Necessary and sufficient condition for quantum adiabatic evolution by unitary control fields

Zhen-Yu Wang and Martin B. Plenio
Institut für Theoretische Physik, Albert-Einstein-Allee 11, Universität Ulm, 89069 Ulm, Germany

We decompose the quantum adiabatic evolution as the products of gauge invariant unitary operators and obtain the exact nonadiabatic correction in the adiabatic approximation. A necessary and sufficient condition that leads to adiabatic evolution with geometric phases is provided and we determine that in the adiabatic evolution, while the eigenstates are slowly varying, the eigenenergies and degeneracy of the Hamiltonian can change rapidly. We exemplify this result by the example of the adiabatic evolution driven by parametrized pulse sequences. For driving fields that are rotating slowly with the same average energy and evolution path, fast modulation fields can have smaller nonadiabatic errors than obtained under the traditional approach with a constant amplitude.

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Introduction. The adiabatic theorem in quantum mechanics concerns the evolution of quantum systems subject to slowly varying Hamiltonians [1]. It states that the transitions between the instantaneous eigenstates of a Hamiltonian are negligible if the change of the Hamiltonian is much slower than the energy gaps between the instantaneous eigenstates. Berry discovered that in addition to the dynamic phase the adiabatic evolution exhibits a geometric phase determined only by the path [2]. Wilczek and Zee generalized the result to non-Abelian geometric phase for degenerate Hamiltonians [3]. While the adiabatic theorem has a wide range of applications, it was found that the widely used adiabatic quantitative condition

$$\left| \frac{\langle n_f | \dot{n}_j(t) \rangle}{E_n(t) - E_m(t)} \right| \ll 1,$$

for adiabatic approximation can be invalid [4][7]. Here $|n_j\rangle$ is the Hamiltonian eigenstate with the eigenenergy $E_n(t)$ and degeneracy label $j$ and the dot means a time derivative. As a consequence of these observations a debate arose and new adiabatic conditions were proposed (e.g., Refs. [8][14]). Those works [4][13] and the debate on the necessity of Eq. (1) [15][18], however, start from the assumption of non-degenerate Hamiltonians with a gap condition (i.e., $|E_n(t) - E_m(t)| > 0$). It has been noted however, that the formulation of an adiabatic theorem with a finite number of energy crossings is possible [19]. To verify the adiabatic conditions in the general setting, it is important to obtain the exact nonadiabatic correction in the adiabatic approximation for Hamiltonians with possible energy crossings.

In this work, we consider Hamiltonians $H(t)$ with possible energy degeneracies and arbitrary number of energy crossings. We decompose the quantum evolution

$$U(t) = U_{\text{Dyn}}(t)U_{\text{Geo}}(t)U_{\text{Dia}}(t),$$

as the products of gauge invariant unitary operators: the dynamic phase operator $U_{\text{Dyn}}(t)$, the geometric phase operator $U_{\text{Geo}}(t)$, and the nonadiabatic correction $U_{\text{Dia}}(t)$ in the adiabatic approximation. In the adiabatic limit, $U_{\text{Dia}}(t) = I$ is the identity operator and $U_{\text{Dia}}(t) = U_{\text{Dyn}}(t)U_{\text{Geo}}(t)$ is the exact adiabatic evolution. From $U_{\text{Dia}}(t)$, we derive an upper bound of the nonadiabatic deviation in the adiabatic approximation and propose a necessary and sufficient condition for adiabatic evolution. Counterintuitively perhaps, we find that the eigenenergies of the Hamiltonian can change rapidly and can have an arbitrary number of energy crossings during the adiabatic evolution. The result presented here reveals that the crucial condition for adiabatic evolution is a slowly varying eigenpath, while the eigenenergies are not required to vary slowly. This finding leads to a new way to realize adiabatic evolution. By applying a sequence of coherent pulses or a fast varying field parameterized by the adiabatic path, we can achieve the adiabatic evolution with accumulated (non-Abelian) geometric phases in a shorter time for a given average energy.

Note that we can achieve $U_{\text{Dia}}(t)$ by using the Hamiltonian $H'(t) = iU_{\text{Dia}}(t)U_{\text{Dia}}(t)^*$, a scheme called transitionless or counterdiabatic quantum driving [20][23]. Since generally $|n_j\rangle$ is not the eigenstate of the driving Hamiltonian $H'(t)$, this driving does not follow the adiabatic evolution and we will not discuss it in this work.

Gauge invariant formalism for adiabatic evolution. Here we obtain the exact nonadiabatic deviation and derive the general condition for adiabatic evolution. Consider a quantum system driven by a time-dependent Hamiltonian $H(t) = H(R) \equiv H(\theta)$, where $R \equiv (R_1(\theta), R_2(\theta), \ldots)$ is parametrized by $\theta = \theta(t)$ and $\omega \equiv d\theta/dt$ describes the speed of traversing a path. The function parameters $t$, $R$, and $\theta$ are used interchangeably in this paper. The evolution of arbitrary quantum states from the moment $t = 0$ (with the parameters $R = R_0$ and $\theta = \theta_0$) to the moment $T$ (i.e., $R_T$ and $\theta_T$) is described by the evolution operator $U(T)$, which satisfies the Schrödinger equation ($\hbar = 1$)

$$i\dot{U}(t) = H(t)U(t).$$

The instantaneous orthonormal eigenstates $|n_f\rangle \equiv |n_j\rangle$ at the moment $t$ satisfy $H(t)|n_f\rangle = E_n(t)|n_f\rangle \equiv E_n(\theta)|n_f\rangle$. Substituting the transformation $U(t) \equiv U_1(t)U_2(t)$ in Eq. (3) with $U_1(t)$ a unitary operator, we obtain $i\dot{U}_2(t) = H_2(t)U_2(t)$ with $H_2(t) = U_1(t)^* \left[ H(t) - iU_1(t)U_1(t)^* \right] U_1(t)$ in the interaction picture. By the transformation $U_1(t) = U_{\text{Dyn}}(t)U_{\text{Geo}}(t)$.

