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General conditions for quantum adiabatic evolution

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Adiabaticity occurs when, during its evolution, a physical system remains in the instantaneous eigenstate of the hamiltonian. Unfortunately, existing results, such as the quantum adiabatic theorem based on a slow down evolution ($H(\epsilon t)$, $\epsilon \rightarrow 0$), are insufficient to describe an evolution driven by the hamiltonian $H(t)$ itself. Here we derive general criteria and exact bounds, for the state and its phase, ensuring an adiabatic evolution for any hamiltonian $H(t)$. As a corollary we demonstrate that the commonly used condition of a slow hamiltonian variation rate, compared to the spectral gap, is indeed sufficient to ensure adiabaticity but only when the hamiltonian is real and non oscillating (for instance containing exponential or polynomial but no sinusoidal functions).

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The "adiabatic" process, from the Greek $\alpha-$ (a-), not, $\delta\iota\alpha$ (dia), through, $\beta\alpha\iota\upsilon\upsilon\upsilon$ (bainen), to pass, was introduced by Carnot (in 1824) and W. J. M. Rankine (in 1858) in thermodynamics, then by Boltzmann (in 1866) in classical mechanics[1]. In 1928, Fritz London applied adiabatic process in chemical kinetics. Concerning the quantum physics, in 1911-1916 Paul Ehrenfest used adiabatic invariance in the development of the 'Old Quantum Theory' and in 1928 Born and Fock [2] demonstrated the quantum adiabatic theorem. By definition, quantum adiabaticity occurs when, during its evolution driven by an hamiltonian $H(t)$, a quantum state $|\Psi(t)\rangle$ prepared in an eigenstate $|n(0)\rangle$ remains close to the instantaneous eigenstate $|n(t)\rangle$ (with a proper phase choice) as time t goes on. The basic concept of adiabaticity in quantum theory has been widely applied in both theories and experiments. Applications range from energy level crossings, such as Landau-Zener transition, Born-Oppenheimer molecular coupling, collisional processes, quantum control or adiabatic quantum computation [3, 4]. Unfortunately, even for the two-level system, no sufficient conditions are known to efficiently describe an adiabatic evolution driven by a general hamiltonian $H(t)$ [5]. For instance, an example as simple as the Schwinger's hamiltonian (solved hereafter) [6] $H(t) = \frac{\hbar\omega_0}{2} \begin{pmatrix} \cos\theta & \sin\theta e^{-i\omega t} \\ \sin\theta e^{i\omega t} & -\cos\theta \end{pmatrix}$, proves that neither the "usual" adiabatic phase evolution $\int_0^t E_n/\hbar - i\langle n|\dot{n}\rangle$ nor the commonly used approximate adiabatic criterion [54] [7]:

$$\sum_{m \neq n} \frac{\hbar}{|E_n - E_m|} \frac{|\langle m|\dot{H}|n\rangle|}{|E_n - E_m|} = \sum_{m \neq n} \left| \frac{\hbar\langle m|\dot{n}\rangle}{E_n - E_m} \right| \ll 1, \quad (1)$$

are sufficient (or necessary) to ensure adiabaticity. This statement may look surprising [8, 9, 10, 11, 12, 13] but is presented in textbooks [14, 15]. It is indeed well known in NMR or in quantum optics (through Rabi oscillation) that resonant terms can lead to population transfer, i.e. to a non adiabatic behavior. This is linked to branch points, connecting the different eigenstates of the adi-

abatic Hamiltonian, and explains for instance that non adiabatic behaviour exist when several successive transitions between pairs of levels occurs [16, 17, 18, 19]. Thus, condition (1) is not valid globally.

It is therefore important to derive general conditions, for a system and its phase evolution, which ensure adiabaticity. This is the goal of this article. As a corollary we will answer the still pending (even in the two-level case) question: why and when the standard condition (1), of a slow hamiltonian variation rate, compared to the frequency associated to the spectral gap $\Delta E_n = \min_{m \neq n} |E_m - E_n|$, is a sufficient adiabatic condition. Indeed, we show that condition (1) is sufficient to ensure adiabaticity but only when the hamiltonian is real and non oscillating.

Because almost all existing results, as the adiabatic criterion (1) are based on the so called adiabatic limit of a slow down evolution, we shall first start by studying the standard results and by explaining why the standard adiabatic theorem can not help to solve the problem. Hopefully this part will also clarify the recent debate concerning the adiabatic phase and adiabatic criterion [5, 11, 12, 13, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30] following the (over-subtle) "rediscovery" by Marzlin and Sanders [31] that condition (1) is not a sufficient one. We shall then derive exact bounds for adiabaticity. We then discussed their validity in a the general two-level case and their simplification in the case of a non oscillating hamiltonian. For clarity some lengthy calculations are reported in an appendix.

STANDARD RESULTS

Quantum adiabatic theorem

The Born and Fock's quantum adiabatic theorem has been rigorously demonstrated, several times and by several different methods (see for instance [2, 4, 7, 32] and references therein), extended to the infinite dimensional

setting by Kato [33], studied as a geometrical holonomy evolution by Berry [34], extended to degenerate cases (without gap condition) [35] and to open quantum system [36].

