Elementary Exponential Error Estimates for the Adiabatic Approximation

George Hagedorn*
Center for Statistical Mechanics and Mathematical Physics
Virginia Polytechnic Institute and State University
Blacksburg, Virginia 24061-0123, U.S.A.

Alain Joye
Institut Fourier
Unité Mixte de Recherche CNRS-UJF 5582
Université de Grenoble I
38402 Saint-Martin d'Hères Cedex, France

July 25, 2001

Abstract

We present an elementary proof that the quantum adiabatic approximation is correct up to exponentially small errors for Hamiltonians that depend analytically on the time variable. Our proof uses optimal truncation of a straightforward asymptotic expansion. We estimate the terms of the expansion with standard Cauchy estimates.

*Partially Supported by National Science Foundation Grant DMS–0071692.

1 Introduction

The adiabatic theorem of quantum mechanics describes the asymptotic behavior of solutions to the time-dependent Schrödinger equation when the Hamiltonian depends slowly on the time variable. By rescaling the time variable by a factor of ϵ, which measures the slowness of the Hamiltonian's variation, the problem is usually restated in the following way: Let $\{H(t)\}_{t\in\mathbb{R}}$ be a smooth family of self-adjoint operators that satisfies the following gap condition: Assume $H(t)$ possesses a smooth non-degenerate eigenvalue $E(t)$ for all times. Then the solution to

$$i\,\epsilon\,\frac{\partial\psi}{\partial t} \;=\; H(t)\,\psi, \qquad \text{for small} \quad \epsilon > 0, \tag{1.1}$$

with initial condition $\psi(t_0)$ in the eigenspace associated with $E(t_0)$, will evolve to a state $\psi(t)$ that belongs to the eigenspace associated with $E(t)$, up to an $O(\epsilon)$ error as $\epsilon \to 0$. The square of the norm of the orthogonal projection of $\psi(t)$ onto the complement of the instantaneous eigenspace defines the non-adiabatic transition probability. According to the adiabatic theorem, it is of order ϵ^2.

The statement that solutions to (1.1) follow the instantaneous eigenspaces of the Hamiltonian was made as early as 1928 by Born and Fock in [4] for discrete, non-degenerate Hamiltonians, and was generalized over the years by several authors. A few milestones in the history of the adiabatic theorem were the following: Kato [16] proved the theorem for Hamiltonians with a non-degenerate eigenvalue separated from the rest of the spectrum, without any assumption on the nature of the rest of the spectrum. In [21], Nenciu showed that the adiabatic theorem holds for bounded Hamiltonians if one replaces the isolated eigenvalue $E(t)$ by an isolated component of the spectrum $\sigma(t)$ and the instantaneous eigenspace associated with $E(t)$ by the instantaneous spectral subspace associated with $\sigma(t)$. This result was further generalized to unbounded Hamiltonians by Avron, Seiler and Yaffe in [2].

At the same time that the adiabatic theorem was qualitatively generalized to handle more situations, it was quantitatively improved to compute transition probabilites more accurately. For discrete Hamiltonians Lenard [18] and Garrido [7] developed techniques that provide asymptotic expressions for certain solutions to (1.1), with $O(\epsilon^\infty)$ error estimates. These techniques have been generalized by Nenciu and Rasche [22, 25, 23] to fit the general setting described above. Typical results say that if all time derivatives of the Hamiltonian at both the initial and final times are zero, then the transition probability is $O(\epsilon^\infty)$. When these derivatives are non–zero, there exists a smooth ϵ–dependent subspace, close to the instantaneous spectral subspace, to which certain solutions belong, up to $O(\epsilon^\infty)$ errors. A scattering theory analog was proved in [2], where the derivatives were assumed to vanish as $t \to \pm\infty$.

