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Singularities of Berry connections inhibit the accuracy of the adiabatic approximation

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Abstract

Adiabatic approximation for quantum evolution is investigated addressing its dependence on the Berry connections that are functions of a slowly-varying parameter R. When the Berry connections have singularities of type $1/R^{\sigma}$ with $\sigma < 1$, the adiabatic fidelity converges to unit according to a power-law; When the singularity index σ becomes larger than one, adiabatic approximation breaks down. Two-level models are used to substantiate our theory.

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The adiabatic theorem, as a fundamental theorem in quantum mechanics, plays a crucial role in our understanding and manipulation of microscopic world [1]. Recent years witness its growing importance in the quantum control of the newly formed matter—Bose–Einstein condensate [2] and adiabatic quantum computation [3].

However, applicability and completeness of the theorem need further study. A warning that the application of the theorem may lead to inconsistency was given recently by Marzlin and Sanders [4]. A subsequent work [5] explicitly formulated a 'counterexample' with a two-level model illustrating that the adiabatic condition widely recognized and commonly used is not sufficient for guaranteeing the adiabatic approximation. In the present Letter, we point out that the above confusions can be avoided when formulating the quantum adiabatic evolution within a parameter domain rather than the time domain. Within this new formulation, we investigate the fidelity of the adiabatic approximation quantitatively. We find that the properties of the Berry connections dramatically affect the behavior of the adiabatic fidelity and conclude that the singularities of the Berry connections inhibit the accuracy of the adiabatic approximation. Because the estimation on the upper bound of adiabatic fidelity is essential for the search time [6,7], our findings have important meaning in the practical adiabatic quantum search algorithms.

The system we consider is a Hamiltonian containing slowly-varying dimensionless parameters $\mathbf{R}(t)$ belonging to a given regime $[\mathbf{R}_0, \mathbf{R}_1]$, say, $H(\mathbf{R}(t))$. Initially we have a state, for example the ground state $|E_0(\mathbf{R}(t_0))\rangle$ with energy $E_0(\mathbf{R}(t_0))$. The wave function $|\Psi(t)\rangle$ fulfills the usual Schrödinger equation, i.e., $i\frac{d\Psi}{dt} = H(\mathbf{R}(t))\Psi(t)$, with $\hbar = 1$. The above problem has a well-known adiabatic approximate solution:

$$|\Psi_{\mathrm{ad}}\rangle = e^{-i\int^t E_0\,dt} e^{i\gamma_0} \big|E_0\big(\mathbf{R}(t)\big)\big\rangle \tag{1}$$

with $\gamma_0 = i\int^t dt\langle E_0|\dot{E}_0\rangle$, the geometric phase term [8,9]. The above equation is the explicit formulation of the adiabatic theorem stating that the initial non-degenerate ground state will remain to be the instantaneous ground state and evolve only in its phase, given by the time integral of the eigenenergy (known as the dynamical phase) and a quantity independent of the time duration (known as the geometric phase).

The problems is, how close is the above adiabatic approximate solution to the actual solution $|\Psi(t)\rangle$. To clarify the above question and formulate it quantitatively, we introduce two phys-

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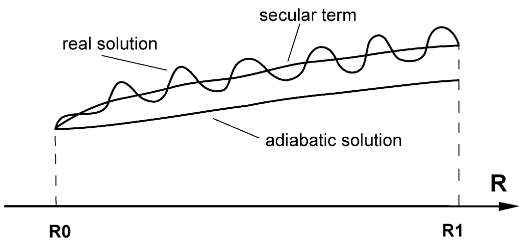

Fig. 1. Schematic illustration of the quantum adiabatic evolution formulated in parameter condition, see text for detailed description.

ical quantities, namely the adiabatic parameter and the adiabatic fidelity.

The dimensionless adiabatic parameter is defined as the ratio between the change rate of the external parameters and the internal characteristic time scale of the quantum system (i.e. the Rabi frequency $|E_m - E_n|$), used to measure how slow the external parameter changes with time:

$$\epsilon = \max \frac{|\dot{\mathbf{R}}|}{|E_n(\mathbf{R}) - E_m(\mathbf{R})|}, \quad m \neq n. \tag{2}$$

$\epsilon \to 0$ corresponds to adiabatic limit.