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with
\[ U_{\text{Dyn}}(t) \equiv \sum_{n,j} e^{-i \int_0^t E_n(t') dt'} |n_j'\rangle \langle n_j'|, \]
\[ U_{\text{G1}}(t) \equiv \sum_{n,j} |n_j\rangle \langle n_j|, \]
we obtain \( H_2(t) = -i \sum_{n=m,n,p,q} |n_p\rangle \langle n_q'| \langle n_q'| \langle n_q| \langle n_q'| E_n(t') dt' + H_{\text{G2}}(t) \) with \( H_{\text{G2}}(t) \equiv -i \sum_{n,m,n,p,q} |n_p\rangle \langle n_q'| \langle n_q'| \langle n_q| \) where \( |n_p\rangle \) are the initial eigenstates. To obtain the nonadiabatic correction \( U_{\text{Dia}}(t) \), we write \( U_2(t) = U_1(t) U_{\text{Dia}}(t) \), where
\[ U_{\text{G2}}(t) \equiv T \exp \left[ -i \int_0^t H_{\text{G2}}(t') dt' \right], \]
with \( T \) the time ordering operator. In the decomposition
\[ U(t) = U_{\text{Dyn}}(t) U_{\text{G1}}(t) U_{\text{G2}}(t) U_{\text{Dia}}(t), \]
\( U_{\text{Dyn}}(t) \) is the dynamic phase operator and \( U_{\text{Geo}}(t) \equiv U_{\text{G1}}(t) U_{\text{G2}}(t) \) is the geometric phase operator. The geometric phase operator
\[ U_{\text{Geo}}(t) = \sum_{n,j} |n_j\rangle \langle n_j'| \mathcal{P} e^{i T_0 \sum_{p} \hat{H}_p \phi_p(t)} e^{i T_0 \sum_{n} |n_n\rangle \langle n_n'| \phi_n(t) - i \frac{d}{dt} \phi_n(t)} dR^n, \]
is generally non-Abelian for degenerate Hamiltonians. Here \( \mathcal{P} \) is the path ordering operator on \( R \) or \( \theta \), and \( \mathcal{N}_R \equiv \left( \frac{\partial}{\partial R^1}, \frac{\partial}{\partial R^2}, \ldots \right) \) acts on \( \hat{R}^3 \). The nonadiabatic correction reads
\[ U_{\text{Dia}}(t) = \mathcal{P} \exp \left[ i \int_{\theta_0}^\theta \sum_{n,m,p,q} F_{n,m}(\theta') G_{n,m}^p(\theta') d\theta' \right], \]
where the geometric functions
\[ G_{n,m}^p(\theta) \equiv U_{\text{Geo}}^{-1}(\theta) |p\rangle \langle p'| \mathcal{P} e^{i T_0 \sum_{p} \hat{H}_p \phi_p(t)} e^{i T_0 \sum_{n} |n_n\rangle \langle n_n'| \phi_n(t) - i \frac{d}{dt} \phi_n(t)} dR^n, \]
describe nonadiabatic transitions \( |m_j\rangle \leftrightarrow |p_j\rangle \), and the modulation functions
\[ F_{n,m}(\theta) \equiv e^{i \int_{E_n(t')} E_n(t') dt'} = e^{i \int_0^\theta \int_0^t E_n(t') dt'} \]
determined by the energy gaps \( E_n(t) - E_m(t) \) and the speed of path sweeping \( \alpha \). We have separated the effects of \( F_{n,m} \) (determined by the eigenenergies \( E_n \)) and \( G_{n,m}^p(\theta) \) (determined by eigenstates \( |n_p\rangle \)) in \( U_{\text{Dia}}(t) \). The decomposition Eq. (12) is obtained, with \( U_{\text{Dia}}(t) \) describing all the nonadiabatic effects.

The system Hamiltonian \( H(t) \) is gauge invariant, that is, \( H(t) \) does not change when we replace \( |n_p\rangle \) with \( |W_j| n_j\rangle \) in the formulas, where \( W_j \) is a time-dependent unitary transformation of degenerate subspaces with the property \( \langle m_j'| W_j | n_j\rangle = 0 \) if \( m \neq n \). An example is the phase-shift operator of the eigenstates, \( W_j = \sum_{n,j} e^{i \phi_{n,j}(t)} |n_j\rangle \langle n_j'| \). An important property of our general formalism is that \( U_{\text{Dyn}}(t), U_{\text{Geo}}(t), \) and \( U_{\text{Dia}}(t) \) are all gauge invariant.

The deviation from the adiabatic evolution is described by
\[ D_{\text{Dia}}(t) \equiv U_{\text{Dia}}(t) - I. \]

When its unitarily invariant norm \( \| D_{\text{Dia}}(t) \| \) \( \approx 0 \), the quantum evolution is adiabatic with \( U_{\text{Dia}}(t) \approx I \). Let the average of the modulation functions be bounded by \( \xi_{\text{avg}} \) during the evolution time \( T \),
\[ \left| \int_0^\theta F_{n,m}(\theta') d\theta' \right| < \xi_{\text{avg}}, \forall \theta \in [\theta_0, \theta_T] \text{ and } n \neq m. \]

For example, if \( \int_0^\theta F_{n,m}(\theta') d\theta' = 0 \) for the intervals \( \theta_j - \theta_j < \eta \) with \( j = 0, 1, \ldots, N \) and \( \theta_{N+1} \equiv \theta_T \), we have \( \xi_{\text{avg}} = \eta \). And an upper bound of the nonadiabatic correction reads
\[ \| D_{\text{Dia}}(T) \| < \xi_{\text{avg}} \left( g_{\text{tot}}^2 + w_{\text{tot}} \right) (\theta_T - \theta_0), \]
where \( g_{\text{tot}} = \sum_{n \neq m} g_{n,m} \) and \( w_{\text{tot}} = \sum_{n \neq m} w_{n,m} \), with the least upper bounds \( g_{n,m} \equiv \sup_{\theta_0 \leq \theta \leq \theta_T} \| \sum_p G_{n,m}^p(\theta) \| \) and \( w_{n,m} \equiv \sup_{\theta_0 \leq \theta \leq \theta_T} \| \sum_p \frac{d}{dt} G_{n,m}^p(\theta) \| \).