When the Hamiltonian is an analytic function of time, one expects the transition probability to be exponentially small in the scattering context mentioned above. This is suggested by non–rigorous analyses of 2×2 matrix Hamiltonians, certain explicitly solvable models (see [28, 17, 5]), and the success of the Landau–Zener formula. It was proved to be true in a general setting only recently by Joye and Pfister in [13]. Earlier works proved it for matrix hamiltonians [6, 9, 12] or for discrete hamiltonians with special time dependence [10]. These papers solve (1.1) for complex values of the time variable along carefully chosen paths in the complex plane. Subsequent works on the exponential accuracy of the adiabatic approximation have been performed by Nenciu [24] who proved the existence of "superadiabatic evolution operators," *i.e.*, exponentially accurate approximations of the evolution generated by (1.1). Superadiabatic evolutions were first introduced and studied in the physics literature by Berry and Lim [3, 19]. Joye and Pfister, [14, 11] used superadiabatic evolutions to set up a reduction theory and to prove the Landau–Zener formula. The method of proof consisted in deriving and achieving sufficient control on asymptotic expansions of the evolution operator so that optimal truncation would yield exponential accuracy. Exponential accuracy of the adiabatic theorem was also tackled using powerful pseudo-differential operator techniques by Sjöstrand [27] and by Martinez [20] who studied the exponential decay rate of the transition probability as a function of the parameters of the problem using this method. Further details and results on other aspects of the adiabatic theorem can be found in the references quoted in the recent reviews [15] and [1].

In the present paper we provide an elementary proof of the exponential accuracy of the adiabatic theorem, in the spirit of the results concerning superadiabatic evolutions for Hamiltonians that have a non–degenerate isolated eigenvalue. Our result is not new, nor the most general, but our proof uses only simple techniques of elementary analysis. Our approach is to use a straightforward asymptotic expansion [8] for the solution to (1.1). We estimate the individual terms in the expansion by using Cauchy estimates. From this, it follows that when the expansion is truncated after an optimal number of terms, the resulting approximation is exponentially accurate.

1.1 The Main Results

We assume two hypotheses. The first one states that the (possibly unbounded) Hamiltonian is analytic in an appropriate sense in a neighboorhood of the real axis.

H1: Let $\{H(t)\}_{t\in I\!\!R}$ be a family of self-adjoint operators in a separable Hilbert space $\mathcal{H}$ with common dense domain $D \subset \mathcal{H}$. We assume that $\{H(t)\}_{t\in I\!\!R}$ admits an extension to the set $S_{\delta_0} = \{t \in \mathbb{C} \,:\, |\mathrm{Im}\, t| < \delta_0\}$ which forms an analytic family of type A.

The second hypothesis asserts the existence of a non-degenerate eigenvalue in the spectrum of $H(t)$ for all times.

H2: For $t \in I\!\!R$, let $E(t)$ be a simple eigenvalue of $H(t)$ that remains a distance $d(t) > d_0 > 0$ away from the rest of the spectrum of $H(t)$.

We let $[\![x]\!]$ denote the greatest integer less than or equal to x, and let $\phi^{\perp}(t)$ denote the projection of any vector $\phi(t)$ onto the orthogonal complement of the instantaneous eigenspace associated with $E(t)$.

Our main result is the following:

Theorem 1.1 *Assume hypotheses H1 and H2. Then, for all* $t \in I\!\!R$, *there exists a sequence* $\{\psi_n(t)\}_{n\in\mathbf{N}}$ *of vectors in* $\mathcal{H}$ *that is determined by an explicit recurrence relation. For each*

$N \in \mathbf{N}$, we construct

$$\Psi_N(t,\epsilon) \;=\; e^{-i\int_{t_0}^t E(s)\,ds/\epsilon}\,\Big(\psi_0(t) \,+\, \epsilon\psi_1(t) \,+\, \cdots \,+\, \epsilon^N\psi_N(t) \,+\, \epsilon^{N+1}\psi_{N+1}^{\perp}(t)\Big).$$

For any t_0 and t in an arbitrary compact interval of $I\!R$, there exist positive G, $C(g)$, and $\Gamma(g)$ (given in (5.9)), such that for all $g \in (0,\,G)$, the vector $\Psi_*(t,\epsilon) \;=\; \Psi_{[\![g/\epsilon]\!]}(t,\epsilon)$ satisfies

$$\|\psi(t,\epsilon) \,-\, \Psi_*(t,\epsilon)\| \;\leq\; C(g)\; e^{-\Gamma(g)/\epsilon},$$

for all $\epsilon \leq 1$. Here $\psi(t,\epsilon)$ is the exact solution to the Schrödinger equation (1.1) with initial condition $\psi(t_0,\epsilon) \;=\; \Psi_*(t_0,\epsilon)$.

