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

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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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I. 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 the 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

$$\left|\frac{\langle n_p^t|\dot{m}_q^t\rangle}{E_n(t)-E_m(t)}\right| \ll 1 \tag{1}$$

for adiabatic approximation can be invalid [4–8]. Here $|n_p^t\rangle$ ($|m_q^t\rangle$) is the Hamiltonian eigenstate with the eigenenergy $E_n(t)$ [$E_m(t)$] and degeneracy label p (q), 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. [9–15]). Those works [4–15] and the debate on the necessity of Eq. (1) [16–20]), however, start from the assumption of nondegenerate 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 finite numbers of energy crossings is possible [21]. 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 paper, we consider Hamiltonians $H(t)$ with possible energy degeneracies and arbitrary numbers of energy crossings. We decompose the quantum evolution

$$U(t)=U_{\rm Dyn}(t)U_{\rm Geo}(t)U_{\rm Dia}(t), \tag{2}$$

as the products of unitary operators: the dynamic phase operator $U_{\rm Dyn}(t)$, the geometric phase operator $U_{\rm Geo}(t)$, and the nonadiabatic correction $U_{\rm Dia}(t)$ in the adiabatic approximation. In the adiabatic limit, $U_{\rm Dia}(t)=I$ is the identity operator and $U_{\rm adia}(t)=U_{\rm Dyn}(t)U_{\rm Geo}(t)$ is the exact adiabatic evolution. From $U_{\rm Dia}(t)$, 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.

II. 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 $H(t)\equiv H(\boldsymbol{R})\equiv H(\vartheta)$, where $\boldsymbol{R}\equiv(R_1(\vartheta),R_2(\vartheta),\dots)$ is parametrized by the dimensionless parameter $\vartheta=\vartheta(t)$, and

$$\omega=\omega(t)\equiv\frac{d\vartheta}{dt} \tag{3}$$

describes the speed of traversing a path. The function parameters t, $\boldsymbol{R}$, and ϑ are used interchangeably in this paper. The evolution of arbitrary quantum states from the moment $t=0$ (with the parameters $\boldsymbol{R}=\boldsymbol{R}_0$ and $\vartheta=\vartheta_0$) to the moment T (i.e., $\boldsymbol{R}_T$ and ϑ_T) is described by the evolution operator $U(T)$, which satisfies the Schrödinger equation ($\hbar=1$)

$$i\dot{U}(t)=H(t)U(t). \tag{4}$$

The instantaneous orthonormal eigenstates $|n_j^{\boldsymbol{R}}\rangle\equiv|n_j^{\vartheta}\rangle\equiv|n_j^t\rangle$ at the moment t satisfy $H(t)|n_j^t\rangle=E_n(t)|n_j^t\rangle\equiv E_n(\vartheta)|n_j^{\vartheta}\rangle$. Substituting the transformation $U(t)\equiv U_1(t)U_2(t)$ in Eq. (4) with $U_1(t)$ a unitary operator, we obtain $i\dot{U}_2(t)=H_2(t)U_2(t)$ with $H_2(t)=U_1^{\dagger}(t)[H(t)-i\dot{U}_1(t)U_1^{\dagger}(t)]U_1(t)$ in the interaction picture [22]. By another transformation $U_1(t)=U_{\rm Dyn}(t)U_{\rm G1}(t)$ with

$$U_{\rm Dyn}(t)\equiv\sum_{n,j}e^{-i\int_0^t E_n(t')dt'}|n_j^t\rangle\langle n_j^t|, \tag{5}$$

$$U_{\rm G1}(t) \equiv \sum_{n,j} |n_j^t\rangle\langle n_j^0|, \tag{6}$$

we obtain $H_2(t) = -i\sum_{n\neq m;p,q} |n_p^0\rangle\langle n_p^t|\dot{m}_q^t\rangle\langle m_q^0| e^{i\int_0^t (E_n-E_m)dt'} + H_{\rm G2}(t)$ with $H_{\rm G2}(t) = -i\sum_{n,p,q} |n_p^0\rangle\langle n_p^t|\dot{n}_q^t\rangle \langle n_q^0|$, where $|n_j^0\rangle$ are the initial eigenstates. To obtain the nonadiabatic correction $U_{\rm Dia}(t)$, we write $U_2(t)$ as $U_2(t) = U_{\rm G2}(t)U_{\rm Dia}(t)$, where

$$U_{\rm G2}(t) \equiv \mathcal{T}\exp\left[-i\int_0^t H_{\rm G2}(t')dt'\right], \tag{7}$$

with $\mathcal{T}$ the time ordering operator. In the decomposition

$$U(t) = U_{\rm Dyn}(t)U_{\rm G1}(t)U_{\rm G2}(t)U_{\rm Dia}(t), \tag{8}$$

$U_{\rm Dyn}(t)$ is the dynamic phase operator and $U_{\rm Geo}(t) \equiv U_{\rm G1}(t)U_{\rm G2}(t)$ is the geometric phase operator. The geometric phase operator

$$U_{\rm Geo}(t) = \sum_{n,j} \left|n_j^{\boldsymbol{R}}\right\rangle\!\left\langle n_j^{\boldsymbol{R}_0}\right| \mathcal{P} e^{i\int_{\boldsymbol{R}_0}^{\boldsymbol{R}} \sum_{n,p,q} \left|n_p^{\boldsymbol{R}_0}\right\rangle\left\langle n_p^{\boldsymbol{R}'}\right| i\nabla_{\boldsymbol{R}'}\left|n_q^{\boldsymbol{R}'}\right\rangle\left\langle n_q^{\boldsymbol{R}_0}\right| \cdot d\boldsymbol{R}'}, \tag{9}$$

is generally non-Abelian for degenerate Hamiltonians. Here $\mathcal{P}$ is the path ordering operator on $\boldsymbol{R}$ or ϑ, and $\nabla_{\boldsymbol{R}} \equiv (\frac{\partial}{\partial R_1}, \frac{\partial}{\partial R_2}, \cdots)$ acts on $|n_q^{\boldsymbol{R}}\rangle$. The nonadiabatic correction reads

$$U_{\rm Dia}(t) = \mathcal{P}\exp\left[i\int_{\vartheta_0}^{\vartheta} \sum_{n\neq m;p,q} F_{n,m}(\vartheta')G_{n,m}^{p,q}(\vartheta')d\vartheta'\right], \tag{10}$$

where the geometric functions

$$G_{n,m}^{p,q}(\vartheta) \equiv U_{\rm Geo}^\dagger(\vartheta)\left|n_p^\vartheta\right\rangle\left(\left\langle n_p^\vartheta\right| i\frac{d}{d\vartheta}\left|m_q^\vartheta\right\rangle\right)\left\langle m_q^\vartheta\right| U_{\rm Geo}(\vartheta) \tag{11}$$

describe nonadiabatic transitions $|m_q^\vartheta\rangle \leftrightarrow |n_p^\vartheta\rangle$, and the modulation functions

$$F_{n,m}(\vartheta) \equiv e^{i\int_0^t [E_n(t')-E_m(t')]dt'} = e^{i\int_{\vartheta_0}^{\vartheta} [E_n(\vartheta')-E_m(\vartheta')]\frac{1}{\omega}d\vartheta'} \tag{12}$$

are determined by the energy gaps $E_n(t) - E_m(t)$ and the speed of path sweeping ω. We have separated the effects of $F_{n,m}$ (determined by the eigenenergies E_n) and $G_{n,m}^{p,q}$ (determined by eigenstates $|n_j^t\rangle$) in $U_{\rm Dia}(t)$. The decomposition Eq. (2) is obtained, with $U_{\rm Dia}(t)$ describing all the nonadiabatic effects.

