\widehat{W}^{-1}(z,-r;\delta)\| \leq w'. \tag{6.93}$$

Now, the set of vectors

$$\left\{\widehat{W}(z',-r;0)\varphi; \quad z' \in C_r^+\right\} \tag{6.94}$$

is a compact set in $\mathcal{H}$ because $\widehat{W}(z',-r;0)$ is continuous in z' so that we apply lemma (3.4) of the introduction of [Kr] to obtain

$$\lim_{\delta\to 0} \sup_{z'\in C_r^+} \| \left(\widehat{K}(z',\delta) - \widehat{K}(z',0)\right) \widehat{W}^{-1}(z',-r;0)\varphi\| = 0. \tag{6.95}$$

As a consequence

$$\begin{aligned}
&\| \left(\widehat{W}(z,-r;0) - \widehat{W}(z,-r;\delta)\right) \varphi\| \leq \\
&\|\widehat{W}(z,-r;\delta)\|\|\| \left(\widehat{W}^{-1}(z,-r;0)\widehat{W}(z,-r;0) - I\!I\right) \varphi\| \leq \\
&w'^2\pi r \sup_{z'\in C_r^+} \| \left(\widehat{K}(z',\delta) - \widehat{K}(z',0)\right) \widehat{W}^{-1}(z,-r;0)\varphi\|
\end{aligned} \tag{6.96}$$

showing that $\widehat{W}(z,-r,\delta)$ is strongly continuous in δ on C_r^+. Moreover, we can construct a normalized eigenvector $\varphi_1(-r,\delta)$ of $H(-r,\delta)$ which is continuous in δ by

$$\varphi_1(-r,\delta) = \frac{P_1(-r,\delta)\varphi_1(-r,0)}{\langle\varphi_1(-r,0)|P_1(-r,\delta)\varphi_1(-r,0)\rangle} \tag{6.97}$$

where $H(-r,0)\varphi_1(-r,0) = e_1(-r,0)\varphi_1(-r,0)$. Hence the estimate

$$\begin{aligned}
&\|\widehat{W}(z,-r;\delta)\varphi_1(-r,\delta) - \widehat{W}(z,-r;0)\varphi_1(-r,0)\| \leq \\
&\| \left(\widehat{W}(z,-r;\delta) - \widehat{W}(z,-r;0)\right) \varphi_1(-r,0)\| + \\
&\|\widehat{W}(z,-r;\delta) \left(\varphi_1(-r,\delta) - \varphi_1(-r,0)\right) \|
\end{aligned} \tag{6.98}$$

from which follows that

$$\widehat{W}(z,-r;\delta)\varphi_1(-r,\delta) \to \widehat{W}(z,-r;0)\varphi_1(-r,0) \tag{6.99}$$

as $\delta \to 0$. Since for $\delta = 0$, $\widehat{W}(z,-r;0)$ is analytic for any z in $D(0,r)$, $\widehat{W}(+r,-r;0)$ integrated along C_r^+ coincides with $\widehat{W}(+r,-r;0)$ integrated along the real axis. Thus this operator is unitary and we have $\|\widehat{W}(+r,-r;0)\varphi_1(-r,0)\| = 1$, which together with (6.90) imply

$$\lim_{\delta\to 0} \mathrm{Im}\theta_1(\delta) = 0. \tag{6.100}$$

□

6.2.4 Expansion in δ

Let us turn finally to the last assertion of theorem (6.1.1) which deals with the actual computation of $\mathrm{Im} \int_\beta e_1(z,\delta)dz$ and $\mathrm{Im}\theta_1(\delta)$ to the lowest order in δ, when hypothesis XI is fulfilled.

Proposition 6.2.5 *Under hypothesis VIII to XI we have*

$$\begin{aligned} 2\mathrm{Im} \int_\beta e_1(z,\delta)dz &= -\delta^2 \frac{\pi}{2}\left(\frac{b^2}{a} - \frac{c^2}{a^3}\right)(1 + \mathcal{O}(\delta)) \\ 2\mathrm{Im}\theta_1(\delta) &= \mathcal{O}(\delta). \end{aligned}$$

Proof: By condition XI we have

$$\rho(z,\delta) = a^2 z^2 + 2c\delta z + b^2\delta^2 + R_3(z,\delta) \tag{6.101}$$

with

$$c^2 < a^2 b^2 \tag{6.102}$$

where $R_3(z,\delta)$ is analytic and satisfies

$$|R_3(z,\delta)| \le k(|z^2| + \delta^2)(|z| + \delta) \tag{6.103}$$

for k some constant. There will appear several other constants in the sequel, which we shall denote generically by the same letter k. Let $C_{x\delta}$ be the circle centered at the origin of radius $x\delta$, where x is some real parameter. We can write

$$\begin{aligned} |a^2z^2 + 2c\delta z + b^2\delta^2| &= \left| a^2\left(z + \frac{c\delta}{a^2}\right)^2 + \left(b^2 - \frac{c^2}{a^2}\right)\delta^2 \right| \\ &\ge \left| a^2\left|z + \frac{c\delta}{a^2}\right|^2 - \left|b^2 - \frac{c^2}{a^2}\right|\delta^2 \right|. \end{aligned} \tag{6.104}$$

If x is large enough, $x\delta > \frac{|c|\delta}{a^2}$, and we have for any $z \in C_{x\delta}$

$$\left|z + \frac{c\delta}{a^2}\right| \ge \left||z| - \left|\frac{c\delta}{a^2}\right|\right| \ge \left(x - \frac{|c|}{a^2}\right)\delta. \tag{6.105}$$

Thus we can always choose x sufficiently large so that

$$a^2\left|z + \frac{c\delta}{a^2}\right|^2 - \left|b^2 - \frac{c^2}{a^2}\right|\delta^2 \ge \left(a^2\left(x - \frac{|c|}{a^2}\right)^2 - \left(b^2 - \frac{c^2}{a^2}\right)\right)\delta^2 \ge k\delta^2 > 0 \tag{6.106}$$

where k is independent of δ and arrive at the conclusion that for any $z \in C_{x\delta}$

$$|a^2z^2 + 2c\delta z + b^2\delta^2| \ge k\delta^2, \tag{6.107}$$

whereas

$$|R_3(z,\delta)| \le k\delta^3. \tag{6.108}$$

on the same circle. By applying Rouché's theorem for δ small enough we have that

$$\zeta_\pm = -\frac{c\delta}{a^2} \pm i\frac{\sqrt{a^2b^2 - c^2}}{a^2}\delta, \tag{6.109}$$

the zeros of $a^2z^2 + 2c\delta z + b^2\delta^2$, and $z_0(\delta)$, $\overline{z_0(\delta)}$ are in $C_{x\delta}$. Moreover, $\forall z \in C_{x\delta}$,

$$\begin{aligned}\sqrt{\rho(z,\delta)} &= \sqrt{a^2z^2 + 2c\delta z + b^2\delta^2\left(1 + \frac{R_3(z,\delta)}{a^2z^2 + 2c\delta z + b^2\delta^2}\right)} \\ &\equiv \sqrt{a^2z^2 + 2c\delta z + b^2\delta^2}(1 + h(z,\delta)) \qquad (6.110)\end{aligned}$$

where $|h(z,\delta)|_{z\in C_{x\delta}} \leq k\delta$, since

$$\left|\frac{R_3(z,\delta)}{a^2z^2 + 2c\delta z + b^2\delta^2}\right| \leq k\delta \quad \forall z \in C_{x\delta}. \qquad (6.111)$$

From these last estimates we can write

$$\begin{aligned}2\text{Im}\int_\beta e_1(z,\delta)dz &= -\text{Im}\int_{C^+_{x\delta}} \sqrt{\rho(z,\delta)}dz \\ &= -\text{Im}\int_{C^+_{x\delta}} \sqrt{a^2z^2 + 2c\delta z + b^2\delta^2}dz + \mathcal{O}(\delta^3). \qquad (6.112)\end{aligned}$$

Finally, we compute by deforming the path of integration to a vertical segment going from $z = \text{Re}\zeta_+$ to $z = \zeta_+$ and back to $z = \text{Re}\zeta_+$,

$$\begin{aligned}-\text{Im}\int_{C^+_{x\delta}} \sqrt{a^2z^2 + 2c\delta z + b^2\delta^2}dz &= -2\int_0^{\frac{1}{a^2}\sqrt{a^2b^2-c^2}\delta} \sqrt{\left(b^2 - \frac{c^2}{a^2}\right)\delta^2 - y^2a^2dy} \\ &= -\delta^2\frac{\pi}{2}\left(\frac{b^2}{a} - \frac{c^2}{a^3}\right). \qquad (6.113)\end{aligned}$$

To bound $\text{Im}\theta_1(\delta)$ by a term of order δ, we need a little more work. The first step is to derive a formula for $\text{Im}\theta_1(\delta)$ of the type given in proposition (4.1.1).

Proposition 6.2.6 *Let $\psi_j(t,\delta)$, $j = 1,2,3$ and $B_k(t,\delta)$ be defined by (6.54) and (6.56) respectively and assume that conditions VIII to X hold. Then*

$$\begin{aligned}&\text{Im}\theta_1(\delta) = \text{Im}\int_\sigma \frac{B_3(z,\delta)\left(B_1(z,\delta)B_2'(z,\delta) - B_2(z,\delta)B_1'(z,\delta)\right)}{2\sqrt{\rho(z,\delta)}\left(B_1^2(z,\delta) + B_2^2(z,\delta)\right)}dz \\ &+\text{Re}\int_\sigma \left(\frac{B_3(z,\delta)}{2\sqrt{\rho(z,\delta)}}(\langle\psi_1(z,\delta)|\psi_1'(z,\delta)\rangle - \langle\psi_2(z,\delta)|\psi_2'(z,\delta)\rangle)\right. \\ &\left.+\frac{B_1(z,\delta) + iB_2(z,\delta)}{2\sqrt{\rho(z,\delta)}}\langle\psi_1(z,\delta)|\psi_2'(z,\delta)\rangle + \frac{B_1(z,\delta) - iB_2(z,\delta)}{2\sqrt{\rho(z,\delta)}}\langle\psi_2(z,\delta)|\psi_1'(z,\delta)\rangle\right)\end{aligned}$$

where the path σ encircles $z_0(\delta)$ and contains no zero of $B_1^2(z,\delta) + B_2^2(z,\delta)$.

Remark:
This formula is of course true when the hamiltonian is independent of δ, as in theorem (5.2.1).
Proof: We introduce the vectors

$$\begin{aligned}\chi_j(t,\delta) &= \left(B_3(t,\delta) + (-1)^j\sqrt{\rho(t,\delta)}\right)\psi_1(t,\delta) + \left(B_1(t,\delta) + iB_2(t,\delta)\right)\psi_2(t,\delta) \\ &\equiv \alpha_j(t,\delta)\psi_1(t,\delta) + \beta(t,\delta)\psi_2(t,\delta), \quad j = 1,2, \qquad (6.114)\end{aligned}$$

which satisfy by construction

$$H(t,\delta)\chi_j(t,\delta) = e_j(t,\delta)\chi_j(t,\delta), \quad j = 1,2. \qquad (6.115)$$

Moreover, their analytic continuations along σ, from the origin back to the origin, are given by

$$\widetilde{\chi_j}(0,\delta) = \chi_k(0,\delta) \tag{6.116}$$

since the components $B_k(t,\delta)$ and the basis vectors $\psi_j(t,\delta)$ have analytic continuations in a neighbourhood of the origin, even at $z = z_0(\delta)$. As in paragraph (4.1.4) we write the eigenvector $\varphi_j(t,\delta)$ satisfying $\langle\varphi_j(t,\delta)|\varphi_j'(t,\delta)\rangle \equiv 0$ under the form

$$\varphi_j(t,\delta) \equiv \exp\{-i\delta_j(t,\delta)\}\,\chi_j(t,\delta), \quad j = 1,2 \tag{6.117}$$

with $\exp\{i\delta_j(0,\delta)\} = \|\chi_j(0,\delta)\|$. It then follows from (6.116) that

$$\mathrm{Im}\theta_1(\delta) = \mathrm{Im}\left(\int_\sigma \delta_1'(z,\delta) + \delta_1(0,\delta) - \delta_2(0,\delta)\right). \tag{6.118}$$

We have by the same argument as in paragraph (4.1.4) (see (4.58))

$$i\delta_j'(t,\delta) = \frac{\langle\chi_j(t,\delta)|\chi_j'(t,\delta)\rangle}{\langle\chi_j(t,\delta)|\chi_j(t,\delta)\rangle} \quad \forall t \in I\!R. \tag{6.119}$$

Due to the time dependence of the basis vectors $\psi_j(t,\delta)$, we obtain here for δ_j' (without expliciting the arguments (t,δ), $t \in I\!R$)

$$\begin{aligned} i\delta_j' &= \frac{1}{|\alpha_j|^2+|\beta|^2}\left(\overline{\alpha_j}\alpha_j' + \overline{\beta}\beta'\right) + \frac{1}{|\alpha_j|^2+|\beta|^2}\left\{|\alpha_j|^2\langle\psi_1|\psi_1'\rangle\right. \\ &+ \left.|\beta|^2\langle\psi_2|\psi_2'\rangle + \overline{\alpha_j}\beta\langle\psi_1|\psi_2'\rangle + \overline{\beta}\alpha_j\langle\psi_2|\psi_1'\rangle\right\}. \end{aligned} \tag{6.120}$$

The first term coincides with the previously computed one in paragraph (4.1.4). Using the self adjointness of $Q(t,\delta)$ for $t \in I\!R$, we check that the functions

$$\langle\psi_j(t,\delta)|\psi_k'(t,\delta)\rangle \quad t \in I\!R \tag{6.121}$$

have analytic continuations close to the origin, even at $z = z_0(\delta)$, which we denote by

$$\langle\psi_j|\psi_k'\rangle(z,\delta). \tag{6.122}$$

Multiplying (6.120) by $\frac{\sqrt{\rho}+B_3}{\sqrt{\rho}+B_3}$, using proposition (4.1.1) and (6.118) we obtain

$$\begin{aligned} \mathrm{Im}\theta_1(\delta) &= \mathrm{Im}\int_\sigma \frac{B_3\,(B_1B_2' - B_2B_1')}{2\sqrt{\rho}\,(B_1^2+B_2^2)}dz \\ &+\mathrm{Re}\int_\sigma\left(\frac{(B_3-\sqrt{\rho})(B_1^2+B_2^2)}{2\sqrt{\rho}(B_1^2+B_2^2)}\langle\psi_1|\psi_1'\rangle - \frac{(B_3+\sqrt{\rho})(B_1^2+B_2^2)}{2\sqrt{\rho}(B_1^2+B_2^2)}\langle\psi_2|\psi_2'\rangle\right) \\ &+\frac{(B_1^2+B_2^2)(B_1+iB_2)}{2\sqrt{\rho}(B_1^2+B_2^2)}\langle\psi_1|\psi_2'\rangle + \frac{(B_1^2+B_2^2)(B_1-iB_2)}{2\sqrt{\rho}(B_1^2+B_2^2)}\langle\psi_2|\psi_1'\rangle\Bigg) \end{aligned} \tag{6.123}$$

for a path σ containing no zero of $(B_1^2 + B_2^2)$. This proves the proposition.

