

## Inconsistency in the Application of the Adiabatic Theorem

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The adiabatic theorem states that an initial eigenstate of a slowly varying Hamiltonian remains close to an instantaneous eigenstate of the Hamiltonian at a later time. We show that a perfunctory application of this statement is problematic if the change in eigenstate is significant, regardless of how closely the evolution satisfies the requirements of the adiabatic theorem. We also introduce an example of a two-level system with an exactly solvable evolution to demonstrate the inapplicability of the adiabatic approximation for a particular slowly varying Hamiltonian.

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**Introduction.**—Since the dawn of quantum mechanics [1–3], the venerable adiabatic theorem (AT) has underpinned research into quantum systems with adiabatically (i.e., slowly) evolving parameters, and has applications beyond quantum physics, for example, to electromagnetic fields. The AT lays the foundation for the Landau-Zener transition (LZT) (including the theory of energy level crossings in molecules) [4], for the Gell-Mann–Low theorem in quantum field theory [5] on which perturbative field theory is constructed, and for Berry’s phase [6]. More recently the AT has renewed its importance in the context of quantum control, for example, concerning adiabatic passage between atomic energy levels [7], as well as for adiabatic quantum computation [8]. Essentially the standard statement of the AT implies that a system prepared in an instantaneous eigenstate of a time-dependent Hamiltonian will remain close to an instantaneous eigenstate of the Hamiltonian provided that the Hamiltonian changes sufficiently slowly. Here we demonstrate that the application of the standard statement of the AT leads to an inconsistency, regardless of how slowly the Hamiltonian changes; although the AT itself is sound provided that deviations from adiabaticity are properly accounted for, the standard statement alone does not ensure that a formal application of it results in correct results. In addition, we present a simple two-level example for the failure of the AT even in a case when all the criteria for the AT seem to be met. The results of this Letter are intended to serve as a warning that the incautious use of the AT may produce seemingly unproblematic results which nevertheless may be grossly wrong.

Before demonstrating the inconsistency arising from the standard statement of the AT, we give a simple exposition of the theorem’s proof as presented in Ref. [9]. The evolution of a quantum state  $|\psi(t)\rangle$  under a unitary evolution  $U(t, t_0)$  is described by  $|\psi(t)\rangle = U(t, t_0)|E_0(t_0)\rangle$ . We assume that the initial state  $|E_0(t_0)\rangle$  is an eigenstate of the initial Hamiltonian  $H(t_0)$ . The time-dependent Hamiltonian is related to  $U(t)$  by  $H(t) = i\dot{U}U^\dagger$  [10],

such that  $|\psi(t)\rangle$  fulfills the usual Schrödinger equation. In the instantaneous eigenbasis  $\{|E_n(t)\rangle\}$  of  $H(t)$ , the state can be expressed as  $|\psi(t)\rangle = \sum_n \psi_n(t) e^{-i \int_{t_0}^t E_n(t') dt'}$ , where we have introduced the shorthand notation  $\int E_n \equiv \int_{t_0}^t E_n(t') dt'$ . Inserting this expansion into the Schrödinger equation leads to the following differential equation for the coefficients:

$$i\dot{\psi}_n = -i \sum_m e^{i \int_{t_0}^t (E_n - E_m) dt'} \psi_m \langle E_n | \dot{E}_m \rangle. \quad (1)$$

The AT relies on the requirement that  $H(t)$  is slowly varying according to

$$|\langle E_n | \dot{E}_m \rangle| \ll |E_n - E_m|, \quad n \neq m. \quad (2)$$

Transitions to other levels are then supposed to be negligible due to the rapid oscillation arising from the phase factor  $\exp(i \int (E_n - E_m))$ , yielding

$$|\psi(t)\rangle \approx e^{-i \int_{t_0}^t E_0 dt'} |E_0(t)\rangle \quad (3)$$

with  $\beta_n = i \langle E_n | \dot{E}_n \rangle$  the geometric phase (GP) [6]. Condition (2) and approximation (3) summarize the standard statements of the AT.

