QUANTUM ADIABATIC EVOLUTION[a]

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ADIABATIC THEOREM OF QUANTUM MECHANICS

The notion of adiabatic evolution or adiabatic process is an important theoretical concept, which occurs at several places in Physics. The main feature of this concept is that although the process is very slow, global changes can take place without local changes. Adiabaticity is at the border between dynamics and statics. This concept was introduced by Boltzmann in Classical Mechanics through the notion of adiabatic invariants. In Thermodynamics adiabatic processes play an important role. In Quantum Mechanics, if the state of the system is an eigenfunction $\psi(t_0)$ for the eigenvalue $e(t_0)$ at $t = t_0$, then in the adiabatic limit the state of the system at time $t = t_1$ is an eigenfunction $\psi(t_1)$ for the eigenvalue $e(t_1)$, provided the energy-level $e(t)$ remains isolated during the time-interval $[t_0, t_1]$. Even if $H(t_0) = H(t_1)$, the eigenfunction $\psi(t_1)$ is generally different from $\psi(t_0)$ by a phase which can be decomposed into a dynamical phase related to the energy-level $e(t)$ and a geometric phase related to the spectral subspaces visited during the adiabatic process. This is the fundamental observation of Berry [1] which gave rise to extensive developments during the last ten years [2],[3],[4].

The adiabatic theorem in Quantum Mechanics has been proven very early by Born and Fock [5]. It was refined at several occasions. We mention in particular the papers of Kato [6] and Garrido [7] which brought new ideas into the subject. In this short paper we describe recent mathematical results obtained during the last four years, mainly in the case of analytic time-dependent quantum systems, where few rigorous results were known before. Let $H(t)$ be the Hamiltonian of a time-dependent system. We suppose that $H(t)$ is a self-adjoint operator, uniformly bounded from below, defined on a dense domain D, independent of t, of a Hilbert space $\mathcal{H}$. We suppose that $H(t)$ is at least of class C^2. The time evolution of the system is governed by the evolution operator

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$U(s,s')$, solution of the Schrödinger equation ($\hbar = 1$)

$$i\frac{d}{ds}U(s,s') = H(\varepsilon s)U(s,s'),\ \ U(s',s') = \mathbb{I} \tag{1}$$

where $1/\varepsilon$ is the typical time-scale over which the Hamiltonian changes significantly. This equation is conveniently studied using a rescaled time, $t = \varepsilon s$, which leads to

$$i\varepsilon\frac{d}{dt}U(t,t') = H(t)U(t,t'),\ \ U(t',t') = \mathbb{I} \tag{2}$$

where, with an abuse of notations, we have again denoted the evolution by U. It should be stressed, although we do not write it explicitly, that $U(t,t')$ is a function of ε. The adiabatic limit corresponds to the limit ε tending to zero which is a singular limit. The adiabatic theorem states that there exists an approximate solution $V(t,t')$ of equation (2), called adiabatic evolution, such that

$$\sup_{t\in[t_0,t_1]} \|U(t,t_0) - V(t,t_0)\| = \mathcal{O}(\varepsilon) \tag{3}$$

The main assumptions needed to prove this result are the smoothness of the Hamiltonian and the
Gap Condition: *there exists $g > 0$ so that for each t the spectrum $\sigma(t)$ of $H(t)$ can be separated into two closed subsets $\sigma_1(t)$, $\sigma_2(t)$ and*

$$\mathrm{dist}(\sigma_1(t), \sigma_2(t)) \geq g$$

By convention $\sigma_1(t)$ is always a bounded subset of $\sigma(t)$. We denote the spectral projector associated with $\sigma_1(t)$ by $Q(t)$. The main feature of $V(t,t')$ is that it is *compatible with the decomposition, or follows the decomposition, of the Hilbert space $\mathcal{H}$* into

$$\mathcal{H} = Q(t)\mathcal{H} \oplus (\mathbb{I} - Q(t))\mathcal{H} \tag{4}$$

which is expressed by the intertwining property

$$V(t,t')Q(t') = Q(t)V(t,t') \tag{5}$$

Let us consider now the consequences of (3) and (5). Let ψ_0 be an initial wave-function at $t = t_0$, such that $Q(t_0)\psi_0 = \psi_0$. At time $t > t_0$ the wave-function is $\psi(t) = U(t,t_0)\psi_0$, and $\phi(t) = V(t,t_0)\psi_0$ is an approximate solution. Because of property (5) $Q(t)\phi(t) = \phi(t)$, i.e. $\phi(t)$ belongs to the spectral subspace $Q(t)\mathcal{H}$ of $H(t)$. This information, combined with (3), implies that the probability that the system makes a transition from the subspace $Q(t_0)\mathcal{H}$ to the subspace $(Q(t)\mathcal{H})^\perp$ is of order ε^2. In the special case $\dim Q(t) \equiv 1$, ψ_0 is an eigenfunction of $H(t_0)$ for the eigenvalue $e(t_0) = \mathrm{tr}Q(t_0)H(t_0)$ and $\phi(t)$ an eigenfunction of $H(t)$ for the eigenvalue $e(t) = \mathrm{tr}Q(t)H(t)$. We can give a more explicit expression for $\phi(t)$,

