Consistency of the Adiabatic Theorem

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The adiabatic theorem provides the basis for the adiabatic model of quantum computation. Recently the conditions required for the adiabatic theorem to hold have become a subject of some controversy. Here we show that the reported violations of the adiabatic theorem all arise from resonant transitions between energy levels. In the absence of fast driven oscillations the traditional adiabatic theorem holds. Implications for adiabatic quantum computation are discussed.

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A statement of the *traditional* adiabatic theorem [1–3], as described in most recent publications, is as follows: Consider a system with a time-dependent Hamiltonian $H(t)$ and a wave function $|\psi(t)\rangle$, which is the solution of the Schrödinger equation ($\hbar = 1$)

$$i|\dot{\psi}(t)\rangle = H(t)|\psi(t)\rangle. \tag{1}$$

Let $|E_n(t)\rangle$ be the instantaneous eigenstates of $H(t)$ with eigenvalues $E_n(t)$. If at an initial time $t = 0$ the system starts in an eigenstate $|E_n(0)\rangle$ of the Hamiltonian $H(0)$, it will remain in the same instantaneous eigenstate, $|E_n(t)\rangle$, at a later time $t = T$, as long as the evolution of the Hamiltonian is slow enough to satisfy

$$\max_{t\in[0,T]} \left| \frac{\langle E_m(t)|\dot{E}_n(t)\rangle}{E_{nm}(t)} \right| \ll 1 \quad \text{for all } m \neq n, \tag{2}$$

where $E_{nm}(t) \equiv E_n(t) - E_m(t)$. One can easily show that: $\langle E_m(t)|\dot{E}_n(t)\rangle = \langle E_m(t)|\dot{H}|E_n(t)\rangle/E_{nm}(t)$. The adiabatic theorem has recently gained renewed attention as it provides the basis for one of the important schemes for quantum computation, i.e., adiabatic quantum computation [4,5].

Recently, the adiabatic condition (2) has become a subject of controversy. It was first shown by Marzlin and Sanders [6] and then by Tong *et al.* [7] that if a first system with Hamiltonian $H(t)$ follows an adiabatic evolution, a second system defined by Hamiltonian

$$\bar{H}(t) = -U^{\dagger}(t)H(t)U(t), \qquad U(t) \equiv \mathcal{T} e^{-i\int_0^t H(t)dt}, \tag{3}$$

cannot have an adiabatic evolution unless

$$|\langle E_n(t)|E_n(0)\rangle| \approx 1, \tag{4}$$

even if both systems satisfy the same condition (2). Here, $\mathcal{T}$ denotes the time ordering operator. Recently, the validity of the adiabatic theorem was experimentally examined [8], and (2) was reported to be neither sufficient nor a necessary condition for adiabaticity.

These inconsistencies have created debates among researchers [9–12] and motivated a search for alternative conditions [13–18], reexamination of some adiabatic algorithms [19], or generalizations of the adiabatic theorem to open quantum systems [20]. While it is valuable to find new conditions that guarantee adiabaticity in general, it is important to understand why the traditional adiabatic condition (2) is sufficient for some Hamiltonians, but not for others. Moreover, from the practical point of view it is much easier to work with a simple condition like (2) than some of the other more sophisticated ones. In this Letter, we relate the reported violations of the traditional adiabatic theorem to resonant transitions between energy levels. We further show that in the absence of such resonant oscillations, the traditional adiabatic condition is sufficient to assure adiabaticity. Our line of thought is close to that of Duki *et al.* [9], but largely extended with rigorous mathematical proofs.

It is well known that fast driven oscillations invalidate the adiabatic theorem [21]. Consider a simple example of a two-state system driven by an oscillatory force:

$$H(t) = -\frac{1}{2}\epsilon\sigma_z - V\sin\omega_0 t\sigma_x. \tag{5}$$

We take V to be a small positive number. The exact instantaneous eigenvalues and eigenstates are

$$E_{0,1} = \mp\frac{1}{2}\Omega, \qquad |E_{0,1}\rangle = \begin{pmatrix} \alpha^{\pm} \\ \pm\alpha^{\mp} \end{pmatrix}, \tag{6}$$