**Proof of inconsistency.**—The inconsistency implied by Eq. (3) is evident by considering the state  $|\tilde{\psi}\rangle := U^\dagger(t, t_0)|E_0(t_0)\rangle$ . Using  $\partial_t(U^\dagger U) = 0$  it is easy to see that this state fulfills an exact Schrödinger equation with Hamiltonian  $\tilde{H}(t) = -U^\dagger(t, t_0)H(t)U(t, t_0)$ . To demonstrate the inconsistency, we commence with a claim that is shown to yield a contradiction.

Claim: The AT (3) implies

$$|\tilde{\psi}\rangle = e^{i \int_{t_0}^t E_0 dt'} |E_0(t_0)\rangle. \quad (4)$$

**Proof of inconsistency:** Because  $U(t_0, t_0) = 1$ , result (4) fulfills the correct initial condition so it remains to show that (4) also fulfills the Schrödinger equation:

$$\begin{aligned}
i\partial_t|\bar{\psi}\rangle &= -E_0(t)|\bar{\psi}\rangle \\
&= -E_0(t)U^\dagger U e^{i\int_{t_0}^t E_0} |E_0(t_0)\rangle \\
&\approx -E_0(t)U^\dagger e^{i\beta_0} |E_0(t)\rangle \\
&= -U^\dagger H(t) e^{i\beta_0} |E_0(t)\rangle \\
&\approx -U^\dagger H(t) U e^{i\int_{t_0}^t E_0} |E_0(t_0)\rangle \\
&= \bar{H}(t)|\bar{\psi}\rangle.
\end{aligned} \tag{5}$$

The AT is explicitly used in the lines with  $\approx$ . However, Eq. (4) implies

$$\begin{aligned}
\langle E_0(t_0)|UU^\dagger|E_0(t_0)\rangle &= \langle E_0(t_0)|U|\bar{\psi}\rangle \\
&\approx e^{i\beta_0}\langle E_0(t_0)|E_0(t)\rangle \neq 1,
\end{aligned} \tag{6}$$

which is false  $\square$ .

Clearly the inconsistency is a consequence of neglecting the deviations of Eq. (3) from the exact time evolution which is free of inconsistencies. Stated another way, approximation (3), without correction terms, could be exact only in the limit of infinitesimally slow evolution, for which the system is constant over finite time and the evolution is indeed given by a multiplicative phase cofactor. However, evolution is not infinitesimally slow, and neglect of the correction terms leads to the inconsistency demonstrated above. To elucidate this point we define the following unitary transformation,

$$U_{\text{AT}}(t, t_0) \equiv \sum_n e^{-i\int_{t_0}^t E_n} e^{i\beta_n(t)} |E_n(t)\rangle\langle E_n(t_0)|. \tag{7}$$

The (exact) time evolution generated by  $U_{\text{AT}}$  is equivalent to the standard statement (3) of the AT for adiabatic motion in a finite-dimensional Hilbert space with non-degenerate energy levels. It is straightforward to write  $\bar{H}_{\text{AT}}(t) = -iU_{\text{AT}}^\dagger \dot{U}_{\text{AT}}$  in the form

$$\begin{aligned}
\bar{H}_{\text{AT}}(t) &= -\sum_n E_n(t) |E_n(t_0)\rangle\langle E_n(t_0)| \\
&\quad -i \sum_{m \neq n} e^{i\int_{t_0}^t (E_n - E_m)} e^{-i(\beta_n - \beta_m)} \langle E_n(t) | \dot{E}_m(t) \rangle \\
&\quad \times |E_n(t_0)\rangle\langle E_m(t_0)|.
\end{aligned} \tag{8}$$

The second sum in this expression has the same structure as those terms that are omitted in the adiabatic approximation, and by omitting these terms one again arrives at the inconsistent result (4). However, evaluating Hamiltonian  $\bar{H}_{\text{AT}}$  in the interaction picture with respect to the first line of  $\bar{H}_{\text{AT}}$ , one finds

$$\tilde{H}_{\text{AT}}(t) = -i \sum_{m \neq n} e^{-i(\beta_n - \beta_m)} \langle E_n(t) | \dot{E}_m(t) \rangle |E_n(t_0)\rangle\langle E_m(t_0)|. \tag{9}$$

In this Hamiltonian the transition matrix elements be-

tween the different initial eigenstates are not rapidly oscillating anymore and therefore cannot be neglected. However, perfunctory use of the standard statement of the AT (3) implicitly neglects such terms.