To be valid for arbitrary finite smooth paths, the averaging condition (13) with vanishing \( \xi_{\text{avg}} \to 0 \) can be shown to be necessary and sufficient for the adiabatic approximation \( U_{\text{Dia}}(t) \to I \) during \( t \in [0, T] \). The condition (13) means that the low-frequency Fourier components \( f_{n,m}(\lambda) \equiv \int_0^\theta F_{n,m}(\theta') e^{-i\lambda \theta'} d\theta' \) of \( F_{n,m}(\theta) \) are negligible when \( \xi_{\text{avg}} \ll 1 \), since for a small \( \lambda \) the factor \( e^{-i\lambda \theta} \) is slowly varying and \( f_{n,m}(\lambda) \approx 0 \) by the generalized Riemann-Lebesgue lemma (22, 28). The condition \( \xi_{\text{avg}} \to 0 \) is sufficient because \( F_{n,m}(\theta) \) are fast oscillating functions and the slowly varying functions \( G_{n,m}^p(\theta) \) are averaged out. If the adiabatic limit \( U_{\text{Dia}}(t) \to I \) is valid for arbitrary finite smooth paths, we can always find some paths which lead to \( \xi_{\text{avg}} \to 0 \) in Eq. (13), and thus Eq. (13) with \( \xi_{\text{avg}} \to 0 \) is also necessary.

\section*{Adiabatic evolution by pulse sequences}

Now we show that adiabatic evolution can be driven by pulsed Hamiltonians. We consider a quantum system driven solely by a sequence of \( N \) unitary pulses
\[ P(R_k) = \sum_{n,j} e^{-i\theta_k(R_k)} |n_j\rangle \langle n_j'|. \]
The idea is illustrated by a two-level system in Fig. 1. Between the pulses there is no control and the system is gapless with \( H(t) = 0 \) \cite{29}, which is not the setting of previous works \cite{4,12,15}. The pulses are applied in the order of the parameters \( R_k = R_1, R_2, \ldots, R_N \), which sample a path gradually, and they induce the modulation functions \( F_{n,n}(\theta) \) to average out the effects of nonadiabatic transitions. The actual time duration of each pulse can be arbitrary (within the coherence time). For \( M \) non-degenerate subspaces, we can choose \( \theta_n(R_k) = 2\pi n/M \) with \( n = 1, \ldots, M \). If the system is a spin-1 system, the pulses are just rotations with an angle \( 2\pi/(2J + 1) \) by a magnetic field that defines the eigensates \( |\theta_k^B \rangle \). If we apply the pulses equidistantly during the parameter range \( [\theta_0, \theta_T] \), the integral \( \int_{\theta_0}^{\theta_T} F_{n,n}(\theta')d\theta' = O(1/N) \) vanishes at large \( N \). The dynamic phase \[42, 43\] we can use equal numbers of \( \theta_n(R_k) \) and the geometric phase factor \( U_{Geo}(T) \) is given by Eq. (8) with the path sampled by the points \( R_k \). Note that this pulse sequence is different from dynamical decoiling pulse sequences \cite{30–32}, which also use pulses to induce modulation functions to average out unwanted evolution \cite{33}. Here the pulses are parametrized by a path sampled by \( (R_k) \) and are used to suppress state transitions caused by the change of system eigenstates, whereas dynamical decoiling uses pulses in some fixed directions and has the purpose to suppress system-environment interactions.

Another way to traverse an adiabatic path is using a sequence of projective measurements \cite{34,35}. If we begin in the ground state of \( H(R_0) \) and successively measure \( H(R_1), H(R_2), \ldots, H(R_N) \), then the final state will be the ground state of \( H(R_N) \) with high probability, assuming the difference between successive points is sufficiently small. The advantages of our method are the following: the control is unitary and is easier to implement in experiments; the states do not collapse and the traversal of the path is deterministic; the (non-Abelian) geometric phases are preserved in the whole state space during the evolution. In addition, similar to dynamical decoiling realized by continuous driving fields in some fixed directions \cite{37,40}, our method works for fields varying continuously in amplitudes and directions (see the later part of this work).