In the non degenerate ($E_m \neq E_n$) case, the adiabatic theorem stipulates that:

$$|\Psi_\epsilon(t)\rangle - e^{-i \int_0^t (E_n/\hbar - i\langle n|\dot{n}_\epsilon\rangle)} |n_\epsilon(t)\rangle = O(\epsilon) \xrightarrow{\epsilon \rightarrow 0} 0, \quad (2)$$

where evolution speed is controlled by ϵ and the subscript stands for the $H_\epsilon(t) = H(\epsilon t)$ evolution [55]. Here the dot designates the time derivative and $\int_0^t f = \int_0^t f(t') dt'$.

To illustrate the limited practical utility of the theorem, let's suppose that an external laser field, with constant angular frequency $R_1(t) = \omega$, is applied to a two-level system that we want to adiabatically drive by experimentally modifying two parameters: the coupling Rabi frequency (proportional to the square-root of the laser intensity) $R_2(t) = \Omega(t)$, and the detuning of the laser from resonance $R_3(t) = \delta(t)$. The hamiltonian is, in the rotating wave approximation: $\frac{\hbar}{2} \begin{pmatrix} \delta(t)+\omega & \Omega(t)e^{-i\omega t} \\ \Omega(t)e^{i\omega t} & -\delta(t)-\omega \end{pmatrix} = H(R_1(t), R_2(t), R_3(t), R_4(t))$. Due to the $R_4(t) = \omega t$ term, slowing down the time would lead to $\omega(\epsilon t) = (\omega\epsilon)t$. When $\epsilon \rightarrow 0$, this would require reducing ω to zero which is experimentally impossible. Moreover, even in the static field ($\omega = 0$) regime, the theorem applies but only if δ and Ω can be slowed down simultaneously. The theorem says nothing about the adiabaticity if $\delta(t)$ and $\Omega(t)$ are varied independently with time.

Although undoubtedly of great theoretical interest, as in the quantum adiabatic computation using interpolating hamiltonian [37], the theorem describes an evolution driven by $H(\epsilon t)$ with $\epsilon \rightarrow 0$ and is obviously of no utility concerning the evolution driven by $H(t)$ itself, as in this case $\epsilon = 1$ and cannot be reduced to zero. The theorem is then better formulated within the parameter domain than within the time domain [9, 38]: an evolution driven by $H(\mathbf{R}(t))$ is adiabatic if the parameter path, between an initial \mathbf{R}_{in} parameter value and a final one \mathbf{R}_{fin} , is followed infinitely slowly.

Approximate adiabatic condition

Contrary to the quantum adiabatic theorem, the approximate adiabatic condition (1) can be applied to $H(t)$ itself. The origin of condition (1) arises [7] from the fact that the error term in Eq. (2) can be written [32] as $O(\epsilon) = \sum_{m \neq n} \frac{\hbar \langle m_\epsilon | \dot{n}_\epsilon \rangle}{E_n - E_m} + O(\epsilon^2)$, where the linear ϵ dependence is here only implicit and, deliberately but confusingly, hidden in $|\dot{n}_\epsilon\rangle$. This has been the source of confusion [8, 9, 10, 11, 12, 13] when used with $\epsilon = 1$ where $|m_\epsilon\rangle = |m\rangle$. The confusion occurs because, even if derived without any proof by using $\epsilon = 1 \rightarrow 0$, the criterion (1) ensures an adiabatic evolution in almost all the

known examples: Landau-Zener(-Stückelberg), Rosen-Zener-Demkov, Nikitin, Zhu-Nakamura models or in the Rapid Adiabatic Passage or STImulated Raman Adiabatic Passage (STIRAP) processes, ... [3, 4, 39]. Important enough, as we shall see, all these examples use non-oscillating (exponential or polynomial) functions. Therefore, the simple idea of adiabaticity, given by the condition (1), of a small but finite variation rate of $H(t)$ (compared to the spectral gap), is broadly used. Similarly, as extracted from equation (2) without any proof by using $\epsilon = 1 \rightarrow 0$, an adiabatic phase evolution of $\int_0^t E_n/\hbar - i\langle n|\dot{n}\rangle$ is widely used [25]. However as mentioned in the introduction the Schwinger's example demonstrates that this "usual" adiabatic condition, as well as this "usual" adiabatic phase, is neither sufficiently nor necessarily to obtain an adiabatic evolution.

To avoid any confusion the term $O(\epsilon^2)$ has to be evaluated. This can be done for instance by giving an exact bound [32] on the adiabatic fidelity $|\langle \Psi | n \rangle|$ such as [56]

$$\frac{1 - |\langle \Psi(t) | n(t) \rangle|}{\hbar} \leq \left\| \frac{\dot{H}(0)}{\Delta E_n(0)^2} \right\| + \left\| \frac{\dot{H}(t)}{\Delta E_n(t)^2} \right\| + \int_0^t \left(\frac{7 \|\dot{H}\|^2}{\Delta E_n^3} + \frac{\|\ddot{H}\|}{\Delta E_n^2} \right). \quad (3)$$

Similar bounds [4, 23, 40] exists. They can be used to restore the usual theorem [55] because $\frac{dH_\epsilon}{dt} = \epsilon \frac{dH_\epsilon}{d(\epsilon t)} = \epsilon \frac{dH}{ds}$ vanishes when $\epsilon \rightarrow 0$. However, they have severe limitations because, due to the integral term, they require a maximal evolution time T to provide an adiabatic evolution when none is needed. This can be easily seen from the Schwinger's $H(t) = \frac{\hbar 10\omega}{2} \begin{pmatrix} \cos \theta & \sin \theta e^{-i\omega t} \\ \sin \theta e^{i\omega t} & -\cos \theta \end{pmatrix}$ example with $\omega = 1 \text{ s}^{-1}$ and $\theta = 0.01$.