An important property of our general formalism is that the unitary operators $U_{\rm Dyn}(t)$, $U_{\rm Geo}(t)$, and $U_{\rm Dia}(t)$ are all gauge invariant (see Appendix A). That is, these unitary operators do not change when we replace $|n_j^t\rangle$ with $W_t|n_j^t\rangle$ in the formulas, where W_t is a time-dependent unitary transformation of degenerate subspaces with the property $\langle m_p^t|W_t|n_q^t\rangle = 0$ if $m \neq n$. An example of W_t is the phase-shift operator of the eigenstates, $W_t = \sum_{n,j} e^{i\phi_{n,j}(t)}|n_j^t\rangle\langle n_j^t|$. Examples of gauge invariant operators are the system Hamiltonian $H(t)$ and the corresponding unitary propagator $U(t)$. Examples of operators that are not gauge invariant are $U_{\rm G1}(t)$ [Eq. (6)] and $U_{\rm G2}(t)$ [Eq. (7)]. Not all decompositions of a gauge invariant unitary operators are gauge invariant. For example, $U_a(t) = U_{\rm Dyn}(t)U_{\rm G1}(t)$ and $U_b(t) = U_{\rm G2}(t)U_{\rm Dia}(t)$, for a different decomposition $U(t) = U_a(t)U_b(t)$ of Eq. (8), are not gauge invariant.

III. CONDITION FOR QUANTUM ADIABATIC EVOLUTION

The deviation from the adiabatic evolution is described by

$$D_{\rm Dia}(t) \equiv U_{\rm Dia}(t) - I. \tag{13}$$

When its unitarily invariant norm [23,24] $\|D_{\rm Dia}(t)\| \approx 0$, the quantum evolution is adiabatic with $U_{\rm Dia}(t) \approx I$.

Let the average of the modulation functions be bounded by $\xi_{\rm avg}$ during the evolution time T,

$$\left|\int_{\vartheta_0}^{\vartheta} F_{n,m}(\vartheta')d\vartheta'\right| < \xi_{\rm avg}, \forall\vartheta \in [\vartheta_0,\vartheta_T] \text{ and } n \neq m. \tag{14}$$

Note that the left-hand side of Eq. (14) is the absolute value of the Fourier component

$$f_{n,m}(\lambda) \equiv \int_{\vartheta_0}^{\vartheta} F_{n,m}(\vartheta')e^{-i\lambda\vartheta'}d\vartheta', \tag{15}$$

at $\lambda = 0$.

If $\int_{\vartheta_j}^{\vartheta_{j+1}} F_{n,m}(\vartheta)d\vartheta = 0$ for the intervals $\vartheta_{j+1} - \vartheta_j < \eta$ with $j = 0,1,\ldots,N$ and $\vartheta_{N+1} \equiv \vartheta_T$, we have $\xi_{\rm avg} = \eta$. For this partition, the upper bound of the nonadiabatic correction reads (see Appendix B)

$$\|D_{\rm Dia}(T)\| < \xi_{\rm avg}\left(g_{\rm tot}^2 + w_{\rm tot}\right)(\vartheta_T - \vartheta_0), \tag{16}$$

where $g_{\rm tot} = \sum_{n\neq m} g_{n,m}$ and $w_{\rm tot} = \sum_{n\neq m} w_{n,m}$ with the least upper bounds $g_{n,m} \equiv \sup_{\vartheta\in[\vartheta_0,\vartheta_T]} \|\sum_{p,q} G_{n,m}^{p,q}(\vartheta)\|$ and $w_{n,m} \equiv \sup_{\vartheta\in[\vartheta_0,\vartheta_T]} \|\sum_{p,q} \frac{d}{d\vartheta}G_{n,m}^{p,q}(\vartheta)\|$. Note that the factor $(g_{\rm tot}^2 + w_{\rm tot})(\vartheta_T - \vartheta_0)$ on the right-hand side of Eq. (16) is only a function of evolution path.

In Appendix B, we also derive two upper bounds in general cases for $\xi_{\rm avg} \ll 1$, i.e.,

$$\|D_{\rm Dia}(t)\| \lesssim 2(\vartheta - \vartheta_0)\sqrt{\xi_{\rm avg}g_{\rm tot}\left(g_{\rm tot}^2 + w_{\rm tot}\right)}, \tag{17}$$

and

$$\begin{aligned}\|D_{\rm Dia}(t)\| <& \sqrt{\xi_{\rm avg}}\left(g_{\rm tot}^2 + w_{\rm tot}\right)(\vartheta - \vartheta_0)^2\\ &+ (\sqrt{\xi_{\rm avg}} + \xi_{\rm avg})g_{\rm tot}.\end{aligned} \tag{18}$$

To be valid for arbitrary finite smooth paths, the averaging condition (14) with vanishing $\xi_{\rm avg} \to 0$ can be shown to be necessary and sufficient for the adiabatic approximation $U_{\rm Dia}(t) \to I$ during $t \in [0,T]$ (see Appendix B). The sufficiency is obvious from the bounds Eqs. (17) or (18), and the physical reason is the following. The condition (14) means that the low-frequency Fourier components $f_{n,m}(\lambda)$ of $F_{n,m}(\vartheta')$ are negligible when $\xi_{\rm avg} \ll 1$, since for a small λ the factor $e^{-i\lambda\vartheta'}$ is slowly varying, and we can show $f_{n,m}(\lambda) \approx 0$ by the generalized Riemann-Lebesgue lemma [25,26]. The condition $\xi_{\rm avg} \to 0$ is sufficient because $F_{n,m}(\vartheta)$ are fast oscillating functions and the slowly varying functions $G_{n,m}^{p,q}(\vartheta)$ are averaged out. If the adiabatic limit $U_{\rm Dia}(t) \to I$ is valid for arbitrary finite smooth paths, we can always find some paths which lead to $\xi_{\rm avg} \to 0$ in Eq. (14), and thus Eq. (14) with $\xi_{\rm avg} \to 0$ is also necessary.

To have a simple picture of the condition Eq. (14), consider as an example the case that the ratios $r_{n,m} \equiv \frac{\hbar\omega}{E_n - E_m}$ of the speed ω for traversing a path to the energy gaps $E_n - E_m$ are constants. By using Eqs. (12) and (14), we obtain $|f_{n,m}(0)| \leqslant 2|r_{n,m}|$. Therefore, we can choose $\xi_{\rm avg} = \max|r_{n,m}| + 0^+$ for the condition Eq. (14). For finite energy gaps $E_n - E_m$, the slow evolution limit $\omega = d\vartheta/dt \to 0$ (i.e., the limit of infinite evolution time $t \to \infty$) gives $\xi_{\rm avg} \to 0$ and hence the quantum adiabatic evolution. Note that since the time and energy are conjugate variables, we can realize the quantum adiabatic evolution by increasing the energy gaps $|E_n - E_m| \to \infty$ for a finite speed ω and finite evolution times t. If we treat $\hbar\omega$ as the energy scale of the excitation caused by path transversal, we have another physical interpretation. The adiabatic approximation is valid when the excitation energy scale $\hbar\omega$ is much smaller than the energy gap $E_n - E_m$. The above arguments apply to situations that the energy gaps and the speed ω change smoothly, since we can split the evolution into pieces and the evolution of each piece has approximately constant ratios $r_{n,m}$.