A spin-1/2 driven by a pulse sequence. An example of the pulses in Eq. (15) for a spin-1/2 is a sequence of equidistant ±\( \pi \) rotations along the directions \( \hat{x} \sin \theta \cos \theta_k + \hat{y} \sin \theta \sin \theta_k + \hat{z} \cos \theta_k \) with \( \vartheta_k = (\theta_T - \vartheta_0)/(2N - 1) + \vartheta_0 \), for \( k = 1, \ldots, N \), (16) and \( \vartheta_0 = 0 \) (see Fig. 1). Since the sampling of \( \vartheta \) is similar to the timing of Carr-Purcell (CP) sequences \cite{41}, we denote our sequence as CP_{Geo} pulse sequence for convenience. Each of the unitary pulse, \( P(\theta_k) = \sum_{\pm} \exp \left[ \pm i(-1)^{\pm} \frac{\pi}{2} \right] |\theta_k^\pm \rangle \langle \theta_k^\pm | \) with \( s_k \in \{ \pm 1 \} \), introduces a ±\( \pi \) phase shift between the instantaneous eigenstates \( |\theta_k^\pm \rangle \). To isolate the geometric phase by cancelling the dynamic phase \cite{42,43}, we can use equal numbers of +\( \pi \) and −\( \pi \) pulses. The geometric (Berry) phase from \( \vartheta_0 \) to \( \vartheta_T \) is \( U_{Geo}(T) = \sum_k |\vartheta_k^+ \rangle \langle \vartheta_k^+ | e^{i\vartheta_k^+ \vartheta_0^+ \cos \vartheta} \) and \( U_{Dia}(T) = \mathcal{P} \exp \left[ \frac{1}{\pi} \int_{\theta_0}^{\theta_T} \sin \theta F_{1,1}(\theta) e^{i \cos \theta} \right] |\langle \uparrow | + \text{H.c.} \rangle d\theta \right] \), where the modulation function \( F_{1,1}(\theta) = (-1)^k \) when \( \vartheta \in (\vartheta_{k-1}, \vartheta_k) \) [see Fig. 2(a)]. Note that if we apply 2\( \pi \) rotations on the spin-1/2, even though the energy gaps are larger during the control, the modulation function \( F_{1,1}(\theta) = 1 \) does not have averaging effects and the adiabatic evolution is not realized.

We measure the nonadiabatic correction at the moment \( T \) numerically by the average deviation \( \Delta_{Dia} = \langle \Psi | D_{Dia}(T) | \Psi \rangle \), where the over bar is the average over all possible states \( |\Psi\rangle \). We plot the deviation \( \Delta_{Dia} \) under the control of CP_{Geo} pulses in Fig. 3, which shows that as the number of pulses increases, the nonadiabatic evolution is smaller because of better averaging. The CP_{Geo} sequences with even number of pulses have better performance than those with odd \( N \). Note that with \( \vartheta = \pi/2 \) and at the moment \( T \), \( D_{Dia}(T) = 0 \) under the CP_{Geo} sequences with any pulse number \( N \geq 1 \).

A spin-1/2 driven by continuously varying fields. Fast varying fields that are changing continuously can also lead to adiabatic evolution and can have better performance than slowly varying fields in traditional adiabatic evolution. Consider the driving fields \( B(t) (\hat{x} \sin \theta \cos \vartheta + \hat{y} \sin \theta \sin \vartheta + \hat{z} \cos \vartheta) \) on a spin-1/2 with \( \vartheta = \omega t \), where \( B(t) \) has the values (i) \( B_2(t) = \Omega (1 + \gamma \cos(\Omega t)) \), (ii) \( B_{2x}(t) = 2B_2(t) \), and (iii) \( B_{const}(t) = \)}
with even number of
though the field amplitude changes rapidly and there are
than the slowly varying field $B_e$. The results are shown at integer numbers of $N'$, with the red squares (black triangles) for the fast varying field $B_f$ ($B_{2f}$) and the green circles for the field $B_{\text{const}}$ of constant amplitude. For other values of $N'$, the results are shown for $B_{\text{const}}$ by blue dots and for $B_f$ by red empty squares from $N' = 1$ to 6.

$$\sqrt{(2 + \gamma^2)/8\Omega},$$

which has the same average energy as $B_e(t)$ [i.e., $\int_0^{2\pi} |B_{\text{const}}| dt = \int_0^{2\pi} |B_f| dt$]. We set $\gamma \approx 2.34$ so that the average of the modulation function $e^{i\int_0^{2\pi} B_f(t) dt}$ vanishes in a half period $\pi/\Omega$ (see Fig. 2). The eigenenergies are $\pm \frac{1}{2} B(t)$. There are degeneracy points for $B_{2\pi e}(t) = 0$. The field $B_{2\pi n_e}$ contributes a $\pi (2\pi)$ phase shift in each period of $2\pi/\Omega$.

In Fig. 4 we plot $\Delta \text{Dua}$ for $B_f$, $B_{2f}$, and $B_{\text{const}}$ as a function of $N' \equiv \Omega/2\pi$ with the total evolution time $T = 1$ and $\omega = 2\pi$. For $B_e$, the integer values of $N'$ is the number of accumulated $\pi$ phases during the evolution. Increasing $N'$ (i.e., increasing the energy) is equivalent to increasing the evolution time in adiabatic evolution. As shown in Fig. 4, the fast varying field $B_f$ realizes the adiabatic evolution even though the field amplitude changes rapidly and there are many energy crossings during the evolution. The field $B_{2f}$ with even number of $\pi$ phase shift is much more efficient than the slowly varying field $B_{\text{const}}$ in traditional adiabatic evolution, because the modulation function $e^{i\int_0^{2\pi} B_{2f}(t) dt}$ is more efficient than $e^{i\int_0^{2\pi} B_{\text{const}} dt}$ (see Fig. 2). Even though $B_{2\pi e}(t)$ has a larger amplitude and energy than $B_e(t)$, it cannot realize adiabatic evolution because the average of the modulation does not vanish. Thus larger field amplitudes do not always lead to better adiabatic evolution.

Note that here the energy crossings are not avoided crossings. With perturbation, multiple avoided crossings can occur, and the effect of multiple Landau-Zener transitions is a topic for future study.