GENERAL BOUNDS

In order to derive a more useful bound than (3), let's study the evolution of $|\Psi(t)\rangle$ driven by a general N -level hamiltonian $H(t)$. For the corresponding eigenvalues $E_m(t)$ of $H(t)$, the eigenvectors $e^{i\theta_m(t)}|m(t)\rangle$, $m = 1, \dots, N$ form a so called adiabatic basis, where $\theta_m(t)$ are arbitrary phases to be chosen conveniently later. To study the adiabatic evolution we assume that $|\Psi(t=0)\rangle = |n(0)\rangle$. The Schrödinger equation for $|\Psi(t)\rangle = \sum_{m=1}^N U_{mn}(t) e^{i\theta_m(t)} |m(t)\rangle$, i.e. with $U(0) = I$, leads to the time-evolution equation: $i\hbar \dot{U} = H'U$, where

$$H'_{mk} = (E_m + \hbar \dot{\theta}_m) \delta_{mk} - i\hbar \langle m | \dot{k} \rangle e^{i(\theta_k - \theta_m)}. \quad (4)$$

As usual, we identify the operators and their matrices in the standard (also called natural or canonical) basis $|m^{\text{st}}\rangle$, $m = 1, \dots, N$. Thus, $H' = P^{-1}HP - i\hbar P^{-1}\dot{P}$

where the columns of P are the eigenvectors $e^{i\theta_m(t)}|m\rangle$: $P_{mk} = \langle m^{\text{st}}|P|k^{\text{st}}\rangle = e^{i\theta_k(t)}\langle m^{\text{st}}|k\rangle$ of H .

The evolution is adiabatic if and only if the fidelity $|U_{nn}(t)|$ is close to unity (or $\|\Psi\rangle\langle\Psi| - |n\rangle\langle n|\| \ll 1$). In order to also study the phase evolution of the state $|\psi\rangle$ we compare the matrix U to another time evolution matrix U' which can be more easily evaluated.

Let's define U' by $U'(0) = 1$ and

$$i\hbar\dot{U}' = P'^{-1}H'P'U', \quad (5)$$

where P' is an auxiliary matrix to be chosen conveniently. Then, the important equality comparing two operators

$$U(t) - U'(t) = (P'(t) - 1)U'(t) - U(t)(P'(0) - 1) - U(t)\int_0^t U^{-1}(t')\dot{P}'(t')U'(t')dt' \quad (6)$$

can be established by multiplying it by U^{-1} and then taking the time derivative.

Several choices are possible but, for simplicity we choose P' to have $P'^{-1}H'P'$ as an eigenvalue value decomposition of H' . In this case U' is diagonal: $U'_{nn} = e^{-i\int_0^t E'_n(t')/\hbar dt'}$ where E'_n is the eigenvalue of the n^{th} eigenvector $|n'\rangle = P'|n^{\text{st}}\rangle$ of H' . P' is unitary, so $\|P'\| = \|U\| = \|U'\| = 1$. We then apply Eq. (6) on $|n^{\text{st}}\rangle$ and take the norm on both sides to have

$$\begin{aligned} \left\| |\Psi(t)\rangle - e^{-i\int_0^t \frac{E'_n}{\hbar}} |n(t)\rangle \right\| &\leq \| |n'(0)\rangle - |n^{\text{st}}\rangle \| + \\ \| |n'(t)\rangle - |n^{\text{st}}\rangle \| &+ \int_0^t \| |\dot{n}'(t')\rangle \| dt' \end{aligned} \quad (7)$$

Eq. (7) gives a bound as well as the correct phase evolution for adiabatic evolution. Sufficient adiabatic conditions are:

$$\| (P'(t) - 1)|n^{\text{st}}\rangle \| = \| |n'(t)\rangle - |n^{\text{st}}\rangle \| \ll 1 \quad (8)$$

$$\int_0^t \| |\dot{P}'(t')|n^{\text{st}}\rangle \| dt' = \int_0^t \| |\dot{n}'(t')\rangle \| dt' \ll 1 \quad (9)$$

To tight these bounds we choose the phase of $|n'\rangle$ to be such that $\langle n^{\text{st}}|n'\rangle \geq 0$. The adiabatic fidelity is bound by the inequality $2(1 - |\langle\Psi(t)|n(t)\rangle|) \leq \| |\Psi(t)\rangle - e^{-i\int_0^t \frac{E'_n}{\hbar}} |n(t)\rangle \|^2$, which should now be tighten as much as possible by choosing the $\theta_m(t)$ phases.