Adiabatic fidelity is introduced to measure how close the adiabatic solution is to the actual one, $F_{ad} = |\langle \Psi(t)|\Psi_{ad}\rangle|^2$. The convergence of the adiabatic fidelity to unit uniformly in the range $\mathbf{R} \in [\mathbf{R}_0, \mathbf{R}_1]$ in the adiabatic limit ($\epsilon \to 0$), indicates the validity of the adiabatic approximation. Evaluating fidelity function will give an estimation on how good the adiabatic approximation is.

In Fig. 1 we schematically illustrate the physical process we describe above. Our main result is that the distance between the adiabatic solution and actual one consists in two parts: the fast oscillation term and the secular term. The time scale of the oscillation is the Rabi period, its amplitude is proportional to the square of the adiabatic parameter. The amplitude of the secular term is exponentially small ($\sim \exp -1/\epsilon$) supposing that the Berry connections of the system are regular, and turn to follow a power-law ($\sim \epsilon^x$, $x < 2$) if the Berry connections have singularity or the external parameters vary in time nonlinearly.

We start our statement with writing the wavefunction as a superposition of the instantaneous eigenstates,

$$\big|\Psi(t)\big\rangle = \sum_n C_n(t) e^{-i\int^t dt (E_n - i\langle E_n(R)|\dot{E}_n(R)\rangle)} \big|E_n\big(\mathbf{R}(t)\big)\big\rangle,$$

and suppose initial state is the ground state, i.e., $C_0(t=0) = 1$, $C_n(t=0) = 0 (n \neq 0)$. Then the adiabatic approximate solution takes the form of Eq. (1) and the adiabatic fidelity $F_{ad} = |\langle \Psi(t)|\Psi_{ad}\rangle|^2 = |C_0|^2 \sim 1 - |\Delta C_n|^2 (n \neq 0)$. To evaluate the adiabatic fidelity we need quantitatively evaluate the change of the coefficients C_n with respect to time.

Substituting the above solution into Schrödinger equation, we have the following differential equation for the coefficients:

$$\frac{d}{dt} C_n = i \sum_{m \neq n} e^{i\int^t ((E_n - \alpha_{nn}\dot{\mathbf{R}}) - (E_m - \alpha_{mm}\dot{\mathbf{R}}))\, dt} \alpha_{nm}(\mathbf{R}) \frac{d\mathbf{R}}{dt} C_m \tag{3}$$

where $\alpha_{nm}(\mathbf{R})$ is the Berry connection. Both off-diagonal and diagonal Berry connections have clear physical meaning and important applications [10]. We first suppose these Berry connections and the gradient of instantaneous eigenenergy are not singular (NS) as the functions of the external parameters, i.e.,

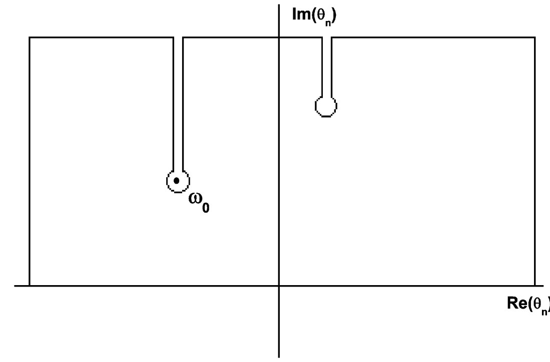

Fig. 2. The integral path and the singular points in the complex plane.

$$\alpha_{nm}(\mathbf{R}) = \langle E_n | i\nabla_{\mathbf{R}} | E_m\rangle; \qquad \beta_n(\mathbf{R}) = \nabla_{\mathbf{R}} E_n(\mathbf{R}), \quad \text{NS}. \tag{4}$$

The right-hand side of Eq. (3) contains unknown C_m, to the first order of approximation, we take $C_0 = 1$ and $C_m = 0, m \neq 0$ in the right-hand side of Eq. (3). Then, Eq. (3) shows that the change consists in two parts: the fast oscillation term and the secular term. The time scale of the oscillation is the Rabi period, its amplitude is proportional to the adiabatic parameter under the condition that the Berry connections are regular with limitation. Whereas the secular term maybe is exponential small of form $e^{-1/\epsilon}$ or a power-law depending on the Berry connections as will be shown in following.

