

Fidelity susceptibility and quantum adiabatic condition in thermodynamic limits

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In this work, we examine the validity of quantum adiabatic theorem in thermodynamic systems. For a d -dimensional quantum many-body system, we show that the duration time τ_0 required by its ground-state adiabatic process does not depend on the microscopic details but the scaling dimension of the fidelity susceptibility d_a . Our result, therefore, provides a quantitative time scale of the quantum adiabatic theorem in thermodynamic systems. The quantum adiabatic theorem might be violated in case that the scaling dimension of the fidelity susceptibility is larger than the system's real dimension ($d_a > d$).

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Quantum phase transition (QPT) [1] is one of the most active research fields in condensed-matter physics. For a quantum many-body system described by a Hamiltonian $H(\lambda)$, a QPT occurs as its ground-state property undergoes a significant change at a transition point λ_c . In order to study QPTs, people usually work on the lowest eigenstate of $H(\lambda)$. In practice, if there is no other mechanisms to change the lowest eigenstate but drive the system from one phase to the another by changing the driving parameter λ directly, one should ensure the validity of the quantum adiabatic theorem.

The quantum adiabatic theorem states that a quantum state will not transit to the system's other states of different eigenenergy if the driving Hamiltonian changes slowly enough in time. The theorem is an extremely intuitive concept because its validity relies on the criterion of the "slowness." This criterion, for an arbitrary D -level system, has been improved step by step in the last several decades [2–10]. However, the relation between the slowness and thermodynamic properties, such as dimensionality and various critical exponents etc., has been paid few attention. Therefore, for a d -dimensional quantum thermodynamic system, how to define the slowness or its relation to statistical quantities remains a fundamentally important question. To answer this question in a quantitative way is the key motivation of the present work.

In this paper, we start from the time-dependent Schrödinger equation and show that the leading transition probability from the ground state to excited states at the perturbation level is proportional to the fidelity susceptibility [11,12], which was proposed recently in the fidelity studies on the QPTs [13–26]. Then we are able to use the scaling dimension of the fidelity susceptibility d_a (called quantum adiabatic dimension hereafter [23]) to quantify the scale of the duration time required by the quantum adiabatic theorem. A general inequality is established for the slowness criterion (in terms of the duration time) in the thermodynamic limit.

We take the linear quench process, in which the driving Hamiltonian is turned on linearly with the time t , as an example. In this case, the duration time τ_0 for sufficient slowness should satisfy $\tau_0 \gg \kappa L^{d_a}$, where κ is independent of L . Therefore, if we require that a physically acceptable duration

time is proportional to the system size, which is about the order of the Avogadro's constant (6.02×10^{23}) for a realistic system, then the two limits of $N(=L^d) \rightarrow \infty$ and $\tau_0(\propto N) \rightarrow \infty$ do not commute with each other in case that the quantum adiabatic dimension $d_a > d$ (in other words $\infty \neq \infty^\mu$ for $\mu \neq 1$), hence the quantum adiabatic theorem might break down. We finally examine the validity of the quantum adiabatic theorem in a few of many-body systems, including the one-dimensional (1D) transverse-field Ising model [1], the Lipkin-Meshkov-Glick (LMG) model [27], and the Kitaev honeycomb model (KHM) [28]. In these models, $d_a > d$ at their corresponding critical point, hence the quantum adiabatic theorem is violated around the critical point. In the Kitaev honeycomb model, moreover, the quantum adiabatic dimension in the gapless phase is $2 + \ln$ (for a size dependence of $N^2 \ln N$), which is still larger than the real dimension 2, so the adiabatic theorem might break down in the whole phase.

To begin with, we consider a general d -dimensional quantum many-body system of length L and size $N=L^d$. Its Hamiltonian reads as

$$H(\lambda) = H_0 + \lambda H_I, \quad (1)$$

where H_I is the driving Hamiltonian, $\lambda = \lambda_i + t/\tau_0$ denotes its time-dependent strength with τ_0 being the duration time scale and λ_i being the starting point. To be consistent with the time-dependent perturbation theory, we let $\{|\phi_n(t)\rangle\}$ define the complete set of eigenstates of the instant Hamiltonian $H(t)$, i.e., $H(t)|\phi_n(t)\rangle = \epsilon_n(t)|\phi_n(t)\rangle$. According to the quantum adiabatic theorem, the ground state of the system is always $|\phi_0(t)\rangle$ if the driving Hamiltonian H_I is turned on slowly enough (here we exclude those cases of the ground-state level crossing). Then we can always use the adiabatic ground state $|\phi_0(t)\rangle$ to study QPTs in the parameter space of λ .