Links and differences, of Eq. (7) with the usual theorem given by Eq. (2) and of Eq. (8) with the usual condition given by Eq. (1), can be inferred by applying standard perturbation theory to Eq. (4):

$$E'_n \approx E_n - i\hbar\langle n|\dot{n}\rangle + \hbar\dot{\theta}_n + \sum_{m \neq n} \frac{|H'_{mn}|^2}{H'_{nn} - H'_{mm}} \quad (10)$$

$$|n'\rangle \approx |n^{\text{st}}\rangle + \sum_{m \neq n} \frac{H'_{mn}}{H'_{nn} - H'_{mm}} |m^{\text{st}}\rangle. \quad (11)$$

Using the equality $\theta_m = \theta_n + \arg(-i\langle m|\dot{n}\rangle)$ for all $m \neq n$, creates (to this second order approximation) reals P'_{mn} , and condition (8) becomes:

$$\sum_{m \neq n} \left| \frac{\langle m|\dot{n}\rangle}{(E_n - E_m)/\hbar - i\langle n|\dot{n}\rangle + i\langle m|\dot{n}\rangle - \frac{d}{dt} \arg\langle m|\dot{n}\rangle} \right| \ll 1 \quad (12)$$

This condition, first derived in [20], generalizes condition (1) when H is not real[57]. However, as (1), it is an insufficient adiabatic criterion for two reasons: it arises from a perturbative approach, and it neglects the condition (9), which is important for oscillating H . Indeed, it is only when the hamiltonian matrix elements are non oscillating functions – in the approximate sens of none of their sum, product, division or combination has a large number of monotonic changes – that the condition (9) can be neglected. More precisely, in the general case when all the $P'_{mn} = \langle m^{\text{st}}|n'\rangle$ are real (or with a time independent phase argument) and monotonic, an important simplification occurs because $\int_0^t |\dot{P}'_{mn}(t')| dt' = |P'_{mn}(t) - P'_{mn}(0)| \leq |P'_{mn}(t) - 1| + |P'_{mn}(0) - 1|$. In this case, we see, by using the 1-norm [56], that the derivative condition (9) essentially reduces to the sole (8) condition. Similarly P'_{mn} piecewise functions with finite number $(M - 1)$ of monotonicity changes[58] would lead to a $\sum_m |P'_{mn} - 1| \ll 1/M$ type of condition.

Multi levels system

We use here an exact perturbation theory [41] to calculate $P'|n^{\text{st}}\rangle$. We write $H' = H_0 + V$ where V is a perturbation. For simplicity, i.e. in order to isolate the n^{th} subspace, we renumber the states to have $n = 1$ and, using the $1 + (N - 1)$ block matrix notation, we choose (see Eq. (4))

$$H' = H_0 + V; \quad H_0 = \begin{pmatrix} H'_{nn} & 0 \\ 0 & H'_{nn} - \hbar\delta' \end{pmatrix}, \quad V = \frac{\hbar}{2} \begin{pmatrix} 0 & \Omega'^{\dagger} \\ \Omega' & 0 \end{pmatrix}.$$

We then apply techniques, detailed in the appendix, to endup with the following simple conditions:

$$\|\delta'^{-1}\|\|\Omega'\| \ll 1 \quad (13)$$

$$\int_0^t \left(\|\Omega'\| \left\| \frac{d}{dt}(\delta'^{-1}) \right\| + \|\delta'^{-1}\| \left\| \frac{d}{dt}\Omega' \right\| \right) \ll 1 \quad (14)$$

which are together sufficient adiabatic conditions because they imply Eqs. (8) and (9).

Eq. (14) is here to prevent the use of oscillating hamiltonian. Indeed, as discussed previously, if H is real and "non-oscillating", meaning that Ω'_{mn} and $(\delta'^{-1})_{mk}$ are (piecewise) real monotonic functions, the condition (14) essentially reduces to condition (13).

Eq. (13) itself can be seen as a generalization of the Eq. (12) which itself generalizes the standard condition (1).

Indeed, if we add to the condition (13) the, fortunately common condition of negligible coupling within the space orthogonal to $|n\rangle$, i.e. negligible [59] δ' off diagonal terms to have $(\delta'^{-1})_{mm} \approx (\delta'_{mm})^{-1}$, we can recover Eq. (12) by choosing $\theta_m = \theta_n + \arg(-i\langle m|\dot{n}\rangle)$ (i.e. Ω' real).

Finally, the appendix indicates that, for a strongly non-oscillating (very few monotonicity changes) real hamiltonian H the sole usual condition (1), which is then condition (13), is sufficient to ensure an adiabatic behavior.