Thus we have shown that the standard statement of the AT may lead to an inconsistency no matter how slowly the Hamiltonian is varied, but so much science rests on the AT that the implications of this inconsistency are important and require exploration. Perhaps the most important application of the AT is the slow evolution of an initial instantaneous eigenstate  $|E_0(t)\rangle$  into a later instantaneous eigenstate  $|E_0(t)\rangle$  that is meant to be quite different; i.e.  $\mathcal{F}_0 = |\langle E_0(t)|E_0(t_0)\rangle| \ll 1$ . For example, the famous LZT [4] evolves a two-level molecule or atom with orthogonal basis states  $|0\rangle$  and  $|1\rangle$  from  $|E_0(t_0)\rangle = |0\rangle$  to  $|E_0(t)\rangle = |1\rangle$  with near-unit probability so that  $\mathcal{F}_0 \approx |\langle 0|1\rangle| = 0$ . On the other hand, the quantity  $\mathcal{F}_1 = |\langle E_0(0)|UU^\dagger|E_0(0)\rangle|$  should always be unity, but (6) implies  $\mathcal{F}_1 \approx \mathcal{F}_0 \approx 0$ . Thus, the deviation of the overlap function  $\mathcal{F}_0$  from unity is an alarm indicator for when the AT is vulnerable to the inconsistency: whenever  $|E_0(t)\rangle$  deviates strongly from the initial state  $|E_0(0)\rangle$ , the inconsistency is a potential problem, *regardless of how slowly  $H(t)$  changes*.

*Counterexample of a two-level system.*—Problems in the application of the AT are not restricted to the inverse time evolution. As a specific example, consider a two-level system with exact time evolution defined by

$$U(t) = \exp(-i\theta(t)\mathbf{n}(t) \cdot \boldsymbol{\sigma}) = \cos\theta \mathbb{1} - i\mathbf{n} \cdot \boldsymbol{\sigma} \sin\theta \tag{10}$$

with  $\theta(t) = \omega_0 t$ ,  $\mathbf{n}(t) = (\cos(2\pi t/\tau), \sin(2\pi t/\tau), 0)$ , and  $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$  denoting the Pauli spin vector operator. The associated Hamiltonian can be calculated using  $H(t) = i\dot{U}U^\dagger$  and can be written in the form  $H(t) = \mathbf{R}(t) \cdot \boldsymbol{\sigma}$ , with

$$\begin{aligned}
\mathbf{R} &= \dot{\theta}\mathbf{n} + \cos\theta \sin\theta \dot{\mathbf{n}} + \sin^2\theta (\mathbf{n} \times \dot{\mathbf{n}}) \\
&= \omega_0 \mathbf{n}(t) + \frac{\sin(\omega_0 t)}{\tau} \tilde{\mathbf{R}}(t),
\end{aligned} \tag{11}$$

where  $\tilde{\mathbf{R}}(t) \equiv 2\pi(-\sin(\frac{2\pi t}{\tau})\cos(\omega_0 t), \cos(\frac{2\pi t}{\tau})\cos(\omega_0 t), \sin(\omega_0 t))$ . This Hamiltonian is similar to that of a spin- $\frac{1}{2}$  system in a magnetic field of strength proportional to  $\omega_0$  that rotates with period  $\tau$  in the  $x$ - $y$  plane. The exact Hamiltonian for the latter case would correspond to  $\tilde{\mathbf{R}}(t) = 0$ ; we discuss the importance of this difference below. The eigenvalues of  $H(t)$  are given by

$$E_{\pm}(t) = \pm|\mathbf{R}(t)| = \pm\sqrt{\dot{\theta}^2 + \sin^2\theta \omega_0^2}. \tag{12}$$

It is easy to show that the evolution operator (10) fulfills requirement (2) for adiabatic evolution as long as the vector  $\mathbf{n}$  changes slowly compared to  $\omega_0$ , i.e., for  $\omega_0 \tau \gg 1$ . The time scale  $\tau$  corresponds to the large time scale which appears in the mathematically more elaborate forms of the AT [2,3,11]. These correction terms are resonant [12] so that a large deviation from the AT predictions can accumulate over time.

