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Absence of geometrical correction to the Landau–Zener formula ☆

Alain Joye
Département de Physique, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

and

Charles-Edouard Pfister
Département de Mathématiques, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

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We consider the transition probability $\mathscr{P}_{21}$ in the adiabatic limit between two levels displaying one avoided crossing of width $O(\delta)$. The geometrical prefactor completing the Dykhne formula for $\mathscr{P}_{21}$ is shown to be of order $1+O(\delta)$, so that the dominant contribution to $\mathscr{P}_{21}$ is given by the well-known Landau–Zener formula.

1. Introduction

The adiabatic theorem of quantum mechanics deals with systems governed by slowly varying time-dependent Hamiltonians. More precisely, if the typical time scale of the Hamiltonian H is $T=1/\epsilon$, the adiabatic theorem describes the singular limit $\epsilon\to 0$ of the rescaled Schrödinger equation

$$\mathrm{i}\epsilon\frac{\partial}{\partial t}\varphi_\epsilon(t)=H(t)\varphi_\epsilon(t)\,. \qquad (1.1)$$

The original statement [1] is that if we prepare the system at $t=t_0$ in an eigenstate $\psi_1(t_0)$ associated with the eigenvalue $e_1(t_0)$ of the Hamiltonian $H(t_0)$, then the solution of (1.1) at any time $t_1\geqslant t_0$ has the form

$$\varphi_\epsilon(t_1)=\exp\left(-\frac{\mathrm{i}}{\epsilon}\int_{t_0}^{t_1} e_1(t)\,\mathrm{d}t\right)\psi_1(t_1)+O(\epsilon)\,, \qquad (1.2)$$

provided $e_1(t)$ remains isolated in the spectrum for all $t_0\leqslant t\leqslant t_1$. As a consequence, the transition probability $\mathscr{P}_{21}(\epsilon)$ to any other eigenstate $\psi_2(t_1)$ of $H(t_1)$ is of order ϵ^2 and vanishes in the limit $\epsilon\to 0$. When the Hamiltonian is analytic in t, the decay of the transition probability is then exponential, provided one takes the limits $t_0\to-\infty$ and $t_1\to+\infty$ [2–4],

$$\mathscr{P}_{21}(\epsilon)\simeq \mathrm{e}^{-\gamma/\epsilon}\,,\quad \gamma>0\,. \qquad (1.3)$$

The adiabatic limit is an important regime in physics which is reached in a wide variety of applications, ranging from atomic and molecular physics (see for example refs. [5–8] to nuclear physics [9], solid state physics [10] or laser physics [11,12]. In such situations, the transition probability $\mathscr{P}_{21}(\epsilon)$ between two isolated levels $e_1(t)$ and $e_2(t)$ expresses the physically relevant quantity of the problem. As a typical example in atomic physics, $\mathscr{P}_{21}(\epsilon)$ gives the probability of a charge transfer during a slow atomic collision [5]. This is the reason why it is important to have explicit formulae for the asymptotic regime $\epsilon\ll 1$ of $\mathscr{P}_{21}(\epsilon)$. In case of an avoided crossing between the two levels of interest, there exists a simple and general formula.

Let $e_1(t)$ and $e_2(t)$ be two neighboring levels isolated in the spectrum displaying an avoided crossing at $t=0$,

$$e_2(t)-e_1(t)=\sqrt{a^2t^2+b^2\delta^2}+O(t^2)\,, \qquad (1.4)$$

with closest approach of order δ. If δ is small but fi-

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nite, the Landau–Zener formula states that the transition probability is explicitly given by

$$\mathscr{P}_{21}(\epsilon)\simeq\exp(-\delta^2 b^2\pi/2\epsilon a) \tag{1.5}$$

as $\epsilon\to 0$. This formula has been obtained by Zener [13] in the case of a particular real symmetric two-level Hamiltonian for which he found an analytic solution to the Schrödinger equation, and it was derived independently by Landau [14] who introduced the idea of integrating the Schrödinger equation in the complex plane on a path surrounding the complex eigenvalue crossing point $t^*\simeq ib\delta/a$, making explicit use of the analyticity of the Hamiltonian. The Landau–Zener formula has been used with success in atomic and molecular physics mainly but also in the other fields quoted above.