Two level system

Let's now illustrate the results in the two-level ($N = 2$) framework. We write, by removing the average diagonal energy, the general hamiltonian in the (spin-magnetic interaction $H = -\gamma\vec{B}\cdot\frac{\hbar}{2}\vec{\sigma}$) form: $H(t) = \frac{\hbar\omega_0(t)}{2} \begin{pmatrix} \cos\theta(t) & \sin\theta(t)e^{-i\varphi(t)} \\ \sin\theta(t)e^{i\varphi(t)} & -\cos\theta(t) \end{pmatrix}$. Using $-\theta_1 = \theta_2 = \theta_1 + \arg(-i\langle 2|\dot{1}\rangle)$, the appendix shows that Eq. (8) and Eq. (9) are equivalent to:

$$\frac{|\dot{\varphi}\sin\theta - i\dot{\theta}|}{\left|\dot{\varphi}\cos\theta - \omega_0 - \frac{d}{dt}\arg(\dot{\varphi}\sin\theta - i\dot{\theta})\right|} = \frac{|\Omega'|}{|\delta'|} \ll 1 \quad (15)$$

$$\int_0^t dt' \left| \frac{d}{dt'} \frac{|\Omega'(t')|}{\delta'(t')} \right| \ll 1 \quad (16)$$

In order to check their validity, or similarly the one of conditions (13) and (14), we first use the simple example due to Schwinger [6], where all the parameters $\omega_0, \theta, \dot{\varphi} = \omega$ are real and time independent. In this case the condition (16) vanishes and $U(t) = e^{-i\int_0^t H'/\hbar} = \begin{pmatrix} \cos\frac{\Omega_R t}{2} - i\frac{\delta'}{\Omega_R} \sin\frac{\Omega_R t}{2} & -i\frac{\Omega'}{\Omega_R} \sin\frac{\Omega_R t}{2} \\ -i\frac{\Omega'}{\Omega_R} \sin\frac{\Omega_R t}{2} & \cos\frac{\Omega_R t}{2} + i\frac{\delta'}{\Omega_R} \sin\frac{\Omega_R t}{2} \end{pmatrix}$ where $\Omega_R = \sqrt{|\Omega'|^2 + \delta'^2}$ is the generalized Rabi frequency. The adiabatic evolution (negligible off-diagonal terms in U) is ensured by the condition $\frac{|\Omega'|}{\Omega_R} = \frac{|\omega \sin\theta|}{\sqrt{(\omega_0 - \omega \cos\theta)^2 + \omega^2 \sin^2\theta}} \ll 1$ which is indeed equivalent to our condition (15): $\frac{|\Omega'|}{|\delta'|} = \frac{|\omega \sin\theta|}{|\omega_0 - \omega \cos\theta|} \ll 1$. Furthermore, our equation (7), including its phase $\int_0^t E_1'/\hbar = \Omega_R t/2$, correctly describes an adiabatic evolution.

On the contrary, using this analytical example (by looking at the resonant $\omega \approx \omega_0$ or small θ cases for instance) it is straightforward to demonstrate that Eq. (1): $\frac{|\Omega'|}{|\omega_0|} = \frac{|\omega \sin\theta|}{|\omega_0|} \ll 1$, as well as the "usual" adiabatic phase evolution $\omega_0 t/2 = \int_0^t E_1/\hbar - i\langle 1|\dot{1}\rangle$ (see Eq. (2)), are not correlated with an adiabatic evolution.

We now add to our study the condition (16) by the use of the real cycling hamiltonian $H = \frac{\hbar}{2} \begin{pmatrix} \delta & \Omega \\ \Omega & -\delta \end{pmatrix}$ where $\delta(t) = \alpha \cos(\varpi t)$ and α, ϖ, Ω are positive constants verifying, for simplicity, weak-coupling ($\Omega \ll \alpha$) and large amplitude ($\alpha \gg \varpi$). For $t \in [0, T_1 = \pi/\varpi]$, $\frac{|\Omega'|}{\delta'} =$

$\frac{|\dot{\theta}|}{\omega_0} = \frac{\dot{\Omega}\delta - \Omega\dot{\delta}}{(\delta^2 + \Omega^2)^{3/2}}$ is real and with a single monotonicity change, so our second condition (16) reduces to condition (15). The non-adiabatic transition probability p_1 (so called single-passage or one-way transition), is given by the Landau-Zener's formula: $p_1 \approx e^{-\frac{\pi}{2} \frac{\Omega^2}{\alpha\varpi}}$ [42] and the adiabatic limit $p_1 \rightarrow 0$ is covered by the condition (15): $\max_{t \in [0, T_1]} \left| \frac{\dot{\theta}}{\omega_0} \right| = \frac{\alpha\varpi}{\Omega^2} \ll 1$. After M (even) multiple passage, for $t = MT_1$, the non-adiabatic transition probability becomes $p_M \approx p_1 \frac{\sin^2 M\Theta}{\cos^2 \Theta}$ and depends of a relative (Stückelberg) phase $\Theta \simeq \frac{\alpha}{\varpi}$ of the wavefunction [42]. For $\Theta \sim \pi/2[\pi]$, p_M can be M^2 times higher than p_1 leading to a full non adiabaticity $p_M \sim 1$ even if $p_1 \ll 1$. This illustrates why, in such an oscillating case, condition (15) ($\frac{\alpha\varpi}{\Omega^2} \ll 1$) is not sufficient and the extra condition (16) ($\frac{\alpha\varpi}{\Omega^2} \ll 1/M$) is needed to ensure an adiabatic evolution. This example shows that, with an oscillating hamiltonian, even if a single passage is quasi-adiabatic constructive interferences might accumulate the small non adiabatic amplitude to result, after multiple passages, in a full non-adiabatic transition [60]. This is very similar to the case of single crossing but with several levels [16, 43], or to multilevel system [19], leading, using stationary phase (saddle-point) theorem or steepest descent WKB type of methods, to sums or products of dephased Landau-Dykhne-Davis-Pechukas's formulas corresponding to several successive transitions between pairs of levels [17, 18]. Finally, this shows that the standard condition (1) breaks down, not only when resonant terms are present, as sometimes believed [11, 21, 22, 44], but more generally when oscillating terms are presents.

