Experimental Study of the Validity of Quantitative Conditions in the Quantum Adiabatic Theorem

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The quantum adiabatic theorem plays an important role in quantum mechanics. However, counterexamples were produced recently, indicating that their transition probabilities do not converge as predicted by the adiabatic theorem [K. P. Marzlin *et al.*, Phys. Rev. Lett. **93**, 160408 (2004); D. M. Tong *et al.*, Phys. Rev. Lett. **95**, 110407 (2005)]. For a special class of Hamiltonians, we examine the standard criterion for adiabatic evolution experimentally and theoretically, as well as three newly suggested adiabatic conditions. We show that the standard criterion is neither sufficient nor necessary.

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In classical physics, adiabatic processes do not involve a transfer of heat between the system and environment. In quantum mechanics, the adiabatic theorem states that a system that is initially in an eigenstate of the Hamiltonian will remain in this eigenstate if the changes of this Hamiltonian are sufficiently slow [1,2]. While this quantum adiabatic theorem (QAT) is a well-established fact, it appears to be difficult to formulate a consistent quantum adiabatic condition (QAC), which unambiguously states when the theorem applies and is both necessary and sufficient.

A QAT is critical for developments in many areas of physics. It provides the foundation and interpretation of the Landau-Zener transition [3], the Gell-Mann–Low theorem [4], and Berry's phase [5]. Quantum adiabatic processes are also used for some quantum algorithms [6,7], the affectivity of which are based on the validity of the QAT [8].

Recently, however, doubts were cast over the consistency of the QAT and the sufficiency of the QAC. Marzlin and Sanders first suggested a possible inconsistency of the QAT [9]. Although there are some questionable points in their deduction [10], their main point triggered an extended discussion [11]. Then Tong *et al.* gave a specific counterexample to show that the traditional QAC is not sufficient for the adiabatic approximation to hold [12]. These discussions about the QAT and the QAC resulted in further investigations, such as modification of the traditional QAC [13–16], reexamination of the quantum adiabatic algorithm [17], and the study of the QAC in different quantum systems [18]. While there is fast progress in the theoretical discussion about the QAC and the QAT, an unambiguous experimental investigation is certainly important here. However, such experiments still remain a real challenge due to the following reasons: (i) the conflict between the sufficiently long time during the adiabatic evolution of the time-dependent Hamiltonian in QAT and the severely short coherent time of the real physical system due to the decoherence; (ii) the suitable technique with good quantum controlling during the quantum adiabatic process.

Considering that the coherent time of nuclei spin inside the atom is relatively longer compared to that of other physical systems and nuclear magnetic resonance (NMR) has been well developed over the past decades, we utilize this technique because there is less room for interpretation than with other potential experimental approaches. We first present a clear-cut experimental investigation of the issue, using a spin-$1/2$ particle in a rotating magnetic field. We show that, depending on the parameters chosen, the traditional QAC is either insufficient or unnecessary. Then we theoretically compare three newly proposed QACs with the traditional one and examine their applicability in our specific system. We also provide further experimental proof to support our theoretical comparison and discuss the character of different adiabatic conditions.

The quantum adiabatic theorem states that if the energy levels of a time-dependent Hamiltonian $H(t)$ are never degenerate and the Hamiltonian varies sufficiently slowly with time, the initial eigenstate of this Hamiltonian will stay close to the instantaneous eigenstate at a later time [2].

The widely used qualitative condition that assures the QAT valid is

$$\left|\frac{\langle E_m(t)|\dot{E}_n(t)\rangle}{E_m(t)-E_n(t)}\right| \ll 1, \qquad m \neq n, \qquad t \in [0, T], \quad (1)$$

where $E_m(t)$ and $|E_m(t)\rangle$ are the instantaneous eigenvalues and eigenstates of $H(t)$, and T is the total evolution time. We define the fidelity as the absolute value of the overlap of the actual state and the instantaneous eigenstate: $F(t) = |\langle\Psi(t)|\phi(t)\rangle|$, where $|\Psi(t)\rangle$ is the instantaneous eigenstate of the Hamiltonian and $|\phi(t)\rangle$ is the state that has evolved under the Hamiltonian $H(t)$ from $|\Psi(0)\rangle$. With this definition, the adiabatic theorem can be formulated such that the fidelity $F(t)$ will stay close to 1 if the variation of the Hamiltonian meets the condition in (1).