The original idea of Landau has been recently reconsidered to compute the transition probability in the adiabatic limit for general two-level systems driven by *Hermitian* Hamiltonians. These results complete the earlier works of Davis and Pechukas [15] and Hwang and Pechukas [16] on a generalization of the Landau–Zener formula for real symmetric two-level Hamiltonians, the so-called Dykhne formula [2]. Berry [17] and Joye, Kunz and Pfister [4] realized independently that the Dykhne formula must be completed by a prefactor of geometrical nature in the case of a general Hermitian two-level Hamiltonian:

$$\mathscr{P}_{21}(\epsilon)=\exp(2\,\mathrm{Im}\,\theta)\times\exp\left(\frac{2}{\epsilon}\mathrm{Im}\int_\gamma e_1(z)\,\mathrm{d}z\right)[1+\mathrm{O}(\epsilon)]\,. \tag{1.6}$$

Here $\int_\gamma e_1(z)\,\mathrm{d}z$ is the integral of the analytic continuation of e_1 in the complex plane along a loop γ based at the origin which encircles a carefully chosen complex eigenvalue crossing point z^* of e_1 and e_2, and $\exp(\mathrm{Im}\,\theta)$ is the geometrical prefactor mentioned above. This geometrical prefactor has been measured experimentally by Zwanziger, Rucker and Chingas [18]. A detailed analysis of the conditions under which this formula holds is given in ref. [4]. See also refs. [19] and [20] for generalizations of this result.

At this point a natural question arises. Does the geometrical prefactor contribute to the Landau–Zener formula giving $\mathscr{P}_{21}(\epsilon)$ in the situation of an avoided crossing described above when the (reduced) Hamiltonian is Hermitian instead of real symmetric? And if not, of what order is the first correction to the Landau–Zener formula? These remarks lead us to a mathematical study of the range of validity of the Landau–Zener formula in the general case. Indeed, despite its wide application in a variety of circumstances, no rigorous proof of this formula under general assumptions on the Hamiltonian can be found in the literature. Concerning this problem, we can mention the work of Hagedorn [21] where he showed that if the minimum gap δ between e_1 and e_2 is rescaled according to $\delta=\sqrt{\epsilon}$, then the transition probability is indeed given by the Landau–Zener formula where δ is replaced by $\sqrt{\epsilon}$:

$$\mathscr{P}_{21}(\epsilon)=\exp(-b^2\pi/2a)[1+\mathrm{O}(\epsilon^p)]\,,\quad p>0\,. \tag{1.7}$$

Due to the importance of the Landau–Zener formula and the presence of geometrical effects in adiabatic evolution we would like to present the results of our mathematical analysis of these problems. We formulate below a theorem establishing the validity of the Landau–Zener formula in the physically relevant regime of one avoided crossing characterized by a small minimum gap δ between $e_1(t)$ and $e_2(t)$, under natural and general conditions on the Hamiltonian. Our analysis of the Landau–Zener formula relies on our recent results [22] where we prove that the transition probability between two levels isolated in the spectrum of the (possibly unbounded) Hamiltonian is still given in the adiabatic limit by formula (1.6) derived for the two-level case. Naturally, the two levels e_1 and e_2 must be sufficiently isolated in the spectrum. This condition is to insure that the transition probability from the two-dimensional subspace to the rest of the space is negligible with respect to the transition between the two levels. Moreover, another technical condition is necessary to prove the result. We exploit here the presence, beside ϵ, of the supplementary parameter δ to show that the hypotheses of ref. [22] are always satisfied when δ is small. Then we perform an asymptotic analysis of the generalized Dykhne formula to obtain, to the lowest order in δ, the Landau–Zener formula. The transition probability $\mathscr{P}_{21}(\epsilon,\delta)$ in the adiabatic limit

$\epsilon \ll 1$ for an avoided crossing described by (1.4) with $\delta \ll 1$ is given by

$$\mathscr{P}_{21}(\epsilon,\delta)=\exp\left(-\frac{\delta^2 b^2 \pi}{2\epsilon a}[1+O(\delta)]\right.$$
$$\times[1+O(\delta)+O(\epsilon)]\,. \qquad (1.8)$$

This result shows that to the leading order in δ, the exponential decay rate in $1/\epsilon$ of the transition probability is given by the Landau–Zener formula whereas the geometrical prefactor is a correction of order $O(\delta)$ to the leading term.