Remarks: **1.** By keeping track of how $\Gamma(g)$ depends on the minimum gap d_0, we recover the expected behavior $\Gamma(g) \simeq d_0$ as $d_0 \to \infty$. See [14] and [20].
2. The theorem implies that the range of the projector $\dfrac{|\Psi_*(t,\epsilon)\rangle\,\langle\Psi_*(t,\epsilon)|}{\|\Psi_*(t,\epsilon)\|^2}$ is a smooth subspace that solutions follow, up to $O(e^{-\Gamma(g)/\epsilon})$ errors.
3. At the cost of some more technicalities, it is possible to get the same result when the analyticity and gap hypotheses only hold in a neighborhood of some bounded interval of the real axis, or when t and t_0 tend to minus and plus infinity, respectively.

The rest of the paper is devoted to the proof of the Theorem 1.1.

2 Adiabatic Expansion in Powers of ϵ

In this section we develop the expansion in powers of ϵ for certain solutions to the evolution determined by

$$i\,\epsilon\,\frac{\partial\psi}{\partial t} \;=\; H(t)\,\psi. \tag{2.1}$$

We assume H1 and H2 so that the resolvent of $H(t)$ and the isolated eigenvalue $E(t)$ of multiplicity 1 are C^∞ in $t \in I\!R$. Without loss of generality, we assume the initial time is $t_0 = 0$.

We prove that $\psi(t,\epsilon)$ has an expansion of the form

$$\psi(t,\epsilon) \;=\; e^{-i\int_0^t E(s)\,ds/\epsilon}\,\Big(\psi_0(t) \,+\, \epsilon\,\psi_1(t) \,+\, \epsilon^2\,\psi_2(t) \,+\, \ldots\Big). \tag{2.2}$$

We choose $\Phi(t)$ to be a smooth normalized eigenvector of $H(t)$ corresponding to $E(t)$, and we assume its phase has been chosen so that

$$\langle\,\Phi(t),\,\Phi'(t)\,\rangle \;=\; 0 \tag{2.3}$$

for each t. The existence of such an eigenvector follows *e.g.*, from Problem 15, Chapter XII of [26].

We substitute the expression (2.2) into (2.1) and equate terms on the two sides of the resulting equation that are formally of the same orders in ϵ.

Order 0. The terms of order zero require

$$[\,H(t) - E(t)\,]\ \psi_0(t) \;=\; 0.$$

This equation forces us to take

$$\psi_0(t) \;=\; f_0(t)\,\Phi(t), \tag{2.4}$$

for some yet to be determined function $f_0(t)$.

Order 1. The terms of order ϵ require

$$i\,\frac{\partial \psi_0}{\partial t} \;=\; [\,H(t) - E(t)\,]\ \psi_1(t).$$

From (2.4) this implies

$$i\,\frac{\partial f_0}{\partial t}(t)\,\Phi(t) \;+\; i\,f_0(t)\,\frac{\partial \Phi}{\partial t}(t) \;=\; [\,H(t) - E(t)\,]\ \psi_1(t).$$

We solve this equation by separately examining those components of this equation that are multiples of $\Phi(t)$ and those that are perpendicular to $\Phi(t)$. Using (2.3), we thus obtain two conditions:

$$i\,\frac{\partial f_0}{\partial t}(t) \;=\; 0, \tag{2.5}$$

and

$$i\,f_0(t)\,\frac{\partial \Phi}{\partial t}(t) \;=\; [\,H(t) - E(t)\,]\ \psi_1(t). \tag{2.6}$$

Equation (2.5) requires that f_0 be constant, and without loss of generality, we choose it to be

$$f_0(t) \;=\; 1. \tag{2.7}$$

Equation (2.6) then forces us to choose

$$\psi_1(t) \;=\; f_1(t)\,\Phi(t) \;+\; \psi_1^{\perp}(t), \tag{2.8}$$

where f_1 is yet to be determined, and

$$\psi_1^{\perp}(t) \;=\; i\,[\,H(t) - E(t)\,]_r^{-1}\,\Phi'(t). \tag{2.9}$$

In this expression we have used $[\,H(t) - E(t)\,]_r^{-1}$ to denote the reduced resolvent operator of $H(t)$ on the orthogonal complement of the span of $\Phi(t)$.