According to quantum mechanics, the system's state can be expressed as a linear combination of the adiabatic eigenstates,

$$|\Psi(t)\rangle = \sum_n a_n(t) |\phi_n(t)\rangle, \quad (2)$$

which is required to satisfy the time-dependent Schrödinger equation, i.e.,

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$$i \frac{\partial}{\partial t} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle. \quad (3)$$

Here we set $\hbar=1$. Introducing the unitary transformation

$$a_n(t) = \tilde{a}_n(t) \exp\left(-i \int^t \epsilon_n t' dt'\right) \quad (4)$$

and combining Eqs. (2) and (3) together, we can obtain

$$\begin{aligned} \frac{\partial \tilde{a}_m}{\partial t} = & -\tilde{a}_m \langle \phi_m | \partial_t \phi_m \rangle - \sum_{n \neq m} \frac{\langle \phi_m | \partial_t H | \phi_n \rangle \tilde{a}_n}{\omega_{nm}} \\ & \times \exp\left(-i \int^t \omega_{nm} dt'\right), \end{aligned} \quad (5)$$

where $\partial_x \phi \equiv \partial \phi / \partial x$ and $\omega_{nm} \equiv \epsilon_n - \epsilon_m$. The quantum adiabatic theorem is based on the approximation that if the second term on the right-hand side of the above equation is small enough compared with the first term, then the m th state will keep its position except for an accumulation of a Berry phase from the first term of Berry connection. Such an approximation holds true for a finite-size system with a finite-size energy gap but should be treated very carefully for a thermodynamic system in which the gap might vanish and long-range correlations appear in various distinct ways.

Now we suppose the Hamiltonian evolves from λ to $\lambda + \delta\lambda$ during a finite time interval Δt that is $\Delta t = \delta\lambda \tau_0$. The $\delta\lambda$ is small enough for the validity of the time-dependent perturbation theory. We will return to this requirement later. At time $t=0$, $\tilde{a}_0=1, \tilde{a}_m=0$ so the system is at the ground state $\phi_0(t=0)$; then at $t=\Delta t$, we have, to the first order,

$$\tilde{a}_0 \approx 1 - \frac{1}{\tau_0} \int_0^{\Delta t} \langle \phi_0 | \partial_\lambda \phi_0 \rangle dt, \quad (6)$$

$$\tilde{a}_m \approx -\frac{1}{\tau_0} \int_0^{\Delta t} \frac{H_I^{m0}}{\omega_{0m}} \exp\left(-i \int^t \omega_{0m} dt'\right) dt, \quad (7)$$

where $H_I^{nm} = \langle \phi_n | \partial_\lambda H | \phi_m \rangle$. To see the validity of the adiabatic theorem, we need to address the fidelity between $|\phi_0(t)\rangle$ and $|\Psi(t)\rangle$. For the normalized states $|\phi_0(t)\rangle$ and $|\Psi(t)\rangle$, the fidelity is

$$F = |\langle \phi_0(t) | \Psi(t) \rangle|. \quad (8)$$

The adiabatic theorem requires that $F \approx 1$.

However, it is not easy to estimate exactly the values of the integrals in Eqs. (6) and (7). To see the qualitative behavior of the leading term of the fidelity, we first make use of $|\phi_n(\lambda)\rangle$ as reference states, then the energy levels vary slowly with time. Under this approximation, the fidelity is the same as the perturbative form of the Loschmidt echo [24]

$$F_1 \approx 1 - (\delta\lambda)^2 \sum_{n \neq 0} \frac{|H_I^{n0}|^2 [1 - \cos(\omega_{0n} \Delta t)]}{\omega_{0n}^2}. \quad (9)$$

Here the second term denotes the transition probability and a phase factor from Eq. (6) has been normalized out.

The second alternative approach is to find the bound of the integral in Eq. (7). Because of

TABLE I. The adiabatic dimensions d_a^+, d_a^c and d_a^- (above, at, and below the critical point) for the 1D Ising model [14], the LMG model [20], and the Kitaev honeycomb model [21,23].

Model (critical point)	d	d_a^c	d_a^+	d_a^-
1D Ising model ($h_c=1$)	1	2	1	1
LMG model ($h_c=1$)	1	4/3	0	1
KHM ($J_c=1/2$)	2	5/2	2	2+ln

$$\left| \exp\left(-i \int^t \omega_{0m} dt'\right) \right| = 1, \quad (10)$$

we have

$$|\tilde{a}_m| \leq \frac{1}{\tau_0} \int_0^{\Delta t} \left| \frac{H_I^{m0}}{\omega_{0m}} \right| dt. \quad (11)$$

Then we obtain a lower bound of the fidelity

$$F_2 \approx 1 - \frac{(\delta\lambda)^2}{2} \sum_{n \neq 0} \frac{|H_I^{n0}|^2}{\omega_{0n}^2}, \quad (12)$$

hence an upper bound of the transition probability.