As a specific Hamiltonian, we choose

$$H(t) = \omega_0 \frac{\sigma_z}{2} + \omega_1\left(\frac{\sigma_x}{2}\cos\omega' t + \frac{\sigma_y}{2}\sin\omega' t\right), \quad (2)$$

where ω_0 is the Larmor frequency, ω_1 is the strength of the coupling to a radio frequency (rf) magnetic field, and ω' is the rotation frequency of the rf magnetic field. We investigate the validity of the adiabatic theorem as a function of the strength and frequency of the rf field.

Experiments were performed on ^{13}C-labeled $CHCl_3$ at room temperature using a Bruker AV-400 spectrometer. The experiments were performed on the ^{13}C nuclear spin, while the ^{1}H nuclear spin was decoupled during the whole experiment.

The initial Hamiltonian $H(0)$ has an eigenstate $|\Psi(0)\rangle = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}|1\rangle$, in which $\theta = \arctan(\omega_1/\omega_0) \approx 0.06$. We can prepare this initial state by applying an rf pulse along the y axis, with a rotation angle arctan0.06, to the thermal equilibrium state.

To realize an evolution determined by the Hamiltonian (2), we use the discrete approach proposed by Steffen *et al.* [7]. The rotation of the rf field, at frequency ω', was performed by applying a sequence of small flip-angle pulses, whose phase was initially set to zero and shifted by $\frac{\pi}{36}$ for every pulse.

In our experiments, we set the rf field strength to $\omega_1 = 100$ Hz and the static field offset to $\omega_0 = 1700$ Hz, corresponding to $\omega_1 = 0.06\omega_0$. For the rate of change of the transverse field component, we consider two specific cases: $\omega' = \omega_0$ and $\omega' = 10\omega_0$. For $\omega' = \omega_0$, the relevant parameter of Eq. (1) is close to $0.03 \ll 1$; i.e., the traditional QAC is fulfilled. For $\omega' = 10\omega_0$, this parameter becomes close to 0.3, which is considered a violation of the QAC.

For the case $\omega' = \omega_0$, the width of each pulse is $\Delta t = \frac{(\pi/36)}{2\pi\omega'} = 8.2\ \mu$s. We can compute the time that the rf field rotates one cycle as $\tau = \frac{2\pi}{\pi/36}\Delta t = 590.4\ \mu$s. We measure the state of the spin after it evolves n circles, in other word, at the time $t = n\tau$, in which n changes from 0 to 15. We can calculate the fidelities at these time points, and the experimental results are summarized as solid black circles in Fig. 1.

By simply changing the pulse width Δt in the above experiment, we can realize the case $\omega' = 10\omega_0$. Here, $\omega' = 10\omega_0 = 17000$ Hz and $\Delta t = 0.82\ \mu$s. The results of this experiment are represented as open red squares in Fig. 1.

An interesting and exciting phenomenon is that when $\omega' = \omega_0$ and the traditional adiabatic condition is satisfied, the state evolves far away from the instantaneous eigenstate and the fidelity falls below 0.1 at $t = 5$ ms. Therefore, we can conclude that the adiabatic condition is not sufficient, which agrees with the theoretical claim in Refs. [9,12]. On the other hand, when $\omega' = 10\omega_0$, even

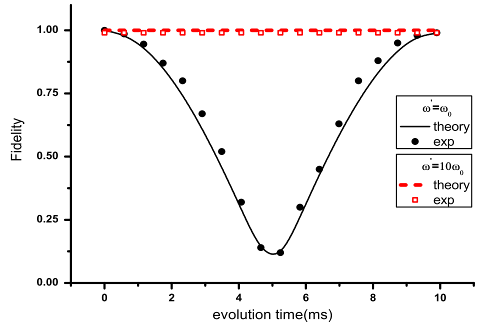

FIG. 1 (color online). Measured fidelity when $\omega' = \omega_0$ compared to the fidelity when $\omega' = 10\omega_0$. The solid black curve and dashed red curve are the theoretical results of $\omega' = \omega_0$ and $\omega' = 10\omega_0$, respectively. The solid black circles and open red squares are the experimental results of $\omega' = \omega_0$ and $\omega' = 10\omega_0$, respectively.

though the traditional adiabatic condition is violated, the state is always next to the instantaneous eigenstate and the fidelity remains close to 1. So the adiabatic condition (1) is not necessary. Synthesizing these two cases, it is evident that the traditional QAC is indeed problematic.