Order $n \geq 2$. We assume inductively that we have solved the equations of order $j \leq n-1$ to obtain

$$\psi_j(t) \;=\; f_j(t)\,\Phi(t) \,+\, \psi_j^{\perp}(t). \tag{2.10}$$

Here, the scalar function f_j has been determined for $j \leq n-2$, and the vector–valued function $\psi_j^{\perp}$ has been determined for $j \leq n-1$.

Equating terms of order n requires

$$i\,\frac{\partial \psi_{n-1}}{\partial t} \;=\; [\,H(t) - E(t)\,]\;\psi_n(t).$$

From (2.10) this implies

$$i\,\frac{\partial f_{n-1}}{\partial t}(t)\,\Phi(t) \,+\, i\,f_{n-1}(t)\,\frac{\partial \Phi}{\partial t}(t) \,+\, i\,\frac{\partial \psi_{n-1}^{\perp}}{\partial t}(t) \;=\; [\,H(t) - E(t)\,]\;\psi_n(t).$$

Using (2.3), we separately examine the components of this equation that are multiples of $\Phi(t)$ and those that are perpendicular to $\Phi(t)$ to obtain two conditions:

$$i\,\frac{\partial f_{n-1}}{\partial t}(t) \,+\, i\,\langle\, \Phi(t),\, \frac{\partial \psi_{n-1}^{\perp}}{\partial t}(t)\,\rangle \;=\; 0, \tag{2.11}$$

and

$$i\,f_{n-1}(t)\,\frac{\partial \Phi}{\partial t}(t) \,+\, i\,P_{\perp}(t)\,\frac{\partial \psi_{n-1}^{\perp}}{\partial t}(t) \;=\; [\,H(t) - E(t)\,]\;\psi_n(t), \tag{2.12}$$

where $P_{\perp}(t) \;=\; I \,-\, |\Phi(t)\rangle\,\langle\Phi(t)|$.

Equation (2.11) is solved simply by integration. It determines f_{n-1} up to a constant of integration that we take to be zero:

$$f_{n-1}(t) \;=\; -\int_0^t \langle\, \Phi(s),\, \frac{\partial \psi_{n-1}^{\perp}}{\partial t}(s)\,\rangle\, ds. \qquad\qquad (n \geq 2) \tag{2.13}$$

Equation (2.12) determines $\psi_n^{\perp}$ to be

$$\psi_n^{\perp}(t) \;=\; i\,[\,H(t) - E(t)\,]_r^{-1}\,\left(\,f_{n-1}(t)\,\Phi'(t) \,+\, P_{\perp}(t)\,\frac{\partial \psi_{n-1}^{\perp}}{\partial t}(t)\,\right). \tag{2.14}$$

We have thus determined f_{n-1} and $\psi_n^{\perp}$, and the induction can proceed.

By using lemma 2.1 of [8], we now easily prove that

$$\Psi_N(t,\epsilon) \;=\; e^{-i\int_0^t E(s)\,ds/\epsilon}\,\Big(\,\psi_0(t) \,+\, \epsilon\,\psi_1(t) \,+\, \epsilon^2\,\psi_2(t) \,+\, \dots \,+\, \epsilon^N\,\psi_N(t) \,+\, \epsilon^{N+1}\,\psi_{N+1}^{\perp}\Big) \tag{2.15}$$

agrees with an exact solution of (2.1) up to an error that is bounded by $A_N\,\epsilon^{N+1}$ for some A_N, as long as t is kept in a fixed compact interval.

Lemma 2.1 of [8] states that if $\chi(t,\epsilon)$ approximatively solves (2.1) in the sense that

$$i\,\epsilon\,\frac{\partial\chi}{\partial t}(t,\epsilon)\;-\;H(t)\,\chi(t,\epsilon)=\zeta(t,\epsilon), \tag{2.16}$$

where $\zeta(t,\epsilon)$ is non-zero but small, then there exists an exact solution $\psi(t,\epsilon)$ to (2.1), such that

$$\|\psi(t,\epsilon)-\chi(t,\epsilon)\|\le\int_0^t\;\|\zeta(s,\epsilon)\|\,ds/\epsilon. \tag{2.17}$$