CONCLUSION

By simply diagonalizing the hamiltonian H' (hamiltonian in the adiabatic basis), we have derived simple conditions, Eqs.(13) and (14) and exact bounds (Eq. (7)) for the state and its phase, ensuring an adiabatic evolution. The usual (or standard) condition (1) is found to be a sufficient adiabatic condition but only for a real and "non-oscillating" hamiltonian evolution. This explains why all the previously cited examples (Landau-Zener, STIRAP, ...) deal with the (real) interaction representation or the dressed state basis, where $\omega = 0$, and use non oscillating functions such as exponential or polynomial ones.

Condition (14) prevents oscillation [61] but unfortunately with no distinction between case with constructive crossings or case with destructive (Stückelberg) interferences. However, the generic most common case concerns a "complex enough" system with small total probability when the single crossing probability is small [45], i.e. where the sole Eq. (13), or Eq. (1) for real hamiltonian, is sufficient to ensure an adiabatic evolution.

This result simply highlight the fact that the standard mathematical technique (so called asymptotic analysis)

to study the adiabaticity consists in extracting, from the global solution of the Schrodinger equation, a set of local solutions which individually covers a region (let say between time 0 and T), with a controlled behavior of the coefficients in the equation. This means that the criterion (1) is local and that in order to study the adiabatic behavior of a given hamiltonian, one should cut its evolution in part where we could apply safely the criterion (1), namely in part with single branching point or with single crossing between pairs of levels. Globally we shall add each local non-adiabatic amplitude to get the global non-adiabatic amplitude [16, 17, 18, 19, 43]. We would stress that all this should be very well known, but seems to be forgot by many physicist if we refer to recent published articles. Our article, demonstrate in a simple way that using non-oscillating function the number of local solution is obviously finite and so the added probability remains small if the criterion (1) is globally fulfilled.

Finally, the adiabatic evolution is strongly related to the (semi-)classical limit $\hbar \rightarrow 0$ of quantum mechanics [55] [46], to the WKB approximation [43], to the Minimal work principle [47], to the quasistatic thermodynamical process [48], and to perturbation theory. Therefore, we hope that this work and the given examples can enable the development of significant techniques, or provide novel insights into these important systems.

Thanks to Sabine Jansen to have pointed out to me Born and Fock's consideration concerning monotonicity.

APPENDIX

Multi levels model

We demonstrate here that conditions (13) and (14) imply the conditions (8) and (9). The techniques are similar to one used in Davis-Kahan $\sin \theta$ theorem or Weyl-Bauer-Fike's types of perturbative bounds [49, 50, 51]. The starting point is the exact Brillouin-Wigner perturbation theory that we demonstrate here for completeness [41].

We define the projector $Q_n = 1 - |n^{st}\rangle\langle n^{st}|$, which in matrix notation is $Q_n = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$, and the eigenvector $|\mathbf{n}'\rangle \propto |n'\rangle$ of $H' = H_0 + V$ with a simple normalization $\langle n^{st}|\mathbf{n}'\rangle = 1$. $H_0 = H' - V$ commutes with Q_n so [62] $(E'_n - H_0)Q_n|\mathbf{n}'\rangle = Q_n(E'_n - H' + V)|\mathbf{n}'\rangle = Q_nV|\mathbf{n}'\rangle$. When multiply by $(E'_n - H_0)^{-1}$ this directly lead, using $Q_n|\mathbf{n}'\rangle = |\mathbf{n}'\rangle - |n^{st}\rangle$, to the Brillouin-Wigner equation: $|\mathbf{n}'\rangle = (1 - (E'_n - H_0)^{-1}Q_nV)^{-1}|n^{st}\rangle$. Using the matrix notation, and the blockwise inversion, this becomes:

$$|\mathbf{n}'\rangle = \begin{pmatrix} 1 \\ (1 + \delta'^{-1}\Delta')^{-1} \frac{\delta'^{-1}\Omega'}{2} \end{pmatrix} \quad (17)$$

where $\hbar\Delta' = E'_n - H'_{nn} = \langle n^{st}|H_0 + V|\mathbf{n}'\rangle - H'_{nn} = \langle n^{st}|V|\mathbf{n}'\rangle$ satisfies

$$\delta'^{-1}\Delta' = \frac{\delta'^{-1}\Omega'^{\dagger}}{2}(1 + \delta'^{-1}\Delta')^{-1}\frac{\delta'^{-1}\Omega'}{2} \quad (18)$$

The idea is now to use the smallness of $\delta'^{-1}\Omega'$ (see Eq. (13)) to evaluate $|n'\rangle = |\mathbf{n}'\rangle/\sqrt{\langle \mathbf{n}'|\mathbf{n}'\rangle}$ and its time derivative, i.e. to study Eqs. (8) and (9).