Now that the traditional QAC is problematic, it is urgent to find a new applicable condition. While there are many theoretical works that propose new quantum adiabatic conditions [13–16], here we apply the QACs to our specific Hamiltonian (2) and examine the validity of the traditional QAC and the three newly proposed QACs from Refs. [13–15]. For the adiabatic evolution, we chose the total time $T = \pi/\sqrt{(\omega_0 - \omega')^2 + \omega_1^2}$. By solving the Schrödinger equation analytically, we calculate $F_{\min}$, the minimal fidelity of $F(t)$ in the process of evolution:

$$F_{\min} = \frac{(\omega_0 - \omega')\cos\theta + \omega_1 \sin\theta}{\sqrt{(\omega_0 - \omega')^2 + \omega_1^2}}, \quad (3)$$

where θ was defined earlier. For the sake of convenience, we define C_1 as the expression in the traditional QAC [2]:

$$C_1 = \left|\frac{\langle E_+(t)|\dot{E}_-(t)\rangle}{E_+ - E_-}\right| = \frac{\omega'\omega_1}{2(\omega_0^2 + \omega_1^2)}. \quad (4)$$

Using fundamental inequalities, Tong *et al.* [13] proposed the sufficient condition shown as Eqs. (17)–(19) therein. The condition for the Hamiltonian in Eq. (2) can be rewritten as

$$C_2 = \int_0^T \left|\left(\frac{\langle E_+(t)|\dot{E}_-(t)\rangle}{E_+ - E_-}\right)'\right| dt = \frac{\pi\omega_0\omega'^3}{(\omega_0^2 + \omega_1^2)^{3/2}\sqrt{(\omega_0 - \omega')^2 + \omega_1^2}}. \quad (5)$$

On the basis of invariant perturbation theory, Wu *et al.* deduced a modified adiabatic condition [14]:

$$\left| \frac{\langle E_m(t)|\dot{E}_n(t)\rangle}{E_m - E_n + \Delta_{nm}} \right| \ll 1, \qquad t \in [0, T], \tag{6}$$

in which Δ_{nm} is defined as geometric potential. For the Hamiltonian (2), we can rewrite the condition above as

$$\begin{aligned} C_3 &= \left| \frac{\langle E_+(t)|\dot{E}_-(t)\rangle}{E_+ - E_- + i\langle E_-(t)|\dot{E}_-(t)\rangle - i\langle E_+(t)|\dot{E}_+(t)\rangle} \right| \\ &= \left| \frac{\omega_1 \omega'}{2(\omega_0^2 + \omega_1^2 - \omega_0 \omega')} \right|. \end{aligned} \tag{7}$$

Ambainis and Regev gave a new proof of the QAT, which states that the following condition can guarantee that the final state is at a distance at most δ from instantaneous eigenstate [15]:

$$T \geq \frac{10^5}{\delta^2} \max\left\{\frac{\|H'\|^3}{\lambda^4}, \frac{\|H'\| \cdot \|H''\|}{\lambda^3}\right\}, \tag{8}$$

where $\|\cdots\|$ is the usual operator norm and λ is the minimum energy gap during the evolution. In the Hamiltonian (2), by neglecting the constant coefficient we can rewrite this QAC as follows:

$$C_4 = \frac{\omega_1^2 \omega'^3}{(\omega_0^2 + \omega_1^2)^{3/2}[(\omega_0 - \omega_\prime)^2 + \omega_1^2]}. \tag{9}$$