We compute the error when (2.15) is substituted into (2.1):

$$\begin{aligned}\zeta_N(t,\epsilon)\;&=\;i\,\epsilon\,\frac{\partial\Psi_N}{\partial t}(t,\epsilon)\;-\;H(t)\,\Psi_N(t,\epsilon)\\ &=\;i\,\epsilon^{N+2}\;e^{-i\int_0^t\,E(s)\,ds/\epsilon}\;\frac{\partial\psi_{N+1}^{\perp}}{\partial t}(t).\end{aligned} \tag{2.18}$$

Then $\Psi_N(t,\epsilon)$ agrees with an exact solution of (2.1) up to an error whose norm is bounded by $A_N\,\epsilon^{N+1}$, where

$$A_N\;\le\;\int_0^t\left\|\frac{\partial\psi_{N+1}^{\perp}}{\partial t}(s)\right\|\,ds. \tag{2.19}$$

Remarks: **1.** For future reference, we note that an integration by parts in (2.13) yields an alternative expression for $f_n(t)$. Since $\psi_{n-1}^{\perp}(s)$ is orthogonal to $\Phi(s)$ for each s, the boundary terms vanish, and

$$f_{n-1}(t)\;=\;\int_0^t\langle\,\Phi'(s),\,\psi_{n-1}^{\perp}(s)\,\rangle\,ds. \tag{2.20}$$

2. So far we have used only smoothness of $H(t)$, rather than analyticity. If $\frac{d^n}{dt^n}(H(t)-i)^{-1}=0$ for all $n\ge1$, then $\psi_0(t)=\Phi(t)$ and $\psi_n(t)\equiv0$ for $n\ge1$. This implies that the transition probability is $O(\epsilon^\infty)$ for initial and final times where the derivatives of the Hamiltonian vanish.

3 Cauchy Estimates

To prove exponential estimates by using optimal truncation of (2.2), we estimate the dependence on N of the quantity A_N in (2.19). In this section we prove a simple lemma that we use to estimate this dependence.

Lemma 3.1 *Define $B(0)=1$ and $B(k)=k^k$ for integers $k\ge1$. Suppose g is an analytic vector–valued function on the strip $S_\delta\;=\;\{\,t\,:\,|\mathrm{Im}\,t|<\delta\,\}$. If g satisfies*

$$\|g(t)\|\;\le\;C\,B(k)\,(\delta\;-\;|\mathrm{Im}\,t|)^{-k},$$

for some $k\ge0$, then g' satisfies

$$\|g'(t)\|\;\le\;C\,B(k+1)\,(\delta\;-\;|\mathrm{Im}\,t|)^{-k-1},$$

for all $t\in S_\delta$.

Proof: Let us first consider the case $k \geq 1$. By Cauchy's formula, we can write

$$g'(t) \;=\; \frac{1}{2\pi i} \int_\Gamma \frac{g(s)}{(t-s)^2}\, ds, \tag{3.1}$$

where Γ is the circular contour with center t and radius $\dfrac{1}{k+1}\,(\delta \,-\, |\mathrm{Im}\, t|)$.

For s on Γ, we have $(\delta - |\mathrm{Im}\, s|) \geq \dfrac{k}{k+1}(\delta \,-\, |\mathrm{Im}\, t|)$. Thus,

$$\begin{aligned} \|g(s)\| &\leq C\, k^k\, (\delta \,-\, |\mathrm{Im}\, s|)^{-k} \\ &\leq C\, k^k \left[\frac{k}{k+1}\,(\delta \,-\, |\mathrm{Im}\, t|) \right]^{-k} \end{aligned}$$

So, by putting the norm inside the integral in (3.1), we have

$$\begin{aligned} \|g'(t)\| &\leq \frac{1}{2\pi}\,\frac{2\pi}{k+1}(\delta \,-\, |\mathrm{Im}\, t|)\; C\, k^k \left[\frac{k}{k+1}(\delta \,-\, |\mathrm{Im}\, t|)\right]^{-k} \left[\frac{1}{k+1}(\delta \,-\, |\mathrm{Im}\, t|)\right]^{-2} \\ &= C\, (k+1)^{k+1}\, (\delta \,-\, |\mathrm{Im}\, t|)^{-k-1}. \end{aligned}$$

For $k=0$ we use the same argument with the radius of Γ replaced by $\alpha\, (\delta \,-\, |\mathrm{Im}\, t|)$ for any $\alpha < 1$. This yields the bound

$$\|g'(t)\| \;\leq\; C\, \alpha^{-1}\, (\delta \,-\, |\mathrm{Im}\, t|)^{-1}.$$

The lemma follows because $\alpha < 1$ is arbitrary. ∎

4 Preliminary Estimates

In this section we derive preliminary estimates for derivatives of the resolvent operator and and the eigenvector $\Phi(t)$.