$$\phi(t) = V(t,t_0)\psi_0 = \mathrm{e}^{-i/\varepsilon\int_{t_0}^t e(s)ds}\varphi(t) \tag{6}$$

where $\varphi(t)$ is the unique eigenfunction of eigenvalue $e(t)$ which is determined by the conditions $\langle \frac{d}{ds}\varphi(s)|\varphi(s)\rangle = 0$, $t_0 \leq s \leq t$, and $\varphi(t_0) = \psi_0$.

The adiabatic evolution $V(t,t')$ is solution of the equation

$$i\varepsilon\frac{d}{dt}V(t,t') = \left(H(t) + i\varepsilon\left[\frac{d}{dt}Q(t), Q(t)\right]\right)V(t,t')\ ,\ \ V(t',t') = \mathbb{I} \tag{7}$$

The result (3) can be improved when $H(t)$ is of class C^{q+2}, $q > 0$. For $j = 1, 2, \ldots, q$ we can construct decompositions of the Hilbert space $\mathcal{H}$ into

$$\mathcal{H} = Q_j(t)\mathcal{H} \oplus (I\!I - Q_j(t))\mathcal{H} \tag{8}$$

and evolutions compatible with these decompositions, which are better approximate solutions of (2). Before doing this let us recall the main result about smooth evolutions (not necessarily unitary), which are compatible with a given decomposition of the Hilbert space (4) [8], [9]. There is a particular evolution $W(t, t')$ satisfying (5), which is a solution of

$$i\frac{d}{dt}W(t, t') = i\left[\frac{d}{dt}Q(t), Q(t)\right] W(t, t'), \quad W(t', t') = I\!I \tag{9}$$

This evolution has a geometric interpretation given below, and it depends only on $Q(t)$. All other smooth evolutions $\widehat{V}$ satisfying the intertwining property (5) are solutions of equations

$$i\frac{d}{dt}\widehat{V}(t, t') = \left(B(t) + i\left[\frac{d}{dt}Q(t), Q(t)\right]\right) \widehat{V}(t, t'), \quad \widehat{V}(t', t') = I\!I \tag{10}$$

where $B(t)$ commutes with $Q(t)$. The structure of equation (7) is now clear, and the best choice [10] of $B(t)$ with respect to (3) is $B(t) = \varepsilon^{-1}H(t)$. It is not difficult to show that the eigenfunction $\varphi(t)$ in (6) is simply $W(t, t')\psi_0$.

We come to the geometric interpretation of W, and give at the same time an illustration of the adiabatic theorem. Let $H(m)$ be a family of Hamiltonians $H(m)$, satisfying the gap condition for each value of the parameter m belonging to some manifold M, and let $\sigma_1(m)$ consist of a single eigenvalue $e(m)$ with $\dim Q(m) \equiv p$. We also suppose that the family of all subspaces $Q(m)\mathcal{H}$, $m \in M$, forms a vector bundle F of base M, whose points are all (m, ϕ) with $m \in M$ and $\phi \in Q(m)\mathcal{H}$, and whose fiber above m' is the set of all points (m', ϕ), $\phi \in Q(m')\mathcal{H}$. The wave-function ψ_0 is an eigenfunction of $H(m_0)$ for the eigenvalue $e(m_0)$. We decide to change the value of the parameter m_0 into m_1 in an adiabatic way, and ask what is the wave-function ψ_1 of the system after this change. To do that we choose a path γ in M, parametrized by $t \in [0, 1]$, with $\gamma(0) = m_0$, and $\gamma(1) = m_1$. The speed of the change of the parameter m is controlled by the parameter $\varepsilon > 0$. Using the *rescaled* time $\psi_1 = \psi(1)$ is the solution of

$$i\varepsilon\frac{d}{ds}\psi(s) = H(\gamma(s))\psi(s), \quad \psi(0) = \psi_0 \tag{11}$$

The adiabatic approximation of ψ_1 is $V(1, 0)\psi_0$ and has an expression like (6),

$$V(1, 0)\psi_0 = \mathrm{e}^{-i/\varepsilon \int_0^1 e(\gamma(s))ds} W(1, 0)\psi_0 \tag{12}$$