We summarize the result of our calculation of the traditional and three newly proposed QACs in Fig. 2. We can easily distinguish whether a QAC is applicable for our Hamiltonian: if the adiabatic condition is satisfied ($C_i \ll 1$) and the adiabatic approximation happens to hold ($F_{\min} \approx 1$), then the condition $C_i \ll 1$ is a valid QAC in our system, and vice versa. From examining these three quantum adiabatic conditions we find the following: (i) For the traditional QAC [Fig. 2(b)], when the QAC is satisfied ($C_1 \ll 1$), $F_{\min}$ falls well below 1; conversely, when the QAC is violated, $F_{\min}$ remains close to 1. Therefore, the traditional QAC is neither necessary nor sufficient. (ii) For the QAC in Ref. [13] [Fig. 2(c)], the adiabatic condition ($C_2 \ll 1$) is satisfied at $\omega' \ll \omega_0$. In this region the adiabatic approximation is valid, so we can conclude that this adiabatic condition is valid for our Hamiltonian. (iii) For the QAC in Ref. [14] [Fig. 2(d)], the adiabatic condition ($C_3 \ll 1$) is satisfied except for $\omega' \approx \omega_0$. In this area the adiabatic approximation is valid, so this adiabatic condition is also applicable to our specific Hamiltonian. (iv) For the QAC in Ref. [15] [Fig. 2(e)], the adiabatic condition ($C_4 \ll 1$) holds at $\omega' \ll \omega_0$. Because the adiabatic approximation is also valid in this region, we can conclude that this adiabatic condition is correct for our Hamiltonian.

Although the three recently proposed QACs seem to be applicable in our specific Hamiltonian, it is important to indicate that they are still not perfect. First, $C_2 \ll 1$ is a strong sufficient condition, but not a necessary condition [13]. For example, when $\omega' \gg \omega_0$ and $\omega_1 \ll \omega_0$, the particle stays in the eigenstate, but the adiabatic condition is not satisfied ($C_2 > 1$). Besides, even though the condition $C_3 \ll 1$ seems to be applicable in our specific system, this adiabatic condition has been proven to be an insufficient and unnecessary condition in general cases [14]. Moreover, $C_4 \ll 1$ is also a too strong condition, because

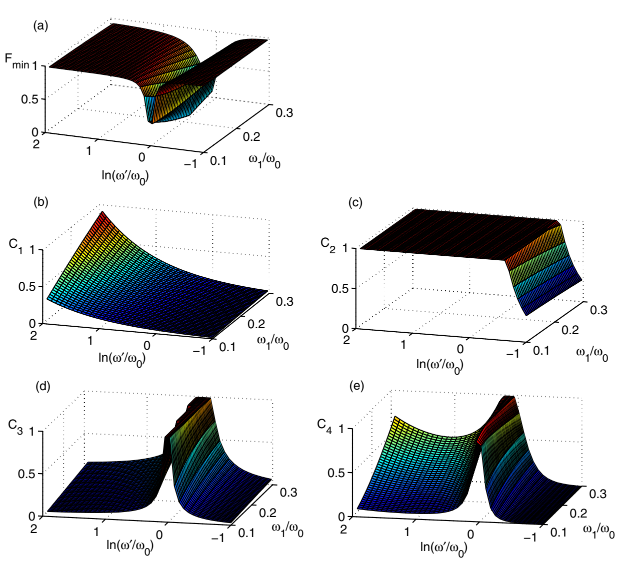

FIG. 2 (color online). $F_{\min}$, C_1, C_2, C_3, and C_4 as functions of ω'/ω_0 and ω_1/ω_0. (a) The minimum fidelity in the process of evolution as a function of $\ln(\omega'/\omega_0)$ and ω_1/ω_0. (b)–(e) The expression of a traditional QAC, the QAC in Ref. [13], the QAC in Ref. [14], and the QAC in Ref. [15] as a function of the same parameters.

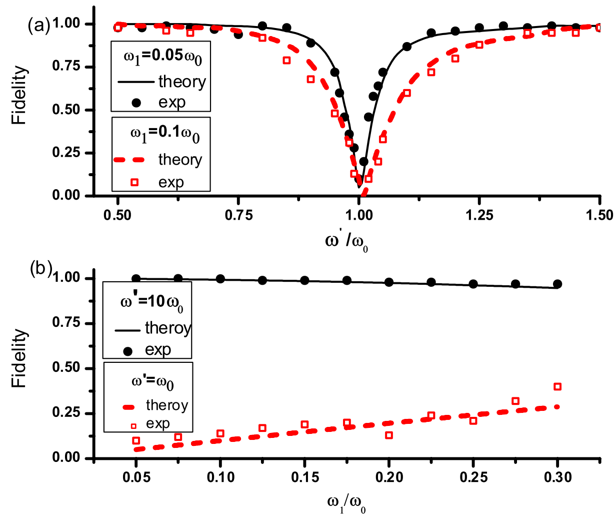

FIG. 3 (color online). (a) Fidelity of the evolution measured as a function of ω'/ω_0. The solid black circles and open red squares are the experimental minimum fidelities for $\omega_1 = 0.05\omega_0$ and $\omega_1 = 0.1\omega_0$, respectively. The solid black curve and the dashed red curve are the theoretical results. (b) The minimum fidelity as a function of ω_1/ω_0. The solid black circles and open red squares represent the experimental data for $\omega' = 10\omega_0$ and $\omega' = \omega_0$, respectively. The solid black curve and the dashed red curve are the theoretical results.