We first take the norm of Eq. (18) and use $\|(1 + \delta'^{-1}\Delta')^{-1}\| \leq \sum_{k=0}^{\infty} \|\delta'^{-1}\Delta'\|^k = (1 - \|\delta'^{-1}\Delta'\|)^{-1}$ to see that: if $\|\delta'^{-1}\|\|\Omega'\| \ll 1$ then $\|\delta'^{-1}\Delta'\| \ll 1$ (see also Eq. (19)). Therefore Eq. (17) shows that Eq. (8) is implied by (it is in fact equivalent to) Eq. (13): $\|\delta'^{-1}\|\|\Omega'\| \ll 1$.

When $\|\delta'^{-1}\|\|\Omega'\| \ll 1$, i.e. $|\mathbf{n}'\rangle \approx |n^{st}\rangle$, the time derivative of $|n'\rangle = |\mathbf{n}'\rangle/\sqrt{\langle \mathbf{n}'|\mathbf{n}'\rangle}$ shows that $\|\dot{|n'}\rangle\| \approx \|\dot{|\mathbf{n}'}\rangle\|$. Time derivative of the equations (17) and (18) can then be used to study Eq. (9). Indeed, using $\delta'^{-1} = -\delta'^{-1}\dot{\delta}'\delta'^{-1}$ and (again) useful estimations on the smallness (see Eq. (18)) of the norm of $\delta'^{-1}\Delta'$ and its time derivative, finally leads to the fact that condition (14) (together with (13)) implies the condition (9).

Two levels model

We derive here, in a simpler way, the conditions (13) and (14). The eigenvectors $e^{i\theta_1}|1\rangle, e^{i\theta_2}|2\rangle$ of the hamiltonian H , corresponding respectively to the eigenvalues $\hbar\omega_0/2$ and $-\hbar\omega_0/2$, are given by the columns of $P = \begin{pmatrix} e^{-i\frac{\varphi}{2}} \cos \frac{\theta}{2} e^{i\theta_1} & -e^{-i\frac{\varphi}{2}} \sin \frac{\theta}{2} e^{i\theta_2} \\ e^{i\frac{\varphi}{2}} \sin \frac{\theta}{2} e^{i\theta_1} & e^{i\frac{\varphi}{2}} \cos \frac{\theta}{2} e^{i\theta_2} \end{pmatrix}$ and $H' = \frac{\hbar}{2} \begin{pmatrix} -\dot{\varphi} \cos \theta + \omega_0 + 2\dot{\theta}_1 & (\dot{\varphi} \sin \theta + i\dot{\theta})e^{i(\theta_2 - \theta_1)} \\ (\dot{\varphi} \sin \theta - i\dot{\theta})e^{i(\theta_1 - \theta_2)} & -\omega_0 + \dot{\varphi} \cos \theta + 2\dot{\theta}_2 \end{pmatrix}$.

With $\theta_2 = -\theta_1$, $H' = \frac{\hbar}{2} \begin{pmatrix} \delta' & \Omega'^{\dagger} \\ \Omega' & -\delta' \end{pmatrix}$. The $N = 2$ case is a very special one because it is always possible to choose H' , and then P' real with $\theta_2 = \theta_1 + \arg(-i\langle 2|\dot{1}\rangle)$. Using the obvious notations $H' = \frac{\hbar\omega'_0}{2} \begin{pmatrix} \cos \theta' & \sin \theta' \\ \sin \theta' & -\cos \theta' \end{pmatrix}$, i.e. $P' = \begin{pmatrix} \cos \frac{\theta'}{2} & -\sin \frac{\theta'}{2} \\ \sin \frac{\theta'}{2} & \cos \frac{\theta'}{2} \end{pmatrix}$. Our conditions (8-9) then read $\theta' \ll 1$ and $\int_0^t |\dot{\theta}'| \ll 1$ which leads to the general conditions of adiabatic evolution: Eqs. (15) and (16).

Non oscillating case

We assume here that the usual condition (1) is fulfilled for a strongly non-oscillating real hamiltonian (i.e. with monotonicity the $P_{mk} = \langle m^{st}|k\rangle = \varphi_{mk}$ functions) and we give here a clue that the evolution is indeed adiabatic.

By using a proof by contradiction, we assume that the evolution is not adiabatic. Thus condition (13) is not fulfilled so non negligible δ' off diagonal terms exists to modify substantively the δ' eigenvalues. The (Weyl-)Bauer-Fike's theorem (19) applied to δ' , implies that one of the off diagonal elements ($\sim \dot{\varphi}_{mk}$) of δ' should then be bigger than the diagonal ones (the gap ΔE_n). But Eq. (20) indicates that a time $T \sim 1/\|\Omega'\|$ is needed to have a non adiabatic evolution. Thus condition (1), which is roughly

$\|\Omega'\| \ll \Delta E_n$, would implies that $\varphi_{mk} \sim \dot{\varphi}_{mk} T \gg 1$ which contradicts $\varphi_{mk} = \langle m^{st} | k \rangle \leq 1$.