To evaluate the predictions of the AT it is convenient to consider projection operators instead of the state itself. Projectors onto eigenstates of  $H(t)$ , which fulfill  $H(t)|\pm(t)\rangle = \pm|\mathbf{R}(t)||\pm(t)\rangle$ , can generally be written as

$$P_{|\pm(t)\rangle} = \frac{1}{2} \left( \mathbf{1} \pm \frac{\mathbf{R}(t) \cdot \boldsymbol{\sigma}}{|\mathbf{R}(t)|} \right). \quad (13)$$

If we consider the evolution at time  $T = \tau/2$  and assume for simplicity that  $\omega_0 T$  is a multiple of  $2\pi$ , we have  $\mathbf{R}(T) = -\mathbf{R}(0)$  and  $U(T) = \mathbf{1}$ . We thus find  $P_{|+(T)\rangle} = P_{|- (0)\rangle}$ , but  $P_{U|+(0)\rangle} = U(T)P_{|+(0)\rangle}U(T)^\dagger = P_{|+(0)\rangle}$ . In other words, the perfunctory prediction

$$U(T)P_{|+(0)\rangle}U(T)^\dagger \approx P_{|+(T)\rangle} \quad (14)$$

of the AT is invalid. Thus, whereas a resonant but weak time-dependent oscillatory term in the evolution represents an unusual application of the AT, this system meets the criteria of the AT and therefore casts doubt on the general applicability of criterion (2).

For two-level systems, it is possible to derive a general criterion on when the AT is bound to fail, i.e., when the quantity  $\mathcal{Q} := |\langle + (t) | U(t) | + (0) \rangle|^2 = \text{Tr} P_{U|+(0)\rangle} P_{|+(t)\rangle}$  strongly deviates from one. It is evident that this criterion depends on  $U(t)$  at time  $t$  only, as well as on the Hamiltonians  $H(t)$  and  $H(0)$ . There is no direct reference to the slow evolution of the Hamiltonian because the criterion does not depend on  $\dot{H}$ . For a unitary transformation of the form (10) with general  $\theta(t)$  and  $\mathbf{n}(t)$  it is straightforward to derive

$$\mathcal{Q} = \frac{1}{2} \left( 1 + \mathbf{n}(0) \cdot \frac{\dot{\theta} \mathbf{n} + \cos \theta \sin \theta \dot{\mathbf{n}} - \sin^2 \theta \mathbf{n} \times \dot{\mathbf{n}}}{|\mathbf{R}|} \right). \quad (15)$$

We have assumed that  $U(0)$  is given by the identity matrix so that  $\theta(0) = 0$  and  $\mathbf{R}(0) = \dot{\theta}(0)\mathbf{n}(0)$ . To examine when  $\mathcal{Q}$  can become small we focus on a special case of adiabatic evolutions, characterized by  $\dot{\theta} \gg |\dot{\mathbf{n}}|$ . In this case we can neglect all terms containing  $\dot{\mathbf{n}}$  such that  $|\mathbf{R}| \approx \dot{\theta}$ . We then arrive at the conclusion that the AT is maximally violated if  $\mathbf{n}(t) \approx -\mathbf{n}(0)$ , as in the case for the example given above. We note that many other adiabatic evolutions do not fulfill  $\dot{\theta} \gg |\dot{\mathbf{n}}|$ , since it implies that  $\dot{\theta} > 0$  so that  $U(t)$  has to become equal to the identity again within the fast time scale  $1/\dot{\theta}$ . For instance, a LZT, for which  $\mathbf{R}(t) = \Omega \mathbf{e}_x - \dot{\Delta}_0 t / 2 \mathbf{e}_z$  for constant real  $\Omega$  and  $\dot{\Delta}_0$ , asymptotically fulfills  $\mathbf{R}(t) \approx -\mathbf{R}(-t)$ , but not  $\dot{\theta} \gg |\dot{\mathbf{n}}|$  so that  $\mathcal{Q} \approx 1$  is still valid.