Mathematically, F_1 defines a distance between $|\phi_0(\lambda)\rangle$ and $|\Psi(t)\rangle$ and F_2 a distance between $|\phi_0(\lambda)\rangle$ and $|\phi_0(\lambda + \delta\lambda)\rangle$. Therefore, F_1 , F_2 , and F in Eq. (8) form a ‘‘triangle’’ in the parameter space. Our concern here is that the transition probabilities in both F_1 and F_2 are determined by the fidelity susceptibility [11,12]

$$\tilde{\chi}_F = \sum_{n \neq 0} \frac{|H_I^{n0}|^2}{\omega_{0n}^2}, \quad (13)$$

which defines also the scale of the original fidelity F defined in Eq. (8). In previous studies on the quantum adiabatic theorem, the formalism given in Eqs. (6)–(12) are familiar to us; however, few attention has been paid to the scaling behavior [29] of the quantity (the fidelity susceptibility) until recently [16,19].

For a d -dimensional system, the fidelity susceptibility of the driving Hamiltonian has its own dimension d_a [23] instead of the system’s real dimension though in many cases both dimensions are equal. That is

$$\tilde{\chi}_F \propto L^{d_a} \quad (14)$$

given that L is larger enough. In the critical region, the quantum adiabatic dimension $d_a = 2d + 2\zeta - 2\Delta_\nu$ [16], with d, ζ , and Δ_ν being the real dimension, dynamic exponent, and scaling dimension of the driving Hamiltonian, respectively. Clearly, in this case, the quantum adiabatic dimension d_a can be larger than d . In the noncritical region, the correlation length is finite, then we usually have $d_a = d$ or $d_a < d$. For instance, in the fully polarized phase of the LMG model, $d_a = 0$ [20] (here the LMG model is considered as a one-dimensional system with infinite-range interactions). In Table I, we show the adiabatic dimension for three exactly solvable models, i.e., the one-dimensional transverse-field Ising model [1], the LMG model [27], and the Kitaev honeycomb

model [28], around their corresponding phase-transition point. These data are collected from the recent fidelity approaches to QPTs, as shown in the caption of the table.

However, the results obtained from the perturbation theory is valid only if the change in the driving Hamiltonian is very small. Physicists are interested in the case that the change in the Hamiltonian, though varies slowly with the time, is not small, then the perturbation method cannot be applied directly. To solve this problem, we first assume, without loss of generality, that the system evolves from λ_i to λ_f during the time interval τ_0 , and the quantum adiabatic dimension in this region is d_a . Second, we divide the interval $\lambda_f - \lambda_i$ into M subintervals (here M defines also the scale of τ_0), that is, $\delta\lambda = (\lambda_f - \lambda_i)/M$. The total leading transition probability to excited states P_t then scales like

$$P_t \sim M \left(\frac{1}{M} \right)^2 \tilde{\chi}_F.$$

Because of $\tilde{\chi}_F \propto L^{d_a}$, M should be *at least* about the order of L^{d_a} to ensure the validity of the perturbation method. The final (minimum) probability of staying in the ground state $|\phi_0\rangle$ at λ_f then becomes

$$P_s \approx \left[1 - \frac{1}{2} \left(\frac{\Delta t}{\tau_0} \right)^2 \tilde{\chi}_F \right]^{L^{d_a}}. \quad (15)$$

The quantum adiabatic theorem requires $P_s \approx 1$. In the thermodynamic limit, we arrive at a simple inequality,

$$\tau_0 \gg \kappa L^{d_a}, \quad (16)$$

where κ is a L -independent quantity. The above inequality concludes the key result of the present work.

Clearly, inequality (16) defines the scale of duration time required by the quantum adiabatic theorem. That is, a sufficient adiabatic condition should defines the duration time in order of L^{d_a} . For a realistic (thermodynamic) system, the only comparable scale is the system size $N = L^d$, which is about the order of the Avogadro's constant (6.02×10^{23}). If we require that a physically acceptable duration time is, at most, proportional to the system size, then the two limits of $N \rightarrow \infty$ and $\tau_0 \rightarrow \infty$ do not commute with each other if $d_a > d$, and the quantum adiabatic theorem might be violated. On the other hand, in case that the starting and ending points are located in two regions with different quantum adiabatic dimensions, say d_{a1} and d_{a2} , the required duration time is determined by $\tau_0 \gg \kappa L^{\max(d_{a1}, d_{a2})}$.