□

Our condition XI implies that the analytic functions $B_j(z,\delta)$ defined by (6.56) have the form

$$B_j(z,\delta) = a_jz + b_j\delta + R_2(z,\delta) \tag{6.124}$$

where the real constants a_j and b_j satisfy

$$\sum_{j=1}^{3} a_j^2 = a^2, \quad \sum_{j=1}^{3} b_j^2 = b^2, \quad \sum_{j=1}^{3} a_j b_j = c \tag{6.125}$$

and $R_2(z,\delta)$ is a rest of order two in (z,δ). Again we shall replace the path σ by $C^+_{x\delta}$ since on the real axis, the integrals in proposition (6.2.6) do not contribute to $\mathrm{Im}\theta_1(\delta)$. But here some care must be taken for the first integral since the integrand has poles at the zeros of $B_1^2(z,\delta)+B_2^2(z,\delta)$. But this is not the case for the other integrals in which the replacement of σ by $C^+_{x\delta}$ is justified. As on $C^+_{x\delta}$ we have (see (6.107))

$$|\sqrt{\rho(z,\delta)}| \geq k\delta, \quad |B_j(z,\delta)| \leq k\delta \quad \text{and} \quad |\langle\psi_j|\psi_k'\rangle(z,\delta)| \leq k, \tag{6.126}$$

we immediately obtain

$$\mathrm{Im}\theta_1(\delta) = \mathrm{Im}\int_\sigma \frac{B_3\,(B_1B_2' - B_2B_1')}{2\sqrt{\rho}\,(B_1^2+B_2^2)}dz + \mathcal{O}(\delta). \tag{6.127}$$

To deal with the first term, we introduce

$$\alpha = \sqrt{a_1^2+a_2^2}, \quad \beta = \sqrt{b_1^2+b_2^2} \quad \text{and} \quad \gamma = a_1b_1 + a_2b_2. \tag{6.128}$$

By the Cauchy-Schwartz inequality these quantities satisfy $|\gamma| \leq \alpha\beta$. Actually, we can assume without loss of generality that

$$0 < |\gamma| < \alpha\beta. \tag{6.129}$$

Indeed, the equality $|\gamma| = \alpha\beta$ implies

$$a_1 = yb_1, \quad a_2 = yb_2 \tag{6.130}$$

for some $y \neq 0$. This cannot be the case for any couple of indices since it would imply $a_3 = yb_3$ as well, in contradiction with the condition $|c| < ab$. Thus we can always perform a change of basis vectors, which amounts to write $H(t,\delta)Q(t,\delta)$ in a new basis $\{S\psi_1(t,\delta), S\psi_2(t,\delta)\}$ instead of $\{\psi_1(t,\delta),\psi_2(t,\delta)\}$, where S is a unitary matrix, so that the components of the new field are such that (6.129) is verified. With these definitions and (6.124) we can rewrite

$$B_1^2(z,\delta) + B_2^2(z,\delta) = \alpha^2z^2 + 2\gamma\delta z + \beta^2\delta^2 + R_3(z,\delta). \tag{6.131}$$

As previously we have, for $z \in C^+_{x\delta}$

$$\left|\alpha^2z^2 + 2\gamma\delta z + \beta^2\delta^2\right| \geq \left|\alpha^2\left|z + \frac{\gamma\delta}{\alpha^2}\right| - \left|\beta^2 - \frac{\gamma^2}{\alpha^2}\right|\delta^2\right| \tag{6.132}$$

where

$$\alpha^2\left|z + \frac{\gamma\delta}{\alpha^2}\right|^2 \geq \alpha^2\left(x - \frac{|\gamma|}{\alpha^2}\right)^2\delta^2 > \left|\beta^2 - \frac{\gamma^2}{\alpha^2}\right|\delta^2, \tag{6.133}$$

provided x is large enough, so that

$$\left|\alpha^2z^2 + 2\gamma\delta z + \beta^2\delta^2\right| \geq k\delta^2. \tag{6.134}$$

Hence,

$$|R_3(z,\delta)| \leq k\delta^3 < k\delta^2 \leq \left|\alpha^2 z^2 + 2\gamma\delta z + \beta^2\delta^2\right| \tag{6.135}$$

for δ small enough, $\forall z \in C^+_{x\delta}$. Then it follows from Rouché's theorem that $B_1^2(z,\delta) + B_2^2(z,\delta)$ has as many zeros in $C^+_{x\delta}$ as $\alpha^2 z^2 + 2\gamma\delta z + \beta^2\delta^2$, i.e. two $\zeta_0(\delta)$ and $\overline{\zeta_0(\delta)}$, counting multiplicities. Indeed, the roots of $\alpha^2 z^2 + 2\gamma\delta z + \beta^2\delta^2$ are given by $\xi_\pm$,

$$\xi_\pm = -\frac{\gamma\delta}{\alpha^2} \pm i\frac{\sqrt{\alpha^2\beta^2 - \gamma^2}}{\alpha^2}\delta \tag{6.136}$$

which belong to $C_{x\delta}$ if x is large enough. Note that due to (6.129), $\mathrm{Im}\xi_+ > 0$. Now we can replace the contour of integration σ in (6.127) by $C^+_{x\delta}$, provided we take the residue at $\zeta_0(\delta)$ into account. Consider first the case where $\zeta_0(\delta) \neq \overline{\zeta_0(\delta)}$. Since $\mathrm{Im}\zeta_0(\delta) > 0$, we have

$$\begin{aligned}\mathrm{Im}\theta_1(\delta) &= 2\pi\mathrm{Re}\left(\mathrm{Res}\left(\frac{B_3\,(B_1B_2' - B_2B_1')}{2\sqrt{\rho}\,(B_1^2 + B_2^2)}, \zeta_0(\delta)\right)\right) \\ &+\mathrm{Im}\int_{C^+_{x\delta}} \frac{(a_3 z + b_3\delta)(a_2b_1 - a_1b_2)\delta + R_3(z,\delta)}{2\sqrt{a^2z^2 + 2c\delta z + b^2\delta^2}(\alpha^2z^2 + 2\gamma\delta z + \beta^2\delta^2 + R_3(z,\delta))(1 + h(z,\delta))}dz\end{aligned} \tag{6.137}$$

where $|h(z,\delta)| \leq k\delta$ (see (6.110)) and $\mathrm{Res}(f, z_0)$ is the residue of $f(z)$ at the point z_0. In view of (6.134) and (6.110), we can estimate the remaining integral by

$$\mathrm{Im}\int_{C^+_{x\delta}} \frac{(a_3z + b_3\delta)(a_2b_1 - a_1b_2)\delta}{2\sqrt{a^2z^2 + 2c\delta z + b^2\delta^2}(\alpha^2z^2 + 2\gamma\delta z + \beta^2\delta^2)} + \mathcal{O}(\delta) \tag{6.138}$$

when δ is small. The integrand is now singular at ζ_+ and ξ_+ only, which both belong to $C^+_{x\delta}$, when x is large. Thus we can replace the contour of integration $C^+_{x\delta}$ by C^+_R, the half circle of radius R, which will ultimately tend to infinity, since on the real axis the integral is real. On C^+_R we have the estimates

$$|a^2z^2 + 2c\delta z + b^2\delta^2| = |z^2|\left|a^2 + \frac{2c\delta}{z} + \frac{b^2\delta^2}{z^2}\right| \geq k(\delta)R^2 \tag{6.139}$$

and

$$|\alpha^2z^2 + 2\gamma\delta z + \beta^2\delta^2| \geq k(\delta)R^2 \tag{6.140}$$

which imply

$$\left|\int_{C^+_R} \frac{(a_3z + b_3\delta)(a_2b_1 - a_1b_2)\delta}{2\sqrt{a^2z^2 + 2c\delta z + b^2\delta^2}(\alpha^2z^2 + 2\gamma\delta z + \beta^2\delta^2)}\right| \leq \frac{k(\delta)}{R}. \tag{6.141}$$

Taking the limit $R \to \infty$ we are left with

$$\mathrm{Im}\theta_1(\delta) = 2\pi\mathrm{Re}\left(\mathrm{Res}\left(\frac{B_3\,(B_1B_2' - B_2B_1')}{2\sqrt{\rho}\,(B_1^2 + B_2^2)}, \zeta_0(\delta)\right)\right) + \mathcal{O}(\delta). \tag{6.142}$$

The residue is given here by the formula

$$\begin{aligned}\left.\frac{B_3\,(B_1B_2' - B_2B_1')}{4\sqrt{\rho}\,(B_1B_1' + B_2B_2')}\right|_{\zeta_0(\delta)} &= \varepsilon_1\left.\frac{(B_1B_2' - B_2B_1')}{4\,(B_1B_1' + B_2B_2')}\right|_{\zeta_0(\delta)} = \\ \varepsilon_1\varepsilon_2\left.\frac{i\,(B_2B_2' + B_1B_1')}{4\,(B_1B_1' + B_2B_2')}\right|_{\zeta_0(\delta)} &= \pm\frac{i}{4}\end{aligned} \tag{6.143}$$

where we have used the fact that

$$B_1^2(\zeta_0(\delta),\delta)+B_2^2(\zeta_0(\delta),\delta)=0, \tag{6.144}$$

so that

$$\sqrt{\rho(\zeta_0(\delta),\delta)}=\sqrt{B_3^2(\zeta_0(\delta),\delta)}=\varepsilon_1 B_3(\zeta_0(\delta),\delta) \tag{6.145}$$

where $\varepsilon_1=\pm 1$ and

$$B_1(\zeta_0(\delta),\delta)=\varepsilon_2 i B_2(\zeta_0(\delta),\delta) \tag{6.146}$$

with $\varepsilon_2=\pm 1$ as well. Hence

$$\text{Im}\theta_1(\delta)=\mathcal{O}(\delta). \tag{6.147}$$

Consider now the case $\zeta_0(\delta)=\overline{\zeta_0(\delta)}$. We come back to (6.127) and we use the fact that $B_j(\overline{z},\delta)=\overline{B_j}(z,\delta)$ by Schwartz's principle and that $z_0(\delta)$ a simple żero $\rho(z,\delta)$ to write

$$\text{Im}\theta_1(\delta)=\frac{1}{2}\text{Im}\int_{\sigma\cup\overline{\sigma}}\frac{B_3\,(B_1B_2'-B_2B_1')}{2\sqrt{\rho}\,(B_1^2+B_2^2)}+\mathcal{O}(\delta) \tag{6.148}$$

where $\sigma\cup\overline{\sigma}$ form a closed path surrounding $\zeta_0(\delta)$ and $\overline{\zeta_0(\delta)}$ (see figure (6.3)). By the same

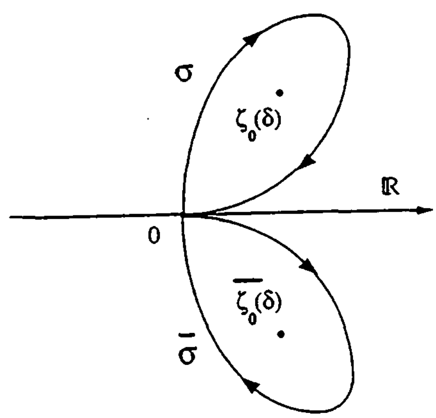

Figure 6.3: The integration path $\sigma\cup\overline{\sigma}$.

argument as before, we have

$$\text{Im}\theta_1(\delta)=\pi\text{Re}\left(\text{Res}\left(\frac{B_3\,(B_1B_2'-B_2B_1')}{2\sqrt{\rho}\,(B_1^2+B_2^2)},\zeta_0(\delta)\right)\right)+\mathcal{O}(\delta). \tag{6.149}$$

The residue is now given by

$$2\frac{d}{dz}\left(\frac{B_3\,(B_1B_2'-B_2B_1')}{2\sqrt{\rho}}\right)\left.\frac{1}{\frac{d^2}{dz^2}\,(B_1^2+B_2^2)}\right|_{\zeta_0(\delta)}, \tag{6.150}$$

since $\zeta_0(\delta)$ is a double zero of $B_1^2+B_2^2$. Moreover, as it located on the real axis, this implies

$$B_1(\zeta_0(\delta))=B_2(\zeta_0(\delta))=0. \tag{6.151}$$

Thus

$$\left.\frac{d}{dz}\left(\frac{B_3\,(B_1B_2'-B_2B_1')}{2\sqrt{\rho}}\right)\right|_{\zeta_0(\delta)}=0 \tag{6.152}$$

and

$$\text{Im}\theta_1(\delta)=\mathcal{O}(\delta). \tag{6.153}$$

This last assertion ends the proof of proposition (6.2.5).

□

To bring the proof of theorem (6.1.1) to an end, it remains to show the existence of the dissipative path γ_δ of proposition (6.2.2).

6.2.5 Existence of a Dissipative Path γ_δ

Proof of proposition (6.2.2): To prove the existence of a dissipative path γ_δ for $\Delta_{12}(z,\delta)$, we first show that there exists a dissipative path γ_0 for $\Delta_{12}(z,0)$. When $\delta = 0$, the function

$$\Delta_{12}(z,0) = \int_0^z e_1(u,0) - e_2(u,0)du = -\int_0^z \sqrt{\rho(u,0)}du \tag{6.154}$$

is analytic in a neighbourhood of the real axis and behaves as z^2 close to the origin. We select the branch of the square root by requiring $\Delta_{12}(t,0) > 0$ if $t < 0$. The Stokes lines given by the level lines

$$\text{Im}\Delta_{12}(z,0) = 0 \tag{6.155}$$

are homeomorphic to the lines depicted in figure (6.4) in a neighbourhood of $z = 0$. As a

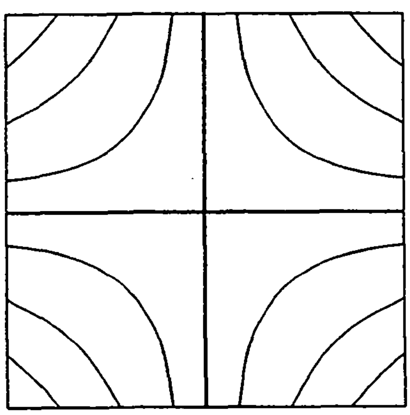

Figure 6.4: The level lines $\text{Im}z^2$ =cst.

consequence, there exist in this neighbourhood two points z_1 and z_2 above the real axis such that

$$\begin{aligned}\text{Im}\Delta_{12}(z_1,0) &= -\alpha \\ \text{Im}\Delta_{12}(z_2,0) &= +\alpha\end{aligned} \tag{6.156}$$

with $\alpha > 0$ small which are connected by the level line

$$\text{Re}\Delta_{12}(z,0) = \text{Re}\Delta_{12}(z_1,0). \tag{6.157}$$

Then, the idea is to take α small enough, and to complete this segment on the left by the level line $\text{Im}\Delta_{12}(z,0) = -\alpha$ and on the right by $\text{Im}\Delta_{12}(z,0) = +\alpha$ which connect z_1 to $-\infty$ in S_a and z_2 to $+\infty$ in S_a. If we can find such an α, we have at hand a path $\gamma_0(t)$, whose parameterization can be chosen such that $\gamma_0(t_1) = z_1$, $\gamma_0(t_2) = z_2$ which is dissipative for $\Delta_{12}(z,0)$ (see figure (6.5)). Indeed, we have for any path

$$\frac{d}{dt}\text{Im}\Delta_{12}(\gamma_0(t),0) = -\text{Re}\dot{\gamma}_0(t)\text{Im}\sqrt{\rho(\gamma_0(t),0)} - \text{Im}\dot{\gamma}_0(t)\text{Re}\sqrt{\rho(\gamma_0(t),0)} \tag{6.158}$$

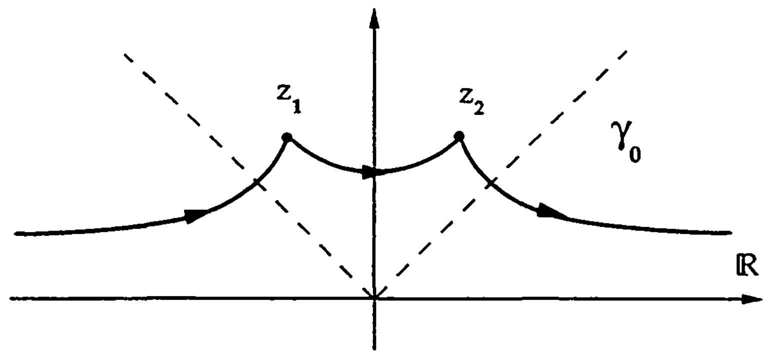

Figure 6.5: The dissipative path γ_0.

and

$$\frac{d}{dt}\mathrm{Re}\Delta_{12}(\gamma_0(t),0) = -\mathrm{Re}\dot{\gamma}_0(t)\mathrm{Re}\sqrt{\rho(\gamma_0(t),0)} + \mathrm{Im}\dot{\gamma}_0(t)\mathrm{Im}\sqrt{\rho(\gamma_0(t),0)}. \tag{6.159}$$

Thus, if we choose for $t \in [t_1, t_2]$

$$\begin{aligned} \mathrm{Re}\dot{\gamma}_0(t) &= -\mathrm{Im}\sqrt{\rho(\gamma_0(t),0)} \\ \mathrm{Im}\dot{\gamma}_0(t) &= -\mathrm{Re}\sqrt{\rho(\gamma_0(t),0)} \end{aligned} \tag{6.160}$$

then equation (6.159) is identically equal to 0 and

$$\frac{d}{dt}\mathrm{Im}\Delta_{12}(\gamma_0(t),0) = |\sqrt{\rho(\gamma_0(t),0)}|^2 > d > 0. \tag{6.161}$$

We can continue this path on the left and on the right as described by using the following

Lemma 6.2.6 *For any $\mu > 0$, there exists $\nu > 0$ such that on*

$$F_\pm = \left\{ z | \mathrm{Re} z \gtrless \pm\mu, \quad |\mathrm{Im} z| \leq \nu \right\}$$

the function $\Delta_{12}(z,0)$ is bijective.