The Marzlin-Sanders inconsistency in degenerate Hamiltonians. The quantitative condition Eq. (1) had been widely used as a criterion for the adiabatic approximation. Unlike the condition in Eq. (13), the condition in Eq. (1) is a function of eigenstates (i.e., the evolution path) in addition to the dependency on eigenenergies. The path dependency may cause failure of adiabatic approximation for some evolution paths. Indeed, it was first discovered by Marzlin and Sanders that this condition (1) is not sufficient for adiabatic approximation. If a system $A$ with the Hamiltonian $H(t)$ follows the adiabatic evolution and $|\langle n'|n'\rangle| \neq 1$, another system $\bar{A}$ driven by the Hamiltonian $\bar{H}(t) = -U^\dagger(t)H(t)U(t)$ with $U(t) = T e^{-i \int_0^t \bar{H}(\tau) d\tau}$ cannot have adiabatic evolution even if both systems satisfy the same condition (1). The inconsistency for non-degenerate Hamiltonians was explained by the resonant transitions between the energy levels in $\bar{H}(t)$ [6]. Here we consider general Hamiltonians with possible degeneracy and show that the unbounded path of $\bar{S}$ violates the adiabatic approximation. The eigenstates of the second system are expressed by the first system as $|n'\rangle = U^\dagger(t)|n\rangle$ with the eigenenergies $\bar{E}_n(t) = -E_n(t)$. For the system $S$ with a bounded path, the geometric function $G_{n,n}(\theta)$ evolves finitely along the path. It is easy to obtain for the system $\bar{A}$ the geometric function $G_{n,n}(\theta) = \bar{F}_{n,n}(\theta)G_{n,n}(\theta)$, which contains the fast oscillating factors $e^{i\int_0^\theta (E_n(t^\prime) - E_n(t)) dt^\prime}$. Therefore in the adiabatic limit, the change of the geometric function $G_{n,n}(\theta)$ is not finite and the path of $\bar{A}$ is not bounded. The effect of nonadiabatic evolution $\bar{U}_{\text{Dua}}(t) = \mathcal{P} \exp \left[ \int_0^t \sum_{m}\bar{G}^p_{n,m}(\theta) d\theta \right]$ does not vanish unless $\langle n'|\bar{U}^\dagger(t)|n\rangle = 0$ in Eq. (10), i.e., $|n'\rangle = e^{i\bar{F}_{n,n}(\theta)}|n\rangle$. Therefore the condition (1) does not guarantee finite eigenpaths and is not sufficient. It was claimed that the condition (1) is necessary when there is no energy degeneracy or crossings [15]. We have shown that energy crossings are possible in the adiabatic evolution. Thus the condition (1) is also not necessary. To have adiabatic evolution, the geometric operator $G_{n,n}(\theta)$ should be slowly varying compared with $F_{n,m}(\theta)$.

Conclusions. We have developed a gauge invariant formalism to obtain the whole nonadiabatic transitions in the adiabatic approximation, and have used this to show that the instantaneous eigenenergies and eigenstates play different roles in the adiabatic evolution. For finite evolution paths, the instantaneous eigenenergies can change rapidly as long as the gap modulations are off-resonant to the excitations generated by the instantaneous eigenstates. We have demonstrated examples of adiabatic evolution by fast changing fields, which can lead to better adiabatic evolution. Arbitrary number of level crossings during the adiabatic evolution is possible. Under an exact and transparent formalism, we have shown by general Hamiltonians with possible degeneracy and crossings that the Marzlin-Sanders inconsistency arises because the evolution path is not slowly varying. Our formalism also clearly show that the quantitative condition Eq. (1) is neither necessary nor sufficient. A necessary and sufficient condition for adiabatic evolution has been provided.

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Gauge invariance

Consider the gauge transformation

\[ |n_j'\rangle \rightarrow |\tilde{n}_j'\rangle = W_t |n_j'\rangle, \]

(17)

where the time-dependent unitary operator \( W_t \) is the transformation within each degenerate subspace with the property

\[ \langle m_p'|W_t|m_q'\rangle = 0, \text{ if } m \neq n. \]

(18)

An example of this transformation is the phase shifts \( W_t = \sum_{n,j} \exp(i \phi_{n,j}^t)|n_j'\rangle\langle n_j'| \) of the eigenstates. The property Eq. (18) leads to

\[ \left[ \sum_j |n_j'\rangle\langle n_j'|, W_t \right] = 0, \]

(19)

which can be verified by using Eq. (18) and inserting the identity operator \( I = \sum_{m,k} |m_k'\rangle\langle m_k'| \) into the commutator:

\[ \sum_j |n_j'\rangle\langle n_j'|W_t \sum_{m,k} |m_k'\rangle\langle m_k'| - \sum_{m,k} |m_k'\rangle\langle m_k'|W_t \sum_j |n_j'\rangle\langle n_j'| = 0. \]

(20)

Using Eq. (19), the system Hamiltonian

\[ \tilde{H}(t) = \sum_{n,j} E_n(t) |\tilde{n}_j'\rangle\langle \tilde{n}_j'| = \sum_n E_n W_t \sum_j |n_j'\rangle\langle n_j'| W_t^\dagger, \]

(21)

\[ = \sum_{n,j} E_n(t) |n_j'\rangle\langle n_j'| = H(t), \]

(22)

is gauge invariant under the transformation of \( W_t \).

Gauge invariance of \( U_{\text{dyn}}(t) \)

Using Eq. (19), the dynamic phase operator

\[ U_{\text{dyn}}(t) = \sum_j e^{-i \int_0^t E_j(t) dt} \sum_j |\tilde{n}_j'\rangle\langle \tilde{n}_j'|, \]

(23)

\[ = \sum_n e^{-i \int_0^t E_n(t) dt} \sum_j W_t |n_j'\rangle\langle n_j'| W_t^\dagger, \]

(24)

\[ = \sum_n e^{-i \int_0^t E_n(t) dt} \sum_j |n_j'\rangle\langle n_j'| = U_{\text{dyn}}(t), \]

(25)

is gauge invariant.