Let us denote $\theta_n = \int^t (E_n - E_0)\, dt$, and then the upper bound of the increment on the coefficients ($n \neq 0$) can be evaluated as follows,

$$\Delta C_n \sim \int_{\theta_n(\mathbf{R}_0)}^{\theta_n(\mathbf{R}_1)} \frac{e^{i\theta_n}}{E_n - E_0} \alpha_{n0} \dot{\mathbf{R}}\, d\theta_n \tag{5}$$

$$= \int_{-\infty}^{\infty} \ldots d\theta_n - \left(\int_{-\infty}^{\theta_n(\mathbf{R}_0)} + \int_{\theta_n(\mathbf{R}_1)}^{\infty} \right) \ldots d\theta_n \tag{6}$$

where we set that in the right-hand side of Eq. (3) the coefficients $C_m \sim 0$ for $m \neq 0$, and $C_0 \sim 1$ since we want to estimate the upper bound of the adiabatic approximation. For simplicity and without loosing generality, in following deductions we regard the slowly-varying parameter as a scalar quantity, and assume that $\frac{dR}{dt} \sim \epsilon g(R)$ with the function $g(R)$ being regular with limitation.

The first term on the right-hand side is an infinite integral; it can be estimated by extending the integral to the upper half-plane with a closed path at infinity as shown in Fig. 2. The integral along the upper horizontal path of the closure is zero because $e^{-\operatorname{Im}\theta_n} \to 0$ there. On the other hand, the integrals along the vertical paths also vanish because of the fast oscillation of the function $e^{-i\operatorname{Re}\theta_n}$ at infinity [11]. Hence, the main contribution to the first term comes from the pole point, $\theta_n^c = \int^{t_c} (E_n - E_0)\, dt \sim \frac{1}{\epsilon} \int^{R_c} (E_n - E_0)/g(R)\, dR$, determined by the equation $E_n(\theta^c{}_n) - E_0(\theta^c{}_n) = 0$. Under the assumption of nondegeneracy, the solutions of the above equation are complex with nonzero imaginary parts. Let ω_0 be the singularity closest to real axis, i.e., the one with the smallest (positive) imaginary part (see Fig. 2). Then, the first term is approximately bounded by $\exp(-\operatorname{Im}\omega_0) \sim e^{-\frac{1}{\epsilon}|\int^{|\operatorname{Im}(R_c)|}(E_n-E_0)/g(R)\,dR|}$, which contributes to the secular term with an exponential small quantity in the adiabatic limit.

The second term on the right-hand side depends on the boundary condition. If the boundary values are large enough the terms in parentheses of Eq. (6) will be small compared to the first term. For an infinite boundary of the parameter domain as that in the well-known Landau–Zener model [12], i.e., $R_{1,0} \to \pm\infty$, the integral vanishes because $\theta_n(R_{1,0}) = \pm\infty$; for a finite boundary condition, it gives a quantity of order ϵ.

Now, we consider the situation that Berry connection has singularity of form $\frac{1}{R^\sigma}$ at $R(t^*) = 0$. We then evaluate the above integral in the neighborhood domain $[-\Delta t + t^*, \Delta t + t^*]$ of the singular point, integral over other regimes is regular and contributes a quantity of order ϵ. Near the singular point,

$$|\Delta C_n| \sim \left| \int_{-\Delta t+t^*}^{\Delta t+t^*} e^{i\int^t (E_n-E_0)\,dt} \alpha_{n0}(R)\dot{R}\,dt \right| = \left| \int_{\Delta R_-}^{\Delta R_+} e^{i\int^t (E_n-E_0)\,dt} \alpha_{n0}(R)\,dR \right| \sim \epsilon^{(1-\sigma)}. \tag{7}$$

In the above deduction we take advantage of the relation $\Delta R_\pm = R(\pm\Delta t + t^*) \propto \pm\epsilon$.

The situation is divided into two cases: $\sigma < 1$ and $\sigma \geqslant 1$. For $\sigma < 1$, this type of singularity can be removed because the integral is finite. The integral in the neighborhood domain $[-\epsilon, \epsilon]$ of the singularity contributes a quantity of order $\epsilon^{(1-\sigma)}$. We thus expect that the adiabatic fidelity approaches to unit uniformly in the $2(1-\sigma)$ power-law of the adiabatic parameter, i.e.,

$$1 - F_{\mathrm{ad}} \sim \epsilon^{2(1-\sigma)}. \tag{8}$$

For the case of $\sigma \geqslant 1$, the singularity is irremovable and the adiabatic approximation is expected to break down.