The phase $\varepsilon^{-1}\int_0^1 e(\gamma(s))ds$ is the *dynamical phase.* It depends on the parametrization of the path γ, and it records how long is the process for changing the value of the parameter. In this approximation $W(s, 0)\psi_0$ is an eigenfunction of $H(\gamma(s))$ for all $s \in [0, 1]$. The operator $W(1, 0)$ depends only on the path γ, and not on its parametrization. Since the bundle F is constructed with the $Q(m)$, we automatically get a natural connection, because we have a natural decomposition of the tangent spaces into a vertical part and an horizontal part. In order to simplify the notations let us suppose that M is embedded in $I\!R^n$, so that F is embedded in $I\!R^n \times \mathcal{H}$. Let $f = (m, \phi) \in F$. Any tangent vector v_f at f can be viewed as a velocity vector of a curve $c(t) = (c_1(t), c_2(t))$ in $I\!R^n \times \mathcal{H}$ with $c(t) \in F$, and $c(0) = f$, i.e. $v_f = (\dot{c}_1(0), \dot{c}_2(0))_f$. The vertical vectors at f are velocity vectors of curves $c(t)$ with $c_1(t) \equiv m$. They are of the form $(0, \dot{c_2}(0))_f$ with $\dot{c_2}(0) = Q(m)\dot{c_2}(0)$. Using the projection $Q(m)$ we have a decomposition of v_f into a vertical vector $(0, Q(m)\dot{c_2}(0))_f$ and an *horizontal* vector $(\dot{c_1}(0), (I\!\!I - Q(m))\dot{c_2}(0))_f$, and thus we have a connection. The operator $W(1,0)$ in (12) is *the holonomy operator describing the parallel transport corresponding to the above connection along the path* γ. To show this we must verify that the velocity vector to the curve $(\gamma(s), W(s,0)\psi_0)$, $s \in [0,1]$, is horizontal for any s and any $\psi_0 \in Q(m_0)$. This is immediate since

$$Q(\gamma(s))\left(\frac{d}{ds}Q(\gamma(s))\right)Q(\gamma(s)) = 0 \tag{13}$$

as a consequence of $Q(\gamma(s))^2 = Q(\gamma(s))$.

Let us now construct new decompositions (8) of $\mathcal{H}$. We define the projections Q_j as approximate solutions of the Heisenberg equation

$$i\varepsilon\frac{d}{dt}A(t) = [H(t), A(t)] \tag{14}$$

They are obtained by an iteration process [11],[12]. We set $Q_0 := Q$, $K_{-1} = 0$ and $K_j := i\left[\frac{d}{dt}Q_j(t), Q_j(t)\right]$, $j = 0, \ldots$. For each t let Γ be a simple closed path in the complex plane, counterclockwise oriented, and encircling $\sigma_1(t)$. We suppose that the distance from Γ to the spectrum $\sigma(t)$ is at least $g/2$. Clearly $Q_0(t)$ is an approximate solution of (14) up to an error term $\mathcal{O}(\varepsilon)$. Let us suppose that we have constructed $Q_k(t)$, $k = 0, \ldots, j-1$. Then $Q_j(t)$ is the spectral projection of the operator $H_j(t) := H(t) - \varepsilon K_{j-1}(t)$, defined by the Riesz formula

$$Q_j(t) = -\frac{1}{2\pi i}\oint_\Gamma (H_j(t) - \lambda)^{-1} d\lambda \tag{15}$$

Provided ε is small enough Q_j is well defined up to $j = q$ if H is C^{q+2}. Using regular perturbation theory it is easy to show that $Q_j(t)$ is an approximate solution of (14) up to an error term $\mathcal{O}(\varepsilon^{j+1})$. If it happens that all derivatives of the resolvent of $H(t_0)$ are zero up to order p, then $Q_j(t_0) = Q(t_0)$, $j \leq p$. We know how to find evolutions V_j compatible with (8) by solving equation (10). The best choice, if we want V_j to give the best approximate solution of (2), which is compatible with the decomposition (8) of $\mathcal{H}$, is

$$B(t) = \varepsilon^{-1}H_j(t) + Q_j(t)K_{j-1}(t)Q_j(t) + (I\!\!I - Q_j(t))K_{j-1}(t)(I\!\!I - Q_j(t)) \tag{16}$$

Notice that $V_0 = V$.