Now we take the one-dimensional transverse-field Ising model as an example to illustrate the validity of the quantum adiabatic theorem according to our criterion. The Hamiltonian of the Ising model reads as

$$H = - \sum_{j=1}^N (\sigma_j^x \sigma_{j+1}^x + h \sigma_j^z), \quad (17)$$

$$\sigma_1^x = \sigma_{N+1}^x, \quad (18)$$

where $h(t < 0) = -t/\tau_0$. Hamiltonian (17) has been used as a prototype model in both studies on the ground-state fidelity

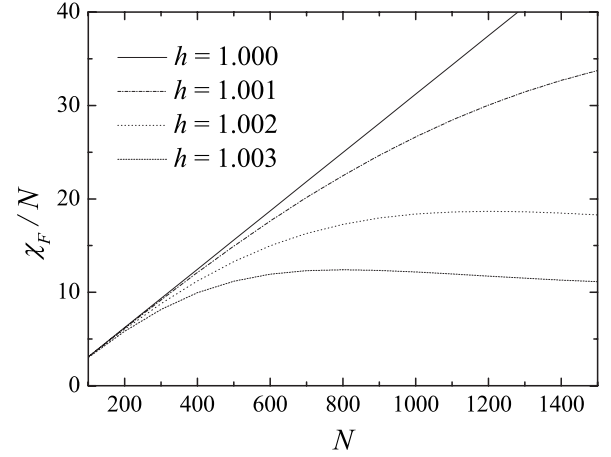


FIG. 1. The scaling behavior of the fidelity susceptibility around the critical point of the one-dimensional transverse-field Ising model.

[14] and dynamics of QPTs [30,31]. If the quantum adiabatic theorem holds true, $t < -\tau_0$ corresponds to the paramagnetic phase and $-\tau_0 < t < 0$ is the ferromagnetic phase. A second-order QPT occurs at $t = -\tau_0$. The fidelity susceptibility in the whole region can be calculated as

$$\tilde{\chi}_F = \sum_{k>0} \left(\frac{d\theta_k}{dh} \right)^2, \quad (19)$$

with $k = \pi/N, 3\pi/N, \dots, \pi(N-1)/N$, and

$$\frac{d\theta_k}{dh} = \frac{1}{2} \frac{\sin k}{1 + h^2 - 2h \cos k}. \quad (20)$$

It can be shown that $\tilde{\chi}_F \propto N^2$ for $h=1$, while $\tilde{\chi}_F \propto N$ for $h \neq 1$. Therefore, according to our criterion, if the starting and ending point are in the same phase, i.e., $t_i(t_f) < -\tau_0$ or $-\tau_0 < t_i(t_f) < 0$, the duration time required by the adiabatic condition is $N \ll \tau_0$. However, if $t_i < -\tau_0$ and $-\tau_0 < t_f < 0$, the system will cross the transition point $h=1$, at which the adiabatic dimension is 2. So the required duration time should satisfy $\tau_0 \gg \kappa N^2$. This observation is consistent with result obtained via the Landau-Zener formula [2,3] in the recent studies on quench dynamics in the Ising model [31]. Therefore, the quantum adiabatic theorem might break down at the critical point.

However, the problem is still subtle because the transition point is not a region but a “point.” Then the large N behavior might be quite different from that of the infinite limit. In Fig. 1, we show the scaling behavior of the fidelity susceptibility around the critical point. We can see that only at the critical point, $\tilde{\chi}_F/N \propto N$. While away from the critical point, though the closer to the critical point, the larger the fidelity susceptibility, the later will be finally saturated to

$$\frac{\chi_F}{N} = \begin{cases} \frac{1}{16(1-h^2)} & \text{for } h < 1 \\ \frac{1}{16h^2(h^2-1)} & \text{for } h > 1, \end{cases} \quad (21)$$

Respectively, as N increases. Therefore, for any simulation on a large but finite sample, the duration time should satisfy $\tau_0 \gg \kappa N^2$ in the region close enough to the critical point. While in the infinite N limit, the condition $\tau_0 \gg \kappa N^2$ is valid rigorously only at the critical point.

Moreover, we can see from Table I that the quantum adiabatic theorem does not hold true at the critical point of both the LMG model and Kitaev honeycomb model also. On the other hand, it has been found recently that the quantum adiabatic dimension in the gapless phase of the Kitaev honeycomb model is $2 + \ln$ [23], which is larger than the real dimension 2. Our quantum adiabatic condition implies that the quantum adiabatic theorem might be violated in the whole gapless phase of the Kitaev honeycomb model.

In summary, we have proposed the quantum adiabatic condition for quantum systems in the thermodynamic limit. A general inequality between duration times required by the quantum adiabatic theorem, the system size, and quantum adiabatic dimension are established. For the commonly studied linear quenches, our results show that the adiabatic condition might be violated if the adiabatic dimension is larger than the real dimension. This phenomenon usually occurs at the quantum critical point and those strange phases of $d_a > d$.

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