The above discussion is readily extended to the case that the slowing-varying parameters change nonlinearly with time, i.e., $R = \epsilon t^\sigma$, where σ is any positive number. The nonlinear time dependent parameter has many physical origins, for example in the molecule spin system the effective field vary in time nonlinearly [13]. Another field of broad examples is quantum optics, Rabi frequency coupling different levels (i.e., stimulated Raman adiabatic passage) has often nonlinear dependence on time [14]. Here we suppose that the Berry connections of quantum system are regular with limitation as the function of the parameter R and the level spacings are of order 1. To apply our theory, we introduce the new parameters R' and ϵ' through the expressions $\epsilon'^{1/\sigma}$ and $R' = \epsilon' t$. Then, $R = R'^\sigma$. As a function of the new parameter R', the singularity of the Berry connections is determined by $\frac{dR}{dR'} \sim 1/R'^{1-\sigma}$. Our discussions are divided into two cases: (i) $\sigma > 1$ and (ii) $\sigma < 1$. In the former case, the Berry connections as functions of the new parameter are regular, so the adiabatic fidelity is determined by the short-term oscillation and is expected to converge to one in a power-law of ϵ'^2. Then we have

$$1 - F_{\mathrm{ad}} \sim \epsilon^{\frac{2}{\sigma}}. \tag{9}$$

In the latter case, the Berry connections as functions of the new parameter are singular, of the type $1/R'^{1-\sigma}$. Fortunately, this singularity is removable, it gives an upper bound of the adiabatic Fidelity as $\epsilon'^{2\sigma}$, i.e.,

$$1 - F_{\mathrm{ad}} \sim \epsilon^2. \tag{10}$$

Notice that in this case, the upper bound of the adiabatic fidelity is independent of the nonlinear index σ.

In following, we use two-level models to substantiate the above discussions. With a model denoted by S^a, let us consider a spin-half particle in a rotating magnetic field; its Hamiltonian reads:

$$H^a\big(R(t)\big) = -\frac{\omega_0}{2}\big(\sin\theta\cos f\big(R(t)\big)\sigma_x + \sin\theta\sin f\big(R(t)\big)\sigma_y + \cos\theta\sigma_z\big), \tag{11}$$

ω_0 is defined by the strength of the magnetic field, and σ_i $(i = x, y, z)$ are Pauli matrices. $f(R)$ is a function of slowly-varying parameter R. The above 2×2 matrix is readily diagonalized for fixed R and we then obtain its instantaneous eigenenergies $E^a_\pm = \pm\frac{\omega_0}{2}$, and instantaneous eigenvectors:

$$\big|E^a_-(R)\big\rangle = \begin{pmatrix} e^{-i\frac{f(R)}{2}}\sin\frac{\theta}{2} \\ -e^{i\frac{f(R)}{2}}\cos\frac{\theta}{2} \end{pmatrix}, \qquad \big|E^a_+(R)\big\rangle = \begin{pmatrix} e^{-i\frac{f(R)}{2}}\cos\frac{\theta}{2} \\ e^{i\frac{f(R)}{2}}\sin\frac{\theta}{2} \end{pmatrix}. \tag{12}$$

The Berry connections are derived as follows,

$$\alpha^c_{--} = \frac{1}{2}\cos\theta\frac{df}{dR}, \qquad \alpha^c_{-+} = \frac{1}{2}\sin\theta\frac{df}{dR}. \tag{13}$$

(i) We first consider the following two cases: $f(R) = \ln|R|$ and $f(R) = |R|^{1-\sigma}$ with $\sigma < 1$, respectively. Here the slowly-varying parameter is supposed to linearly change with time, i.e., $R(t) = \omega t$. ω is the rotating frequency of the magnetic field. Apparently, the Berry connection has a singularity of the form $1/R^\sigma$ at point $R = 0$. These systems are complicated and analytic solutions are not reachable. We thus make numerical simulations on the adiabatic fidelity by directly solving the Schrödinger equation with the 4th–5th Runge–Kutta adaptive step method. Our results are shown in Figs. 3 and 4. In Fig. 3, it is clearly shown that, without the singularity (left panel of Fig. 3), the distance between adiabatic solution and solution is determined by the fast oscillation, therefore gives the upper bound of square adiabatic parameter. With the singularity (right panel of Fig. 3), the upper bound is determined by the type of the singularity of the Berry connections as we discussed above. In case that the Berry connections have an irremovable singularity (i.e., $\sigma = 1$, see Fig. 4b) the adiabatic fidelity converges to 0.53 rather than one, implying the failure of adiabatic approximation. For the case of the removable singularity of the Berry