Adiabatic Theorem

A) *Let $H(t)$ be of class C^{q+2}, $q \geq 0$, and let the gap condition be satisfied for all $t \in [t_0, t_1]$. Then there exists $\varepsilon_j > 0$ so that for all $\varepsilon < \varepsilon_j$, the evolution V_j, $0 \leq j \leq q$ is defined in $[t_0, t_1]$, and*

$$\sup_{t \in [t_0, t_1]} \|U(t, t_0) - V_j(t, t_0)\| = \mathcal{O}\left(\varepsilon^{j+1}\right)$$

B) *Let $H(t)$ have an analytic continuation in the strip $S_\alpha = \{t + is \in \mathbb{C} : |s| < \alpha\}$. Let the gap condition be satisfied for all $t \in \mathbb{R}$, and let $c(t)$ be an integrable function, with $\lim_{t\to\pm\infty} c(t) = 0$, and H^+, H^- be two self-adjoint operators such that for all $\varphi \in D$*

$$\sup_{|s|<\alpha} \|(H(t+is) - H^\pm)\varphi\| \leq c(t)(\|\varphi\| + \|H^\pm\varphi\|) \ , \ \ \pm t >> 1$$

Then there exist $\varepsilon^* > 0$ and a positive constant κ, such that for all $\varepsilon < \varepsilon^*$ and for all $t, t' \in I\!R$ we have a decomposition of $\mathcal{H}$ into $\mathcal{H} = Q_*(t)\mathcal{H} \oplus (I\!I - Q_*(t))\mathcal{H}$ and a compatible evolution $V_*(t,t')$ such that,

$$\|U(t,t') - V_*(t,t')\| = \mathcal{O}\left(\mathrm{e}^{-\kappa/\varepsilon}\right)$$

In both cases

$$\|Q(t) - Q_j(t)\| = \mathcal{O}(\varepsilon) \ , \ \|Q(t) - Q_*(t)\| = \mathcal{O}(\varepsilon)$$

Moreover $\lim_{t\to\pm\infty} \|Q(t) - Q_*(t)\| = 0$.

Comments:

1) The proof [12] of the theorem is to give an explicit lower bound for ε_j or ε^* by proving the following estimate. By hypothesis we can find a, b and c such that for all $\lambda \in \Gamma$

$$\|\frac{d^p}{dt^p}(\lambda - H(t))^{-1}\| \leq ac^p \frac{p!}{(1+p^2)} \ , \ \|\frac{d^p}{dt^p}K_0(t)\| \leq bc^p \frac{p!}{(1+p^2)} \tag{17}$$

with $p = 0, \ldots, q+1$ in case A), all p in case B), and in that case $b = b(t)$ is a bounded integrable function. Then there exist $\varepsilon(a, \|b\|_\infty)$, a constant $d = d(a, \|b\|_\infty)$ such that for all j, $j = 0, \ldots, q$ in case A) or $j \leq q^* = [1/ecd\varepsilon]$ in case B), all $\varepsilon \leq \varepsilon(a, \|b\|_\infty)$,

$$\|K_j(t) - K_{j-1}(t)\| \leq b\varepsilon^j d^j c^j \frac{j!}{(1+j^2)} \tag{18}$$

In case A), using this information we can repeat the proof of Theorem 3.1 in [14]. In case B) we set $Q_*(t) := Q_{q^*}(t)$ and choose as evolution V_* the solution of (10) with $B(t) = \varepsilon^{-1}H_{q^*}$. By writing the differential equation for $V_*^{-1}(t,t')U(t,t')$ the proof is immediate. Notice that we have an explicit simple upper bound for the error term in that case

$$\|U(t,t') - V_*(t,t')\| \leq \left|\int_{t'}^{t} b(s)ds\right| 2(\pi[1/ecd\varepsilon])^{1/2} \exp(-2[1/ecd\varepsilon]) \tag{19}$$

The condition on the asymptotic behaviour of $H(t)$ is not needed to establish (19), but is used in the application of remark 2) below. Of course, if it is not verified, then $b(t)$ is in general not integrable.

2) In case B) if $\psi(t)$ is a normalized solution of the Schrödinger equation such that $\lim_{t\to-\infty} \|(I\!I - Q(t))\psi(t)\| = 0$, then the transition probability to the spectral subspace $(I\!I - Q(+\infty))\mathcal{H}$ at time $t = +\infty$ is exponentially small

$$\lim_{t\to+\infty} \|(I\!I - Q(t))\psi(t)\|^2 = \mathcal{O}\left(\mathrm{e}^{-2\kappa/\varepsilon}\right) \tag{20}$$

This result was first obtained in [13] in the case of matrices, and in the general case in [14]. The method of the proof is quite different than the above mentioned method. The evolution is studied along special complex paths in the complex time-plane. The method gives good estimations of κ in the case of matrices and even optimal values of κ in the case of 2×2 matrices. Recently Martinez [15] has rederived result (20) by a microlocal analysis. We also mention [16], however the results are weaker.