2. Main result

Let us state our results in a precise form. We consider a family of time-dependent Hamiltonians $H(t, \delta)$, $t\in\mathbb{R}$, which also depend on a small parameter $\delta\in I_\Delta=[0, \Delta]$. They are defined on the same separable Hilbert space $\mathscr{H}$. We suppose that the Hamiltonians $H(t, \delta)$ satisfy three natural conditions. The first condition is that the Hamiltonian is analytic in time and sufficiently smooth in t and δ.

(I) *Self-adjointness, analyticity and smoothness.* For any vector φ, $H(z, \delta)\varphi$ is analytic in z in a strip including the real axis for δ fixed [#1] and $H(z, \delta)\varphi$ is C^1 as a function of both variables (z, δ).

The second 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.

(II) *Behaviour at infinity.* There exist $H^+(\delta)$ and $H^-(\delta)$, C^1 in δ, such that

$$\lim_{t\to\pm\infty} H(t+is)=H^\pm(\delta) \qquad (2.1)$$

uniformly in s and δ [#2].

The third hypothesis states that the two levels of interest $e_1(t, \delta)$ and $e_2(t, \delta)$ lie in a gap and when the parameter $\delta=0$, these levels have a crossing at $t=0$ and when $\delta>0$, the crossing becomes an avoided crossing. The parameter δ is to be considered as controlling a perturbation which lifts the degeneracy of $e_1(t, 0)$ and $e_2(t, 0)$ at $t=0$ and turns the genuine crossing into an avoided crossing of minimum gap of order δ.

(III) *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 $H(t, \delta)$, $t\in\mathbb{R}$, $\delta\in I_\Delta$, 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

$$\mathrm{dist}[\sigma_1(t,\delta),\sigma_2(t,\delta)]\geq g>0\,,\quad \forall t\in\mathbb{R},\ \delta\in I_\delta\,.$$

Moreover,

$$e_2(t,\delta)-e_1(t,\delta)>0\,,\quad \forall t\in\mathbb{R}\ \text{and}\ \delta>0 \qquad (2.2)$$

and if $\delta=0$,

$$e_2(t,0)-e_1(t,0)>0\,,\quad \forall t<0\,,$$

$$e_2(t,0)-e_1(t,0)<0\,,\quad \forall t>0\,,$$

$$e_2(0,0)=e_1(0,0)\,, \qquad (2.3)$$

where $t=0$ is a simple zero of the function $e_2(t, 0)-e_1(t, 0)$ (see fig. 1).

This condition implies that for $\delta>0$ there is a *complex* eigenvalue crossing point $z^*(\delta)$ together with its complex conjugate in a neighbourhood of $z=0$, if δ is small enough and that $z^*(\delta)$ is a square root type branch point for the eigenvalues. The one-dimensional projectors corresponding to $e_1(t, \delta)$ and

[#1] More precisely, there exist a strip $S_a=\{z: |\mathrm{Im}\, z|\leq a\}$ and a dense domain D of $\mathscr{H}$ such that for each $z\in S_a$ and $\delta\in I_\Delta$ $H(z, \delta)$ is a self-adjoint holomorphic family for δ fixed [23], and $H(t, \delta)$ is bounded from below if $t\in\mathbb{R}$.

[#2] More precisely again, there exist two families of self-adjoint operators $H^\pm(\delta)$, defined on D, strongly C^1 in δ and bounded from below and a function $b(t)$ independent of δ, behaving as $1/|t|^{1+\alpha}$, $\alpha>0$, $t\to\pm\infty$, such that $\sup_{|s|<a}\|[H(t+is,\delta)-H^\pm(\delta)]\varphi\|\leq b(t)[\|\varphi\|+\|H^\pm(\delta)\varphi\|]$, $t\gtrless 0$, for all $\varphi\in D$ and $\delta\in I_\Delta$. Moreover, for each $\varphi\in D$, $\|(\partial/\partial\delta)H(z,\delta)\varphi\|\leq N$, $\forall (z,\delta)\in S_a\times I_\Delta$.