IV. 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

$$P(\boldsymbol{R}_k) = \sum_{n,j} e^{-i\theta_n(\boldsymbol{R}_k)} |n_j^{\boldsymbol{R}_k}\rangle\langle n_j^{\boldsymbol{R}_k}|. \tag{19}$$

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 $H(t) = 0$ [27], which is not the setting of previous works [4–6,8–13,16]. The pulses are applied in the order of the parameters $\boldsymbol{R}_k = \boldsymbol{R}_1, \boldsymbol{R}_2, \ldots, \boldsymbol{R}_N$, which sample a path gradually, and they induce the modulation functions $F_{n,m}(\vartheta)$ to average out the effects of nonadiabatic transitions. The actual time duration of each pulse can be arbitrary (within the coherence time). For M nondegenerate subspaces, we can choose $\theta_n(\boldsymbol{R}_k) = 2\pi n/M$ with $n = 1, \ldots, M$. If the system is a spin-J system, the pulses are just rotations with an angle $2\pi/(2J+1)$ by a magnetic field that defines the eigenstates $|n_j^{\boldsymbol{R}_k}\rangle$. If we apply the pulses equidistantly during the parameter range $[\vartheta_0, \vartheta_T]$, the integral $\int_{\vartheta_0}^{\vartheta} F_{n,m}(\vartheta')d\vartheta' = O(1/N)$ vanishes at large N. The dynamic phase is $\sum_k \theta_n(\boldsymbol{R}_k)$ and the geometric phase factor $U_{\rm Geo}(T)$ is given by Eq. (9) with the path sampled by the points $\boldsymbol{R}_k$.

Note that this pulse sequence is different from dynamical decoupling pulse sequences [28–30], which also use pulses to induce modulation functions to average out unwanted evolutions [31]. Here the pulses are parametrized by a path sampled by $\{\boldsymbol{R}_k\}$ and are used to suppress state transitions caused by the change of system eigenstates, whereas dynamical decoupling uses pulses to suppress unwanted terms in the original Hamiltonians (e.g., interactions from environments). Additionally, to suppress unwanted terms, the control Hamiltonian used in dynamical decoupling generally does not commute with the original system Hamiltonian. For example, in using dynamical decoupling to suppress the pure dephasing (caused by the noise along the z direction) of a qubit, the control fields are required to have components perpendicular to z (the control fields along the z direction cannot suppress the noise along the z direction). In contrast, the Hamiltonian to generate the pulse sequences for adiabatic evolution is the total Hamiltonian (in the rotating frame of the bare Hamiltonian).

Another way to traverse an adiabatic path is the use of a sequence of projective measurements [32,33], which can be simulated by evolution randomization [34,35]. If we begin in the ground state of $H(\boldsymbol{R}_0)$ and successively measure $H(\boldsymbol{R}_1), H(\boldsymbol{R}_2), \ldots, H(\boldsymbol{R}_N)$, then the final state will be the ground state of $H(\boldsymbol{R}_N)$ with high probabilities, assuming that the difference between successive points is sufficiently small. Unlike those methods [32–35], our protocol represents a deterministic quantum algorithm to stroboscopically sample an intended path and is easier to implement in experiments.

A. A spin-$\frac{1}{2}$ driven by a pulse sequence

An example of the pulses in Eq. (19) for a spin-$\frac{1}{2}$ is a sequence of equidistant $\pm\pi$ rotations along the directions $\hat{\boldsymbol{x}} \sin\theta \cos\vartheta_k + \hat{\boldsymbol{y}} \sin\theta \sin\vartheta_k + \hat{\boldsymbol{z}} \cos\theta$ with

$$\vartheta_k = (\vartheta_T - \vartheta_0)\left(\frac{2k-1}{2N}\right) + \vartheta_0, \text{ for } k = 1, \ldots, N, \tag{20}$$

and $\vartheta_0 = 0$ (see Fig. 1). Since the sampling of ϑ is similar to the timing of Carr-Purcell (CP) sequences [36], we denote our sequence as $\text{CP}_{\rm Geo}$ pulse sequence for convenience. Each of

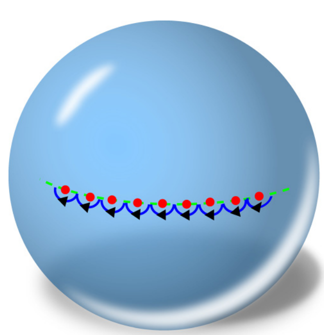

FIG. 1. Illustration of a sequence of pulses applied to a spin-$\frac{1}{2}$. The red dots indicate the directions of the pulses on the Bloch sphere. The blue semicircles illustrate the directions of spin rotation. The green dashed line shows the effective path of adiabatic evolution. These successive rotations induce a geometric phase.

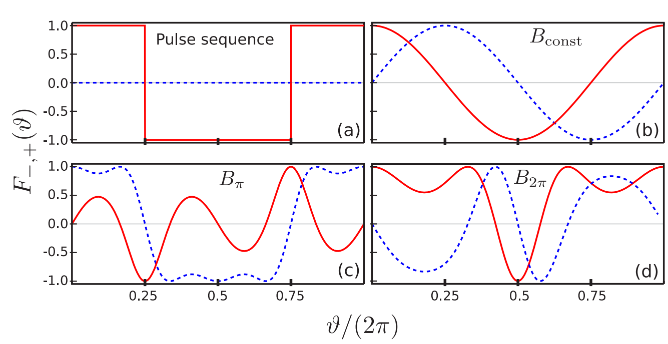

FIG. 2. The modulation functions $F_{-,+}(\vartheta)$ of a spin-$\frac{1}{2}$ in a scaled period. Red solid (blue dashed) lines for the real (imaginary) part of $F_{-,+}(\vartheta)$. (a) for the modulation function of a pulse sequence, (b) for a constant field $B_{\rm const}$, and (c) and (d) for fast varying fields B_π and $B_{2\pi}$, respectively.

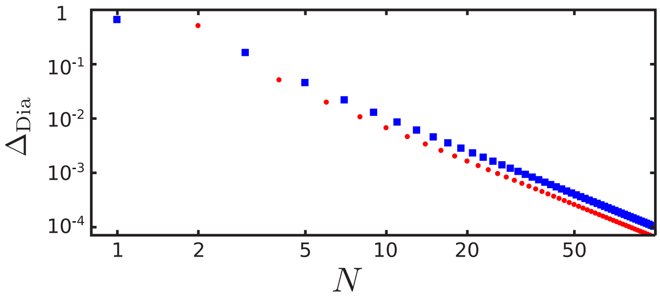

FIG. 3. The average deviation $\Delta_{\rm Dia}$ as a function of $\mathrm{CP_{Geo}}$ pulse number N, with red circles (blue squares) for even (odd) N. Here $\vartheta_0 = 0$, $\vartheta_T = 2\pi$, and $\theta = \pi/6$.