Proof: Let $\mu > 0$. By continuity of $\rho(z,0)$ and condition X, we can chose ν sufficiently small to insure $\mathrm{Re}\sqrt{\rho(z,0)} > R > 0$ for any $z \in F_-$. Let us consider the rectangle $R_-(L)$ whose border is defined by

$$\partial R_-(L) = \partial\left(F_- \backslash \{z \,:\, \mathrm{Re} z \leq -L\}\right). \tag{6.162}$$

Along its horizontal segments we have that

$$\mathrm{Re}\Delta_{12}(t \pm i\nu) = \mathrm{Re}\Delta_{12}(-\mu \pm i\nu) + \int_{-\mu}^{t} dx \mathrm{Re}\sqrt{\rho(x \pm i\nu)} \tag{6.163}$$

is strictly monotonic. Similarly, along its vertical segments

$$\mathrm{Im}\Delta_{12}(-\mu \pm is) = \mathrm{Im}\Delta_{12}(-\mu) \pm \int_{0}^{s} dy \mathrm{Re}\sqrt{\rho(-\mu \pm iy)} \tag{6.164}$$

and $\mathrm{Im}\Delta_{12}(-L \pm is)$ are strictly monotonic as well. Thus the image by $\Delta_{12}(z,0)$ of $\partial R_-(L)$ is a simple closed curve so that we can apply the argument principle which shows that

$\Delta_{12}(z,0)$ is bijective on $R_-(L)$. Since the length L of the rectangle is arbitrary, this proves the first assertion of the lemma.

We proceed similarly for the positive part of the real axis and F_+.

□

We shall assume from now on that the width a of the strip S_a is smaller than ν. Now that we have constructed a dissipative path for $\Delta_{12}(z,0)$, we show that there exists a dissipative path for $\Delta_{12}(z,\delta)$ close to it. Let $D(0,r)$ be the disc centered at the origin whose radius r is such that $D(0,r)\cap\gamma_0=\emptyset$ and let $S_+(v)$ and $S_-(v)$ be tubular neighbourhoods of $\gamma_0(t)$ for $t>t_2$ and $t<t_1$ respectively, defined by their boundaries. These boundaries are given by the level lines

$$\begin{aligned}\partial S_-(v) &= \{z|\mathrm{Re}\Delta_{12}(z,0)\geq \mathrm{Re}\Delta_{12}(z_1,0),\ \ \mathrm{Im}\Delta_{12}(z,0)=-\alpha\pm v\}\\ &\cup\ \{z|\mathrm{Re}\Delta_{12}(z,0)=\mathrm{Re}\Delta_{12}(z_1,0),\ \ |\mathrm{Im}\Delta_{12}(z,0)+\alpha|\leq v\}\end{aligned}\qquad(6.165)$$

and $\partial S_+(v)$ is defined similarly (see figure (6.6)). We choose v sufficiently small so that

$$S_\pm(v)\cap D(0,r)=\emptyset.\qquad(6.166)$$

Consider the multivalued function

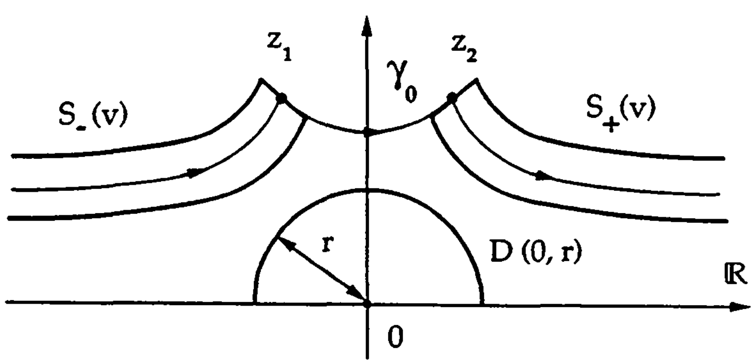

Figure 6.6: The disc $D(0,r)$ and the tubular neighbourhoods $S_-(v)$ and $S_+(v)$ of γ_0.

$$\Delta_{12}(z,\delta)=-\int_0^z\sqrt{\rho(u,\delta)}du.\qquad(6.167)$$

When restricted to

$$S_a^+\backslash D(0,r)\equiv(S_a\backslash D(0,r))\cap\{z|\mathrm{Im}z\geq 0\},\qquad(6.168)$$

$\Delta_{12}(z,\delta)$ is an analytic univalued function provided δ is so small that

$$|z_0(\delta)|<r.\qquad(6.169)$$

We fix a branch of $\Delta_{12}(z,\delta)$ by requiring that the path of integration in (6.167) follows the real axis from 0 to $-r$ and that $\Delta_{12}(t,\delta)>0$ for $t<-r$.

Lemma 6.2.7 *Let $\Delta_{12}(z,0)$ and $\Delta_{12}(z,\delta)$ be defined as above, and let $z\in S_a^+\backslash D(0,r)$.*

$$\lim_{\delta\to 0}\mathrm{Im}\Delta_{12}(z,\delta)=\mathrm{Im}\Delta_{12}(z,0)$$

uniformly in $z\in S_a^+\backslash D(0,r)$.

Proof: We first show that $\rho(z,\delta)$ tends to $\rho(z,0)$ uniformly in z. Let $\varepsilon > 0$ and consider

$$\begin{aligned}|\rho(z,\delta)-\rho(z,0)| &\leq |\rho(z,\delta)-\rho(\pm\infty,\delta)| + \\ |\rho(\pm\infty,\delta)-\rho(\pm\infty,0)| &+ |\rho(\pm\infty,0)-\rho(z,0)|.\end{aligned} \tag{6.170}$$

It follows from (6.59) that there exists $T(\varepsilon) > 0$ such that for any $t \gtrless \pm T(\varepsilon)$

$$\begin{aligned}|\rho(t+is,\delta)-\rho(\pm\infty,\delta)| &< \frac{\varepsilon}{3} \\ |\rho(\pm\infty,0)-\rho(t+is,0)| &< \frac{\varepsilon}{3}.\end{aligned} \tag{6.171}$$

Since $\rho(\pm\infty,\delta)$ is continuous in δ, there exists $\delta_1(\varepsilon)$ such $\delta < \delta_1(\varepsilon)$ implies

$$|\rho(z,\delta)-\rho(z,0)| < \frac{\varepsilon}{3}+\frac{\varepsilon}{3}+\frac{\varepsilon}{3} \tag{6.172}$$

for any $|t| \geq T(\varepsilon)$. Now the set

$$S_a \backslash (D(r,0) \cup D_\pm(T(\varepsilon))) \tag{6.173}$$

where

$$D_\pm(T(\varepsilon)) = \left\{z | \mathrm{Re} z \gtrless T(\varepsilon)\right\} \tag{6.174}$$

is a compact set, so that $\rho(z,\delta)$ is uniformly continuous in (z,δ) for z in this set and $\delta \in I_\Delta$. Thus there exists $\delta_2(\varepsilon, T(\varepsilon))$ such that if $|\mathrm{Re} z| \leq T(\varepsilon)$,

$$|\rho(z,\delta)-\rho(z,0)| < \varepsilon \tag{6.175}$$

if $\delta < \delta_2(\varepsilon, T(\varepsilon))$. Since $S_a^+ \backslash D(0,r)$ is simply connected and contains no zero of $\rho(z,\delta)$ for any small δ (see (6.169)), the analytic function $\sqrt{\rho(z,\delta)}$ tends to $\sqrt{\rho(z,0)}$ uniformly in $z \in S_a^+ \backslash D(0,r)$, provided we select the suitable branches for the square roots. Our choice is $\sqrt{\rho(t,\delta)}$ and $\sqrt{\rho(t,0)}$ positive if $t < -r$. Consider now

$$|\ \mathrm{Im}\Delta_{12}(z,\delta) - \ \mathrm{Im}\Delta_{12}(z,0)| = \left| \mathrm{Im} \int_0^z \sqrt{\rho(u,\delta)} - \sqrt{\rho(z,0)} du \right|. \tag{6.176}$$

Let $z = t+is \in S_a^+ \backslash D(0,r)$. If $t \leq -r$ we can choose a path of integration going from 0 to $t < -r$ along the real axis and then vertically to $t+is$. If $t \geq -r$ we take a path from $-r$ to t following the boundary of $D(0,r)$ and the real axis, if necessary, and then a vertical path to $t+is$, see figure (6.7). Along the second path for $t > r$, for example, we have

$$\begin{aligned}|\ \mathrm{Im}\Delta_{12}(z,\delta) - \ \mathrm{Im}\Delta_{12}(z,0)| &\leq \pi r \sup_{\theta \in [0,\pi]} |\sqrt{\rho(r \exp\{i\theta\},\delta)} - \sqrt{\rho(r \exp\{i\theta\},0)}| \\ &+ a \sup_{|s| \leq a} |\sqrt{\rho(t+is,\delta)} - \sqrt{\rho(t+is,0)}|\end{aligned} \tag{6.177}$$

where the second member tends to zero uniformly in $z = t+is$ as δ tends to zero. The result is the same when $t \leq r$.

□

As a consequence of this lemma we can assume that δ is small enough so that we have

$$|\rho(z,\delta)-\rho(z,0)| \leq \frac{R}{3} \quad \forall z \in S_a \backslash D(0,r) \tag{6.178}$$

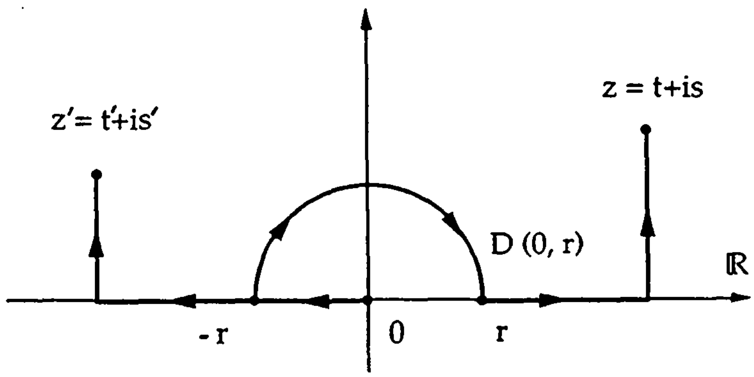

Figure 6.7: Particular integration paths.

where $0 < R = \inf_{z \in S_a \backslash D(0,r)} \rho(z,0)$ and

$$|\operatorname{Im}\Delta_{12}(z,\delta) - \operatorname{Im}\Delta_{12}(z,0)| < \frac{v}{3} \quad \forall z \in S_a^+ \backslash D(0,r). \tag{6.179}$$

Hence the level line

$$\operatorname{Im}\Delta_{12}(z,\delta) = \operatorname{Im}\Delta_{12}(z_1,\delta) \tag{6.180}$$

cannot cross the level lines

$$\operatorname{Im}\Delta_{12}(z,0) = -\alpha \pm v \tag{6.181}$$

since this would imply

$$|\operatorname{Im}\Delta_{12}(z_1,\delta) - \operatorname{Im}\Delta_{12}(z_1,0)| = v > \frac{v}{3}. \tag{6.182}$$

Moreover, the line

$$\operatorname{Im}\Delta_{12}(z,\delta) = \operatorname{Im}\Delta_{12}(z_1,\delta) \tag{6.183}$$

cannot cross the segment

$$\{z | \operatorname{Re}\Delta_{12}(z,0) = \operatorname{Re}\Delta_{12}(z_1,0), \ |\operatorname{Im}\Delta_{12}(z,0) + \alpha| \leq v\} \tag{6.184}$$

if δ is small, except at $z = z_1$. Indeed, for δ small enough $\Delta_{12}'(z_1,\delta) \neq 0$, so that $\Delta_{12}(z,\delta)$ is bijective in a δ-independent neighbourhood V of z_1. Moreover $\Delta_{12}(z,\delta)$ tends to $\Delta_{12}(z,0)$ which has the same property in V so that we can conclude. Note that a level line

$$\operatorname{Im}\Delta_{12}(z,\delta) = \text{cst} \tag{6.185}$$

is given by the solution $\gamma(t)$ of the following differential equation

$$\frac{d}{dt} \operatorname{Im}\Delta_{12}(\gamma(t),\delta) = 0 \tag{6.186}$$

i.e.

$$\begin{aligned} \operatorname{Re}\dot{\gamma}(t) &= \operatorname{Re}\sqrt{\rho(\gamma(t),\delta)} \\ \operatorname{Im}\dot{\gamma}(t) &= -\operatorname{Im}\sqrt{\rho(\gamma(t),\delta)}. \end{aligned} \tag{6.187}$$

Thus

$$\left| \frac{d}{dt} \operatorname{Re}\Delta_{12}(\gamma(t),\delta) \right| = |\rho(\gamma(t),\delta)| > R > 0 \tag{6.188}$$

which implies that $|\,\mathrm{Re}\Delta_{12}(\gamma(t),\delta)|$ is strictly increasing along $\gamma(t)$. Hence the level line $\mathrm{Im}\Delta_{12}(z,\delta) = \mathrm{Im}\Delta_{12}(z_1,\delta)$ leads from z_1 to $-\infty$ in $S_-(v)$. Moreover, $|\dot{\gamma}(t)| = |\sqrt{\rho(\gamma(t),\delta)}|$ is uniformly bounded in δ. Finally, we have along $\gamma_0(t)$ for $t \in [t_1, t_2]$

$$\begin{aligned} &\frac{d}{dt}\,\mathrm{Im}\Delta_{12}(\gamma_0(t),\delta) = \\ &-\left(\mathrm{Re}\dot{\gamma}_0(t)\mathrm{Im}\sqrt{\rho(\gamma_0(t),\delta)} + \mathrm{Im}\dot{\gamma}_0(t)\mathrm{Re}\sqrt{\rho(\gamma_0(t),\delta)}\right) \end{aligned} \tag{6.189}$$

which is strictly greater than zero if δ is sufficiently small, since $\sqrt{\rho(z,\delta)} \to \sqrt{\rho(z,0)}$ and by construction $\frac{d}{dt}\,\mathrm{Im}\Delta_{12}(\gamma_0(t),0) > d > 0$ (see (6.161). Hence, the path γ_δ defined by

$$\gamma_\delta = \begin{cases} \mathrm{Im}\Delta_{12}(z,\delta) = \mathrm{Im}\Delta_{12}(z_1,\delta) & \text{from } -\infty \text{ to } z_1 \\ \gamma_0 & \text{from } z_1 \text{ to } z_2 \\ \mathrm{Im}\Delta_{12}(z,\delta) = \mathrm{Im}\Delta_{12}(z_2,\delta) & \text{from } z_2 \text{ to } +\infty \end{cases} \tag{6.190}$$

is dissipative for $\Delta_{12}(z,\delta)$ and has all the properties announced in the proposition.

□

This completes the proof of theorem (6.1.1) as well.

□

Appendix A

Exponential Bounds via Complex Time Method

We investigate here the possibility to get exponential bounds on the transition probability by integrating the Schrödinger equation in the complex plane, without having to consider the pattern of Stokes lines in S_a. We will show that this can indeed be done and not for two-level systems only since we shall consider bounded hamiltonians in this appendix. Actually, the method we shall develop can be generalized to deal with unbounded hamiltonians as well and yields the same result, but we will treat here the bounded case only in order not to burden the main ideas of the proof under technical problems. We refer the interested reader to [JP4] for the extension of the proof to the unbounded case.