Gauge invariance of \( U_{\text{Geo}}(t) \)

We first find the Hamiltonian \( H_w(t) = i U_w(t) U_w^\dagger(t) \) of the propagator

\[ U_w(t) \equiv \left( \sum_{n,p} |n_p^0\rangle\langle n_p|^t \right) \left( \sum_{m,q} |\tilde{m}_q^0\rangle\langle \tilde{m}_q| \right), \]

(26)

\[ = \sum_{n,p,q} |n_p^0\rangle\langle n_p|^t W_t |n_q^0\rangle W_t^\dagger, \]

(27)

where we have used Eq. (18). We have \( U_w(0) = I \) and \( U_w(t) = T \ e^{-i \int_0^t H_w(t) dt} \). Using Eqs. (18) and (19), we obtain

\[ H_w(t) = i \sum_{n,p,q} |n_p^0\rangle\langle n_p|^t W_t |n_q^0\rangle W_t^\dagger |n_q^0\rangle W_t^\dagger + \]

\[ i \sum_{n,p,q,j} |n_p^0\rangle\langle n_p|^t W_t |\tilde{n}_j\rangle W_t^\dagger |\tilde{n}_j\rangle.W_t^\dagger \]

(28)

The geometric phase factor

\[ \tilde{U}_{\text{Geo}}(t) = \tilde{U}_{\text{G1}}(t) \tilde{U}_{\text{G2}}(t), \]

(29)

where

\[ \tilde{U}_{\text{G1}}(t) = \sum_{n,j} |\tilde{n}_j\rangle\langle \tilde{n}_j| = W_t \sum_{n,j} |n_j\rangle\langle n_j| W_t^\dagger, \]

(30)

\[ = U_{\text{G1}}(t) U_w(t), \]

(31)

and

\[ \tilde{U}_{\text{G2}}(t) = T \exp \left[ -i \int_0^t \sum_{n,p,q} |\tilde{n}_p^0\rangle\langle \tilde{n}_p^0| \tilde{n}_q^0 \langle \tilde{n}_q^0| dt' \right]. \]

(32)

We rewrite \( \tilde{U}_{\text{G2}}(t) \) as

\[ \tilde{U}_{\text{G2}}(t) = U_w(t) T \exp \left[ -i \int_0^t H_{\text{WG2}}(t') dt' \right], \]

(33)

where the Hamiltonian

\[ H_{\text{WG2}}(t) = -i U_w(t) \sum_{n,p,q} |n_p^0\rangle\langle n_p| W_t |\tilde{n}_q^0\rangle U_w^\dagger(t) + H_w(t). \]

(34)

Using Eqs. (18) and (19), we obtain

\[ H_{\text{WG2}}(t) = -i \sum_{n,p,q} \sum_{n,j} |n_p^0\rangle\langle n_p| W_t |\tilde{n}_j\rangle W_t^\dagger |\tilde{n}_j\rangle W_t^\dagger + H_w(t) \]

\[ - i \sum_{n,p,q,j} |n_p^0\rangle\langle n_p| W_t |\tilde{n}_j\rangle W_t^\dagger |\tilde{n}_j\rangle W_t^\dagger. \]

(35)

Substitute Eq. (28) into Eq. (35), we have

\[ H_{\text{WG2}}(t) = i \sum_{n,p,q} |n_p^0\rangle\langle n_p| W_t |\tilde{n}_j\rangle |n_q^0\rangle W_t^\dagger + H_w(t). \]

(36)

From Eqs. (29), (31), (33), and (36), we can see that

\[ \tilde{U}_{\text{Geo}}(t) = U_{\text{G1}}(t) U_{\text{G2}}(t) = U_{\text{Geo}}(t) \]

(37)

is gauge invariant.
Gauge invariance of \( U_{\text{Dia}}(t) \)

As \( U_{\text{Geo}}(t) \) is gauge invariant, we just need to show

\[
\sum_{p,q} |n_p^i\rangle\langle n_p^i| \tilde{\omega}_q^i\rangle\langle \tilde{\omega}_q^i| m_q^i\rangle\langle m_q^i|, \text{ for } n \neq m, \tag{38}
\]

is gauge invariant. For \( n \neq m \),

\[
\sum_{p,q} |n_p^i\rangle\langle n_p^i| \tilde{\omega}_q^i\rangle\langle \tilde{\omega}_q^i| m_q^i\rangle\langle m_q^i| = \sum_{p,q} W_p |n_p^i\rangle\langle n_p^i| \tilde{\omega}_q^i\rangle\langle \tilde{\omega}_q^i| m_q^i\rangle\langle m_q^i| \tilde{W}_m^i \times \left( \langle n_p^i| W_p^i \tilde{\omega}_q^i\rangle \langle \tilde{\omega}_q^i| m_q^i\rangle + \langle n_p^i| \tilde{\omega}_q^i\rangle \langle \tilde{\omega}_q^i| m_q^i\rangle \right) m_q^i W_m^i. \tag{39}
\]

Using Eq. (19), we have

\[
\sum_{p,q} |n_p^i\rangle\langle n_p^i| \tilde{\omega}_q^i\rangle\langle \tilde{\omega}_q^i| m_q^i\rangle\langle m_q^i| = \sum_{p,q} |n_p^i\rangle\langle n_p^i| W_p |m_q^i\rangle\langle m_q^i| W_m^i + \sum_{p,q} |n_p^i\rangle\langle n_p^i| W_p |\tilde{\omega}_q^i\rangle\langle \tilde{\omega}_q^i| m_q^i\rangle\langle m_q^i| \tilde{W}_m^i. \tag{40}
\]

The time derivative of Eq. (18) gives

\[
\langle n_p^i| W_p |m_q^i\rangle = -\langle n_p^i| W_p |\tilde{\omega}_q^i\rangle - \langle n_p^i| \tilde{\omega}_q^i\rangle, \text{ for } n \neq m. \tag{41}
\]