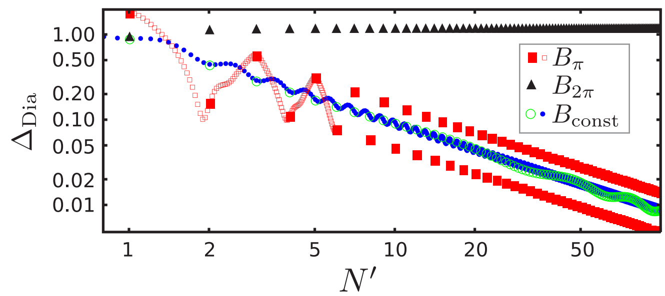

FIG. 4. The plot of $\Delta_{\rm Dia}$ as a function of N' for the continuous driving with $\vartheta_0 = 0$, $\vartheta_T = 2\pi$, and $\theta = \pi/2$. The integer values of N' correspond to the numbers of applied π pulses for the field B_π. The results are shown at integer numbers of N', with the red squares (black triangles) for the fast varying field B_π ($B_{2\pi}$) and the green circles for the field $B_{\rm const}$ of constant amplitude. For other values of N', the results are shown for $B_{\rm const}$ by blue dots and for B_π by red empty squares from $N' = 1$ to 6.

the unitary pulses, $P(\vartheta_k) = \sum_\pm \exp[\pm i(-1)^{s_k}\frac{\pi}{2}]|\vartheta_k^\pm\rangle\langle\vartheta_k^\pm|$ with $s_k \in \{\pm 1\}$, introduces a $\pm\pi$ phase shift between the instantaneous eigenstates $|\vartheta_k^\pm\rangle$. To isolate the geometric phase by canceling the dynamic phase [37,38], we can use equal numbers of $+\pi$ and $-\pi$ pulses or even numbers of π pulses. The geometric (Berry) phase from ϑ_0 to ϑ_T is $U_{\rm Geo}(T) = \sum_\pm |\vartheta_T^\pm\rangle\langle\vartheta_0^\pm| e^{\pm i\frac{1}{2}\vartheta_T\cos\theta}$, and $U_{\rm Dia}(T) = \mathcal{P}\exp[\frac{-i}{2}\int_{\vartheta_0}^{\vartheta_T}(\sin\theta F_{-,+}(\vartheta)e^{i\cos\theta\vartheta}|\vartheta_0^-\rangle\langle\vartheta_0^+| + \text{H.c.})d\vartheta]$, where the modulation function $F_{-,+}(\vartheta) = (-1)^k$ when $\vartheta \in (\vartheta_{k-1},\vartheta_k]$ [see Fig. 2(a)]. Note that if we apply 2π rotations on the spin-$\frac{1}{2}$, even though the energy gaps are larger during the control, the modulation function $F_{-,+}(\vartheta) = 1$ 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 $\Delta_{\rm Dia} \equiv \overline{|\langle\Psi|D_{\rm Dia}(T)|\Psi\rangle|}$, where the over bar is the average over all possible states $|\Psi\rangle$. We plot the deviation $\Delta_{\rm Dia}$ under the control of $\mathrm{CP_{Geo}}$ pulses in Fig. 3, which shows that as the pulse number increases, the nonadiabatic evolution is smaller because of better averaging. The $\mathrm{CP_{Geo}}$ sequences with even pulse numbers have better performance than those with odd N. Note that when $\theta = \pi/2$, $D_{\rm Dia}(T) = 0$ for the $\mathrm{CP_{Geo}}$ sequences with any pulse numbers $N \geqslant 1$.

B. A spin-$\frac{1}{2}$ 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 $B(t)(\hat{\boldsymbol{x}}\sin\theta\cos\vartheta + \hat{\boldsymbol{y}}\sin\theta\sin\vartheta + \hat{\boldsymbol{z}}\cos\theta)$ on a spin-$\frac{1}{2}$ with $\vartheta = \omega t$, where $B(t)$ has the values (i) $B_\pi(t) = \frac{\Omega}{2}[1 + \gamma\cos(\Omega t)]$, (ii) $B_{2\pi}(t) = 2B_\pi(t)$, and (iii) $B_{\rm const}(t) = \sqrt{(2+\gamma^2)/8}\Omega$, which has the same average energy as $B_\pi(t)$ [i.e., $\int_0^{\frac{2\pi}{\Omega}}|B_{\rm const}|^2 dt = \int_0^{\frac{2\pi}{\Omega}}|B_\pi|^2 dt$]. We set $\gamma \approx 2.34$ so that the average of the modulation function $e^{i\int_0^t B_\pi(s)ds}$ vanishes in a half period π/Ω (see Fig. 2). The eigenenergies are $\pm\frac{1}{2}B(t)$. There are degeneracy points for $B_{\pi(2\pi)}(t) = 0$. The field $B_{\pi(2\pi)}$ contributes a π (2π) phase shift in each period of $2\pi/\Omega$.

In Fig. 4, we plot $\Delta_{\rm Dia}$ for B_π, $B_{2\pi}$, and $B_{\rm const}$ as a function of $N' \equiv \Omega T/2\pi$ with $\omega T = 2\pi$ and the total evolution time $T = 1$. For B_π, the integer values of N' are the numbers of accumulated π 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_π realizes the adiabatic evolution even though the field amplitude changes rapidly and there are many energy crossings during the evolution. The field B_π with even numbers of π phase shifts is much more efficient than the slowly varying field $B_{\rm const}$ in traditional adiabatic evolution, because the modulation function $e^{i\int B_\pi dt}$ is more efficient than $e^{i\int B_{\rm const}dt}$ (see Fig. 2). Even though $B_{2\pi}(t)$ has a larger amplitude and energy than $B_\pi(t)$, 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 [39] is a topic for future study.

V. 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. (14), 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 [4,5]. If a system A with the Hamiltonian $H(t)$ follows the adiabatic evolution and $|\langle n^0|n^t\rangle| \neq 1$, another system $\bar{A}$ driven by the Hamiltonian $\bar{H}(t) = -U^\dagger(t)H(t)U(t)$ with $U(t) = \mathcal{T}e^{-i\int_0^t H(s)ds}$ cannot have adiabatic evolution even if both systems satisfy the same condition (1). Here the overbar denotes quantities for the system $\bar{A}$. The inconsistency for nondegenerate Hamiltonians was explained by the resonant transitions between the energy levels in $\bar{H}(t)$ [8].