We know that $H(t)$ is a self-adjoint analytic family in S_{δ_0}. We arbitrarily choose $\delta \in (0,\, \delta_0)$. Taking δ_0 small enough, we can assume that for each $t \in S_{\delta_0}$, the analytic function $E(t)$ is a distance $d(t) > d > 0$ from the rest of the spectrum of $H(t)$, where $d \geq d_0/2$. We can further assume that for $t \in S_{\delta_0}$,

$$\left\| (z + E(t) - H(t))^{-1} \right\| \leq C_1 \tag{4.1}$$

whenever $|z| = d/2$.

The reduced resolvent $[\, H(t) - E(t)\,]_r^{-1}$ can be written as

$$[\, H(t) - E(t)\,]_r^{-1} \;=\; \frac{1}{2\pi i} \int_{|z|=d/2} (H(t) - E(t) - z)^{-1}\, \frac{dz}{z}.$$

From this representation, we see that

$$\left\| [\, H(t) - E(t)\,]_r^{-1} \right\| \;\leq\; C_1, \tag{4.2}$$

for $t \in S_{\delta_0}$.

Similarly, the spectral projection associated with eigenvalue $E(t)$ is given by

$$P(t) \;=\; \frac{-1}{2\pi i} \int_{|z|=d/2} (H(t) - E(t) - z)^{-1}\, dz.$$

From this representation, we see that there exists C_2, such that both $P(t)$ and $P_\perp(t) = I - P(t)$ satisfy

$$\|\, P(t)\, \| \;\le\; C_2, \tag{4.3}$$

and

$$\|\, P_\perp(t)\, \| \;\le\; C_2, \tag{4.4}$$

for $t \in S_{\delta_0}$.

Assumption (4.1) also implies estimates on the derivatives of the vector $\Phi(t)$ of Section 2. To prove these estimates, we note that Problem 15, Chapter XII of [26] and (4.1) imply the existence of an analytic vector-valued function $\Phi(t)$ that never vanishes in S_{δ_0}, which is bounded and analytic in S_{δ_0}, normalized for real $t \in S_{\delta_0}$, and satisfies (2.3) for real $t \in S_{\delta_0}$. We choose C_3, such that

$$\|\, \Phi(t)\, \| \;\le\; C_3, \tag{4.5}$$

for $t \in S_{\delta_0}$.

Since $\delta < \delta_0$, $\Phi'(t)$ is bounded and analytic in S_δ, so there exists C_4, such that

$$\|\, \Phi'(t)\| \;\le\; C_4, \tag{4.6}$$

for $t \in S_\delta$.

Remark: It is not difficult to see by means of the second resolvent identity that $C_1 \simeq 1/d_0$, whereas the other constants are uniform d_0.

5 The Main Estimates

In this section we prove estimates for $f_n(t)$ and $\psi_n^\perp(t)$ that lead to exponential results in an optimal truncation strategy. The idea is to use an induction based on formulas (2.13) and (2.14) with technical help from Sections 3 and 4. Let us introduce the set $S_{\delta,T} = \{t \in S_\delta \;:\; |t| \le T\}$, for any $T > 0$.

Lemma 5.1 *Assume the hypotheses of Section 4 and the notation of Sections 2 and 3. Define* $C_5 \;=\; C_1\,(\,C_3\,C_4\,T \,+\, C_2\,)$. *Then for* $t \in S_{\delta,T}$ *and* $n \ge 1$, *we have*

$$|f_n(t)| \;\le\; T\,C_1\,C_3\,C_4\,C_5^{n-1}\,B(n)\,(\delta - |\mathrm{Im}\, t|)^{-n}. \tag{5.1}$$

and

$$\left\|\, \psi_n^\perp(t)\, \right\| \;\le\; C_1\,C_4\,C_5^{n-1}\,B(n-1)\,(\delta - |\mathrm{Im}\, t|)^{-n+1}. \tag{5.2}$$

Proof: We prove this by induction on n.