where $\Omega = \sqrt{\epsilon^2 + 4V^2\sin^2\omega_0 t}$ and $\alpha^{\pm} = \sqrt{(\Omega \pm \epsilon)/2\Omega}$. To the lowest order in V, $\Omega \approx \epsilon + (2V^2/\epsilon)\sin^2\omega_0 t$, $\alpha^{+} \approx 1 - (V^2/2\epsilon^2)\sin^2\omega_0 t$, and $\alpha^{-} \approx (V/\epsilon)\sin\omega_0 t$. The traditional adiabatic condition (2) leads to

$$\frac{|\langle E_1|\dot{E}_0\rangle|}{E_{10}} \approx \frac{V\omega_0}{\epsilon^2}|\cos\omega_0 t| \ll 1, \tag{7}$$

which is satisfied if $V\omega_0 \ll \epsilon^2$. Near resonance ($\omega_0 \approx \epsilon$), this requires $V \ll \epsilon, \omega_0$. The adiabatic theorem therefore states that if at $t = 0$ the system starts in its ground state $|E_0(0)\rangle = (1, 0)^T$, it will stay in the instantaneous ground state at later times. This, however, is not true as we shall see below.

Using the rotating wave approximation, the wave function of the system at resonance ($\epsilon = \omega_0$) is given by

$$|\psi(t)\rangle = \begin{pmatrix} e^{i\omega_0 t/2}\cos Vt/2 \\ e^{-i\omega_0 t/2}\sin Vt/2 \end{pmatrix}. \tag{8}$$

Therefore, the ground state probability

$$P_0(t) = |\langle E_0(t)|\psi(t)\rangle|^2 \approx (\cos Vt + 1)/2 \tag{9}$$

oscillates with the Rabi frequency $f_R = V/2\pi$. At time $T = T_R/2 = \pi/V$, the system will be in the excited state with probability $P_1 = 1$, violating the adiabatic theorem. Reducing the oscillation amplitude V would only increase the Rabi period T_R, and does not keep the system in the ground state. Therefore, adiabaticity is only satisfied for a time $T \ll T_R$. Indeed some new versions of adiabatic condition set an upper bound on the time T in order to guarantee adiabaticity [15,16]. However, as we shall see, this is not necessary in general. Before that, let us take a close look at the inconsistency discussed in [6,7].

Let us assume that $H(t)$ is a slowly varying Hamiltonian for which the adiabatic theorem holds. This means that if at time $t = 0$, the system starts in an eigenstate $|E_n^0\rangle$ ($\equiv |E_n(0)\rangle$) of $H(0)$, at time t, the wave function of the system will be (see below for proof)

$$|\psi_n(t)\rangle = U(t)|E_n^0\rangle \approx e^{-i\int_0^t E_n(t')dt'}|E_n(t)\rangle. \tag{10}$$

Hereafter, we use a gauge in which $\langle E_n(t)|\dot{E}_n(t)\rangle = 0$.

Now consider another system with Hamiltonian (3). The eigenvalues and eigenstates of the new Hamiltonian are $\bar{E}_n(t) = -E_n(t)$ and $|\bar{E}_n(t)\rangle = U^\dagger(t)|E_n(t)\rangle$, respectively. From (10), we have

$$|\bar{E}_n(t)\rangle \approx e^{i\int_0^t E_n(t')dt'}|E_n^0\rangle. \tag{11}$$

It was shown in Refs. [6,7] that for system $\bar{H}$ the adiabatic theorem holds only when (4) holds, even if the adiabatic condition (2) is satisfied. To understand this, let us write $\bar{H}$ in the basis $|E_n^0\rangle$:

$$\bar{H}(t) = \sum_{m,n}\langle E_m^0|\bar{H}(t)|E_n^0\rangle|E_m^0\rangle\langle E_n^0|. \tag{12}$$

However

$$\begin{aligned}\langle E_m^0|\bar{H}(t)|E_n^0\rangle &= -\langle E_m^0|U^\dagger H(t)U(t)|E_n^0\rangle \\ &= -i\langle\psi_m(t)|\dot{\psi}_n(t)\rangle.\end{aligned} \tag{13}$$