Here we consider general Hamiltonians with possible degeneracy and show that the unbounded path of the second system $\bar{A}$ violates the adiabatic approximation. It can be shown that the eigenstates of the system $\bar{A}$ are expressed by the first system A as

$$|\bar{n}_j^t\rangle = U^\dagger(t)|n_j^t\rangle, \tag{21}$$

with the eigenenergies $\bar{E}_n(t) = -E_n(t)$. For the system A with a bounded path, the geometric function $G_{n,m}^{p,q}(\vartheta)$ evolves finitely along the path. In Appendix C, we obtain

$$\bar{G}_{n,m}^{p,q}(\vartheta) = \bar{F}_{n,m}^*(\vartheta)G_{n,m}^{p,q}(\vartheta), \tag{22}$$

which contains the fast oscillating factors $\bar{F}_{n,m}^*(\vartheta) = e^{i\int_0^t [E_n - E_m]dt'}$. Therefore in the adiabatic limit, the change of the geometric function $\bar{G}_{n,m}^{p,q}(\vartheta)$ is not finite and the path of $\bar{A}$ is not bounded. The nonadiabatic evolution

$$\bar{U}_{\text{Dia}}(t) = \mathcal{P}\exp\left[i\int_{\vartheta_0}^{\vartheta}\sum_{n\neq m;p,q}G_{n,m}^{p,q}(\vartheta')d\vartheta'\right] \tag{23}$$

becomes purely geometric and the effect of nonadiabatic evolution $\bar{U}_{\text{Dia}}(t)$ of the system $\bar{A}$ does not vanish for general paths. Therefore the condition (1) does not grantee finite eigenpaths and is not sufficient.

It was claimed that the condition (1) is necessary when there is no energy degeneracy or crossings [16]. 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 $G_{n,m}^{p,q}(\vartheta)$ should be slowly varying compared with $F_{n,m}(\vartheta)$.

VI. CONCLUSIONS AND DISCUSSIONS

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. An 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 shows that the quantitative condition Eq. (1) is neither necessary nor sufficient. A necessary and sufficient condition for adiabatic evolution has been provided.

Note that we can achieve $U_{\text{adia}}(t)$ by using the Hamiltonian $H'(t) = i\dot{U}_{\text{adia}}(t)U_{\text{adia}}^\dagger(t)$, a scheme called transitionless or counterdiabatic quantum driving [40–43]. Since generally $|n_j^t\rangle$ is not the eigenstate of the driving Hamiltonian $H'(t)$, this driving does not follow the adiabatic evolution.

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APPENDIX A: GAUGE INVARIANCE

Consider the gauge transformation

$$|n_j^t\rangle \rightarrow |\tilde{n}_j^t\rangle = W_t|n_j^t\rangle, \tag{A1}$$

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

$$\langle m_p^t|W_t|n_q^t\rangle = 0, \text{ if } m\neq n. \tag{A2}$$

An example of this transformation is the phase shifts $W_t = \sum_{n,j}\exp(i\phi_{n,j}^t)|n_j^t\rangle\langle n_j^t|$ of the eigenstates. The property Eq. (A2) leads to

$$\left[\sum_j |n_j^t\rangle\langle n_j^t|, W_t\right] = 0, \tag{A3}$$

which can be verified by using Eq. (A2) and inserting the identity operator $I = \sum_{m,k}|m_k^t\rangle\langle m_k^t|$ into the commutator:

$$\sum_j |n_j^t\rangle\langle n_j^t|W_t\sum_{m,k}|m_k^t\rangle\langle m_k^t| - \sum_{m,k}|m_k^t\rangle\langle m_k^t|W_t\sum_j|n_j^t\rangle\langle n_j^t| = 0. \tag{A4}$$

Using Eq. (A3), the system Hamiltonian

$$\tilde{H}(t) = \sum_{n,j}E_n(t)|\tilde{n}_j^t\rangle\langle\tilde{n}_j^t| = \sum_n E_n W_t\sum_j|n_j^t\rangle\langle n_j^t|W_t^\dagger, \tag{A5}$$

$$= \sum_{n,j}E_n(t)|n_j^t\rangle\langle n_j^t| = H(t), \tag{A6}$$

is gauge invariant under the transformation of W_t.

1. Gauge invariance of $U_{\text{Dyn}}(t)$

Using Eq. (A3), the dynamic phase operator

$$\tilde{U}_{\text{Dyn}}(t) = \sum_{n,}e^{-i\int_0^t E_n(\tau)d\tau}\sum_j|\tilde{n}_j^t\rangle\langle\tilde{n}_j^t|, \tag{A7}$$

$$= \sum_n e^{-i\int_0^t E_n(\tau)d\tau}\sum_j W_t|n_j^t\rangle\langle n_j^t|W_t^\dagger, \tag{A8}$$

$$= \sum_n e^{-i\int_0^t E_n(\tau)d\tau}\sum_j|n_j^t\rangle\langle n_j^t| = U_{\text{Dyn}}(t), \tag{A9}$$

is gauge invariant.

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

We first find the Hamiltonian $H_W(t) = i\dot{U}_W(t)U_W^\dagger(t)$ of the propagator

$$U_W(t) \equiv \left(\sum_{n,p}|n_p^0\rangle\langle n_p^t|\right)\left(\sum_{m,q}|\tilde{m}_q^t\rangle\langle\tilde{m}_q^0|\right), \tag{A10}$$

$$= \sum_{n,p,q}|n_p^0\rangle\langle n_p^t|W_t|n_q^t\rangle\langle n_q^0|W_0^\dagger, \tag{A11}$$

where we have used Eq. (A2). We have $U_W(0)=I$ and $U_W(t)=\mathcal{T}e^{-i\int_0^t H_W(s)ds}$. Using Eqs. (A2) and (A3), we obtain

$$H_W(t)=i\sum_{n,p,q}|n_p^0\rangle\langle\dot{n}_p^t|n_q^t\rangle\langle n_q^0|+i\sum_{n,p,q}|n_p^0\rangle\langle n_p^t|\dot{W}_tW_t^\dagger|n_q^t\rangle\langle n_q^0|$$
$$+i\sum_{n,p,q,j}|n_p^0\rangle\langle n_p^t|W_t|\dot{n}_q^t\rangle\langle n_q^t|W_t^\dagger|n_j^t\rangle\langle n_j^0|. \quad \text{(A12)}$$

The geometric phase factor

$$\tilde{U}_{\mathrm{Geo}}(t)=\tilde{U}_{\mathrm{G1}}(t)\tilde{U}_{\mathrm{G2}}(t), \quad \text{(A13)}$$

where

$$\tilde{U}_{\mathrm{G1}}(t)=\sum_{n,j}|\tilde{n}_j^t\rangle\langle\tilde{n}_j^0|=W_t\sum_{n,j}|n_j^t\rangle\langle n_j^0|W_0^\dagger, \quad \text{(A14)}$$
$$=U_{\mathrm{G1}}(t)U_W(t), \quad \text{(A15)}$$

and

$$\tilde{U}_{\mathrm{G2}}(t)=\mathcal{T}\exp\left[-\int_0^t\sum_{n,p,q}|\tilde{n}_p^0\rangle\langle\tilde{n}_p^{t'}|\dot{\tilde{n}}_q^{t'}\rangle\langle\tilde{n}_q^0|dt'\right]. \quad \text{(A16)}$$