A.1 Bounded Case

We assume that $H(z)$ is a bounded operator satisfying conditions I, II and III. The part $\sigma_1(z)$ of its spectrum is associated with the projector $P_1(z)$ and we define $P_2(z) = \mathbb{I} - P_1(z)$. The various evolutions $U_\varepsilon(z,0)$, $W(z,0)$ and $\Phi_\varepsilon(z,0)$ given by

$$\begin{aligned} i\varepsilon U_\varepsilon'(z,0) &= H(z)U_\varepsilon(z,0), \quad U_\varepsilon(0,0) = \mathbb{I} \\ iW'(z,0) &= K(z)W(z,0), \quad W(0,0) = \mathbb{I} \\ i\varepsilon \Phi_\varepsilon'(z,0) &= W^{-1}(z,0)H(z)W(z,0)\Phi_\varepsilon(z,0), \quad \Phi_\varepsilon(0,0) = \mathbb{I} \end{aligned} \tag{A.1}$$

are now all analytic in S_a, provided the width $2a$ of the strip is small enough (see paragraph (2.2.2)), and they are given by Dyson series analogous to (2.27). Let us consider the operator $A(z,-\infty)$ satisfying

$$A'(z,-\infty) = \mathbb{I} + i\int_{-\infty}^{z} \Phi_\varepsilon^{-1}(z',0)W^{-1}(z',0)K(z')W(z',0)\Phi_\varepsilon(z',0)A(z',-\infty)dz'. \tag{A.2}$$

It allows the transition probability $\mathcal{P}_{21}(\varepsilon)$ to be expressed in a convenient way (see lemma (3.1.1)) by

$$\mathcal{P}_{21}(\varepsilon) = \|P_2(0)A(+\infty,-\infty)P_1(0)\|^2. \tag{A.3}$$

To stress the similarity with the two-level case we have treated in chapter (4), we define

$$\begin{aligned} C_1(z) &= P_1(0)A(z,-\infty)P_1(0) \\ C_2(z) &= P_2(0)A(z,-\infty)P_1(0) \end{aligned} \tag{A.4}$$

with initial conditions $C_1(-\infty) = P_1(0)$, $C_2(-\infty) = 0$. The transition probability thus takes the form

$$\mathcal{P}_{21}(\varepsilon) = \|C_2(+\infty)\|^2. \tag{A.5}$$

We also introduce

$$\Phi_1(z) = P_1(0)\Phi_\varepsilon(z,0)P_1(0), \quad \Phi_2(z) = P_2(0)\Phi_\varepsilon(z,0)P_2(0) \tag{A.6}$$

and for an operator $Y(z)$ we define

$$\begin{aligned} \widetilde{Y}_{12}(z) &= P_1(0)W^{-1}(z,0)Y(z)W(z,0)P_2(0) \\ \widetilde{Y}_{21}(z) &= P_2(0)W^{-1}(z,0)Y(z)W(z,0)P_1(0). \end{aligned} \tag{A.7}$$

We recall that due to $[\Phi_\varepsilon(z,0), P_j(0)] = 0$ and $P_j(z)K(z)P_j(z) = 0$ for $j = 1,2$, we have the identities

$$\begin{aligned} \Phi_\varepsilon(z,0) &= \Phi_1(z) + \Phi_2(z) \\ W^{-1}(z,0)K(z)W(z,0) &= \widetilde{K}_{12}(z) + \widetilde{K}_{21}(z) \quad \forall z \in S_a. \end{aligned} \tag{A.8}$$

Equation (A.2) is equivalent to the system of equations for the C_j's

$$\begin{aligned} C_1(z) &= P_1(0) + i\int_{-\infty}^{z} \Phi_1^{-1}(z')\widetilde{K}_{12}(z')\Phi_2(z')C_2(z')dz' \\ C_2(z) &= i\int_{-\infty}^{z} \Phi_2^{-1}(z')\widetilde{K}_{21}(z')\Phi_1(z')C_1(z')dz'. \end{aligned} \tag{A.9}$$

We can apply the integration by parts formula (lemma (3.1.2)) to equation (A.2) to obtain for $z \in I\!R$ with our definitions

$$\begin{aligned} C_1(z) &= P_1(0) + \varepsilon\Phi_1^{-1}(z)\widetilde{\mathcal{R}}_{12}(K)(z)\Phi_2(z)C_2(z) \\ &- \varepsilon\int_{-\infty}^{z} \Phi_1^{-1}(z')\widetilde{\mathcal{R}}'_{12}(K)(z')\Phi_2(z')C_2(z')dz' \\ &- i\varepsilon\int_{-\infty}^{z} \Phi_1^{-1}(z')\widetilde{\mathcal{R}}_{12}(K)(z')\widetilde{K}_{21}(z')\Phi_1(z')C_1(z')dz' \\ C_2(z) &= -\varepsilon\Phi_2^{-1}(z)\widetilde{\mathcal{R}}_{21}(K)(z)\Phi_1(z)C_1(z) \\ &+ \varepsilon\int_{-\infty}^{z} \Phi_2^{-1}(z')\widetilde{\mathcal{R}}'_{21}(K)(z')\Phi_1(z')C_1(z')dz' \\ &+ i\varepsilon\int_{-\infty}^{z} \Phi_2^{-1}(z')\widetilde{\mathcal{R}}_{21}(K)(z')\widetilde{K}_{12}(z')\Phi_2(z')C_2(z')dz' \end{aligned} \tag{A.10}$$

where we have used the notation

$$\widetilde{\mathcal{R}}'_{21}(K)(z) \equiv (I\!I - P(0))W^{-1}(z,0)\frac{d}{dz}\mathcal{R}(K)(z)W(z,0)P(0). \tag{A.11}$$

Moreover, it is not difficult to see that these equations hold along any path in the complex plane as well since the gap hypothesis is true for any $z \in S_a$ when a is small enough. The point now is to find generalized dissipative paths in the complex plane along which we can control the ε-dependence of the dynamical phases $\Phi_j(z)$, $j = 1,2$. In order to do this we introduce a fictitious level e_0 in the gap of the spectrum of H, which will be used as a reference level. Under hypotheses I to III, there exists a positive constant δ and real valued smooth function $r_0(t)$, $t \in I\!R$ such that

$$\begin{aligned} &\text{dist}(r_0(t), \sigma_j(t)) \geq \delta, \\ &\sup_{\mu_1 \in \sigma_1(t)} \mu_1 < r_0(t) < \inf_{\mu_2 \in \sigma_2(t)} \mu_2 \quad \forall t \in I\!R \end{aligned} \tag{A.12}$$

and

$$|r_0(t) - r_0(\pm\infty)| \le b(t)$$
$$|r_0'(t)| \le b(t), \quad t \gtrless 0, \tag{A.13}$$

where $b(t)$ is an integrable decay function. Actually, we can even take $r_0(t) = r_0(\pm\infty)$ if $|t|$ is large enough. We define for $t \in \mathbb{R}$ and $|s| < a$ two complex-valued functions by

$$\begin{aligned} e_0(t,s) &= r_0(t) + isr_0'(t) \\ \lambda_0(t,s) &= isr_0(t). \end{aligned} \tag{A.14}$$

These functions are obviously not analytic but we can assume that they are defined in the complex plane considered as $\mathbb{R}^2$. Thus we shall make the abuses of notation $e_0(z) \equiv e_0(\text{Re}z, \text{Im}z)$ and $\lambda_0(z) \equiv \lambda_0(\text{Re}z, \text{Im}z)$. We introduce new operators $X_j(z)$, $j = 1, 2$, by

$$\begin{aligned} X_1(z) &= \Phi_1(z) \exp\left\{\frac{i}{\varepsilon}\lambda_0(z)\right\} C_1(z) \\ X_2(z) &= \Phi_2(z) \exp\left\{\frac{i}{\varepsilon}\lambda_0(z)\right\} C_2(z) \end{aligned} \tag{A.15}$$

which satisfy the equations (see (A.10))

$$\begin{aligned} &X_1(z) = \Phi_1(z)\exp\left\{\frac{i}{\varepsilon}\lambda_0(z)\right\} + \varepsilon\widetilde{\mathcal{R}}_{12}(K)(z)X_2(z) \\ &-\varepsilon\int_{-\infty}^{z}\left(\Phi_1(z)\exp\left\{\frac{i}{\varepsilon}\lambda_0(z)\right\}\Phi_1^{-1}(z')\exp\left\{-\frac{i}{\varepsilon}\lambda_0(z')\right\}\right)\widetilde{\mathcal{R}}_{12}'(K)(z')X_2(z')dz' \\ &-i\varepsilon\int_{-\infty}^{z}\left(\Phi_1(z)\exp\left\{\frac{i}{\varepsilon}\lambda_0(z)\right\}\Phi_1^{-1}(z')\exp\left\{-\frac{i}{\varepsilon}\lambda_0(z')\right\}\right)\widetilde{\mathcal{R}}_{12}(K)(z')\widetilde{K}_{21}(z')X_1(z')dz' \\ &X_2(z) = -\varepsilon\widetilde{\mathcal{R}}_{21}(K)(z)X_1(z) \\ &+\varepsilon\int_{-\infty}^{z}\left(\Phi_2(z)\exp\left\{\frac{i}{\varepsilon}\lambda_0(z)\right\}\Phi_2^{-1}(z')\exp\left\{-\frac{i}{\varepsilon}\lambda_0(z')\right\}\right)\widetilde{\mathcal{R}}_{21}'(K)(z')X_1(z')dz' \\ &+i\varepsilon\int_{-\infty}^{z}\left(\Phi_2(z)\exp\left\{\frac{i}{\varepsilon}\lambda_0(z)\right\}\Phi_2^{-1}(z')\exp\left\{-\frac{i}{\varepsilon}\lambda_0(z')\right\}\right)\widetilde{\mathcal{R}}_{21}(K)(z')\widetilde{K}_{12}(z')X_2(z')dz'. \end{aligned} \tag{A.16}$$

A *dissipative path* for $\Phi_j(z)\exp\left\{\frac{i}{\varepsilon}\lambda_0(z)\right\}$ is a path $\gamma^{(j)}(t) = \gamma_1^{(j)}(t) + i\gamma_2^{(j)}(t)$, $t \in [a,b]$, defined by the property :

$$\begin{aligned} &\left\|\Phi_j(\gamma^{(j)}(t))\exp\left\{\frac{i}{\varepsilon}\lambda_0(\gamma^{(j)}(t))\right\}\left(\Phi_j(\gamma^{(j)}(s))\exp\left\{\frac{i}{\varepsilon}\lambda_0(\gamma^{(j)}(s))\right\}\right)^{-1}\right\| \le 1 \\ &\forall a \le s \le t \le b. \end{aligned} \tag{A.17}$$

We have introduced indices on the dissipative paths because in general it is not possible to find one path in the complex plane along which (A.17) is satisfied for both $\Phi_1\exp\left\{\frac{i}{\varepsilon}\lambda_0\right\}$ and $\Phi_2\exp\left\{\frac{i}{\varepsilon}\lambda_0\right\}$. The real axis is of course a dissipative path for both operators.

Lemma A.1.1 *There exists a dissipative path $\gamma^{(2)}(t) \subset S_a$, $t \in \mathbb{R}$, such that*

$$\gamma_1^{(2)}(t) = t$$
$$\inf_{t\in\mathbb{R}} \gamma_2^{(2)}(t) \ge h > 0.$$

Moreover, in a neighbourhood of the real axis, any vertical path with upward, respectively downward, orientation is dissipative for $\Phi_1\exp\left\{\frac{i}{\varepsilon}\lambda_0\right\}$, respectively $\Phi_2\exp\left\{\frac{i}{\varepsilon}\lambda_0\right\}$.

We postpone the proof of this lemma to give the main proposition of this section.

Proposition A.1.1 *Let $\Omega \subset S_a$ be defined by the simply connected domain bordered by $\gamma^{(2)}$ and the real axis and let the norm $\|\cdot\|_\Omega$ be define by*

$$\|A\|_\Omega = \sup_{z\in\Omega} \|A(z)\| \quad \forall A(z) \in \mathcal{B}(\mathcal{H}).$$

Then

$$\begin{aligned} \|X_1\|_\Omega &= \mathcal{O}(1) \\ \|X_2\|_\Omega &= \mathcal{O}(\varepsilon) \quad as \ \varepsilon \to 0. \end{aligned}$$

Proof: Let $z \in \Omega$. By lemma (A.1.1), the path $\alpha(t)$ defined by

$$\alpha(t) = \begin{cases} t & t \le \mathrm{Re} z \\ \mathrm{Re} z + i(t - \mathrm{Re} z) & \mathrm{Re} z < t \le \mathrm{Re} z + \mathrm{Im} z \end{cases} \tag{A.18}$$

(see figure (A.1)), is dissipative for $\Phi_1 \exp\left\{\frac{i}{\varepsilon}\lambda_0\right\}$ and $\beta(t)$ defined by

$$\beta(t) = \begin{cases} \gamma^{(2)}(t) & t \le \mathrm{Re} z \\ \gamma^{(2)}(\mathrm{Re} z) - i(t - \mathrm{Re} z) & \mathrm{Re} z < t \le \mathrm{Re} z + \mathrm{Im}\gamma^{(2)}(\mathrm{Re} z) - \mathrm{Im} z \end{cases} \tag{A.19}$$

is dissipative for $\Phi_2 \exp\left\{\frac{i}{\varepsilon}\lambda_0\right\}$. In particular we have along α

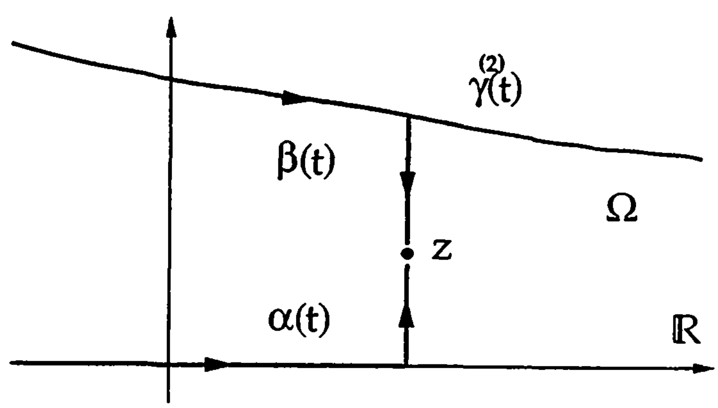

Figure A.1: The dissipative paths α and β.

$$\begin{aligned} \|\Phi_1(z)\exp\left\{\frac{i}{\varepsilon}\lambda_0(z)\right\}\| \ \le \ & \|\Phi_1(z)\exp\left\{\frac{i}{\varepsilon}\lambda_0(z)\right\}\left(\Phi_1(\mathrm{Re} z)\exp\left\{\frac{i}{\varepsilon}\lambda_0(\mathrm{Re} z)\right\}\right)^{-1}\| \times \\ & \|\Phi_1(\mathrm{Re} z)\exp\left\{\frac{i}{\varepsilon}\lambda_0(\mathrm{Re} z)\right\}\| \le 1. \end{aligned} \tag{A.20}$$

Thus considering the first of the equations (A.16) along the same path α and using the integrability of $\|K\|$ (see lemma (2.2.3)), we obtain

$$\begin{aligned} &\|X_1(z)\| \le 1 + \varepsilon\|\tilde{\mathcal{R}}_{12}(K)\|_\Omega\|X_2\|_\Omega \\ &+\varepsilon\left(\int_{-\infty}^{+\infty} dt\|\tilde{\mathcal{R}}'_{12}(K)(t)\| + a\|\tilde{\mathcal{R}}'_{12}(K)\|_\Omega\right)\|X_2\|_\Omega \\ &+\varepsilon\left(\int_{-\infty}^{+\infty} dt\|\tilde{\mathcal{R}}_{12}(K)(t)\|\|\widetilde{K}_{21}(t)\| + a\|\tilde{\mathcal{R}}_{12}(K)\|_\Omega\|\widetilde{K}_{21}\|_\Omega\right)\|X_1\|_\Omega \\ &= 1 + \varepsilon k(\|X_1\|_\Omega + \|X_2\|_\Omega) \end{aligned} \tag{A.21}$$

where k is a constant independent of ε and $z \in \Omega$. The two terms in the factors of ε come from estimating the integral over α by an integral over the whole real line and over a vertical path up to the boundary of S_a. Similarly we get from the second equation along the path β

$$\begin{aligned}
&\|X_2(z)\| \leq \varepsilon\|\tilde{\mathcal{R}}_{21}(K)\|_\Omega\|X_1\|_\Omega \\
&+\varepsilon\left(\int_{-\infty}^{+\infty} dt|\dot{\gamma}^{(2)}(t)|\|\tilde{\mathcal{R}}'_{21}(K)(\gamma^{(2)}(t))\| + a\|\tilde{\mathcal{R}}'_{21}(K)\|_\Omega\right)\|X_1\|_\Omega \\
&+\varepsilon\left(\int_{-\infty}^{+\infty} dt|\dot{\gamma}^{(2)}(t)|\|\tilde{\mathcal{R}}_{21}(K)(\gamma^{(2)}(t))\|\|\widetilde{K}_{12}(\gamma^{(2)}(t))\| + a\|\tilde{\mathcal{R}}_{21}(K)\|_\Omega\|\widetilde{K}_{12}\|_\Omega\right)\|X_2\|_\Omega \\
&= \varepsilon k(\|X_1\|_\Omega + \|X_2\|_\Omega) \qquad (A.22)
\end{aligned}$$

for any $z \in \Omega$. Summing the two inequalities and taking the supremum over $z \in \Omega$ gives

$$\|X_1\|_\Omega + \|X_2\|_\Omega \leq 1 + 2\varepsilon k(\|X_1\|_\Omega + \|X_2\|_\Omega) \qquad (A.23)$$

from which follows

$$\|X_1\|_\Omega + \|X_2\|_\Omega \leq \frac{1}{1-2\varepsilon k} \leq k' \qquad (A.24)$$

if ε is small enough.

□

This proposition allows the desired result to be proven.