3) Nenciu [17] gave a closely related proof of B), which precedes the above sketched proof [12], and Sjöstrand [18] obtained similar results by a microlocal analysis.

4) The evolution V_* is called *superadiabatic* because of the exponential estimate.

TWO-LEVEL SYSTEMS

We consider here only the case of analytic systems with two energy levels $e_1(t)$ and $e_2(t)$, which have the same permanent degeneracy. As above $Q(t)$ is the spectral projection associated with $e_1(t)$. The paradigm model when $\dim Q(t) \equiv 1$ is a spin 1/2 in an external time-dependent magnetic field [13], and when $\dim Q(t) \equiv 2$ it is a spin 3/2 in a time-dependent quadrupole electric field [19]. We suppose that $\mathrm{tr} H(t) \equiv 0$, so that $H(t)^2 = \rho(t)I\!I$ with $\rho(t) \geq g^2/4$ in order that the gap condition be satisfied. We have

$$e_1(t) = -\sqrt{\rho(t)}, \quad \sqrt{1} = 1 \quad \text{and} \quad Q(t) = \frac{1}{2}\left(I\!I + \frac{H(t)}{e_1(t)}\right) \tag{21}$$

We suppose that the conditions of part B) of the adiabatic theorem are satisfied. For these simple systems the adiabatic evolution can be written explicitly as

$$\begin{aligned} V(t,t') &= \exp\left(-i/\varepsilon \int_{t'}^{t} e_1(s)ds\right) W(t,t')Q(t') \\ &+ \exp\left(-i/\varepsilon \int_{t'}^{t} e_2(s)ds\right) W(t,t')(I\!I - Q(t')) \end{aligned} \tag{22}$$

where $W(t,t')$ is given by (9).

Let $\chi_- \in Q(-\infty)\mathcal{H}$ and $\chi_+ \in (I\!I - Q(+\infty))\mathcal{H}$ be two normalized eigenvectors of H^- and H^+. The transition probability from χ_- to χ_+ is

$$\mathcal{P}(\varepsilon, \chi_-, \chi_+) = \lim_{\substack{t_0 \to -\infty \\ t_1 \to +\infty}} |\langle \chi_+ | U(t_1,t_0)\chi_- \rangle|^2 \tag{23}$$

In order to derive an asymptotic formula for $\mathcal{P}(\varepsilon, \chi_-, \chi_+)$, we observe that the evolution U is analytic in the strip S_α, whereas V is in general multivalued and has singularities at the zeros of ρ in S_α. Indeed, let us assume that there exists a complex eigenvalue crossing at z_j (and by symmetry at $\overline{z_j}$), i.e. $\rho(z_j) = 0$. The eigenvalues and eigenprojections have a singularity at z_j and $\overline{z_j}$ (see (21)). We further suppose that z_j is a zero of order one for $\rho(z)$ with $\mathrm{Im} z_j > 0$. We can continue analytically $e_i(t)$, $i = 1, 2$, and $Q(t)$ in the punctured strip S_α, which is defined by removing the zeros of ρ from S_α, but the analytic continuation is not unique. We fix a point t of the real axis and make the analytic continuation of e_1 and Q along a clockwise oriented simple loop γ_j based at t, encircling z_j and no other zero of ρ. After analytic continuation we obtain the values $e_1(t|\gamma_j) = e_2(t)$, and $Q(t|\gamma_j) = (I\!I - Q(t))$. A simple computation shows that

$$i\left[\frac{d}{dt}Q(t), Q(t)\right] = \frac{i}{4\rho(t)}\left[\frac{d}{dt}H(t), H(t)\right] \tag{24}$$

and therefore the generator of W is a single-valued analytic function in the punctured strip. W itself is multi-valued and $W(t|\gamma_j)$, the analytic continuation of $W(t,t)$ along γ_j, is such that

$$W(t|\gamma_j)Q(t) = (I\!I - Q(t))W(t|\gamma_j) \tag{25}$$

The operator $W(t|\gamma_j)$, which describes the transport of vectors along γ_j, is not unitary anymore since γ_j is a path in the complex plane and the projection $Q(z)$ is not self-adjoint when $z \notin I\!R$. If we start with a vector in $Q(t)$, then, at the end of the loop γ_j, we get a vector in the orthogonal subspace. When the eigenvalues are not degenerate, we can thus define a *complex* phase $\theta_j(t)$ by the relation

$$W(t|\gamma_j)\phi_1(t) = \exp(-i\theta_j(t))\phi_2(t) \tag{26}$$

where $\phi_i(t)$ is a (normalized) eigenvector of $H(t)$ for the eigenvalue $e_i(t)$, $i = 1, 2$. The important point is that $W(t|\gamma_j)$ and $\theta_j(t)$ depend only on the homotopy class of the closed path γ_j based at t in the punctured strip. Moreover, $\mathrm{Im}\theta_j(t)$ is independent of the base point t of γ_j since t is *real*.