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

$$\tilde{U}_{\mathrm{G2}}(t)=U_W^\dagger(t)\mathcal{T}\exp\left[-i\int_0^t H_{W\mathrm{G2}}(t')dt'\right], \quad \text{(A17)}$$

where the Hamiltonian

$$H_{W\mathrm{G2}}(t)\equiv -iU_W(t)\sum_{n,p,q}|\tilde{n}_p^0\rangle\langle\tilde{n}_p^{t'}|\dot{\tilde{n}}_q^{t'}\rangle\langle\tilde{n}_q^0|U_W^\dagger(t)+H_W(t). \quad \text{(A18)}$$

Using Eqs. (A2) and (A3), we obtain

$$H_{W\mathrm{G2}}(t)=-i\sum_{n,p,q}|n_p^0\rangle\langle n_p^t|\dot{W}_tW_t^\dagger|n_q^t\rangle\langle n_q^0|+H_W(t)$$
$$-i\sum_{n,p,q,j}|n_p^0\rangle\langle n_p^t|W_t|\dot{n}_q^t\rangle\langle n_q^t|W_t^\dagger|n_j^t\rangle\langle n_j^0|. \quad \text{(A19)}$$

Substituting Eq. (A12) into Eq. (A19), we have

$$H_{W\mathrm{G2}}(t)=i\sum_{n,p,q}|n_p^0\rangle\langle\dot{n}_p^t|n_q^t\rangle\langle n_q^0|=H_{\mathrm{G2}}(t). \quad \text{(A20)}$$

From Eqs. (A13), (A15), (A17), and (A20), we can see that

$$\tilde{U}_{\mathrm{Geo}}(t)=U_{\mathrm{G1}}(t)U_{\mathrm{G2}}(t)=U_{\mathrm{Geo}}(t) \quad \text{(A21)}$$

is gauge invariant.

3. Gauge invariance of $U_{\mathrm{Dia}}(t)$

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

$$\sum_{p,q}|n_p^t\rangle\langle n_p^t|\dot{m}_q^t\rangle\langle m_q^t|,\ \text{for } n\neq m, \quad \text{(A22)}$$

is gauge invariant. For $n\neq m$,

$$\sum_{p,q}|\tilde{n}_p^t\rangle\langle\tilde{n}_p^t|\dot{\tilde{m}}_q^t\rangle\langle\tilde{m}_q^t|$$
$$=\sum_{p,q}W_t|n_p^t\rangle\left(\langle n_p^t|W_t^\dagger\dot{W}_t|m_q^t\rangle+\langle n_p^t|\dot{m}_q^t\rangle\right)\langle m_q^t|W_t^\dagger. \quad \text{(A23)}$$

Using Eq. (A3), we have

$$\sum_{p,q}|\tilde{n}_p^t\rangle\langle\tilde{n}_p^t|\dot{\tilde{m}}_q^t\rangle\langle\tilde{m}_q^t|=\sum_{p,q}|n_p^t\rangle\langle n_p^t|\dot{W}_t|m_q^t\rangle\langle m_q^t|W_t^\dagger$$
$$+\sum_{p,q}|n_p^t\rangle\langle n_p^t|W_t|\dot{m}_q^t\rangle\langle m_q^t|W_t^\dagger. \quad \text{(A24)}$$

The time derivative of Eq. (A2) gives

$$\langle n_p^t|\dot{W}_t|m_q^t\rangle=-\langle\dot{n}_p^t|W_t|m_q^t\rangle-\langle n_p^t|W_t|\dot{m}_q^t\rangle,\ \text{for } n\neq m. \quad \text{(A25)}$$

By substitution of Eq. (A25) into Eq. (A24), we get

$$\sum_{p,q}|\tilde{n}_p^t\rangle\langle\tilde{n}_p^t|\dot{\tilde{m}}_q^t\rangle\langle\tilde{m}_q^t|=-\sum_{p,q}|n_p^t\rangle\langle\dot{n}_p^t|W_t|m_q^t\rangle\langle m_q^t|W_t^\dagger. \quad \text{(A26)}$$

Using Eq. (A3) and $\frac{d}{dt}(\langle n_p^t|m_q^t\rangle)=\langle\dot{n}_p^t|m_q^t\rangle+\langle n_p^t|\dot{m}_q^t\rangle=0$, we obtain for $n\neq m$,

$$\sum_{p,q}|\tilde{n}_p^t\rangle\langle\tilde{n}_p^t|\dot{\tilde{m}}_q^t\rangle\langle\tilde{m}_q^t|=\sum_{p,q}|n_p^t\rangle\langle n_p^t|\dot{m}_q^t\rangle\langle m_q^t|. \quad \text{(A27)}$$

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

APPENDIX B: THE PROOFS OF NECESSITY AND SUFFICIENCY

1. Sufficiency

For simplicity, we define $F_\mu\equiv F_{n,m}$ and $G_\mu\equiv\sum_{p,q}G_{n,m}^{p,q}$ in $U_{\mathrm{Dia}}(t)$ and write it as $U_{\mathrm{Dia}}(\vartheta)\equiv U_{\mathrm{Dia}}(t)=\mathcal{P}\exp[i\int_{\vartheta_0}^{\vartheta}\sum_\mu F_\mu(\vartheta')G_\mu(\vartheta')d\vartheta']$ by using μ to indicate the summation over $n\neq m$. The nonadiabatic deviation Eq. (13) reads

$$D_{\mathrm{Dia}}(t)=i\int_{\vartheta_0}^{\vartheta}\sum_\mu F_\mu G_\mu U_{\mathrm{Dia}}d\vartheta'. \quad \text{(B1)}$$

We use a partition for the interval $[\vartheta_0,\vartheta]$ by $N-1$ points ϑ_j, such that $\vartheta_0<\vartheta_1<\vartheta_2<\cdots<\vartheta_{N-1}<\vartheta\equiv\vartheta_N$ with the interval

$$\eta_{\min}\leqslant\vartheta_{j+1}-\vartheta_j\leqslant\eta, \quad \text{(B2)}$$

for all $j=0,1,\ldots,N-1$. Let

$$g_{\mathrm{tot}}\equiv\sum_\mu g_\mu, \quad \text{(B3)}$$

with the least upper bound of the unitarily invariant norm

$$g_\mu\equiv\sup_{\vartheta'\in[\vartheta_0,\vartheta]}||G_\mu(\vartheta')||. \quad \text{(B4)}$$

The change of $G_\mu(\vartheta')$ is continuous, with a finite time derivative for $\vartheta'\in[\vartheta_0,\vartheta]$, and we define

$$w_{\mathrm{tot}}\equiv\sum_\mu w_\mu, \quad \text{(B5a)}$$

$$w_\mu\equiv\sup_{\vartheta'\in[\vartheta_0,\vartheta]}\left\|\frac{d}{d\vartheta'}G_\mu(\vartheta')\right\|. \quad \text{(B5b)}$$