Using (10) we find

$$\begin{aligned}\bar{H}(t) = &-\sum_n E_n(t)|E_n^0\rangle\langle E_n^0| \\ &- i\sum_{n,m} e^{-i\omega_{nm}(t)}\langle E_m(t)|\dot{E}_n(t)\rangle|E_m^0\rangle\langle E_n^0|,\end{aligned} \tag{14}$$

where $\omega_{nm}(t) \equiv \frac{1}{t}\int_0^t E_{nm}(t')dt'$. The second line in (14) involves rapidly oscillating terms that cause resonant transitions between the levels. The amplitude of each oscillatory term is $|\langle E_m(t)|\dot{E}_n(t)\rangle|$. Hence satisfying (2) will only reduce this amplitude and, as we saw before, it does not eliminate Rabi oscillations and therefore does not keep the system in its original eigenstate beyond half a Rabi period. Notice that Eq. (4) is equivalent to $|E_n(t)\rangle \approx e^{i\phi(t)}|E_n^0\rangle$, where $\phi(t)$ is some time-dependent phase. This leads to $\langle E_m(t)|\dot{E}_n(t)\rangle \propto \langle E_m^0|E_n^0\rangle = 0$. Therefore, the oscillatory terms in (14) will all vanish if (4) is satisfied, leading to an adiabatic evolution in agreement with [6,7].

We now provide a general proof for the adiabatic theorem emphasizing the role of resonant transitions. Let us write the wave function of the system as:

$$|\psi(t)\rangle = \sum_n a_n(t)e^{-i\int_0^t E_n(t')dt'}|E_n(t)\rangle. \tag{15}$$

For a time-independent Hamiltonian, $a_n(t)$ is a constant while for a slowly varying Hamiltonian it is a slow function of time. Substituting (15) into the Schrödinger equation (1), we find

$$\dot{a}_m(t) = -\sum_{n\neq m} a_n(t)\langle E_m(t)|\dot{E}_n(t)\rangle e^{-i\int_0^t E_{nm}(t')dt'}.$$

Integrating over t, we get

$$\begin{aligned}a_m(T) - a_m(0) = &-\sum_{n\neq m}\int_0^T dt a_n(t) \\ &\times\langle E_m(t)|\dot{E}_n(t)\rangle e^{-i\int_0^t E_{nm}(t')dt'}.\end{aligned} \tag{16}$$

To assure adiabaticity, the right-hand side of this equation should be small. With the initial condition $a_m(0) = \delta_{mn}$, this would immediately yield (10). Since the exponential term in the integrand of (16) is a rapidly oscillating function, if the rest of the terms vary very slowly, the integral will be small. To make this statement more quantitative, let us define the right-hand side of the above equation as the error $\varepsilon_m = -\sum_{n\neq m}\varepsilon_{nm}$ for the adiabatic evolution, where

$$\varepsilon_{nm} \equiv \int_0^T dt A_{nm}(t)E_{nm}(t)e^{-i\int_0^t E_{nm}(t')dt'}, \tag{17}$$

and

$$A_{nm}(t) \equiv a_n(t)\frac{\langle E_m(t)|\dot{E}_n(t)\rangle}{E_{nm}(t)}. \tag{18}$$

Using the Fourier transformation: $\tilde{A}_{nm}(\omega) = \int_0^T dt e^{i\omega t}A_{nm}(t)$, we find

$$\varepsilon_{nm} = \int\frac{d\omega}{2\pi}\int_0^T dt\tilde{A}_{nm}(\omega)E_{nm}(t)e^{i[\omega-\omega_{nm}(t)]t}. \tag{19}$$

The integral in (19) is suppressed by the oscillatory exponential in the integrand, except along a path in the two-dimensional t-ω plane defined by the equation $\omega = \omega_{nm}(t)$, where there is no oscillation. In the presence of resonant oscillations, $\tilde{A}_{nm}(\omega)$ has finite components at frequencies $\omega_{nm}(t)$; hence, the contribution from such a

dominant path becomes

$$\varepsilon_{nm} \sim \int_0^T dt \tilde{A}_{nm}(\omega_{nm}(t)) E_{nm}(t) \leq T \max_t |\tilde{A}_{nm}(\omega_{nm}(t)) E_{nm}(t)|. \quad (20)$$

The error therefore grows as a function of T. As a result, to assure adiabaticity one needs an upper limit for T, as expected for the case of resonant oscillations. However, this is not the case for a general system without resonant oscillations, as we shall see below.