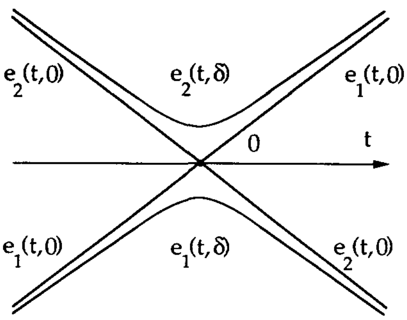

Fig. 1. The levels $e_j(t,\delta)$ and $e_j(t,0)$.

$e_2(t,\delta)$ are denoted by $P_1(t,\delta)$ and $P_2(t,\delta)$. We also define the two-dimensional projector $P(t,\delta)=P_1(t,\delta)+P_2(t,\delta)$.

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 $P(t,\delta)\mathscr{H}$. 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.

(IV) *Behaviour at the avoided crossing.* There exist constants $a>0$, $b>0$ and c with $c^2<a^2b^2$, such that

$$e_2(t,\delta)-e_1(t,\delta)=\sqrt{a^2t^2+2ct\delta+b^2\delta^2+R_3(t,\delta)}\,, \tag{2.4}$$

where $R_3(t,\delta)$ is a rest of order 3 in (t,δ) [#3].

The avoided crossings considered can be rewritten as

$$e_2(t,\delta)-e_1(t,\delta)=\sqrt{a^2t^2+2ct\delta+b^2\delta^2}\,[1+R_2(t,\delta)]\,, \tag{2.5}$$

with closest approach at $t_0(\delta)=-c\delta/a^2+\mathrm{O}(\delta^2)$ given by

$$e_2(t_0(\delta),\delta)-e_1(t_0(\delta),\delta)=\delta\sqrt{b^2-c^2/a^2}\,[1+\mathrm{O}(\delta)]\,. \tag{2.6}$$

[#3] We also assume that if φ_1 and φ_2 form a basis of $P(0,0)\mathscr{H}$, the matrix elements $\langle\varphi_j|P(t,\delta)\varphi_k\rangle$ and $\langle\varphi_j|H(t,\delta)P(t,\delta)\varphi_k\rangle$, $k,j=1,2$, are C^2 as functions of the two real variables (t,δ).

Let δ be fixed and let η be a closed loop based at the origin which encloses the complex eigenvalue $z^*(\delta)$ ($\mathrm{Im}\,z^*(\delta)>0$) as in fig. 2. We fix the phases of the eigenvectors $\psi_1(t,\delta)$ and $\psi_2(t,\delta)$ of $H(t,\delta)$ associated with $e_1(t,\delta)$ and $e_2(t,\delta)$ by the condition

$$\langle\psi_j(t,\delta)\,|\,(\partial/\partial t)\psi_j(t,\delta)\rangle\equiv 0\,,\quad \forall t\in\mathbb{R}\,. \tag{2.7}$$

Consider $e_1(0,\delta)$ and $\psi_1(0,\delta)$ and their analytic continuations along η. If we denote by $\tilde{e}_1(0,\delta)$ and $\tilde{\psi}_1(0,\delta)$ the results of these analytic continuations at the end of the loop η, we have

$$\tilde{e}_1(0,\delta)=e_2(0,\delta)\,,$$
$$\tilde{\psi}_1(0,\delta)=\exp[-\mathrm{i}\theta(\delta)]\psi_2(0,\delta)\,, \tag{2.8}$$

because $z^*(\delta)$ is a square root branch point for the energies. The phase $\theta(\delta)$, which is an analog of the Berry phase, is in general complex and is now δ-dependent.