By substitution of Eq. (18) into Eq. (40), we get

\[
\sum_{p,q} |n_p^i\rangle\langle n_p^i| \tilde{\omega}_q^i\rangle\langle \tilde{\omega}_q^i| m_q^i\rangle\langle m_q^i| = - \sum_{p,q} |n_p^i\rangle\langle n_p^i| W_p |m_q^i\rangle\langle m_q^i| \tilde{W}_m^i. \tag{42}
\]

Using Eq. (19) and \( \frac{d}{dt} \left( \langle n_p^i| \tilde{\omega}_q^i\rangle \right) = \langle n_p^i| \tilde{\omega}_q^i\rangle + \langle n_p^i| \tilde{\omega}_q^i\rangle = 0 \), we obtain for \( n \neq m \),

\[
\sum_{p,q} |n_p^i\rangle\langle n_p^i| \tilde{\omega}_q^i\rangle\langle \tilde{\omega}_q^i| m_q^i\rangle\langle m_q^i| = \sum_{p,q} |n_p^i\rangle\langle n_p^i| \tilde{\omega}_q^i\rangle\langle \tilde{\omega}_q^i| m_q^i\rangle. \tag{43}
\]

Therefore \( U_{\text{Dia}}(t) \) is gauge invariant.

The gauge invariance of \( U_{\text{Dia}}(t) \) can also be verified by the facts that \( U_{\text{Dia}}(t) = [U_{\text{Dyn}}(t)U_{\text{Geo}}(t)]^\dagger U(t) \) and \( U_{\text{Dyn}}(t) \), \( U_{\text{Geo}}(t) \), and \( U(t) \) are gauge invariant.

The proofs of necessity and sufficiency

Sufficiency

For simplicity, we define \( F_\mu \equiv F_{n,m} \) and \( G_\mu \equiv \sum_{p,q} G_{n,m} \) in \( U_{\text{Dia}}(t) \) and write it as \( U_{\text{Dia}}(\theta) \equiv U_{\text{Dia}}(t) = \mathcal{P} \exp \left[ i \int_{\theta_0}^{\theta} \sum_\mu F_\mu(\theta') G_\mu(\theta') d\theta' \right] \) by using \( \mu \) to indicate the summation over \( n \neq m \). The nonadiabatic deviation Eq. (12) reads

\[
D_{\text{Dia}}(t) = i \int_{\theta_0}^{\theta} \sum_\mu F_\mu G_\mu U_{\text{Dia}} d\theta'. \tag{44}
\]

We use a partition for the interval \( [\theta_0, \theta] \) by \( N - 1 \) points \( \theta_j \), such that \( \theta_0 < \theta_1 < \theta_2 < \cdots < \theta_{N-1} < \theta \equiv \theta_N \) with the interval

\[
\eta_{\text{min}} \leq \theta_{j+1} - \theta_j \leq \eta, \tag{45}
\]

for all \( j = 0, 1, \cdots, N - 1 \). Let

\[
g_{\text{tot}} \equiv \sum_\mu g_\mu, \tag{46}
\]

with the least upper bound of the unitarily invariant norm

\[
g_\mu \equiv \sup_{\theta' \in [\theta_0, \theta]} \| G_\mu(\theta') \|. \tag{47}
\]

The change of \( G_\mu(\theta') \) is continuous, with a finite time derivative for \( \theta' \in [\theta_0, \theta] \), and we define

\[
w_{\text{tot}} \equiv \sum_\mu w_\mu, \tag{48a}
\]

\[
w_\mu \equiv \sup_{\theta' \in [\theta_0, \theta')} \| \frac{d}{d\theta'} G_\mu(\theta') \|. \tag{48b}
\]

Any bounded operator \( A(\theta') \) has an associate step function \( \bar{A}(\theta') = A(\theta_j) \) when \( \theta' \in [\theta_j, \theta_{j+1}] \). For \( \theta' \in [\theta_j, \theta_{j+1}] \), the difference

\[
\| G_\mu(\theta') - \bar{G}_\mu(\theta') \| = \| G_\mu(\theta') - G_\mu(\theta_j) \|, \tag{49}
\]

\[
= \left\| \int_{\theta_j}^{\theta'} \frac{d}{d\theta'} G_\mu(\theta) d\theta \right\|, \tag{50}
\]

\[
\leq (\theta' - \theta_j) w_\mu, \tag{51}
\]

\[
< \eta w_\mu, \tag{52}
\]

For \( \theta' \in [\theta_j, \theta_{j+1}] \), the difference

\[
\| U_{\text{Dia}}(\theta') - \bar{U}_{\text{Dia}}(\theta') \| = \| U_{\text{Dia}}(\theta') - U_{\text{Dia}}(\theta_j) \|, \tag{53}
\]

\[
= \left\| \int_{\theta_j}^{\theta'} \frac{d}{d\theta} U_{\text{Dia}}(\theta) d\theta \right\|, \tag{54}
\]

\[
\leq \sum_\mu \left\| \int_{\theta_j}^{\theta'} F_\mu(\theta) G_\mu(\theta) U_{\text{Dia}}(\theta) d\theta \right\|, \tag{55}
\]

\[
\leq (\theta' - \theta_j) g_{\text{tot}}, \tag{56}
\]

\[
< \eta g_{\text{tot}}, \tag{57}
\]

where we have used \( |F_\mu(\theta')| = 1 \). From Eqs. (52) and (57), we have the norm

\[
\| G_\mu U_{\text{Dia}} - \bar{G}_\mu U_{\text{Dia}} \| = \| G_\mu (U_{\text{Dia}} - \bar{U}_{\text{Dia}}) + (\bar{G}_\mu - G_\mu) \bar{U}_{\text{Dia}} \|, \tag{58}
\]

\[
< \eta \left( g_{\text{tot}} + w_\mu \right). \tag{59}
\]