It is natural to write the evolution $U(t, 0)$ as $U(t, 0) := V(t, 0)A(t)$. Using the fact that the evolution U is analytic in the strip, i.e. path independent, whereas V is path dependent, we can derive a useful identity for A by considering the Schrödinger equation along two different paths, the real axis and a path η_j in the complex plane going above z_j [19]. This identity allows us to express the transition probability (23) in terms of the analytic continuations of the eigenvalues and eigenprojections along the path γ_j and of A along the path η_j [19]. We can perform the asymptotic analysis of the transition probability (23) as $\varepsilon \to 0$ whenever we have a good control of the analytic continuation of A along η_j. At this step it is necessary to impose further conditions on the behaviour of the multi-valued function $\Phi(z) := -2\int_t^z \sqrt{\rho}(z')dz'$. These conditions specify the global behaviour in the strip of the so-called Stokes lines, which are the level-lines $\mathrm{Im}\Phi(\cdot) = \mathrm{Im}\Phi(z_j)$, where z_j is a zero of ρ [13,19]. The results of the analysis are given in Table 1 when the above mentioned conditions are satisfied for one (and then necessarily unique) simple zero z_j of ρ. This case is generic. In the table we have dropped the index j.

Table 1. Asymptotic transition probability in the generic case.

Characteristics of $H(t)$	**Transition probability $\mathcal{P}(\varepsilon, \chi_-, \chi_+)$**
General formula[19] Complex hermitian $\mathrm{dim}Q(t)\mathcal{H} > 1$	$\left(\lvert\langle\chi_+\lvert W(+\infty,t)W(t\lvert\gamma)W(t,-\infty)\chi_-\rangle\rvert^2 + \mathcal{O}(\varepsilon)\right)\times$ $\exp\left(\frac{2}{\varepsilon}\ \mathrm{Im}\int_\gamma e_1(z)dz\right)$, $\quad \varepsilon \to 0$
Dykhne formula[20] Real symmetric $\mathrm{dim}Q(t)\mathcal{H} = 1$	$(1 + \mathcal{O}(\varepsilon))\exp\left(\frac{2}{\varepsilon}\ \mathrm{Im}\int_\gamma e_1(z)dz\right),\ \ \varepsilon \to 0$
Geometrical prefactor[21, 13, 22] Complex hermitian $\mathrm{dim}Q(t)\mathcal{H} = 1$	$(1 + \mathcal{O}(\varepsilon))\exp\left(\frac{2}{\varepsilon}\ \mathrm{Im}\int_\gamma e_1(z)dz + 2\mathrm{Im}\theta\right),\ \ \varepsilon \to 0$
Landau-Zener formula[23, 24] Complex hermitian $\mathrm{dim}Q(t)\mathcal{H} = 1$ Avoided crossing: $e_2(t) - e_1(t) \overset{\delta\to 0}{\simeq} \sqrt{a^2t^2 + 2ct\delta + b^2\delta^2}$	$(1 + \mathcal{O}(\delta) + \mathcal{O}(\varepsilon))\exp\left(-\frac{\pi\delta^2}{2\varepsilon}\left(\frac{b^2}{a} - \frac{c^2}{a^3}\right)(1 + \mathcal{O}(\delta))\right),$ $\quad \varepsilon, \delta \to 0$
Accurate formula[25] Complex hermitian $\mathrm{dim}Q(t)\mathcal{H} = 1$	$\left(1 + \mathcal{O}\left(\mathrm{e}^{-\kappa/\varepsilon}\right)\right)\exp\left(\frac{2}{\varepsilon}\mathrm{Im}\int_\gamma e_1^*(z,\varepsilon)dz + 2\ \mathrm{Im}\theta^*(\varepsilon)\right),$ $\quad \kappa > 0,\ \ \varepsilon \to 0$

Remarks:

We can express the decay rate as

$$2\ \mathrm{Im}\int_{\gamma_j} e_1(z)dz = 2\mathrm{Im}\int_t^{z_j}(e_1(z)-e_2(z))dz = 2\ \mathrm{Im}\Phi(z_j) < 0 \tag{27}$$

with the integration path from t to z inside γ_j. There is a geometric interpretation of the Stokes lines as particular geodesics in a metric naturally associated with the quadratic differential $\rho(z)d^2z$ [13]. In this metric $|\ \mathrm{Im}\Phi(z_j)|$ is the distance of z_j to the real axis, and always in this metric it is the nearest complex-eigenvalue crossing in the upper half-plane to the real axis. Except for the real case and the Landau-Zener formula, we have a nontrivial prefactor of geometric nature which is

$$0 \le |\langle\chi_+|W(+\infty,t)W(t|\gamma)W(t,-\infty)\chi_-\rangle|^2 \le \|W(t|\gamma)\|^2 \tag{28}$$

and which reduces to $\exp(2\mathrm{Im}\theta)$ when $\mathrm{dim}Q(t)\mathcal{H}=1$. The geometric nature of the prefactor is evident in (28): we transport the vector χ_- along the real axis from $-\infty$ to t, then along the path γ around the complex-eigenvalue crossing, and finally again along the real axis up to $+\infty$. We get a vector in $(\mathbb{I}-Q(+\infty))\mathcal{H}$ and we compare this transported vector with χ_+. The geometric prefactor was measured recently in a spin experiment[22]. The case of the avoided crossing leading to the Landau-Zener formula is important in Physics. The last row of the Table 1 yields an asymptotic formula accurate up to exponentially small *relative* errors. The expressions e_1^* and θ^* are defined as e_1 and θ with H_{q^*} in place of H (see comment 1 on the adiabatic theorem).

Table 2. Asymptotic transition probability in non generic cases.

Characteristics of $H(t)$	**Transition probability $\mathcal{P}(\varepsilon,\chi_-,\chi_+)$**
High order degeneracy[26,27] Real symmetric $\mathrm{dim}Q(t)\mathcal{H}=1$ $\rho(z)\simeq(z-z_1)^n$ $H(z)\simeq(z-z_1)^m$, $2m\le n$	$\left(4\sin^2\left(\frac{\pi(n-2m)}{2(n+2)}\right)+\mathcal{O}(\varepsilon^p)\right)\times$ $\exp\left(\frac{2}{\varepsilon}\mathrm{Im}\int_t^{z_1}(e_1(z)-e_2(z))dz\right),\quad p>0,\quad \varepsilon\to 0$
Stückelberg oscillations[28,25] Complex hermitian $\mathrm{dim}Q(t)\mathcal{H}=1$ q simple zeros z_j of $\rho(z)$ contribute	$\left\|\sum_{j=1}^q \exp\left(-i\theta_j-\frac{i}{\varepsilon}\int_{\gamma_j}e_1(z)dz\right)\right\|^2+$ $\mathcal{O}(\varepsilon)\exp\left(-\frac{2}{\varepsilon}\|\ \mathrm{Im}\int_{\gamma_1}e_1(z)dz\|\right),\quad \varepsilon\to 0$
Conjugated effects[26] Real symmetric $\mathrm{dim}Q(t)\mathcal{H}=1$ q zeros z_j characterized by (n_j,m_j) as above contribute	$\left\|\sum_{j=1}^q A_j(n_j,m_j)\exp\left(-\frac{i}{\varepsilon}\int_t^{z_j}(e_1(z)-e_2(z))dz\right)\right\|^2+$ $\mathcal{O}(\varepsilon^p)\exp\left(-\frac{2}{\varepsilon}\|\mathrm{Im}\int_t^{z_1}(e_1(z)-e_2(z))dz\|\right),$ $A_j(n_j,m_j)=2\sigma_j\sin\left(\frac{\pi(n_j-2m_j)}{2(n_j+2)}\right),\quad \sigma_j=\pm1,\quad \varepsilon\to 0$
Accurate formula[25] Complex hermitian $\mathrm{dim}Q(t)\mathcal{H}=1$ q simple zeros z_j of $\rho(z)$ contribute	$\left\|\sum_{j=1}^q \exp\left(-i\theta_j^*(\varepsilon)-\frac{i}{\varepsilon}\int_{\gamma_j}e_1^*(z,\varepsilon)dz\right)\right\|^2+$ $\mathcal{O}\left(\mathrm{e}^{-\kappa/\varepsilon}\right)\exp\left(-\frac{2}{\varepsilon}\|\ \mathrm{Im}\int_{\gamma_1}e_1(z)dz\|\right),\quad \kappa>0,\quad \varepsilon\to 0$

In Table 2 we have given the results in the non generic case, when there is an eigenvalue crossing, which is a zero of $\rho(z)$ of higher order and/or when several eigenvalue crossings (say q) determine the asymptotics of the transition probability. These cases give rise to different prefactors and/or interference phenomena in the transition probability. The above outlined method must be slightly modified. The conditions on the Stokes lines, which are needed to prove the results below are given in the quoted references.