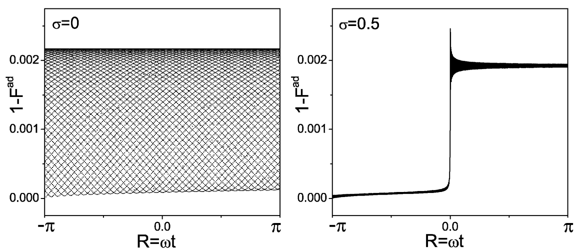

Fig. 3. Adiabatic fidelity evolves for different type of singularity.

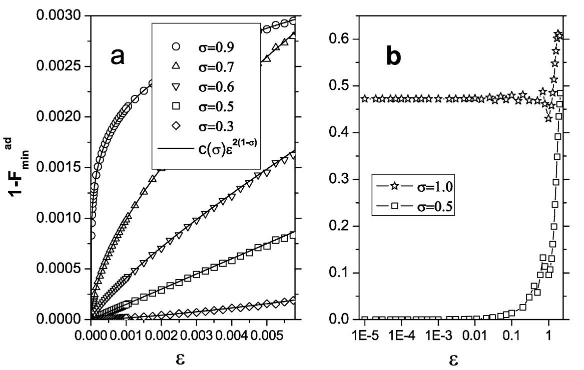

Fig. 4. Upper bound of the adiabatic fidelity in system S^c for different type of singularity. $F^{\mathrm{ad}}_{\mathrm{min}}$ is the minimum fidelity in the parameter range $\mathbf{R} \in [-2\pi, 2\pi]$.

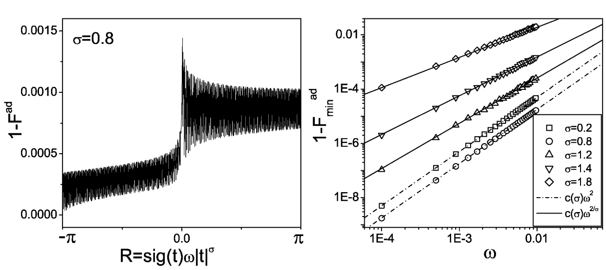

Fig. 5. Upper bound of the adiabatic fidelity for different type of the nonlinearly-varying external parameters.

connection ($\sigma < 1$) the adiabatic fidelity converges to unit in the power-law dependence of the adiabatic parameters as we expect (see Fig. 4a).

(ii) We then set $f(R) = R$ where R varies in time nonlinearly, i.e., $R = \epsilon\,\mathrm{sign}(t)|t|^\sigma$. In this case, from Fig. 5 we see that, for $\sigma > 1$, the adiabatic fidelity converges to unit in a power-law of exponent $2/\sigma$; for $\sigma < 1$, it clearly demonstrates that the exponent turns to be two, independence of the nonlinear index σ. These numerical simulations corroborate our theory.

In the above studies we discussed quantum adiabatic issue in the parameter domain. It requires that the Hamiltonian explicitly depends on time only through the slowly-varying parameter of the form $H(R(t))$. Within this formulation, the initial and the final Hamiltonians are fixed, namely, $H(R_0)$ and $H(R_1)$ are independent of the adiabatic parameter ϵ. We then can well depict how slowly the system varies in time using either $\dot{R}$ or the time duration $T = t_1 - t_0$, i.e., $\dot{R} \to 0$ or $T \to \infty$ indicates the adiabatic limit.

However, things becomes much confusing when people discuss adiabatic issue in a time domain $[t_0, t_1]$ with introducing a small parameter ϵ to describe the change rate of the system. For this case both final $H(t_1, \epsilon)$ and initial $H(t_1, \epsilon)$ depend on the parameter ϵ even though initial time t_0 and final time t_1 are fixed. Therefore it is much illegible to depict the "slowly-varying" for the system through the parameter ϵ because the distance to the target varies in the parameter ϵ.