Theorem A.1.1 *Let $H(t)$ be a bounded operator satisfying conditions I, II and III, and let $\psi_\varepsilon(t)$ be a normalized solution of the Schrödinger equation $i\varepsilon\psi'_\varepsilon = H\psi_\varepsilon$ such that $\lim_{t\to-\infty}\|P_1(t)\psi_\varepsilon(t)\| = 1$. Then, there exist two positive constants M and τ such that the transition probability $\mathcal{P}_{21}(\varepsilon) = \lim_{t\to+\infty}\|P_2(t)\psi_\varepsilon(t)\|^2$ satisfies*

$$\mathcal{P}_{21}(\varepsilon) \leq \varepsilon^2 M \exp\{-2\tau/\varepsilon\}$$

if ε is small enough.

Proof: From the preceding proposition we can write

$$\begin{aligned}
\|C_2(+\infty)\| &\leq \|\Phi_2^{-1}(\gamma^{(2)}(+\infty))\exp\left\{-\frac{i}{\varepsilon}\lambda_0((\gamma^{(2)}(+\infty)))\right\}\|\|X_2(\gamma^{(2)}(+\infty))\| \\
&\leq \varepsilon k k'\|\Phi_2^{-1}(\gamma^{(2)}(+\infty))\|\exp\left\{\frac{1}{\varepsilon}(\gamma^{(2)}(+\infty))r_0(+\infty)\right\}. \qquad (A.25)
\end{aligned}$$

The operator $\Phi_2^{-1}(z)$ satisfies the differential equation (see (A.1) and (A.6))

$$i\varepsilon\frac{d}{dz}\Phi_2^{-1}(z) = -\Phi_2^{-1}(z)P_2(0)W^{-1}(z,0)H(z)W(z,0)P_2(0), \quad \Phi_2^{-1}(0) = P_2(0). \qquad (A.26)$$

In particular, along a vertical path oriented upwards we have

$$\varepsilon\frac{d}{ds}\Phi_2^{-1}(t+is) = i\varepsilon\left.\frac{d}{dz}\Phi_2^{-1}(z)\right|_{t+is} = -\Phi_2^{-1}(t+is)\tilde{H}_2(t+is) \qquad (A.27)$$

with $\tilde{H}_2(z) = P_2(0)W^{-1}(z,0)H(z)W(z,0)P_2(0)$. Let us compare $\Phi_2^{-1}(t+is)$ with $\exp\left\{-\frac{s}{\varepsilon}\tilde{H}_2(t)\right\}$. From

$$\varepsilon\frac{d}{ds}\left(\Phi_2^{-1}(t+is)\exp\left\{\frac{s}{\varepsilon}\tilde{H}_2(t)\right\}\right) = \Phi_2^{-1}(t+is)\left(\tilde{H}_2(t) - \tilde{H}_2(t+is)\right)\exp\left\{\frac{s}{\varepsilon}\tilde{H}_2(t)\right\} \qquad (A.28)$$

we get by integration and by using lemma (2.2.4)

$$\|\Phi_2^{-1}(t+is)\exp\left\{\frac{s}{\varepsilon}\widetilde{H}_2(t)\right\} - P_2(0)\| \leq$$
$$\frac{a}{\varepsilon}\sup_{z\in\Omega}\|\Phi_2^{-1}(z)\| \sup_{t\in\mathbb{R}}\|\exp\left\{\frac{s}{\varepsilon}\widetilde{H}_2(t)\right\}\|\widetilde{b}(t) \quad (A.29)$$

where $\widetilde{b}(t) \to 0$ when $t \to +\infty$. As the spectral theorem implies

$$\|\exp\left\{-\frac{s}{\varepsilon}\widetilde{H}_2(t)\right\}P_2(0)\| = \exp\left\{-\frac{s}{\varepsilon}\inf_{\mu\in\sigma_2(t)}\mu\right\} \quad (A.30)$$

we can write

$$\lim_{t\to+\infty}\|\Phi_2^{-1}(\gamma^{(2)}(t))\| = \exp\left\{-\frac{\gamma^{(2)}(+\infty)}{\varepsilon}\inf_{\mu\in\sigma_2(+\infty)}\mu\right\}. \quad (A.31)$$

Now, since $\inf_{\mu\in\sigma_2(+\infty)}\mu - r_0(+\infty) > \delta > 0$ by construction of r_0, we eventually obtain with (A.5) and (A.25)

$$\mathcal{P}_{21}(\varepsilon) \leq \varepsilon^2 k^2 k'^2 \exp\left\{-\frac{2\gamma_2^{(2)}(+\infty)\delta}{\varepsilon}\right\} \quad (A.32)$$

□

Remarks:

- When the hamiltonian is a 2×2 matrix, there is no need to introduce the fictitious level e_0 and the notion of dissipative path is the same as the one defined previously. In this case, the exponential decay rate 2τ is given by $2|\mathrm{Im}\Delta(\gamma^{(2)}(+\infty))|$, where Δ is the function $\int_0^z e_1(u) - e_2(u)du$ defined in Ω.
- In the case of an unbounded hamiltonian H, we consider bounded approximations H_n of H for which we prove the theorem above by the same method. Then we show that the bounds thus obtained are uniform in n (see [JP4]).

A.2 Existence of the Dissipative Path $\gamma^{(2)}$

Proof of proposition (A.1.1): In order to prove the existence of dissipative paths for $\Phi_j\exp\left\{\frac{i}{\varepsilon}\lambda_0\right\}$, $j=1,2$, we consider the differential equation these operators satisfy along a path $\gamma(t)=\gamma_1(t)+i\gamma_2(t)$.

$$i\varepsilon\frac{d}{dt}\Phi_j(\gamma(t))\exp\left\{-\frac{\gamma_2(t)}{\varepsilon}r_0(\gamma_1(t))\right\} = i\varepsilon\dot\gamma(t)\Phi_j'(\gamma(t))\exp\left\{-\frac{\gamma_2(t)}{\varepsilon}r_0(\gamma_1(t))\right\} -$$
$$i\Phi_j(\gamma(t))\left(\dot\gamma_2(t)r_0(\gamma_1(t)) + \gamma_2(t)r_0'(\gamma_1(t))\dot\gamma_1(t)\right)\exp\left\{-\frac{\gamma_2(t)}{\varepsilon}r_0(\gamma_1(t))\right\} =$$
$$\left(\dot\gamma(t)\widetilde{H}_j(\gamma(t)) - i\dot\gamma_2(t)r_0(\gamma_1(t)) - i\dot\gamma_1(t)\gamma_2(t)r_0'(\gamma_1(t))\right)\Phi_j(\gamma(t))\exp\left\{-\frac{\gamma_2(t)}{\varepsilon}r_0(\gamma_1(t))\right\} \quad (A.33)$$

with initial condition $\Phi_j(z)\exp\left\{\frac{i}{\varepsilon}\lambda_0(z)\right\}\Big|_{z=0} = P_j(0)$. This equation can be viewed as an evolution equation in the subspace $P_j(0)\mathcal{H}$

$$\frac{d}{dt}\left(\Phi_j(\gamma(t))\exp\left\{\frac{i}{\varepsilon}\lambda_0(\gamma(t))\right\}\right) = -\frac{i}{\varepsilon}\widetilde{G}_j(\gamma(t))\left(\Phi_j(\gamma(t))\exp\left\{\frac{i}{\varepsilon}\lambda_0(\gamma(t))\right\}\right),$$
$$\Phi_j(0)\exp\left\{\frac{i}{\varepsilon}\lambda_0(0)\right\} = \mathbb{I}_{P_j(0)\mathcal{H}} \quad (A.34)$$

with

$$\widetilde{G}_j(\gamma(t)) = \dot{\gamma}(t)\widetilde{H}_j(\gamma(t)) - i\left(\dot{\gamma}_2(t)r_0(\gamma_1(t)) + \dot{\gamma}_1(t)\gamma_2(t)r_0'(\gamma_1(t))\right)I\!I_{P_j(0)\mathcal{H}}. \tag{A.35}$$

This form is very convenient because showing that the estimate (A.17) holds amounts to prove that $\frac{i}{\epsilon}\widetilde{G}_j(\gamma(t))$ generates a contraction semigroup on $P_j(0)\mathcal{H}$ for any $t \in I\!R$ and that 0 belongs to its resolvent set (see theorem X.70 in [RS] and the first remark below it). These conditions are verified if

$$\text{Re}\langle\varphi|i\widetilde{G}_j(\gamma(t))\varphi\rangle \geq 0 \quad \forall\varphi \in P_j(0)\mathcal{H}, \quad \|\varphi\| = 1. \tag{A.36}$$

and $0 \in T(\widetilde{G}_j(\gamma(t)))$, the resolvent set of $\widetilde{G}_j(\gamma(t))$ considered in $P_j(0)\mathcal{H}$. This means that we have to control the numerical range of $\widetilde{G}_j(\gamma(t))$. Along γ we must have

$$\begin{aligned} \text{Re}\langle\varphi|i\widetilde{G}_j(\gamma(t))\varphi\rangle &= -\dot{\gamma}_1(t)\left(\text{Im}\langle\varphi|\widetilde{H}_j(\gamma(t))\varphi\rangle - \gamma_2(t)r_0'(\gamma_1(t))\right) \\ &+ \dot{\gamma}_2(t)\left(r_0(\gamma_1(t)) - \text{Re}\langle\varphi|\widetilde{H}_j(\gamma(t))\varphi\rangle\right) \geq 0. \end{aligned} \tag{A.37}$$

Consider the case $j = 2$, and set $\gamma(t) = \gamma_1(t) + i\gamma_2(t)$ with $\gamma_1(t) = t$ and $\gamma_2(t) > 0$. We get the condition

$$\dot{\gamma}_2(t)\text{Re}\langle\varphi|\left(\widetilde{H}_2(\gamma(t)) - r_0(t)\right)\varphi\rangle \leq -\left(\text{Im}\langle\varphi|\widetilde{H}_2(\gamma(t))\varphi\rangle - \gamma_2(t)r_0'(\gamma_1(t))\right). \tag{A.38}$$

By lemma (2.2.4) there exists an integrable decay function $\tilde{b}(t)$ such that

$$\|\widetilde{H}_2(\gamma(t)) - \widetilde{H}_2(t)\| \leq \gamma_2(t)\tilde{b}(t) \tag{A.39}$$

so that

$$\begin{aligned} &\left|\langle\varphi|\widetilde{H}_2(\gamma(t))\varphi\rangle - \langle\varphi|\widetilde{H}_2(t)\varphi\rangle\right| \leq \\ &\gamma_2(t)\tilde{b}(t). \end{aligned} \tag{A.40}$$

Thus if $\sup_{t\in I\!R}\gamma_2(t)$ is small enough and by applying the spectral theorem to the self-adjoint operator $\widetilde{H}_2(t)$ considered in $P_2(0)\mathcal{H}$, we obtain

$$\begin{aligned} &\text{Re}\langle\varphi|\left(\widetilde{H}_2(\gamma(t)) - r_0(t)\right)\varphi\rangle > \\ &\langle\varphi|\left(\widetilde{H}_2(t) - r_0(t)\right)\varphi\rangle - \sup_{t\in I\!R}\gamma_2(t)\tilde{b}(t) > \frac{\delta}{2} \end{aligned} \tag{A.41}$$

where δ is the constant of (A.13). Similarly, we obtain from (A.40) and (A.13) the estimate

$$\left|\text{Im}\langle\varphi|\widetilde{H}_2(\gamma(t))\varphi\rangle - \gamma_2(t)r_0'(t)\right| \leq \gamma_2(t)\hat{b}(t) \tag{A.42}$$

where $\hat{b}(t)$ is an integrable decay function. We define $\gamma_2(t)$ by the differential equation

$$\dot{\gamma}_2(t) = -\frac{2}{\delta}\hat{b}(t)\gamma_2(t), \quad \gamma_2(-\infty) = s_- > 0 \tag{A.43}$$

with s_- small. Its solution is given by

$$\gamma_2(t) = s_-\exp\left\{-\frac{2}{\delta}\int_{-\infty}^{t}\hat{b}(s)ds\right\} > 0 \quad \forall t \tag{A.44}$$

so that if s_- is small enough (A.41) is satisfied and consequently, (A.38) holds as well for any $t \in I\!R$. We have thus proven the first part of lemma (A.1.1). Consider now a path given by $\gamma(t) = \gamma_0 - it$, where γ_0 is a constant. Condition (A.37) for $j = 2$ now reads

$$- \operatorname{Re}\langle\varphi| \left(r_0(\gamma_0) - \tilde{H}_2(\gamma(t))\right) \varphi\rangle \geq 0 \tag{A.45}$$

and it holds sufficiently close to the real axis by (A.41). The corresponding assertion with $j = 1$ is proven in the same way.

□

Remark:
In this proof we have used the fact that $\tilde{H}_j$ were bounded to prove that $\tilde{G}_j$ generate contraction semigroups on $P_j(0)\mathcal{H}$, $j = 1, 2$. But the analysis of the numerical range of $\tilde{H}_j$ can be performed without resorting to the boundedness of H and there exists a definition of $\gamma^{(2)}(t)$ depending only on the function $b(t)$ of condition II. These aspects are treated in details in [JP4].

Appendix B

Proof of Lemma (2.2.1)

Let Ω be a convex compact subset in S_a and consider the map form $\Omega \times \Omega \to I\!R$ defined by $(z, z') \mapsto |||H(z)|||_{z'}$. We first show that this map is continuous in z and z'. Let $z \in \Omega$. Then there exists a constant $M(z)$ such that for any $\varphi \in D$ and z' in Ω

$$\|H'(z')\varphi\| \leq M(z)\|\varphi\|_z. \tag{B.1}$$

Therefore, if z_1 and $z_2 \in \Omega$,

$$\|(H(z_1) - H(z_2))\varphi\| \leq M(z)|z_1 - z_2|\|\varphi\|_z. \tag{B.2}$$

Let us choose $z = z_1$. Then for any $z_2 \in \Omega$ such that $|z_2 - z_1|$ is small enough

$$\begin{aligned} \|\varphi\|_{z_2} &\leq (1 + M(z_1)|z_1 - z_2|)\|\varphi\|_{z_1} \\ \|\varphi\|_{z_1} &\leq \|\varphi\|_{z_2} + M(z_1)|z_1 - z_2|\|\varphi\|_{z_1} \end{aligned} \tag{B.3}$$

hence

$$\frac{1}{1 + M(z_1)|z_1 - z_2|}\|\varphi\|_{z_2} \leq \|\varphi\|_{z_1} \leq \frac{1}{1 - M(z_1)|z_1 - z_2|}\|\varphi\|_{z_2}. \tag{B.4}$$

From (B.4) we prove that $|||\cdot|||_z$ is continuous in z. Indeed, if $A \in \mathcal{L}(X_{z_2}, \mathcal{H})$ then

$$\begin{aligned} \|A\varphi\| &\leq |||A|||_{z_2}\|\varphi\|_{z_2} \\ &\leq |||A|||_{z_2}(1 + M(z_1)|z_1 - z_2|)\|\varphi\|_{z_1}. \end{aligned} \tag{B.5}$$

Thus we get from (B.5) an upper bound for $|||A|||_{z_1}$. In a similar way we derive a lower bound. We have

$$|||A|||_{z_2}(1 - M(z_1)|z_1 - z_2|) \leq |||A|||_{z_1} \leq |||A|||_{z_2}(1 + M(z_1)|z_1 - z_2|) \tag{B.6}$$

so that

$$\left| |||A|||_{z_2} - |||A|||_{z_1} \right| \leq |||A|||_{z_1}\frac{M(z_1)|z_1 - z_2|}{1 - M(z_1)|z_1 - z_2|} \tag{B.7}$$

which tends to zero as z_2 tends to z_1. Using the estimate (B.6) we prove that the function $(z, z') \mapsto |||H(z)|||_{z'}$ is continuous.

$$\begin{aligned} \left| |||H(z_2)|||_{z_2'} - |||H(z_1)|||_{z_1'} \right| &\leq \\ |||H(z_2)|||_{z_1'}\frac{M(z_1')|z_1' - z_2'|}{1 - M(z_1')|z_1' - z_2'|} &+ M(z_1')|z_2 - z_1| \end{aligned} \tag{B.8}$$

going to zero as $(z_2, z_2') \to (z_1, z_1')$. Let Ω be any compact subset of S_a. Then

$$\sup_{\varphi \in D} \sup_{z_1, z_2 \in \Omega} \frac{\|H(z_1)\varphi\|}{\|\varphi\|_{z_2}} = \sup_{z_1, z_2 \in \Omega} |||H(z_1)|||_{z_2} \leq K < \infty \tag{B.9}$$

and

$$\|\varphi\|_{z_1} \leq (K+1)\|\varphi\|_{z_2}, \quad z_1, z_2 \in \Omega. \tag{B.10}$$

On the other hand, using condition II, we can compare any norm $\|\varphi\|_z$ with $\|\varphi\|_+$ or $\|\varphi\|_-$ when $|\text{Re}z|$ is large enough. Thus for any r, $0 < r < a$, using (B.10) we show that there exist constants M_1 and M_2 such that

$$M_1\|\varphi\|_+ \leq \|\varphi\|_z \leq M_2\|\varphi\|_+, \quad |\text{Im}z| \leq r. \tag{B.11}$$

The operator $H(z) \in \mathcal{L}(X_+, \mathcal{H})$ has limits when $|\text{Re}z|$ diverges. Hence, for any r, $0 < r < a$, there exists a constant M_+ such that

$$|||H(z)|||_+ \leq M_+, \quad |\text{Im}z| \leq r + \frac{(a-r)}{2}. \tag{B.12}$$

By similar consideration about $|||H(z)|||_-$ we get the first assertion of the lemma. Now using Cauchy formula and (B.12) we have

$$\|H'(t+is)\varphi\| \leq M_+'\|\varphi\|_+, \quad |s| \leq r. \tag{B.13}$$

On the other hand, if $|t|$ is large enough, we can use condition II instead of (B.12), and apply Cauchy formula to the applications $(H(z) - H^+)\varphi$ or $(H(z) - H^-)\varphi$ as above. We get for $|t|$ large enough

$$\|H'(t+is)\varphi\| \leq C'b(t)\|\varphi\|_+, \quad |s| \leq r \tag{B.14}$$

and

$$\|H'(t+is)\varphi\| \leq C'b(t)\|\varphi\|_-, \quad |s| \leq r. \tag{B.15}$$

In (B.13), (B.14) and (B.15) the constants depend on r only. Since we can compare any norm with $\|\varphi\|_+$ by (B.11), we have finished the proof of the lemma.