(Weyl-)Bauer-Fike's theorem

Let H'_d be the diagonal part of $H' = H'_d + H'_{\text{non diag}}$. Multiplying $H'_{\text{non diag}}|n'\rangle = (E'_n - H'_d)|n'\rangle$ by $(E'_n - H'_d)^{-1}$ and taking norm on both sides leads to the (Weyl-Lidskii)-Bauer-Fike's theorem (applied to H'):

$$\min_m |E'_n - H'_{mm}| \leq \|H'_{\text{non diag}}\| \quad (19)$$

Universal optimal bound

Using the following choice $\theta_m = \int_0^t i \langle m | \dot{m} \rangle - \int_0^t E_m / \hbar$ of a geometrical phase (Berry Phase for cyclic evolution) plus a dynamical phase simplifies the H' matrix elements (see Eq. 4). Using $-\frac{d|U_{nn}|}{dt} \leq \left| \frac{dU_{nn}}{dt} \right|$ and the norm [56] equality $\sqrt{1 - |U_{nn}^2|} = \sqrt{\sum_{m \neq n} |U_{mn}|^2} = \|U_{\bullet n}\|$, when integrating the (Schrödinger) equation ($i\hbar \dot{U}_{nn} = \Omega^\dagger U_{\bullet n}$) leads to the (quantum Zeno's type of) adiabatic condition:

$$1 - |U_{nn}(t)| \leq 1 - \cos(\|\Omega'\|t/2) \leq \frac{\|\Omega'/2\|^2}{2} t^2. \quad (20)$$

This optimal bound is reached by the Schwinger system for $\delta' = 0$.

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- [53] Milena Grifoni and Peter Hänggi. Driven quantum tunneling. *Physics Reports*, 304:229–354, 1998.
- [54] $\langle m|\dot{n}\rangle = \frac{\langle m|\dot{H}|n\rangle}{E_n - E_m}$ comes from the time derivative of $\langle m|n\rangle = \delta_{mn}$ and of $\langle m|H|n\rangle = E_n\delta_{mn}$, where δ_{mk} is Kronecker’s delta.
- [55] The path parametrization is here $s(t) = t/T = \epsilon t \in [0, 1]$ and $H_\epsilon(t) = H(s(t))$ where T is the evolution time. The Schrödinger equation is then $i\hbar \frac{d|\Psi_\epsilon(t)\rangle}{dt} = H_\epsilon(t)|\Psi_\epsilon(t)\rangle$ or $i\hbar \epsilon \frac{d|\Psi(s)\rangle}{ds} = H(s)|\Psi(s)\rangle$. More generally a local control of the speed is possible: $H_s(t) = H(s(t))$ by using a monotonic function $s(t) \in [0, 1]$ [52]. An example is the interpolating hamiltonian $H(s) = H_{\text{in}}(1 - s) + H_{\text{fin}}s$.
- [56] In this article we use $\|x\| = \sqrt{x^\dagger x} = \sqrt{\sum_{i=1}^N |x_i|^2}$ and $\|x\|_1 = \sum_{i=1}^N |x_i|$. They verify $\|x\|_2 \leq \|x\|_1 \leq \sqrt{N}\|x\|_2$. For the matrix norm $\|M\| = \max_{x \neq 0} \frac{\|Mx\|}{\|x\|}$.
- [57] For real hamiltonian H , $|m\rangle$ is real, so the (Pancharatnam’s phase) $\arg\langle m|\dot{n}\rangle$ is zero, and $\frac{d}{dt}\langle m|m\rangle = 2\langle m|\dot{m}\rangle = 0$.
- [58] Interestingly enough, very similar considerations have been used by Born and Fock in their seminal paper [2].
- [59] Simple condition (similar to Weyl’s theorem), for the smallness of δ'^{-1} off diagonal terms exists. For instance by choosing H_0 as the diagonal part of H' in the Brillouin-Wigner equation we can replace conditions (13) essentially by $\frac{\|\dot{H}(t)\|_1}{\Delta E(t)} \ll \frac{\Delta E_n(t)}{\hbar}$. However, this may be of small practical interest because it contains not only ΔE_n , the gap relative to $|n\rangle$, as in Eq. (1), but also the global energy spectral gap $\Delta E = \min_{m \neq k} |E_k - E_m|$.
- [60] Interestingly enough, the reverse case, namely the diabatic limit ($p_1 \approx 1$) can lead (for instance when α/ω annul the Bessel J_0 function) to the reverse phenomenon of adiabaticity created after multiple passages ($p_M \approx 0$) known as suppression of the tunneling, coherent destruction of tunneling, dynamical localization or population trapping depending on the context [42, 53].
- [61] More practical definition of a ”non-oscillating” hamiltonian than based on the small number of monotonicity change of the adiabatic hamiltonian H' would be useful. We conjecture (and hope that someone could demonstrate it) that real hamiltonian containing sum, product, multiplication or division of composition of (real) exponential or polynomial functions are of this type. A possible clue for this proof may be based on iterative used of Eq. (6) with the iterative $U'', P'', U^{(3)}, P^{(3)} \dots$ matrices converging toward the wanted diagonalization, as done in the Jacobi algorithm which iterates the $N = 2$ case. During each Jacobi step, the $P^{(m)}$ elements are still of the sum, product, multiplication or division of composition of (real) exponential or polynomial types. The exponent of the polynomial functions grows, as well as the number of monotonicity changes, but slowly enough to be always bounded (they never reach infinity due to the isolated zero theorem).
- [62] We wrote $E'_n 1$ simply as E'_n