Any bounded operator $A(\vartheta')$ has an associate step function $\overline{A}(\vartheta') = A(\vartheta_j)$ when $\vartheta' \in [\vartheta_j,\vartheta_{j+1})$. For $\vartheta' \in [\vartheta_j,\vartheta_{j+1})$, the difference

$$\|G_\mu(\vartheta') - \overline{G}_\mu(\vartheta')\| = \|G_\mu(\vartheta') - G_\mu(\vartheta_j)\|, \tag{B6}$$

$$= \left\| \int_{\vartheta_j}^{\vartheta'} \frac{d}{d\theta} G_\mu(\theta) d\theta \right\|, \tag{B7}$$

$$\leqslant (\vartheta' - \vartheta_j) w_\mu, \tag{B8}$$

$$< \eta w_\mu. \tag{B9}$$

For $\vartheta' \in [\vartheta_j,\vartheta_{j+1})$, the difference

$$\|U_{\text{Dia}}(\vartheta') - \overline{U}_{\text{Dia}}(\vartheta')\| = \|U_{\text{Dia}}(\vartheta') - U_{\text{Dia}}(\vartheta_j)\|, \tag{B10}$$

$$= \left\| \int_{\vartheta_j}^{\vartheta'} \frac{d}{d\theta} U_{\text{Dia}}(\theta) d\theta \right\|, \tag{B11}$$

$$\leqslant \sum_\mu \left\| \int_{\vartheta_j}^{\vartheta'} F_\mu(\theta) G_\mu(\theta) U_{\text{Dia}}(\theta) d\theta \right\|, \tag{B12}$$

$$\leqslant (\vartheta' - \vartheta_j) g_{\text{tot}}, \tag{B13}$$

$$< \eta g_{\text{tot}}, \tag{B14}$$

where we have used $|F_\mu(\vartheta')| = 1$. From Eqs. (B9) and (B14), we have the norm

$$\|G_\mu U_{\text{Dia}} - \overline{G}_\mu \overline{U}_{\text{Dia}}\| = \|G_\mu(U_{\text{Dia}} - \overline{U}_{\text{Dia}}) + (G_\mu - \overline{G}_\mu)\overline{U}_{\text{Dia}}\|, \\ < \eta(g_\mu g_{\text{tot}} + w_\mu). \tag{B15}$$

We write the deviation Eq. (B1) as $D_{\text{Dia}}(\vartheta) \equiv D_{\text{Dia}}^{(1)} + D_{\text{Dia}}^{(2)}$, where the error caused by the partition

$$D_{\text{Dia}}^{(1)} = i \int_{\vartheta_0}^{\vartheta} \sum_\mu F_\mu [G_\mu U_{\text{Dia}} - \overline{G}_\mu \overline{U}_{\text{Dia}}] d\vartheta' \tag{B16}$$

has the norm

$$\left\| D_{\text{Dia}}^{(1)} \right\| < \eta\left(g_{\text{tot}}^2 + w_{\text{tot}}\right)(\vartheta - \vartheta_0), \tag{B17}$$

and

$$D_{\text{Dia}}^{(2)} = i \int_{\vartheta_0}^{\vartheta} \sum_\mu F_\mu \overline{G}_\mu \overline{U}_{\text{Dia}} d\vartheta'. \tag{B18}$$

Under the averaging condition 14

$$\left| \int_{\vartheta_0}^{\vartheta'} F_{n,m}(\vartheta') d\vartheta' \right| < \xi_{\text{avg}}, \text{ for } \vartheta' \in [\vartheta_0,\vartheta] \text{ and } n \neq m, \tag{B19}$$

we have the norm

$$\left\| D_{\text{Dia}}^{(2)} \right\| = \left\| \sum_\mu \sum_j \overline{G}_\mu \overline{U}_{\text{Dia}} \int_{\vartheta_j}^{\vartheta_{j+1}} F_\mu d\vartheta \right\|, \tag{B20}$$

$$\leqslant \sum_\mu \sum_j \left\| \overline{G}_\mu \overline{U}_{\text{Dia}} \int_{\vartheta_j}^{\vartheta_{j+1}} F_\mu d\vartheta \right\|, \tag{B21}$$

$$< \xi_{\text{avg}} N g_{\text{tot}}. \tag{B22}$$

The nonadiabatic deviation

$$\|D_{\text{Dia}}\| \leqslant \left\| D_{\text{Dia}}^{(1)} \right\| + \left\| D_{\text{Dia}}^{(2)} \right\|. \tag{B23}$$

For sufficiently small $\xi_{\text{avg}} \ll (\vartheta - \vartheta_0)^2 (g_{\text{tot}}^2 + w_{\text{tot}})/g_{\text{tot}}$, we choose the partition with $\eta \approx \eta_{\min} \approx \sqrt{\xi_{\text{avg}} g_{\text{tot}}/(g_{\text{tot}}^2 + w_{\text{tot}})} \ll (\vartheta - \vartheta_0)$. With this partition, we obtain $\|D_{\text{Dia}}^{(1)}\| \approx \|D_{\text{Dia}}^{(2)}\|$ and the upper bound Eq. (17).

We may choose other partitions to obtain other bounds. For example, for $\xi_{\text{avg}} \ll 1$, we choose $\eta_{\min} = \eta = (\vartheta - \vartheta_0)/N$ with N the smallest integer greater than $1/\sqrt{\xi_{\text{avg}}}$. We have for this partition

$$\eta < \sqrt{\xi_{\text{avg}}}(\vartheta - \vartheta_0), \tag{B24}$$

$$N \leqslant (1/\sqrt{\xi_{\text{avg}}}) + 1. \tag{B25}$$

Using Eqs. (B17), (B22), (B23), (B24), and (B25), we obtain the upper bound Eq. (18) for $\xi_{\text{avg}} \ll 1$. Therefore

$$\lim_{\xi_{\text{avg}} \to 0} U_{\text{Dia}}(t) = I, \tag{B26}$$

and the averaging condition 14 with $\xi_{\text{avg}} \ll 1$ is sufficient.

Derivation of Eq. (16)

For the partition that the average

$$\int_{\vartheta_j}^{\vartheta_{j+1}} F_{n,m}(\vartheta') d\vartheta' = 0, \quad \text{for } n \neq m, \tag{B27}$$

vanishes for all the intervals $j = 0,1,\ldots,N-1$, we have $D_{\text{Dia}}^{(2)} = 0$, $\xi_{\text{avg}} = \eta$, and

$$\|D_{\text{Dia}}(t)\| < \xi_{\text{avg}}\left(g_{\text{tot}}^2 + w_{\text{tot}}\right)(\vartheta - \vartheta_0), \tag{B28}$$

which is simpler than the bounds Eqs. (17) and (18).