when $\omega' \gg \omega_0$ and ω_1 is not much less than ω_0, the adiabatic condition is not satisfied ($C_4 \sim 1$) but the system evolves adiabatically.

To support our discussion above, we have experimentally verified the calculation in Fig. 2(a). In the experiment, we measured the minimum fidelity as a function of ω'/ω_0 (or ω_1/ω_0) at fixed ω_1/ω_0 (or ω'/ω_0). In this experiment, the average rf field strength was $\omega_1 = 100$ Hz, and we used the same discrete method for the implementation of the time-dependent Hamiltonian as in the previous experiment. We changed ω' from $0.5\omega_0$ to $1.5\omega_0$ by varying the flip angle of the rf pulses, and we varied ω_1 from $0.05\omega_0$ to $0.3\omega_0$ by varying the frequency offset ω_0. The most important difference from the previous experiment is that here we did not measure the state after a cyclic evolution, at $t = n\tau$, but at the time of the minimum fidelity $t_{\min} = \frac{\pi}{\sqrt{(\omega_0-\omega')^2+\omega_1^2}}$. As an example, for the parameters $\omega_1 = 0.05\omega_0$ and $\omega' = 0.75\omega_0$, $t_{\min} = 980.6\ \mu$s. The experimental points were not chosen equidistant as a function of ω'/ω_0, but denser around $\omega' = \omega_0$, where the minimum fidelity changes rapidly. The experimental results are represented in Fig. 3. The agreement between these experimental results (solid black circles and open red squares) and the theoretical predictions of Fig. 2(a) (the curves in Fig. 3) is more than satisfactory.

Qualitatively, the observed behavior for the case of $\omega' = \omega_0$ can be understood as a resonant phenomenon. Although the ratio ω_1/ω_0 is very small, it can seriously affect the evolution if it contains a frequency component that matches a transition frequency of the system. The traditional QAC and the QAC in Ref. [13] do not account for resonant effects, but the QAC in Refs. [14,15] include this effect.

In the experiment, the ratio ω_1/ω_0 reflects the angle between the rotating magnetic field and the z axis, and ω'/ω_0 reflects the deviation of resonance. Figure 3(a) shows that if the magnetic field is very close to the z axis, the resonance region is narrow. If the angle increases (ω_1/ω_0 increases), the region of "resonance" becomes wider. Figure 3(b) shows that the particle evolves far from the eigenstate of our Hamiltonian when the resonance happens during the evolution ($\omega' = \omega_0$).

In conclusion, by using a special class of Hamiltonians, we examined the validity of the standard criterion of the adiabatic theorem experimentally and theoretically. And we show that this standard criterion C_1 is neither sufficient nor necessary while the quantum adiabatic theorem is physically correct. The clear-cut experiment showed that the failure of standard criterion cannot be ignored even in well-known experimental setups. And our results are also applicable to other experiments. We then examined three recent conditions and found that all conditions are valid for the adiabatic theorem in our special Hamiltonian. Although these three conditions are better than a traditional condition, their sufficiency and/or necessity cannot be verified here because one specific example cannot prove that a condition is sufficient and/or necessary. In fact, up to now, no sufficient and necessary condition for the quantum adiabatic theorem has been proposed. In our opinion, a sufficient and necessary condition is important in both fundamental and application. For example, in a quantum adiabatic algorithm, its efficiency and speed are guaranteed by the sufficiency and necessity of the adiabatic condition, respectively; a sufficient condition can enable an algorithm to get the right answer, while a necessary condition can make an adiabatic algorithm avoid the cost of unwanted long time. Thus, the sufficient and necessary condition for a quantum adiabatic theorem is still worthy of further investigation.

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