□

Appendix C

Proof of Lemma (2.2.4)

The first part of the proof of this lemma is essentially given in [Kr] p. 308. We prove the lemma for $z_0 = 0$. Let $0 < r < a$. We consider first the operator $H'(z)R(z,\lambda)$ where $\lambda \in T(z)$ for all z in the strip, with $|\text{Im}z| \leq r$. (e.g. λ is negative and $|\lambda|$ large enough). We show that for all z with $|\text{Im}z| \leq r$ $H'(z)R(z,\lambda)$ is a bounded holomorphic operator. Moreover, there exists a constant N such that

$$\|H'(z)R(z,\lambda)\| \leq Nb(t), \quad |\text{Im}z| \leq r \tag{C.1}$$

with $b(t)$ the integrable function of lemma (2.2.1). We decompose the operator as

$$H'(z)R(z,\lambda) = H'(z)R(0,\lambda)(H(0)-\lambda)R(z,\lambda) \tag{C.2}$$

The factor $H'(z)R(0,\lambda)$ is a bounded holomorphic operator by condition I and lemma (2.2.1). The other factor $(H(0)-\lambda)R(z,\lambda)$ is a bounded operator, locally uniformly bounded in z. Since $(H(0)-\lambda)R(z,\lambda)$ is the inverse of the operator $(H(z)-\lambda)R(0,\lambda)$ which is a holomorphic bounded operator, the operator $(H(0)-\lambda)R(z,\lambda)$ is itself holomorphic and bounded. From lemma (2.2.1) we have

$$\begin{aligned} \|H'(z)R(z,\lambda)\varphi\| &\leq b(t)\|R(z,\lambda)\varphi\|_z \\ &\leq b(t)\left(\|R(z,\lambda)\| + 1 + |\lambda|\|R(z,\lambda)\|\right)\|\varphi\| \end{aligned} \tag{C.3}$$

The result follows therefore from (C.3) and (2.11). Let us denote in the rest of this proof $P(t)$ by $P_1(t)$ and $\mathbb{I}- P(t)$ by $P_2(t)$, for notational convenience. It follows from the foregoing that the operator

$$G(z) = [P_1'(z), P_1(z)] + P_1(z)H'(z)R(z,\lambda)P_1(z) + P_2(z)H'(z)R(z,\lambda)P_2(z) \tag{C.4}$$

is a bounded holomorphic operator, provided that λ is negative and $|\lambda|$ is large enough. Moreover, there exists a constant N' so that for $|s| \leq r$

$$\|G(t+is)\| \leq N'b(t) \tag{C.5}$$

with $b(t)$ the integrable decay function of lemma (2.2.1). Therefore we can define $S(z)$ by the holomorphic solution of the equation

$$S'(z) = G(z)S(z), \quad S(0) = \mathbb{I}. \tag{C.6}$$

Besides $S(z)$ we also introduce the operator

$$F(z) = R(z,\lambda)S(z). \tag{C.7}$$

Let us compute the derivative of $F(z)$,

$$F'(z) = R'(z,\lambda)S(z) + R(z,\lambda)G(z)S(z). \tag{C.8}$$

We know that

$$P_k(z)R(z,\lambda) = R(z,\lambda)P_k(z), \quad k = 1,2 \tag{C.9}$$

so that by differentiating this identity we get

$$P_k'(z)R(z,\lambda) + P_k(z)R'(z,\lambda) = R'(z,\lambda)P_k(z) + R(z,\lambda)P_k'(z) \tag{C.10}$$

Now, using (C.9), (C.10) and $R'(z,\lambda) = -R(z,\lambda)H'(z)R(z,\lambda)$ we have

$$\begin{aligned} &R(z,\lambda)P_k'(z) + R(z,\lambda)P_k(z)H'(z)R(z,\lambda) = \\ &R(z,\lambda)P_k'(z) - P_k(z)R'(z,\lambda) = \\ &P_k'(z)R(z,\lambda) - R'(z,\lambda)P_k(z). \end{aligned} \tag{C.11}$$

Hence we can write

$$\begin{aligned} R(z,\lambda)G(z) &= R(z,\lambda)\left(\sum_{k=1}^{2} P_k'(z)P_k(z) + P_k(z)H'(z)R(z,\lambda)P_k(z)\right) \\ &= \sum_{k=1}^{2} P_k'(z)P_k(z)R(z,\lambda) - R'(z,\lambda). \end{aligned} \tag{C.12}$$

Therefore the operator $F(z)$ satisfies the differential equation

$$\begin{aligned} F'(z) &= \left(\sum_{k=1}^{2} P_k'(z)P_k(z)\right) F(z) \\ &= [P_1'(z), P_1(z)]F(z). \end{aligned} \tag{C.13}$$

At $z = 0$ we have $F(0) = R(0,\lambda)$ and by the uniqueness of the solution of (C.13) we have

$$\begin{aligned} F(z) &= W(z,0)R(0,\lambda) \\ &= R(z,\lambda)S(z). \end{aligned} \tag{C.14}$$

Therefore $W(z,0)$ leaves the domain D invariant.

By definition

$$S(z) - S(t) = \int_t^z G(y)S(y)dy \tag{C.15}$$

where $\int_t^z dy$ is a shorthand for $\int_0^1 ds \frac{d}{ds} y(s)$ with $y(s) = t + s(z-t) \in \mathbb{C}$. Iterating this equality we have

$$\begin{aligned} &S(z) - S(t) = \\ &\sum_{n\geq 1} \int_t^z dy_1 \cdots \int_t^{y_{n-1}} dy_n G(y_1)\cdots G(y_n)S(t) \end{aligned} \tag{C.16}$$

and by (C.5) there exists a constant N'' such that

$$\|(S(z) - S(t))\varphi\| \leq |z-t|N''b(t)\exp\{|z-t|N''b(t)\}\|S(t)\varphi\|. \tag{C.17}$$

Using (C.14) we have

$$\begin{aligned}
&\|(\tilde{H}(z) - \tilde{H}(t))R(0,\lambda)\varphi\| = \\
&\|(W(0,z)S(z) - W(0,t)S(t))\varphi\| \leq \\
&\|W(0,z) - W(0,t)\|\|S(t)\varphi\| + \|W(0,z)\|\|(S(z) - S(t))\varphi\|.
\end{aligned} \qquad \text{(C.18)}$$

Since we can write

$$W(0,z) - W(0,t) = -i\int_t^z dyW(0,y)[P_1'(y), P_1(y)] \qquad \text{(C.19)}$$

we have by lemma (2.2.3) and estimate (C.17) the existence of a constant N''' such that

$$\begin{aligned}
\|(\tilde{H}(z) - \tilde{H}(t))R(0,\lambda)\varphi\| &\leq |z-t|b(t)N'''\|S(t)\varphi\| \\
&= |z-t|b(t)N'''\|(H(t)-\lambda)R(t,\lambda)S(t)\varphi\| \\
&= |z-t|b(t)N'''\|(H(t)-\lambda)W(t,0)R(0,\lambda)\varphi\| \\
&= |z-t|b(t)N'''\|W(t,0)(\tilde{H}(t)-\lambda)R(0,\lambda)\varphi\| \\
\leq |z-t|b(t)N'''(\|\tilde{H}(t)R(0,\lambda)\varphi\| &+ |\lambda|\|R(0,\lambda)\varphi\|).
\end{aligned} \qquad \text{(C.20)}$$

Finally, if $\varphi \in D$,

$$\tilde{H}(z)\varphi = W(0,z)S(z)\psi + W(0,z)\lambda R(z,\lambda)S(z)\psi \qquad \text{(C.21)}$$

for a $\psi \in \mathcal{H}$, and this application is holomorphic because $W(0,z)$, $S(z)$ and $R(z,\lambda)$ are bounded, holomorphic operators.

□

Appendix D

Proof of Lemma (3.1.2)

In this appendix we derive the formula of integration by parts which is used in section (3.1.1) and we give a generalization of this formula at the end of the appendix. Let us also denote $P(t)$ by $P_1(t)$ and $\mathbb{I} - P(t)$ by $P_2(t)$ in this proof.

1) $\mathcal{R}B(t)$ is strongly C^1 because $R(t,\lambda)$ is C^1 (see [Kr] chap. II) and $B(t)$ is C^1. This operator maps $\mathcal{H}$ into D because

$$R(t,\lambda) = R(t,\mu)\left(\mathbb{I} + (\lambda-\mu)R(t,\lambda)\right), \quad \text{if } \mu \in T(t). \tag{D.1}$$

Indeed, since we can find $\mu \in T(t)$ for all $t \in \mathbb{R}$ we have

$$\oint_\Gamma R(t,\lambda)B(t)R(t,\lambda)d\lambda = R(t,\mu)\oint_\Gamma \left(\mathbb{I} + (\lambda-\mu)R(t,\lambda)\right)B(t)R(t,\lambda)d\lambda. \tag{D.2}$$

By definition

$$P_1(t)\mathcal{R}B(t)P_1(t) = \frac{1}{(2\pi i)^3}\oint_\Gamma\oint_{\Gamma'}\oint_{\Gamma''} R(t,\lambda')R(t,\lambda)B(t)R(t,\lambda)R(t,\lambda'')d\lambda d\lambda' d\lambda'' \tag{D.3}$$

where the paths Γ , Γ' and Γ'' are given in figure (D.1). We can write the integrand under

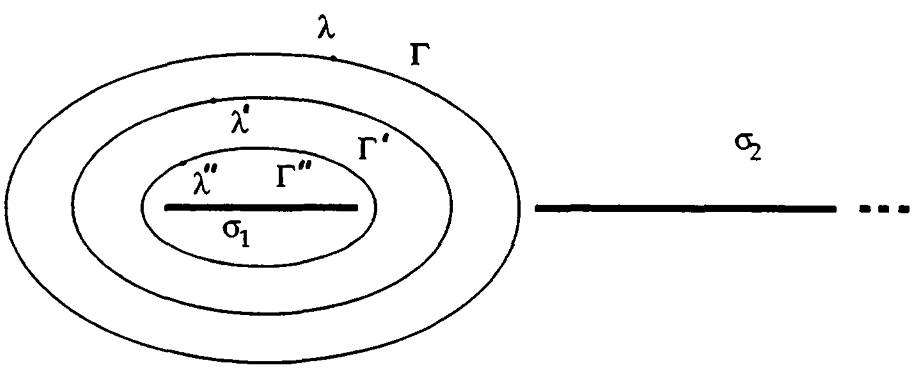

Figure D.1: The paths Γ , Γ' and Γ''.

the following form, using (D.1)

$$\frac{R(t,\lambda')B(t)R(t,\lambda)}{(\lambda'-\lambda)(\lambda-\lambda'')} - \frac{R(t,\lambda')B(t)R(t,\lambda'')}{(\lambda'-\lambda)(\lambda-\lambda'')}$$

$$-\frac{R(t,\lambda)B(t)R(t,\lambda)}{(\lambda'-\lambda)(\lambda-\lambda'')}+\frac{R(t,\lambda)B(t)R(t,\lambda'')}{(\lambda'-\lambda)(\lambda-\lambda'')}. \tag{D.4}$$

Now, integrating each term over the variable that does not appear in the resolvents, we obtain the result by the Cauchy formula. For the term $P_2(t)\mathcal{R}B(t)P_2(t)$ we use the definition of $P_2(t)$ and the above result to obtain

$$P_2(t)\mathcal{R}B(t)P_2(t) = \mathcal{R}B(t) - P_1(t)\mathcal{R}B(t) - \mathcal{R}B(t)P_1(t). \tag{D.5}$$

With the same paths as in figure (D.1) we compute

$$-P_1(t)\mathcal{R}B(t) = \frac{1}{(2\pi i)^2}\oint_\Gamma\oint_{\Gamma'} \frac{R(t,\lambda')B(t)R(t,\lambda)}{(\lambda'-\lambda)} - \frac{R(t,\lambda)B(t)R(t,\lambda)}{(\lambda'-\lambda)}d\lambda d\lambda' \tag{D.6}$$

and

$$-\mathcal{R}B(t)P_1(t) = \frac{1}{(2\pi i)^2}\oint_\Gamma\oint_{\Gamma'} \frac{R(t,\lambda)B(t)R(t,\lambda')}{(\lambda'-\lambda)} - \frac{R(t,\lambda)B(t)R(t,\lambda)}{(\lambda'-\lambda)}d\lambda d\lambda' \tag{D.7}$$

where the last term in (D.6) and (D.7) drops after an integration over λ'. Let us perform the integration over λ in the first term of (D.6)

$$\begin{aligned}&\frac{1}{2\pi i}\oint_\Gamma \frac{R(t,\lambda')B(t)R(t,\lambda)}{(\lambda'-\lambda)}d\lambda = \\ &\frac{1}{2\pi i}\oint_{\Gamma''} \frac{R(t,\lambda')B(t)R(t,\lambda'')}{(\lambda'-\lambda'')}d\lambda'' - R(t,\lambda')B(t)R(t,\lambda')\end{aligned} \tag{D.8}$$

by the Cauchy formula. Thus it remains

$$\begin{aligned}&P_2(t)\mathcal{R}B(t)P_2(t) = \\ &\frac{1}{(2\pi i)^2}\oint_{\Gamma'}\oint_{\Gamma''} \frac{R(t,\lambda')B(t)R(t,\lambda'')}{(\lambda'-\lambda'')}d\lambda' d\lambda'' - \\ &\frac{1}{(2\pi i)^2}\oint_{\Gamma}\oint_{\Gamma'} \frac{R(t,\lambda)B(t)R(t,\lambda')}{(\lambda-\lambda')}d\lambda d\lambda' - \\ &\frac{1}{2\pi i}\oint_{\Gamma'} R(t,\lambda')B(t)R(t,\lambda')d\lambda' + \mathcal{R}B(t)\end{aligned} \tag{D.9}$$

where the first two terms vanish by the Cauchy formula and the last two by definition of $\mathcal{R}B(t)$.