We write the deviation Eq. (44) as \( D_{\text{Dia}}(\theta) \equiv D^{(1)}_{\text{Dia}} + D^{(2)}_{\text{Dia}} \), where the error caused by the partition

\[
D^{(1)}_{\text{Dia}} = i \int_{\theta_0}^{\theta} \sum_\mu F_\mu \left[ G_\mu U_{\text{Dia}} - \bar{G}_\mu \bar{U}_{\text{Dia}} \right] d\theta' \tag{59}
\]

has the norm

\[
\| D^{(1)}_{\text{Dia}} \| < \eta \left( \eta^2 + w_{\text{tot}} \right) (\theta - \theta_0). \tag{60}
\]
and

\[ D_{\text{Dia}}^{(2)} = i \int_{\theta_0}^\theta \sum_{\mu} F_{\mu} \mathcal{U}_{\text{Dia}} d\theta'. \] (61)

Under the averaging condition [13]

\[ \left| \int_{\theta_0}^\theta F_{n,m}(\theta') d\theta' \right| < \epsilon_{\text{avg}}, \text{ for } \theta' \in [\theta_0, \theta] \text{ and } n \neq m, \] (62)

we have the norm

\[ \| D_{\text{Dia}}^{(2)} \| = \left\| \sum_{\mu} \sum_{j} G_{\mu} \mathcal{U}_{\text{Dia}} \int_{\theta_j}^{\theta_{j+1}} F_{\mu} d\theta \right\|, \] (63)

\[ \leq \sum_{\mu} \sum_{j} \left\| G_{\mu} \mathcal{U}_{\text{Dia}} \int_{\theta_j}^{\theta_{j+1}} F_{\mu} d\theta \right\| , \] (64)

\[ < \epsilon_{\text{avg}} N g_{\text{tot}}. \] (65)

The nonadiabatic deviation \( \| D_{\text{Dia}} \| \leq \| D_{\text{Dia}}^{(1)} \| + \| D_{\text{Dia}}^{(2)} \| \).

For sufficiently small \( \epsilon_{\text{avg}} \ll (\theta - \theta_0)^2 \left( \frac{g_{\text{tot}}^2 + w_{\text{tot}}}{g_{\text{tot}}} \right), \) we choose the partition with \( \eta \approx \eta_{\text{min}} \approx \sqrt{\epsilon_{\text{avg}} g_{\text{tot}} / \left( g_{\text{tot}}^2 + w_{\text{tot}} \right)} \ll (\theta - \theta_0). \) With this partition, we obtain

\[ \| D_{\text{Dia}} \| \leq 2(\theta - \theta_0) \sqrt{\epsilon_{\text{avg}} g_{\text{tot}} \left( g_{\text{tot}}^2 + w_{\text{tot}} \right)}. \] (66)

and

\[ \lim_{\epsilon_{\text{avg}} \to 0} U_{\text{Dia}}(t) = I. \] (67)

Therefore the averaging condition [13] with \( \epsilon_{\text{avg}} \ll 1 \) is sufficient.

If the average

\[ \int_{\theta_j}^{\theta_{j+1}} F_{n,m}(\theta') d\theta' = 0, \text{ for } n \neq m, \] (68)

vanishes for all the intervals \( j = 0, 1, \ldots, N - 1, \) we have

\[ D_{\text{Dia}}^{(2)} = 0, \epsilon_{\text{avg}} = \eta, \text{ and } \]

\[ \| D_{\text{Dia}} \| < \epsilon_{\text{avg}} \left( g_{\text{tot}}^2 + w_{\text{tot}} \right) (\theta - \theta_0). \] (69)

**Necessity**

A general condition for adiabatic evolution should be universal and works for all bounded paths. We choose a path that satisfies \( \frac{d}{d\theta} m_0 = 0 \) if \( n_p \neq N, M \) and the states \( |N^0\rangle = \cos(b\theta) |N^0\rangle - i \sin(b\theta) |M^0\rangle \) and \( |M^\theta\rangle = -i \sin(b\theta) |N^0\rangle + \cos(b\theta) |M^0\rangle \) with \( b = O(1) \). We have \( \frac{d}{d\theta} N^0 = -ib|N^0\rangle, \) \( \frac{d}{d\theta} M^0 = -ib|N^0\rangle, \) and thus \( U_{G2}(\theta) = I \) by using Eq. (6). The deviation from the adiabatic evolution is

\[ D_{\text{Dia}}(\theta) = i \int_{\theta_0}^{\theta} b \left[ F_{N,M}(\theta') |N^0\rangle \langle M^0| + \text{H.c.} \right] U_{\text{Dia}}(\theta') d\theta'. \] (70)

Using \( U_{\text{Dia}}(\theta') = D_{\text{Dia}}(\theta') + I, \) we write

\[ \int_{\theta_0}^{\theta} b \left[ F_{N,M}(\theta') |N^0\rangle \langle M^0| + \text{H.c.} \right] d\theta' = \]

\[ iD_{\text{Dia}}(\theta) - \int_{\theta_0}^{\theta} b \left[ F_{N,M}(\theta') |N^0\rangle \langle M^0| + \text{H.c.} \right] D_{\text{Dia}}(\theta') d\theta'. \] (71)

For a good adiabatic approximation, the correction \( \| D_{\text{Dia}}(\theta') \| < \epsilon \) is small for all bounded paths \( \theta' \in [\theta_0, \theta]. \) Here \( \epsilon \) is a small value. By choosing other paths with different \( |N^0\rangle \) and \( |M^0\rangle \) in Eq. (71), we have for \( n \neq m, \)

\[ \left| \int_{\theta_0}^{\theta} F_{n,m}(\theta') d\theta' \right| < \epsilon, \] (72)

with a finite \( \kappa. \) In the adiabatic limit

\[ \lim_{\| D_{\text{Dia}} \| \to 0} \left| \int_{\theta_0}^{\theta} F_{n,m}(\theta') d\theta' \right| = 0, \] (73)

for \( n \neq m. \)