To get the induction started, we estimate $\psi_1^\perp$ and $f_1(t)$. The function $\psi_1^\perp$ is given by (2.9). By (4.2) and (4.6), we have

$$\left\| \psi_1^\perp(t) \right\| \;\leq\; C_1\, C_4. \tag{5.3}$$

By Lemma 3.1, this implies

$$\left\| \frac{\partial \psi_1^\perp}{\partial t}(t) \right\| \;\leq\; C_1\, C_4\; B(1)\, (\delta - |\mathrm{Im}\, t|)^{-1}.$$

Using this and integrating along a straight contour in (2.13), we see that

$$|f_1(t)| \;\leq\; T\, C_1\, C_3\, C_4\, B(1)\, (\delta - |\mathrm{Im}\, t|)^{-1}. \tag{5.4}$$

Note that we have used the estimate $(\delta - |\mathrm{Im}\, s|)^{-1} \leq (\delta - |\mathrm{Im}\, t|)^{-1}$, as s goes from 0 t0 t along the straight contour.

For the induction step, suppose for some $N \geq 2$, that the lemma's conclusion is true for all $n < N$. Lemma 3.1 then implies

$$\left\| \frac{\partial \psi_{N-1}^\perp}{\partial t}(t) \right\| \;\leq\; C_1\, C_4\, C_5^{N-2}\, B(N-1)\, (\delta - |\mathrm{Im}\, t|)^{-N+1}. \tag{5.5}$$

From this, the estimate on f_{N-1}, and (2.14), we easily see that

$$\begin{aligned}\left\| \psi_N^\perp(t) \right\| \;&\leq\; C_1\, C_4\, C_5^{N-2} \\ &\qquad \times\; [\, C_1\, C_3\, C_4\, T \;+\; C_1\, C_2\,]\;\; B(N-1)\;(\delta - |\mathrm{Im}\, t|)^{-N+1}.\end{aligned}$$

This is (5.2). It and (2.13) imply (5.1) for $n = N$. ∎

We now obtain an exponential bound on the error in the adiabatic theorem by combining Lemma 5.1 and formula (2.19). From the extimates above and the estimate

$$(N+1)^{N+1} \;\leq\; N^N\, (N(1+1/N)^{N+1}) \;\leq\; 2\,(2e)^N\, N^N, \tag{5.6}$$

we see that $\Psi_N(t)$ agrees with an exact solution up to an error that is bounded by

$$A_N\, \epsilon^{N+1} \;\leq\; C_6\, (C_7\, N\, \epsilon)^N \tag{5.7}$$

where $C_6 = 2\, C_1\, C_4/\delta$ and $C_7 = 2\, e\, C_5/\delta$. By choosing $N = [\![g/\epsilon]\!]$, with $g < 1/C_7$, we obtain

$$C_6\, (C_7\, N\, \epsilon)^N \;\leq\; C_6\; (C_7\, g)^{[\![g/\epsilon]\!]} \;\leq\; C_6\; e^{|\ln(C_7 g)|}\; e^{-\, g\, |\ln(C_7 g)|/\epsilon}. \tag{5.8}$$

This yields Theorem 1.1 with

$$G \;=\; 1/C_7, \quad \Gamma(g) \;=\; g\; |\ln(C_7 g)|, \quad \text{and} \quad C(g) \;=\; C_6\; e^{|\ln(C_7 g)|}. \tag{5.9}$$

∎

Remarks: **1.** By further assuming that the Hamiltonian tends sufficiently rapidly to limiting values at plus and minus infinity, it is possible to replace the factor of T in Lemma 5.1 by some constant that is uniform in t_0 and t. That allows us to prove exponential decay of the transition probability between times $-\infty$ and $+\infty$.

2. According to the remark below (4.6), we see that $C_7 \simeq 1/d_0$. Therefore, by choosing $g = G/2 = 1/2C_7$, we obtain $\Gamma(g) \simeq d_0$.

References

[1] J.E. Avron and A. Elgart, An Adiabatic Theorem without a Gap Condition, in *Operator theory advances and Applications, vol 108.* J. Dittrich, P. Exner, and M. Tater editors, Birkhauser, 1999.

[2] J.E. Avron, R. Seiler and L.G. Yaffe, Adiabatic theorems and applications to the quantum Hall effect, *Commun. Math. Phys.* **110**, 33-49 (1987).