2) We have the following identities for $k \neq j$

$$\begin{aligned}&\frac{d}{ds}\left(P_k(0)V(s)^{-1}\mathcal{R}B(s)V(s)P_j(0)\right) = \\ &\left(P_k(0)V(s)^{-1}\left(\frac{d}{ds}\mathcal{R}B(s)\right)V(s)P_j(0)\right) + \\ &i\epsilon^{-1}P_k(0)V(s)^{-1}[H(s),\mathcal{R}B(s)]V(s)P_j(0) + \\ &iP_k(0)V(s)^{-1}[E(s),\mathcal{R}B(s)]V(s)P_j(0)\end{aligned} \tag{D.10}$$

and

$$\begin{aligned}[H(s),\mathcal{R}B(s)] &= \frac{1}{2\pi i}\oint_\Gamma [H(s)-\lambda, R(s,\lambda)B(s)R(s,\lambda)]d\lambda \\ &= -B(s)P_1(s) + P_1(s)B(s).\end{aligned} \tag{D.11}$$

Therefore we get

$$\begin{aligned}
&\int_{t'}^{t} P_1(0)V(s)^{-1}B(s)V(s)P_2(0)x(s)ds = \\
&\int_{t'}^{t} V(s)^{-1}P_1(s)B(s)P_2(s)V(s)x(s)ds = \\
&\int_{t'}^{t} P_1(0)V(s)^{-1}[H(s),\mathcal{R}B(s)]V(s)P_2(0)x(s)ds = \\
&-i\epsilon\int_{t'}^{t}\frac{d}{ds}\left(P_1(0)V(s)^{-1}\mathcal{R}B(s)V(s)P_2(0)\right)x(s) + \\
&i\epsilon\int_{t'}^{t} P_1(0)V(s)^{-1}\left(\frac{d}{ds}\mathcal{R}B(s)\right)V(s)P_2(0)x(s)ds - \\
&\epsilon\int_{t'}^{t} V(s)^{-1}P_1(s)[E(s),\mathcal{R}B(s)]P_2(s)V(s)x(s)ds = \\
&-i\epsilon P_1(0)V(s)^{-1}\mathcal{R}B(s)V(s)P_2(0)x(s)\Big|_{t'}^{t} + \\
&i\epsilon\int_{t'}^{t} P_1(0)V(s)^{-1}\left(\frac{d}{ds}\mathcal{R}B(s)\right)V(s)P_2(0)x(s)ds + \\
&i\epsilon\int_{t'}^{t} P_1(0)V(s)^{-1}\mathcal{R}B(s)V(s)P_2(0)\frac{d}{ds}x(s)ds - \\
&\varepsilon\int_{t'}^{t} P_1(0)V(s)^{-1}[E(s),\mathcal{R}B(s)]V(s)P_2(0)x(s)ds \qquad \text{(D.12)}
\end{aligned}$$

where we have used the intertwining property $V(s)P_k(0) = P_k(s)V(s)$.

□

Remark:
It is not difficult to generalize this formula to the following case:

Lemma D.0.1 *Let $V(t)$ be defined by*

$$i\varepsilon\frac{d}{dt}V(t) = (H(t) + \varepsilon E(t))V(t)$$

and $V(0) = \mathbb{I}$ where $H(t)$ is a strongly C^2 self-adjoint operator densely defined on D and $E(t)$ is a bounded, strongly C^2, self-adjoint operator. Let $B(t)$ be a closed operator defined on D which is strongly C^1 on D and leaves the domain D invariant. Let $x(t)$ a vector of $\mathcal{H}$ which belongs to D for all t and which is C^1 Then
1) $\mathcal{R}B(t)$ is a bounded operator, strongly C^1 which maps $\mathcal{H}$ into D. Moreover

$$P_k(t)\mathcal{R}B(t)P_k(t) \equiv 0, \quad k = 1,2$$

2)

$$\begin{aligned}
&\int_{t'}^{t} V(s)^{-1}P_1(s)B(s)P_2(s)V(s)x(s)ds = \\
&-i\epsilon V(s)^{-1}P_1(s)\mathcal{R}B(s)P_2(s)V(s)x(s)\Big|_{t'}^{t} + \\
&i\epsilon\int_{t'}^{t} V(s)^{-1}P_1(s)\left(\frac{d}{ds}\mathcal{R}B(s)\right)P_2(s)V(s)x(s)ds + \\
&i\epsilon\int_{t'}^{t} V(s)^{-1}P_1(s)\mathcal{R}B(s)P_2(s)V(s)\frac{d}{ds}x(s)ds -
\end{aligned}$$

$$\epsilon \int_{t'}^{t} V(s)^{-1} P_1(s)[E(s), \mathcal{R}B(s)] P_2(s) V(s) x(s) ds +$$
$$i\epsilon \int_{t'}^{t} V(s)^{-1} P_2(s) \left(\frac{d}{ds} P_1(s)\right) \mathcal{R}B(s) P_2(s) V(s) x(s) ds +$$
$$i\epsilon \int_{t'}^{t} V(s)^{-1} P_1(s) \mathcal{R}B(s) \left(\frac{d}{ds} P_2(s)\right) P_1(s) V(s) x(s) ds.$$

We have an analogous formula for $\int_{t'}^{t} V(s)^{-1} P_2(s) B(s) P_1(s) V(s) x(s) ds$ *which is obtained by exchanging* $P_1(s)$ *and* $P_2(s)$ *and changing the sign on the right hand side in the above formula.*

Note that $V(t)$ in this case does not necessarily follow the decomposition of the Hilbert space.

Appendix E

Proof of Proposition (4.1.1)

We perform here the last step to obtain an explicit formula for the phase $\theta_1(0|\gamma)$ defined by

$$W(0|\gamma)\varphi_1(0) = e^{-i\theta_1(0|\gamma)}\varphi_2(0) \tag{E.1}$$

in terms of the components $B_j(z)$ of the magnetic field. In order to do that we have to insert the definition

$$\psi_j(z) = \left(B_3(z) + (-1)^j\sqrt{\rho(z)}\,,\ B_1(z) + iB_2(z)\right)\quad ;\ j = 1,2 \tag{E.2}$$

into the expression

$$e^{-i\theta_j(0|\gamma)} = \frac{\|\psi_k(0)\|}{\|\psi_j(0)\|}\exp\left\{-i\int_\gamma \frac{\langle\psi_j(z)|P_j(z)\psi_j'(z)\rangle}{\|\psi_j(z)\|^2}\right\}. \tag{E.3}$$

On the real axis, $P_j(z)$ is self-adjoint, so that

$$i\delta_j'(t) = \frac{\langle\psi_j(t)|\psi_j'(t)\rangle}{\langle\psi_j(t)|\psi_j(t)\rangle}\quad t \in \mathbb{R}. \tag{E.4}$$

As $\frac{d}{dt}\langle\psi_j(t)|\psi_j(t)\rangle = 2\mathrm{Re}\langle\psi_j(t)|\psi_j'(t)\rangle$ we can write

$$i\delta_j'(t) = \frac{1}{2}\frac{d}{dt}\ln\langle\psi_j(t)|\psi_j(t)\rangle + i\mathrm{Im}\frac{\langle\psi_j(t)|\psi_j'(t)\rangle}{\langle\psi_j(t)|\psi_j(t)\rangle}. \tag{E.5}$$

From the expression (E.2) we compute

$$\langle\psi_j(t)|\psi_j(t)\rangle = 2\sqrt{\rho(t)}\left(\sqrt{\rho(t)} + (-1)^j B_3(t)\right) \tag{E.6}$$

and

$$\mathrm{Im}\langle\psi_j(t)|\psi_j'(t)\rangle = B_1(t)B_2'(t) - B_2(t)B_1'(t). \tag{E.7}$$

Since both expressions possess an analytic continuation obtained by putting $z \in \mathbb{C}$ in place of $t \in \mathbb{R}$ we eventually obtain

$$\begin{aligned} i\delta_j'(z) &= \frac{1}{2}\frac{d}{dz}\ln 2\sqrt{\rho(z)}\left(\sqrt{\rho(z)} + (-1)^j B_3(z)\right) \\ &+ i\frac{B_1(z)B_2'(z) - B_2(z)B_1'(z)}{2\sqrt{\rho(z)}\left(\sqrt{\rho(z)} + (-1)^j B_3(z)\right)} \\ &= \frac{1}{2}\frac{d}{dz}\ln 2\sqrt{\rho(z)}\left(\sqrt{\rho(z)} + (-1)^j B_3(z)\right) + i\frac{d}{dz}\ln\left(\frac{B_1(z) - iB_2(z)}{B_1(z) + iB_2(z)}\right) \\ &- i(-1)^j\frac{B_3(z)\left(B_1(z)B_2'(z) - B_2(z)B_1'(z)\right)}{2\sqrt{\rho(z)}\left(B_1^2(z) + B_2^2(z)\right)}. \end{aligned} \tag{E.8}$$

Using (E.8) we get for the logarithm of (E.3)

$$\begin{aligned} - & i \int_\gamma \frac{B_3 (B_1 B_2' - B_2 B_1')}{2\sqrt{\rho}\,(B_1^2 + B_2^2)}(z)dz - i \int_\gamma \frac{d}{dz} \ln\left(\frac{B_1 - iB_2}{B_1 + iB_2}\right)(z)dz \\ - & \frac{i}{2} \arg 2\sqrt{\rho}(\sqrt{\rho} - B_3)(z)\Big|_0^{(0|\gamma)} . \end{aligned} \tag{E.9}$$

Here $(0|\gamma)$ denotes the endpoint of γ. We have assumed a square root branch point for $\sqrt{\rho}$ at the eigenvalue-crossing z_0 so that $B_1(z_0) \pm iB_2(z_0) \neq 0$ and $\sqrt{\rho(z_0)} \pm B_3(z_0) \neq 0$. Hence we can choose a path γ encircling neither singularities nor zeros of $(B_1 - iB_2)/(B_1 + iB_2)$ and such that $\arg 2\sqrt{\rho}\,(\sqrt{\rho} - B_3)\,(z)|_0^{(0|\gamma)} = n2\pi$, n an integer. Thus we obtain for $\theta_1(0|\gamma)$

$$\begin{aligned} &\exp\{-i\theta_1(0|\gamma)\} = \\ &\exp\left\{ in\pi - i \int_\gamma \frac{B_3(z)\,(B_1(z)B_2'(z) - B_2(z)B_1'(z))}{2\sqrt{\rho(z)}\,(B_1^2(z) + B_2^2(z))} dz \right\} \end{aligned} \tag{E.10}$$

where $B_1^2 + B_2^2 \neq 0$ on γ.

□

Appendix F

Proof of Lemma (6.2.1)

By definition

$$|||H(z,\delta)|||_{z',\delta'} = \sup_{\varphi\in D} \frac{\|H(z,\delta)\varphi\|}{\|\varphi\|_{z',\delta'}}. \tag{F.1}$$

We first show that

$$|||H(z,\delta)|||_{z',\delta'} \leq M(z',\delta'). \tag{F.2}$$

where $M(z',\delta')$ is independent of z and δ. As $H(z,\delta)$ is strongly C^1 in $\mathcal{B}(X_{z',\delta'},\mathcal{H})$, $\|H(z,\delta)\varphi\|$ is continuous in $(z,\delta) \in S_a \times I_\Delta$, so that

$$\|H(z,\delta)\varphi\| \leq M_1(\varphi) \quad \forall (z,\delta) \in \omega \times I_\Delta \tag{F.3}$$

where $\omega = \{z \in S_a : |\mathrm{Re} z| \leq T\}$ is compact. By applying the uniform boundedness principle [Kr] we obtain the estimate

$$\|H(z,\delta)\varphi\| \leq M_1(z',\delta')\|\varphi\|_{z',\delta'} \quad \forall (z,\delta) \in \omega \times I_\Delta. \tag{F.4}$$

Suppose z does not belong to ω. Then by condition IX and by the uniform boundedness principle again we have

$$\begin{aligned} \|H(z,\delta)\varphi\| &\leq b(t)\left(\|\varphi\| + \|H^\pm(\delta)\varphi\|\right) + \|H^\pm(\delta)\varphi\| \\ &\leq \sup_{t\in \mathbb{R}} b(t)\left(\|\varphi\| + M^\pm(\varphi)\right) + M^\pm(\varphi) \leq M_2(\varphi) \end{aligned} \tag{F.5}$$

for some $M_2(\varphi)$. Here we have used the compactness of I_Δ. As a consequence, there exists $M_2(z',\delta')$ such that

$$\|H(z,\delta)\varphi\| \leq M_2(z',\delta')\|\varphi\|_{z',\delta'} \tag{F.6}$$

and it remains to take $M(z',\delta') = \max(M_1(z',\delta'), M_2(z',\delta'))$ to obtain (F.2). Note that z' can be replaced by $+$ or $-$ in (F.2). Using Cauchy formula, we immediately get

$$\|H'(z,\delta)\varphi\| \leq N(z',\delta')\|\varphi\|_{z',\delta'} \tag{F.7}$$

so that

$$\|(H(z_1,\delta) - H(z_2,\delta))\varphi\| \leq |z_1 - z_2| N(z',\delta')\|\varphi\|_{z',\delta'} \tag{F.8}$$

for any z_1, z_2 in a convex subset of S_a. We need a similar estimate for the variations of δ. By assumption, $\frac{\partial}{\partial\delta}H(z,\delta)\varphi$ is continuous in $(z,\delta) \in S_a \times I_\Delta$ and we show that $\frac{\partial}{\partial\delta}H(z,\delta)R(z',\delta',\lambda)$ is bounded as an operator from $\mathcal{H}$ to $\mathcal{H}$, if $\lambda \in T(z',\delta')$. Indeed, by the closed graph theorem $H(z,\delta)R(z',\delta',\lambda)$ is bounded and strongly continuously differentiable in δ, so that Banach Steinhaus theorem [Kr] implies that $\frac{\partial}{\partial\delta}H(z,\delta)R(z',\delta',\lambda)$ is bounded as well. Thus we have

$$\begin{aligned}\|\frac{\partial}{\partial\delta}H(z,\delta)\varphi\| &= \|\frac{\partial}{\partial\delta}H(z,\delta)R(z',\delta',\lambda)(H(z',\delta')-\lambda)\varphi\| \\ &\leq \|\frac{\partial}{\partial\delta}H(z,\delta)R(z',\delta',\lambda)\| \left(\|H(z',\delta')\varphi\| + |\lambda|\|\varphi\|\right) \\ &\leq \|\frac{\partial}{\partial\delta}H(z,\delta)R(z',\delta',\lambda)\|(1+|\lambda|)\|\varphi\|_{z',\delta'} \end{aligned} \tag{F.9}$$

so that

$$\frac{\partial}{\partial\delta}H(z,\delta) \in \mathcal{B}(X_{z',\delta'},\mathcal{H}). \tag{F.10}$$

Then, by condition IX and the uniform boundedness principle again, there exists $\tilde{N}(z',\delta')$ such that

$$\|\frac{\partial}{\partial\delta}H(z,\delta)\varphi\| \leq \tilde{N}(z',\delta')\|\varphi\|_{z',\delta'} \tag{F.11}$$

which implies

$$\|(H(z,\delta_1)-H(z,\delta_2))\varphi\| \leq |\delta_1-\delta_2|\tilde{N}(z',\delta')\|\varphi\|_{z',\delta'}. \tag{F.12}$$

From (F.8) and (F.12) follows the estimate

$$\|(H(z_1,\delta_1)-H(z_2,\delta_2))\varphi\| \leq (|z_1-z_2|+|\delta_1-\delta_2|)\,C(z',\delta')\|\varphi\|_{z',\delta'} \tag{F.13}$$

where $C(z',\delta') = \max(N(z',\delta'),\tilde{N}(z',\delta'))$. Putting $(z',\delta') = (z_1,\delta_1)$ we get

$$\begin{aligned}\|\varphi\|_{z_2,\delta_2} &\leq \|\varphi\|_{z_1,\delta_1} + (|z_1-z_2|+|\delta_1-\delta_2|)\,C(z_1,\delta_1)\|\varphi\|_{z_1,\delta_1} \\ \|\varphi\|_{z_1,\delta_1} &\leq \|\varphi\|_{z_2,\delta_2} + (|z_1-z_2|+|\delta_1-\delta_2|)\,C(z_1,\delta_1)\|\varphi\|_{z_1,\delta_1}\end{aligned} \tag{F.14}$$

hence

$$\frac{\|\varphi\|_{z_2,\delta_2}}{1+(|z_1-z_2|+|\delta_1-\delta_2|)\,C(z_1,\delta_1)} \leq \|\varphi\|_{z_1,\delta_1} \leq \frac{\|\varphi\|_{z_2,\delta_2}}{1-(|z_1-z_2|+|\delta_1-\delta_2|)\,C(z_1,\delta_1)}. \tag{F.15}$$

These relations show that the application $|||\cdot|||_{z,\delta}$ is continuous in (z,δ). Let A belong to $\mathcal{B}(X_{z,\delta},\mathcal{H})$.

$$\begin{aligned}\|A\varphi\| &\leq |||A|||_{z_2,\delta_2}\|\varphi\|_{z_2,\delta_2} \\ &\leq |||A|||_{z_2,\delta_2}\left(1+(|z_1-z_2|+|\delta_1-\delta_2|)\,C(z_1,\delta_1)\right)\|\varphi\|_{z_1,\delta_1}\end{aligned} \tag{F.16}$$

so that

$$|||A|||_{z_1,\delta_1} \leq |||A|||_{z_2,\delta_2}\left(1+(|z_1-z_2|+|\delta_1-\delta_2|)\,C(z_1,\delta_1)\right). \tag{F.17}$$