In the absence of such oscillations, $A_{nm}(t)$ can be made as slow as desired by making the evolution slow. In Fourier space, this makes $\tilde{A}_{nm}(\omega)$ sharply peaked at low frequencies with a cutoff frequency ω_c proportional to the rate of change of the Hamiltonian. To see this, let us introduce a new variable $s = t/T$. Since $a_n(t) = a_n(0) + O(\varepsilon_n)$, to the lowest order in the small error ε_n we have [22]

$$\tilde{A}_{nm}(\tilde{\omega}) \approx a_n(0) \int_0^1 ds e^{i\tilde{\omega}s} \frac{\langle E_m(s)|d/ds|E_n(s)\rangle}{E_{nm}(s)}, \quad (21)$$

where $\tilde{\omega} = \omega T$ is the dimensionless frequency. The integral on the right-hand side is independent of T. Let $\tilde{\omega}_c$ be the largest dimensionless frequency of $\tilde{A}_{nm}(\tilde{\omega})$. Therefore, $\omega_c = \tilde{\omega}_c/T$ can be made arbitrarily small by making T large. Notice that $\tilde{\omega}_c$ is a constant that only depends on the properties of the Hamiltonian and does not depend on the evolution time T.

If $\omega_c \ll \omega_{nm}(t)$, one can neglect ω in the exponential in the integrand of (19) and therefore perform the t and ω integrations independently, yielding

$$\varepsilon_{nm} \sim \omega_c |\tilde{A}_{nm}(0)| \leq \omega_c \int_0^T |A_{nm}(t)| dt \leq \omega_c T \max_t |A_{nm}(t)| \leq \tilde{\omega}_c \max_t \left| \frac{\langle E_m(t)|\dot{E}_n(t)\rangle}{E_{nm}(t)} \right|. \quad (22)$$

Therefore, ε_{nm} can be made arbitrarily small by only satisfying the adiabatic condition (2).

The same conclusion can also be reached from a different angle. Using integration by parts, Eq. (17) becomes

$$\varepsilon_{nm} = [A_{nm}(T) e^{-i\int_0^T E_{nm}(t')dt'} - A_{nm}(0)] - \int_0^T dt \dot{A}_{nm}(t) e^{-i\int_0^t E_{nm}(t')dt'} \leq |A_{nm}(T)| + |A_{nm}(0)| + \int_0^T dt |\dot{A}_{nm}(t)|. \quad (23)$$

The last term above is responsible for the breakdown of the adiabatic theorem. Let us define t_i, $i = 1, \ldots, M_{nm}$, as the solutions to $\dot{A}_{nm}(t_i) = 0$, where M_{nm} is the number of zeros of $\dot{A}_{nm}(t)$ in the interval $[0,T]$. Since $\dot{A}_{nm}(t)$ is monotonic between t_i and t_{i+1}, we can write

$$\int_0^T dt |\dot{A}_{nm}(t)| = \sum_{i=0}^{M_{nm}} \left| \int_{t_1}^{t_{i+1}} dt \dot{A}_{nm}(t) \right| = \sum_{i=0}^{M_{nm}} |A_{nm}(t_{i+1}) - A_{nm}(t_i)|, \quad (24)$$

where we have defined $t_0 = 0$ and $t_{M_{nm}+1} = T$. Thus

$$\varepsilon_{nm} \leq 2 \sum_{i=0}^{M_{nm}} |A_{nm}(t_i)| \leq 2 M_{nm} \max_{t\in[0,T]} |A_{nm}(t)| \leq 2 M_{nm} \max_{t\in[0,T]} \left| \frac{\langle E_m(t)|\dot{E}_n(t)\rangle}{E_{nm}(t)} \right|. \quad (25)$$

Since the error depends on M_{nm}, it is important to understand how M_{nm} depends on the evolution time T.

Let us first consider a Hamiltonian that has an oscillatory term with frequency ω_0. Oscillations of the Hamiltonian will create oscillations in $A_{nm}(t)$ and therefore the number of zeros of $\dot{A}_{nm}(t)$ will grow with time as $M_{nm} \sim \omega_0 T$. In that case, without putting an upper bound on T, it is not possible to limit the error ε_{nm}. This is in agreement with our previous observation for cases involving resonant transitions, as well as the additional conditions introduced in Refs. [15,16]. On the other hand, if M_{nm} does not grow with time, one can always reduce ε_{nm} by just satisfying (2) without a need to limit T. To see this, let us again use the dimensionless parameter $s = t/T$. If by slowing down the evolution, we only change T and not other parameters in the Hamiltonian, then the Hamiltonian $H(s)$ and its eigenvalue $E_n(s)$ and eigenfunctions $|E_n(s)\rangle$ will all be independent of T. Again to the lowest order in ε_n, $a_n(t) \approx a_n(0)$ and therefore from (18), $A_{nm}(t) \approx a_n(0) \times \langle E_m(t)|\dot{E}_n(t)\rangle/E_{nm}(t)$ [22]. The times t_i can therefore be obtained by solving