Remarks:

For the precise definition of σ_j, as well as the paths of integration in the first and third line see [26]. Notice also that in the second and third lines

$$\mathrm{Im}\int_{\gamma_j} e_1(z)dz < 0 \ , \ \mathrm{Im}\int_t^{z_j}(e_1(z)-e_2(z))dz < 0 \tag{29}$$

are independent of $j = 1,\ldots,q$. In the last line the energy e_1^*, or the phases θ_j^* are defined using H_{q^*}, and we have

$$\mathrm{Im}\int_{\gamma_j} e_1^*(z,\varepsilon)dz = \mathrm{Im}\int_{\gamma_j} e_1(z)dz + \mathcal{O}(\varepsilon^2) \tag{30}$$

In the discussion the eigenvalue-crossings in the upper half-plane only play a role, because we consider the transition from the lower energy-level to the higher energy-level.

Finally we mention that these methods, the iteration scheme and the analysis in the complex plane, can be applied to study similar problems, like the semi-classical limit of the above barrier reflection coefficient for the stationary Schrödinger equation, or the adiabatic invariant of a time-dependent classical oscillator [25].

REFERENCES

1. M.V. Berry, quantal phase factors accompanying adiabatic changes, *Proc.Roy.Soc.Lond.A* 392: 45 (1984).

2. A. Shapere and F. Wilczek, "Geometric Phases in Physics", World Scientific, Singapore, New Jersey, London, Hong Kong (1989).

3. J.W. Zwanziger, M. Koenig and A. Pines, Berry's phase, *Annu.Rev.Phys.Chem.* 41: 601 (1990).

4. C.A. Mead, The geometric phase in molecular systems, *Rev.Mod.Phys.* 64: 51 (1992).

5. M. Born and V. Fock, Beweis des Adiabatensatzes, *Zeit.f.Phys.* 51: 165 (1928).

6. T. Kato, On the adiabatic theorem of quantum mechanics, *J.Phys.Soc.Japan*5:435 (1950).

7. L.M. Garrido, Generalized adiabatic invariance, *J.Math.Phys.* 5: 335 (1964).

8. T. Kato, "Perturbation theory for linear operators", Springer Berlin, Heidelberg, New-York (1966).

9. S.G. Krein, "Linear differential equations in Banach spaces", Providence, R.I.: Transl. Math.Mon. 29 (1971).

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

11. A. Joye and C.-E. Pfister, Full asymptotic expansion of transition probabilities in the adiabatic limit, *J.Phys.A* 24: 753 (1991).

12. 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 (1993).

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

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

15. A. Martinez, Precise exponential estimates in adiabatic theory, *Preprint* (1993).

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

17. G. Nenciu, Linear adiabatic theory. Exponential estimates, *Commun.Math.Phys.* 152: 479 (1993).

18. J. Sjöstrand, Remarque sur des projecteurs adiabatiques du point de vue pseudodifférentiel *Preprint* (1993).

19. A. Joye and C.-E. Pfister, Non-abelian geometric effect in quantum adiabatic transitions, *Phys.Rev.A* to appear (1993).

20. 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 (1977).

21. M.V. Berry, Geometric amplitude factors in adiabatic quantum transitions, *Proc.Roy. Soc.London A* 430: 405 (1990).

22. J.W. Zwanziger, S.P. Rucker and G.C. Chingas, Measuring the geometric component of the transition probability in a two-level system, *Phys.Rev.A* 43: 323 (1991).

23. A. Joye and C.-E. Pfister, Absence of geometrical correction to the Landau-Zener formula, *Phys.Lett.A* 169: 62 (1992).

24. A. Joye, Proof of the Landau-Zener formula, *Asymptotic Analysis* to appear (1993).

25. A. Joye and C.-E. Pfister, Semi-classical asymptotics beyond all orders for simple scattering systems, *Preprint* (1993).

26. A. Joye, Non-trivial prefactors in adiabatic transition probabilities induced by high order complex degeneracies *J.Phys.A* to appear (1993).

27. M.V. Berry and R. Lim, Universal transition prefactors derived by superadiabatic renormalization, *Preprint* (1993).

28. A. Joye, G. Mileti and C.-E. Pfister, Interferences in adiabatic transition probabilities mediated by Stokes lines, *Phys.Rev.A* 44: 4280 (1991).