Similarly

$$|||A|||_{z_2,\delta_2} \leq |||A|||_{z_1,\delta_1}\frac{1}{1-(|z_1-z_2|+|\delta_1-\delta_2|)\,C(z_1,\delta_1)} \tag{F.18}$$

so that

$$\left||||A|||_{z_2,\delta_2} - |||A|||_{z_1,\delta_1}\right| \leq |||A|||_{z_1,\delta_1}\frac{(|z_1-z_2|+|\delta_1-\delta_2|)\,C(z_1,\delta_1)}{1-(|z_1-z_2|+|\delta_1-\delta_2|)\,C(z_1,\delta_1)} \tag{F.19}$$

which tends to zero as $(z_2,\delta_2)\to(z_1,\delta_1)$. Finally, from (F.19), (F.2) and (F.13) follows the estimate

$$\begin{aligned}
&\Big| |||H(z_1,\delta_1)|||_{z_1',\delta_1'} - |||H(z_2,\delta_2)|||_{z_2',\delta_2'}\Big| \leq \\
&\Big| |||H(z_2,\delta_2)|||_{z_1',\delta_1'} - |||H(z_2,\delta_2)|||_{z_2',\delta_2'}\Big| + \\
&\Big| |||H(z_1,\delta_1)|||_{z_1',\delta_1'} - |||H(z_2,\delta_2)|||_{z_1',\delta_1'}\Big| \leq \\
&|||H(z_2,\delta_2)|||_{z_1',\delta_1'} \frac{(|z_2'-z_1'|+|\delta_2'-\delta_1'|)\,C(z_1',\delta_1')}{1-(|z_2'-z_1'|+|\delta_2'-\delta_1'|)\,C(z_1',\delta_1')} + \\
&|||H(z_1,\delta_1)-H(z_2,\delta_2)|||_{z_1',\delta_1'} \leq \\
&M(z_1',\delta_1')\frac{(|z_2'-z_1'|+|\delta_2'-\delta_1'|)\,C(z_1',\delta_1')}{1-(|z_2'-z_1'|+|\delta_2'-\delta_1'|)\,C(z_1',\delta_1')} + \\
&(|z_2-z_1|+|\delta_2-\delta_1|)\,C(z_1',\delta_1').
\end{aligned} \tag{F.20}$$

The last term in this inequality tends to zero as $(z_2,\delta_2)\to(z_1,\delta_1)$ and $(z_2',\delta_2')\to(z_1',\delta_1')$ which shows that the application $|||H(z,\delta)|||_{z',\delta'}$ in continuous as a function of (z,z',δ,δ'). Thus, on the compact set $\omega^2\times I_\Delta^2$ we have

$$\sup_{(z,z',\delta,\delta')\in\omega^2\times I_\Delta^2} |||H(z,\delta)|||_{z',\delta'} \leq M' \tag{F.21}$$

It remains to control this application when $|z|,|z'|\to\infty$ in S_a. If $|\mathrm{Re}|\geq T$, T large, we have by condition IX

$$\|\varphi\|_{z,\delta} \leq (1+b(\pm T))\,\|\varphi\|_{\pm,\delta} \leq K_1\|\varphi\|_{\pm,\delta} \tag{F.22}$$

for K_1 some constant, and similarly

$$\|\varphi\|_{\pm,\delta} \leq \frac{\|\varphi\|_{z,\delta}}{1-b(\pm T)} \leq K_2\|\varphi\|_{z,\delta}. \tag{F.23}$$

Moreover, from (F.12)

$$\begin{aligned}
\|\varphi\|_{\pm T,\delta} &\leq \left(1+\Delta\tilde{N}(\pm T,0)\right)\|\varphi\|_{\pm T,0} \leq K_3\|\varphi\|_{\pm T,0} \\
\|\varphi\|_{\pm T,\delta} &\leq \frac{\|\varphi\|_{\pm T,0}}{\left(1-\Delta\tilde{N}(\pm T,0)\right)} \leq K_4\|\varphi\|_{\pm T,0}
\end{aligned} \tag{F.24}$$

provided Δ is small enough. Thus if $|\mathrm{Re}z|\geq T$, $|\mathrm{Re}z'|\leq T$ we can write with (F.21)

$$\begin{aligned}
\|H(z,\delta)\varphi\| &\leq (1+b(\pm T))\|\varphi\|_{\pm,\delta} \leq \\
(1+b(\pm T))K_2\|\varphi\|_{\pm T,\delta} &\leq (1+b(\pm T))K_2(1+M')\|\varphi\|_{\pm T',\delta'}
\end{aligned} \tag{F.25}$$

showing that

$$|||H(z,\delta)|||_{z',\delta'} \leq (1+b(\pm T))K_2(1+M'). \tag{F.26}$$

Now if $|\mathrm{Re}z'|\geq T$ and $|\mathrm{Re}z|\leq T$

$$\begin{aligned}
\|H(z,\delta)\varphi\| &\leq M'\|\varphi\|_{\pm T,\delta'} \leq \\
M'K_1\|\varphi\|_{\pm,\delta'} &\leq M'K_1K_2\|\varphi\|_{z',\delta'}
\end{aligned} \tag{F.27}$$

from which follows

$$|||H(z,\delta)|||_{z',\delta'} \leq M'K_1K_2. \tag{F.28}$$

Finally if both $|\mathrm{Re} z|$ and $|\mathrm{Re} z'|$ are $\geq T$, we use (F.24) as well to get

$$\begin{aligned} \|H(z,\delta)\varphi\| &\leq (1+b(\pm T))K_2\|\varphi\|_{\pm T,\delta} \\ &\leq (1+b(\pm T))K_2K_3K_4\|\varphi\|_{\pm T,\delta'} \\ &\leq (1+b(\pm T))K_2K_3K_4K_1K_2\|\varphi\|_{z',\delta'}. \end{aligned} \tag{F.29}$$

Gathering these estimates, we eventually obtain

$$\sup_{(z,z',\delta,\delta')\in S_a^2\times I_\Delta^2} |||H(z,\delta)|||_{z',\delta'} \leq M < \infty. \tag{F.30}$$

The result is true if z, or z' or both are replaced either by $+$ or $-\infty$.

The last assertions of the lemma are proven as follows. By condition IX and (F.30) we have for $z = t + is$ and any (z', δ')

$$\|(H(z,\delta) - H^{\pm}(\delta))\varphi\| \leq b(t)\|\varphi\|_{\pm,\delta} \leq b(t)(1+M)\|\varphi\|_{z',\delta'} \tag{F.31}$$

and we conclude by Cauchy formula that

$$\|H'(z,\delta)\varphi\| \leq \bar{b}(t)\|\varphi\|_{z',\delta'} \tag{F.32}$$

for any $z = t + is$ with $|s| < r < a$, where $\bar{b}(t)$ is another integrable decay function. Similarly, (F.11) implies

$$\|\frac{\partial}{\partial\delta}H(z,\delta)\varphi\| \leq \tilde{N}(0,0)\|\varphi\|_{0,0} \tag{F.33}$$

so that by (F.30) again

$$\|\frac{\partial}{\partial\delta}H(z,\delta)\varphi\| \leq \tilde{N}(0,0)M\|\varphi\|_{z',\delta'}. \tag{F.34}$$

This finishes the proof of the lemma.

□

Appendix G

Proof of Lemma (6.2.3)

For a fixed $z \in S_a$ and $\lambda \in T(z,\delta)$ we have the strong derivative (see e.g. [Kr] paragraph (1), chapter II.)

$$\frac{\partial}{\partial\delta}R(z,\delta,\lambda) = -R(z,\delta,\lambda)\frac{\partial}{\partial\delta}H(z,\delta)R(0,0,i)(H(0,0)-i)R(z,\delta,\lambda) \tag{G.1}$$

where the bounded operators $R(z,\delta,\lambda)$, $\frac{\partial}{\partial\delta}H(z,\delta)R(0,0,i)$ and $(H(0,0)-i)R(z,\delta,\lambda)$ are strongly continuous in z and δ. Indeed, this is easily seen for $R(z,\delta,\lambda)$ by considering identities analogous to (6.18) and this is true by hypothesis for $\frac{\partial}{\partial\delta}H(z,\delta)R(0,0,i)$. Finally, $(H(0,0)-i)R(z,\delta,\lambda)$ is the inverse of the bounded operator $(H(z,\delta)-\lambda)R(0,0,i)$ which is continuous in norm, as can be seen from estimates of the type (6.14). Thus, by lemma (3.7) of the introduction of [Kr], $(H(0,0)-i)R(z,\delta,\lambda)$ is bounded and even continuous in norm. Hence the strong continuity of $\frac{\partial}{\partial\delta}R(z,\delta,\lambda)$ and of $\frac{\partial}{\partial z}R(z,\delta,\lambda)$, by similar considerations. These properties are true for the projector $Q(z,\delta)$ as well by passing the derivatives under the integral of the formula in lemma (6.2.2). We now turn to the second part of the lemma. Consider the identity

$$R(z,\delta,\lambda) - R(\pm,\delta,\lambda) = -R(z,\delta,\lambda)(H(z,\delta) - H^{\pm}(\delta))R(\pm,\delta,\lambda). \tag{G.2}$$

With condition IX and lemma (6.2.1) we obtain

$$\|R(z,\delta,\lambda) - R(\pm,\delta,\lambda)\| \le \|R(\pm,\delta,\lambda)\|\frac{b(t)d(\pm,\delta,\lambda)}{1-b(t)d(\pm,\delta,\lambda)} \tag{G.3}$$

for $z = t + is$, $|t|$ large with the definition

$$d(\pm,\delta,\lambda) = \|R(\pm,\delta,\lambda)\| + \|H^{\pm}(\delta)R(\pm,\delta,\lambda)\|. \tag{G.4}$$

This defines the integrable decay function $b_{\lambda,\delta}(t)$. The estimate on the derivatives are consequences of the Cauchy formula. We define the projector $Q(z,\lambda)$ by using the finite set of paths Γ_j, introduced in the proof of lemma (6.2.2). If $\lambda \in \Gamma_j$ we obtain from (G.3) and (6.30)

$$\|R(z,\delta,\lambda) - R(\pm,\delta,\lambda)\| \le \frac{\overline{K}^2 b(t)}{1-b(t)\overline{K}} \le K'b(t) \tag{G.5}$$

if $|t|$ is large enough. This estimate and Cauchy formula again finish the proof of the lemma.

□

Appendix H

Proof of Lemma (6.2.5)

We prove here that the coefficients $a^*_{kj}(z,\delta)$ defined by

$$a^*_{kj}(z,\delta) = -\langle\varphi^*_k(0,\delta)|\widehat{W_*}^{-1}(z,\delta)\widehat{K_*}(z,\delta)\widehat{W_*}(z,\delta)\varphi^*_j(0,\delta)\rangle \tag{H.1}$$

are uniformly bounded by an integrable decay function $b(t)$, independent of δ for any $z = t + is \in S^+_a \backslash D(0,r)$. Remembering that

$$\widehat{P^*_j}(z,\delta) = \widehat{W_*}^{-1}(z,\delta)P^{N^*}_j(z,\delta)\widehat{W_*}(z,\delta) \tag{H.2}$$

we have

$$\begin{aligned}\widehat{P^*_j}'(z,\delta) &= \widehat{W_*}^{-1}(z,\delta)P^{N^*\prime}_j(z,\delta)\widehat{W_*}(z,\delta)\\ &+ \frac{1}{i}\widehat{W_*}^{-1}(z,\delta)[P^{N^*}_j(z,\delta),K_{N^*}(z,\delta)]\widehat{W_*}(z,\delta).\end{aligned} \tag{H.3}$$

As the operators are restricted to $Q_{N^*}(0,\delta)\mathcal{H}$, the last term vanishes,

$$\begin{aligned}&Q_{N^*}(0,\delta)\widehat{W_*}^{-1}(z,\delta)[P^{N^*}_j(z,\delta),K_{N^*}(z,\delta)]\widehat{W_*}(z,\delta)Q_{N^*}(0,\delta) \equiv\\ &\widehat{W_*}^{-1}(z,\delta)[P^{N^*}_j(z,\delta),Q_{N^*}(z,\delta)K_{N^*}(z,\delta)Q_{N^*}(z,\delta)]\widehat{W_*}(z,\delta) \equiv 0,\end{aligned} \tag{H.4}$$

and we obtain using (6.41)

$$\begin{aligned}\|\widehat{P^*_j}(z,\delta)\| &\leq w^2\|P^{N^*}_j(z,\delta)\|\\ \|\widehat{K_*}(z,\delta)\| &\leq 4w^2\|P^{N^*}_1(z,\delta)\|\|P^{N^*\prime}_1(z,\delta)\| \quad z \neq z_0(\delta)\end{aligned} \tag{H.5}$$

where w is independent of z, δ, and ε. It remains to show that $P^{N^*}_1(z,\delta)$ is uniformly bounded in ε and δ along the dissipative path $\gamma_\delta(t)$. By construction (proposition (6.2.2)), $\gamma_\delta \in S^+_a\backslash D(0,r)$ if r is small enough, where there is no eigenvalue crossing point of $e^*_j(z,\delta)$ and $e_j(z,\delta)$. Hence for any $z \in S^+_a\backslash D(0,r)$ the projections $P^{N^*}_j(z,\delta)$ are given by means of a Riesz formula

$$P^{N^*}_j(z,\delta) = -\frac{1}{2\pi i}\oint_{\gamma_j} R_{N^*}(z,\delta,\lambda)d\lambda \tag{H.6}$$

where γ_j, encircles both $e^*_j(z,\delta)$ and $e_j(z,\delta)$, a finite distance away from the spectra of $H_{N^*}(z,\delta)$ and $H(z,\delta)$. By an argument similar to the one given in lemma (6.2.2), we see that we can pick γ_j, for any $z \in S^+_a\backslash D(0,r)$, among a finite set of paths which are all of finite length and bounded away from the spectra of $H_{N^*}(z,\delta)$ and $H(z,\delta)$. Then in view of

$$R_{N^*}(z,\delta,\lambda) - R(z,\delta,\lambda) = -R_{N^*}(z,\delta,\lambda)(H_{N^*}(z,\delta) - H(z,\delta))R(z,\delta,\lambda) \tag{H.7}$$

and (6.38) we obtain the estimate

$$\|R_{N^*}(z,\delta,\lambda)\| \leq \|R(z,\delta,\lambda)\| \frac{1}{1-\varepsilon\frac{e}{e-1}b(t)} \tag{H.8}$$

provided ε is small enough, and $\lambda \in T(z,\delta)$. By the continuity in norm of $R(z,\delta,\lambda)$ in δ, there exists δ^* such that $\|R(z,\delta,\lambda)\|$ is uniformly bounded in $\delta < \delta^*$ if $\lambda \in \gamma_j$, and $z \in S_a^+ \backslash D(0,r)$. When $z = t + is$, with $|t|$ large, we use (G.3),

$$\|R(z,\delta,\lambda) - R(\pm,\delta,\lambda)\| \leq \|R(\pm,\delta,\lambda)\| \frac{b(t)d(\pm,\delta,\lambda)}{1-b(t)d(\pm,\delta,\lambda)} \tag{H.9}$$

and the fact that if $\lambda \in \gamma_j \subset T(\pm,0)$, there exists a constant $\overline{k}$ independent of δ such that

$$d(\pm,\delta,\lambda) \leq \overline{k}. \tag{H.10}$$

Hence the estimate

$$\|R(z,\delta,\lambda) - R(\pm,\delta,\lambda)\| \leq \overline{k}\frac{b(t)\overline{k}}{1-b(t)\overline{k}} \leq k'b(t). \tag{H.11}$$

As a consequence of (H.7), (H.8), (H.11) and $R(\pm,\delta,\lambda) = R_{N^*}(\pm,\delta,\lambda)$ we have

$$\begin{aligned}
\|R_{N^*}(z,\delta,\lambda) - R(\pm,\delta,\lambda)\| &\leq \\
\|R_{N^*}(z,\delta,\lambda) - R(z,\delta,\lambda)\| &+ \|R(z,\delta,\lambda) - R(\pm,\delta,\lambda)\| \leq \\
\|R(z,\delta,\lambda)\|^2 \frac{\varepsilon\frac{e}{e-1}b(t)}{1-\varepsilon\frac{e}{e-1}b(t)} &+ k'b(t) \\
&\leq k''b(t)
\end{aligned} \tag{H.12}$$

where k'' is independent of ε and δ. Thus we eventually obtain

$$\|\widehat{K_*}(z,\delta)\| \leq kb(t) \quad \forall z = t + is \in S_a^+ \backslash D(0,r) \tag{H.13}$$

and

$$\|\widehat{W_*}(z,\delta)\| \leq \hat{w} \quad \forall \delta \leq \delta^* \tag{H.14}$$

so that

$$|a_{kj}^*(z,\delta)| \leq \hat{w}^2 kb(t) \tag{H.15}$$

where $b(t)$ is an integrable decay function.

□

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Contents

List of Figures

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