[3] M.V. Berry, Histories of adiabatic quantum transitions, *Proc. Roy. Soc. Lond. A* **429**, 61-72, (1990).

[4] M. Born and V. Fock, Beweis des Adiabatensatzes, *Z. Phys.* **51**, 165-180 (1928).

[5] A.M. Dykhne, Adiabatic perturbation of discrete spectrum states, *Sov. Phys. JETP.* **14**, 941-943 (1962).

[6] M. Fedoriuk, *Méthodes Asymptotiques pour les Equations Différentielles Ordinaires Linéaires*, Mir Moscou, 1987.

[7] L.M. Garrido, Generalized adiabatic invariance, *J. Math. Phys.* **5**, 335-362 (1964).

[8] G. A. Hagedorn, Adiabatic Expansions near Eigenvalue Crossings. *Ann. Phys.* **196**, 278-295 (1989).

[9] J.-T. Hwang and P. Pechukas, The adiabatic theorem in the complex plane and the semi-classical calculation of non-adiabatic transition amplitudes, *J. Chem. Phys.* **67**, 4640-4653 (1977).

[10] V. Jaksic and J. Segert, Exponential approach to the adiabatic limit and the Landau-Zener formula, *Rev. Math. Phys.* **4**, 529-574 (1992).

[11] A. Joye, Proof of the Landau-Zener formula, *Asymptotic Analysis* **9**, 209-258, (1994).

[12] A. Joye, H. Kunz, and C.-E. Pfister, Exponential decay and geometric aspect of transition probabilities in the adiabatic limit, *Ann. Phys.* **208**, 299-332 (1991).

[13] A. Joye and C.-E. Pfister, Exponentially small adiabatic invariant for the Schrödinger equation, *Commun.Math.Phys.* **140**, 15-41 (1991).

[14] A. Joye and C.-E. Pfister, Superadiabatic evolution and adiabatic transition probability between two non-degenerate levels isolated in the spectrum, *J. Math. Phys.* **34**, 454-479 (1993).

[15] A. Joye and C.-E. Pfister, Exponential Estimates in Adiabatic Quantum Evolution, in *XIIth International Congress of Mathematical Physics, ICMP '97*, p. 309-315, De Wit, Bracken, Gould and Pearce Eds, International Press, Cambridge, 1999.

[16] T. Kato, On the adiabatic theorem of quantum mechanics, *J. Phys. Soc. Japan* **5**, 435-439 (1950).

[17] L.D. Landau, *Collected Papers of L.D.Landau*, Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfurt, 1965.

[18] A. Lenard, Adiabatic invariance to all orders, *Ann. Phys.* **6**, 261-276 (1959).

[19] R. Lim, M.V. Berry, Superadiabatic tracking of quantum evolution, *J. Phys. A* **24**, 3255-3264 (1991).

[20] A. Martinez, Precise exponential estimates in adiabatic theory, *J. Math. Phys.* **35** (8), 3889-3915 (1994).

[21] G. Nenciu, On the adiabatic theorem of quantum mechanics, *J. Phys. A* **13** L15-L18 (1980).

[22] G. Nenciu, Adiabatic theorems and spectral concentration, *Commun. Math. Phys.* **82** 121-135 (1981).

[23] G. Nenciu, Asymptotic invariant subspaces, adiabatic theorems and block diagonalisation, in *Recent developments in quantum mechanics (Poiana Braşov, 1989)*, *Math. Phys. Stud.*, **12**, 133-149, Kluwer Acad. Publ., Dordrecht, 1991.

[24] G. Nenciu, Linear adiabatic theory. Exponential estimates, *Commun. Math. Phys.* **152**, 479-496 (1993).

[25] G. Nenciu and G. Rasche: Adiabatic theorem and the Gell-Mann–Low formula, *Helv. Phys. Acta* **62**, 372-388 (1989).

[26] M. Reed and B. Simon, *Methods of Modern Mathematical Physics IV: Analysis of Operators.* New York, San Francisco, London: Academic Press 1978.

[27] J. Sjöstrand, Remarque sur des projecteurs adiabatiques du point de vue pseudodifférentiel, *C. R. Acad. Sci. Paris* **317** Sér. I **22**, 217-220 (1993).

[28] C. Zener: Non-adiabatic crossing of energy levels, *Proc. Roy. Soc. London* **137**, 696-702 (1932).