$$\dot{A}_{nm}(t) = \frac{a_n(0)}{T^2} \frac{d}{ds} \frac{\langle E_m(s)|d/ds|E_0(s)\rangle}{E_{nm}(s)} = 0. \quad (26)$$

The number of zeros of this equation, i.e. M_{nm}, is therefore finite and independent of T. In that case, (25) assures that by just satisfying the adiabatic condition (2), the error ε_{nm} can be made as small as desired.

From the above proof it becomes evident that the following way of stating the adiabatic theorem removes all of the inconsistencies: For a Hamiltonian $H(s)$, where $s = t/T \in [0, 1]$, the evolution of the system starting from an eigenstate $|E_n(0)\rangle$ is adiabatic provided that

$$T \gg \max_{s\in[0,1]} \frac{|\langle E_m|dH/ds|E_n\rangle|}{E_{nm}^2} \quad \text{for all } m \neq n. \quad (27)$$

It should be emphasized that our goal in this Letter was just to study the sufficiency of the adiabatic condition (2) for adiabatic evolution without worrying about the scaling issue. In other words, we do not discuss dependence of the error ε_{nm} on the system size. Scaling becomes important

for determining the performance of an adiabatic quantum computer. The exponentially large number of states involved in the sum in (16) requires ε_{nm} to be exponentially small in order to keep the sum small. Fortunately, this does not put a stringent limitation on the time T. To understand this, let us write the error as

$$\varepsilon_{nm} \lesssim \frac{1}{T} \max_{s\in[0,1]} \frac{|\langle E_m|dH/ds|E_n\rangle|}{E_{nm}^2}. \tag{28}$$

Typically $\langle E_m|dH/ds|E_n\rangle$ is exponentially small, otherwise the curvature of the energy levels

$$\frac{d^2E_n}{ds^2} = 2\sum_{m\neq n} \frac{|\langle E_m|dH/ds|E_n\rangle|^2}{E_{nm}} + \left\langle E_n \left| \frac{d^2H}{ds^2} \right| E_n \right\rangle$$

becomes extremely large due to the sum over an exponentially large number of terms. For the simple example of adiabatic Grover search [23], it is easy to show that $\langle E_m|\dot{H}|E_0\rangle = 0$ for $m > 1$, therefore only the first two energy levels contribute to the adiabatic evolution. For problems with local interactions, the matrix elements typically decay exponentially with the energy separation between the states. This can be checked perturbatively near the beginning and the end of the evolution (using similar techniques as in Ref. [24]). It can also be tested numerically for systems with not very large size [25]. Such exponential suppression of the matrix elements allows only a few energy levels to participate in the calculation of the error. Especially, in adiabatic quantum computation when the gap between the ground state and the first excited state becomes much smaller than other energy separations, those two states dominantly determine the error of the computation and the evolution time can be determined by the minimum gap between those, as has been confirmed numerically for up to 20 qubits [26]. More work is needed to make these statements mathematically rigorous. Moreover, a realistic adiabatic quantum computer will always couple to an environment. Therefore, other methods [20,26] are necessary to study the evolution of such open quantum systems.

To summarize, we have shown that the inconsistencies in the traditional adiabatic theorem reported in the literature are all closely related to the fact that for systems subject to fast driven oscillations, resonant transitions between energy levels cannot be suppressed by just reducing the amplitude of oscillations, although the adiabatic condition (2) can be satisfied. Since the amplitude of oscillations determines the Rabi frequency, reducing the amplitude would only increase the Rabi period. Within a time of the order of half a Rabi period, the system will undergo a transition out of its original state. Thus, the Rabi period sets an upper limit for the total time of the adiabatic evolution. On the other hand, if the Hamiltonian of the system does not involve any driven oscillations, there is no such mechanism to take the system out of its original state and the traditional adiabatic condition is adequate to guarantee adiabaticity.

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