In following we address this point with an example raised recently [5]. It is constructed from S^a for the case of $f(R) = R$, $R = \omega t$ through following relation,

$$H^{\mathrm{ce}} = -U^{a\dagger}(t) H^a(t) U^a(t) \tag{14}$$

with $U^a(t) = T \exp(\int_0^t H^a(t')\,dt')$ the time evolution operator of system S^a. Its explicit analytic expression is readily obtained [5]. After lengthy deduction, we obtain the explicit expression of the Hamiltonian $H^{\mathrm{ce}} = \frac{\omega_0}{2}\mathbf{L}(t)\cdot\sigma$, where $\mathbf{L}(t) = (\sin\theta(\omega_0^2 + 2\omega\omega_0\cos\theta\cos^2\varpi t/2 + \omega^2\cos\varpi t)/\varpi^2, \frac{\omega\sin\theta}{\varpi}\sin\varpi t, \cos\theta + \frac{2\omega\omega_0\sin\theta}{\varpi^2}\sin^2\theta\sin^2\varpi t/2)$, and $\varpi = \sqrt{\omega_0^2 + \omega^2 + 2\omega\omega_0\cos\theta}$.

It is easy to verify that $\mathbf{L}(t)$ is a unit vector, i.e., $|\mathbf{L}(t)| = 1$. The eigenvalues and eigenvectors for this system are,

$$E^{\mathrm{ce}}_{\pm} = \pm\frac{\omega_0}{2}, \qquad \left|E^{\mathrm{ce}}_{\pm}(\mathbf{L})\right\rangle = \begin{pmatrix} \sqrt{\frac{1\pm L_3}{2}}e^{-i\phi} \\ \mp\sqrt{\frac{1\mp L_3}{2}}e^{i\phi} \end{pmatrix}, \tag{15}$$

where $\phi = \frac{1}{2}\arctan(L_2/L_1)$. We then can obtain the Berry connections as follows,

$$\alpha^{\mathrm{ce}}_{--} = \left(\frac{L_2 L_3}{2(1-L_3^2)}, -\frac{L_1 L_3}{2(1-L_3^2)}, 0\right),$$
$$\alpha^{\mathrm{ce}}_{-+} = \left(-\frac{L_2}{2\sqrt{1-L_3^2}}, \frac{L_1}{2\sqrt{1-L_3^2}}, -\frac{i}{2\sqrt{1-L_3^2}}\right). \tag{16}$$

As $L_3 < 1$, the Berry connections are not singular. For $d|\mathbf{L}|/dt \sim \omega$, the adiabatic parameter of this system is $\epsilon = \omega/\omega_0$.

The controversy is that, even though in the adiabatic limit of $\epsilon \to 0$, the adiabatic fidelity calculated in the time domain $t \in [-2\pi, 2\pi]$ does not converge to unit [5]. Moreover, with changing the sign of the above Hamiltonian and re-calculating the adiabatic fidelity in the time domain $[-2\pi, 2\pi]$, we find that the adiabatic fidelity converges to unit in the adiabatic limit. The above result is rather confusing. The reason for the above controversy is that the problem is discussed in time domain rather in parameter domain.

To resolve the above controversy, we check the above system in the parameter domain. First, after transformation (14), $R = \omega t$ acted as the slowly-varying parameter in $H^a(t)$ system no longer should be chosen as the slowly-varying parameter for the new system H^{ce}, because the Hamiltonian H^{ce} depends explicitly on the time not only through R. Instead, $\mathbf{L}(t)$ can serve as the slowly-varying parameters. However, the range of the parameters keeps the same order of the adiabatic parameter (i.e., $|\mathbf{L}_1(t = t_1) - \mathbf{L}_0(t = t_0)| \sim \omega$) and tends to zero in the adiabatic limit no matter how long the evolution time $t_1 - t_0$ is. This completely counters to our picture schematically plotted in Fig. 1. Above analysis indicates that the system H_{ce} cannot be well formulated in the parameter domain, it essentially not a system that adiabatic theory can applies to. If one discuss the dynamics of this system in the time domain as shown the above, any strange things can happen.

In summary, we investigate the fidelity for quantum evolution in the parameter domain addressing the adiabatic approximation quantitatively. Within this framework, we clarify the confusion in applying quantum adiabatic theory and figure out that the singularities of Berry connections inhibit the accuracy of the adiabatic approximation. Our estimation on the adiabatic fidelity has important meaning in the practical adiabatic quantum search algorithms.

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