Theorem 2.1 (*Landau–Zener formula*). Let $H(t,\delta)$ be a self-adjoint operator analytic in t satisfying conditions I–III. Let $\varphi(t)$ be a normalized solution of the Schrödinger equation

$$\mathrm{i}\epsilon\frac{\partial}{\partial t}\varphi(t)=H(t,\delta)\varphi(t)\,,\quad \varphi(0)=\varphi^*\in\mathrm{D}\,,$$

such that

$$\lim_{t\to-\infty}\|P_1(t,\delta)\varphi(t)\|=1\,.$$

If ϵ and δ are small enough,

$$\mathscr{P}_{21}(\epsilon,\delta)=\lim_{t\to+\infty}\|P_2(t,\delta)\varphi(t)\|^2$$
$$=\exp[2\,\mathrm{Im}\,\theta(\delta)]\exp\left(\frac{2}{\epsilon}\mathrm{Im}\int_\eta e_1(z,\delta)\,\mathrm{d}z\right)$$
$$\times[1+\mathrm{O}(\epsilon)]\,,$$

where $\mathrm{O}(\epsilon)$ is independent of δ and where $\mathrm{Im}\,\theta(\delta)$

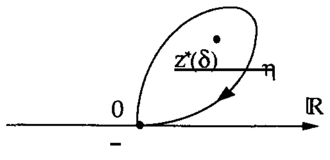

Fig. 2. The loop η and the eigenvalue crossing $z^*(\delta)$.

and $\mathrm{Im} \int_\eta e_1(z, \delta)\,dz \to 0$ if $\delta \to 0$. Moreover, if condition IV is satisfied, we have

$$\mathscr{P}_{21}(\epsilon, \delta) = \exp\left[-\frac{\delta^2 \pi}{2\epsilon}\left(\frac{b^2}{a} - \frac{c^2}{a^3}\right)[1+\mathrm{O}(\delta)]\right] \times [1+\mathrm{O}(\delta)+\mathrm{O}(\epsilon)]\,,$$

where $\mathrm{O}(\epsilon)$ and $\mathrm{O}(\delta)$ are independent of δ and ϵ respectively.

We can recover the results obtained by Hagedorn [21] specialized to our setting as a direct corollary:

Corollary 2.1. If the width δ of the avoided crossing is rescaled according to $\delta = \sqrt{\epsilon}$, then

$$\mathscr{P}_{21}(\epsilon, \sqrt{\epsilon}) = \exp\left[-\frac{\pi}{2}\left(\frac{b^2}{a} - \frac{c^2}{a^3}\right)\right][1+\mathrm{O}(\sqrt{\epsilon})]\,.$$

Remarks. If we set $\delta = 0$ in the above results, we get $\mathscr{P}_{21}(\epsilon, 0) = 1 + \mathrm{O}(\epsilon)$. This apparent contradiction with the adiabatic theorem comes from the fact that the eigenvectors undergo a change of labels when $\delta \to 0$. Indeed when $\delta > 0$, $e_2(t, \delta) > e_1(t, \delta)$ for any time t whereas if $\delta = 0$, $e_2(t, 0) < e_1(t, 0)$ for positive times t as shown in fig. 1 (see (2.2) and (2.3)). Thus $\psi_1(t, \delta)$, associated with the lower level for any t, tends to $\psi_1(t, 0)$ if $t < 0$ and to a vector proportional to $\psi_2(t, 0)$ if $t > 0$. From this remark it follows that the quantity $\mathscr{P}_{21}(\epsilon, 0)$ gives the probability *to stay* in the eigenstate associated with $e_1(t, 0)$, which must be close to 1 according to the adiabatic theorem. Moreover, we get the correct behaviour for that probability since it was in shown in ref. [1] that when a genuine crossing occurs between the levels, the transition probability is of order ϵ instead of ϵ^2.

The proof of the theorem is a combination of two kinds of techniques. We reduce the complete problem to an effective two-level system by means of a "superadiabatic evolution" (a word introduced by Berry [24]) which approximates the true evolution up to exponentially small correction terms. Then we go to the complex plane and perform an analysis similar to the one presented in ref. [4]. One of the main difficulties is to obtain a uniform control in the parameter δ for the correction terms. The details of the analysis can be found in ref. [25].

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