2. Necessity

A general condition for adiabatic evolution should be universal and works for all bounded paths. We choose a path that satisfies $\frac{d}{dt}|n_p^\vartheta\rangle = 0$ if $n_p \neq N,M$ and the states $|N^\vartheta\rangle = \cos(b\vartheta)|N^{\vartheta_0}\rangle - i\sin(b\vartheta)|M^{\vartheta_0}\rangle$ and $|M^\vartheta\rangle = -i\sin(b\vartheta)|N^{\vartheta_0}\rangle + \cos(b\vartheta)|M^{\vartheta_0}\rangle$ with $b = O(1)$. We have $|\frac{d}{d\vartheta}N^\vartheta\rangle = -ib|M^\vartheta\rangle$, $|\frac{d}{d\vartheta}M^\vartheta\rangle = -ib|N^\vartheta\rangle$, and thus $U_{\text{G2}}(\vartheta) = I$ by using Eq. (7). The deviation from the adiabatic evolution is

$$D_{\text{Dia}}(\vartheta) = i \int_{\vartheta_0}^{\vartheta} b[F_{N,M}(\vartheta')|N^{\vartheta_0}\rangle\langle M^{\vartheta_0}| + \text{H.c.}] U_{\text{Dia}}(\vartheta') d\vartheta'. \tag{B29}$$

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

$$\int_{\vartheta_0}^{\vartheta} b\big[F_{N,M}(\vartheta')|N^{\vartheta_0}\rangle\langle M^{\vartheta_0}| + \text{H.c.}\big] d\vartheta' \\ = i D_{\text{Dia}}(\vartheta) - \int_{\vartheta_0}^{\vartheta} b\big[F_{N,M}(\vartheta')|N^{\vartheta_0}\rangle\langle M^{\vartheta_0}| + \text{H.c.}\big] D_{\text{Dia}}(\vartheta') d\vartheta'. \tag{B30}$$

For a good adiabatic approximation, the correction $\|D_{\text{Dia}}(\vartheta')\| < \epsilon$ is small for all bounded paths $\vartheta' \in [\vartheta_0,\vartheta]$.

Here ϵ is a small value. By choosing other paths with different $|N^{\vartheta_0}\rangle$ and $|M^{\vartheta_0}\rangle$ in Eq. (B30), we have for $n \neq m$,

$$\left|\int_{\vartheta_0}^{\vartheta} F_{n,m}(\vartheta')d\vartheta'\right| < \epsilon\kappa, \tag{B31}$$

with a finite κ. In the adiabatic limit

$$\lim_{\|D_{\rm Dia}\|\to 0}\left|\int_{\vartheta_0}^{\vartheta} F_{n,m}(\vartheta')d\vartheta'\right| = 0, \tag{B32}$$

for $n \neq m$.

APPENDIX C: DERIVATION OF EQ. (22)

We express the geometric function for the system $\bar{A}$ ($n \neq m$)

$$\bar{G}^{p,q}_{n,m}(\vartheta) = \bar{U}^{\dagger}_{\rm Geo}(\vartheta)\left|\bar{n}^{\vartheta}_{p}\right\rangle\left(\left\langle\bar{n}^{\vartheta}_{p}\right|i\frac{d}{d\vartheta}\left|\bar{m}^{\vartheta}_{q}\right\rangle\right)\left\langle\bar{m}^{\vartheta}_{q}\right|\bar{U}_{\rm Geo}(\vartheta) \tag{C1}$$

by the time parameter t as

$$\bar{G}^{p,q}_{n,m}(t) = i\bar{U}^{\dagger}_{\rm Geo}(t)\left|\bar{n}^{t}_{p}\right\rangle\left\langle\bar{n}^{t}_{p}\right|\dot{\bar{m}}^{t}_{q}\right\rangle\left\langle\bar{m}^{t}_{q}\right|\bar{U}_{\rm Geo}(t)\frac{dt}{d\vartheta}. \tag{C2}$$

By using $\bar{U}_{\rm Geo}(t) = \bar{U}_{\rm G1}(t)\bar{U}_{\rm G2}(t)$, $\bar{U}_{\rm G1}(t) = \sum_{n,j}|\bar{n}^{t}_{j}\rangle\langle\bar{n}^{0}_{j}|$, and $\bar{U}_{\rm G2}(t) = \mathcal{T}\exp[-i\int_0^t \bar{H}_{\rm G2}(t')dt']$ with $\bar{H}_{\rm G2}(t) = -i\sum_{n,p,q}|\bar{n}^{0}_{p}\rangle\langle\bar{n}^{t}_{p}|\dot{\bar{n}}^{t}_{q}\rangle\langle\bar{n}^{0}_{q}|$ for the system $\bar{A}$, we get

$$\bar{G}^{p,q}_{n,m}(t) = i\bar{U}^{\dagger}_{\rm G2}(t)\left|\bar{n}^{0}_{p}\right\rangle\left\langle\bar{n}^{t}_{p}\right|\dot{\bar{m}}^{t}_{q}\right\rangle\left\langle\bar{m}^{0}_{q}\right|\bar{U}_{\rm G2}(t)\frac{dt}{d\vartheta}. \tag{C3}$$

To relate the expressions to the quantities of system A, we use Eq. (21) to obtain

$$\left|\bar{n}^{0}_{j}\right\rangle = \left|n^{0}_{j}\right\rangle, \tag{C4}$$

and

$$\left|\dot{\bar{m}}^{t}_{q}\right\rangle = \left[\frac{d}{dt}U^{\dagger}(t)\right]\left|m^{t}_{q}\right\rangle + U^{\dagger}(t)\left|\dot{m}^{t}_{q}\right\rangle \tag{C5}$$

$$= iU^{\dagger}(t)H(t)\left|m^{t}_{q}\right\rangle + U^{\dagger}(t)\left|\dot{m}^{t}_{q}\right\rangle \tag{C6}$$

$$= iE_m(t)U^{\dagger}(t)\left|m^{t}_{q}\right\rangle + U^{\dagger}(t)\left|\dot{m}^{t}_{q}\right\rangle. \tag{C7}$$

By using Eqs. (21), (C4) and (C7), Eq. (C3) becomes

$$\bar{G}^{p,q}_{n,m}(t) = i\bar{U}^{\dagger}_{\rm G2}(t)\left|n^{0}_{p}\right\rangle\left\langle n^{t}_{p}\right|\dot{m}^{t}_{q}\right\rangle\left\langle m^{0}_{q}\right|\bar{U}_{\rm G2}(t)\frac{dt}{d\vartheta}, \tag{C8}$$

for $n \neq m$. Similarly,

$$\bar{H}_{\rm G2}(t) = -i\sum_{n,p,q}\left|n^{0}_{p}\right\rangle\left\langle n^{t}_{p}\right|\dot{n}^{t}_{q}\right\rangle\left\langle n^{0}_{q}\right| + \sum_{n,j}E_n(t)\left|n^{0}_{j}\right\rangle\left\langle n^{0}_{j}\right|. \tag{C9}$$

and hence

$$\bar{U}_{\rm G2}(t) = \sum_{n,j}e^{-i\int_0^t E_n dt'}\left|n^{0}_{j}\right\rangle\left\langle n^{0}_{j}\right|U_{\rm G2}(t). \tag{C10}$$

Substituting Eq. (C10) into (C8) and using the geometric function for the system A [cf. Eq. (C3)],

$$G^{p,q}_{n,m}(t) = iU^{\dagger}_{\rm G2}(t)\left|n^{0}_{p}\right\rangle\left\langle n^{t}_{p}\right|\dot{m}^{t}_{q}\right\rangle\left\langle m^{0}_{q}\right|U_{\rm G2}(t)\frac{dt}{d\vartheta}, \tag{C11}$$

we obtain

$$\bar{G}^{p,q}_{n,m}(t) = e^{i\int_0^t(E_n-E_m)dt'}G^{p,q}_{n,m}(t) \tag{C12}$$

$$= F_{n,m}(t)G^{p,q}_{n,m}(t) = \bar{F}^{*}_{n,m}(t)G^{p,q}_{n,m}(t), \tag{C13}$$

which is Eq. (22).

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