Equation (15) is a universal criterion for the failure of the AT for two-level systems. Although it is likely that the small but resonant terms in our counterexample (CE) are the cause for this failure, a nonresonant CE to the consistency of the standard statement of the AT is not necessarily excluded. This is because Eq. (15) depends only on the initial and final Hamiltonians and the final unitary matrix  $U$ , and therefore makes no reference to the behavior during the evolution.

It is worthwhile to examine whether a resonant behavior as in our CE is excluded by the conditions imposed on the Hamiltonian in more rigorous forms of the AT. The two cases we do consider both require the usual gap condition for the energy levels, which is fulfilled in the CE. In addition, Kato [3] demands  $dH(s)/ds$  to be finite for  $\tau \rightarrow \infty$ , where  $s = t/\tau$  is a scaled time variable. This is the case for the CE [13]. In another proof of the AT, Avron *et al.* [11] require the Hamiltonian to be at least twice continuously differentiable, which is also fulfilled by the CE [14]. In this case the AT (Theorem 2.8 of Ref. [11]) is slightly different and states that  $P_{U|+(0)\rangle}$  stays close to  $P_{U_A|+(0)\rangle}$ , where the unitary operator  $U_A(t)$  is generated by the modified Hamiltonian

$$H_A(t) = H(t) + i[\dot{P}_{|+(t)\rangle}, P_{|+(t)\rangle}] \quad (16)$$

[cf. Eq. (1.0) and Lemma 2.2 of Ref. [11]]. For the CE presented above, we have numerically solved the Schrödinger equation (in the scaled time  $s = t/\tau$ ) for the propagator  $U_A$  and calculated the fidelity (or overlap)

$$\mathcal{F} = \text{Tr} \sqrt{P_{U|+(0)\rangle}^{1/2} P_{U_A|+(0)\rangle} P_{U|+(0)\rangle}^{1/2}} \quad (17)$$

between the exact time evolution and the eigenvector subspace propagated with  $H_A$ . The result is shown in Fig. 1. As in our analytical results the overlap becomes zero for  $t/\tau = 1/2$  where the maximal violation occurs.

Thus it seems that the conditions on the AT are not strict enough to exclude the CE. A way to exclude resonant but small behavior may be to demand continuous differentiability of  $H(s)$  even in the limit  $\tau \rightarrow \infty$ . However, while this would be a sufficient criterion to exclude resonances, it may not be a necessary criterion and thus could exclude other cases in which the AT works well. Also, since it is not proven that resonances are the cause of problems, this criterion might not exclude other cases where the AT may become problematic.

*Remarks on the validity of the AT.*—Although the standard statement of the AT may be problematic in certain applications, previous results based on the AT are generally not necessarily affected. The reason is that the inconsistency is not related to the validity of the AT as an approximation but to its application in formal derivations.

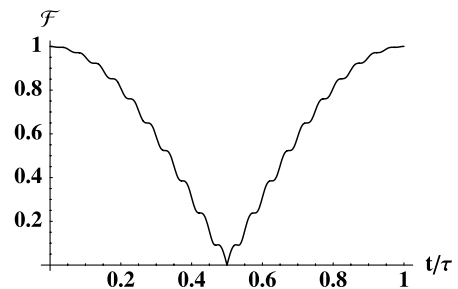


FIG. 1. Fidelity  $\mathcal{F}$  of Eq. (17) for  $\omega_0 = 1 \text{ s}^{-1}$  and  $\tau = 2\pi \times 10 \text{ s}^{-1}$ .

In addition, most applications of the AT as an approximation do not include resonant perturbations, so that the AT should provide an excellent approximation to the exact time evolution. This is the case, for instance, for a real spin- $\frac{1}{2}$  system in a slowly rotating magnetic field ( $\tilde{\mathbf{R}} = 0$  in the Hamiltonian above) and for LZTs. The correctness of the LZT may also guarantee that the results of adiabatic quantum computation [8] remain valid because, for a two-level system, the latter can be mapped to the first. However, if the reversed time evolution  $U^\dagger(t, t_0)$  were to be computed using Eq. (4), the inconsistency could yield an incorrect state.

An example where the inconsistency associated with the AT poses a significant problem is a perturbative treatment of the GP. For brevity we refer to Refs. [6,9,15] for explanations of the technical terms and the GP used in this paragraph. Under the condition of parallel transport [15] the GP of an evolving state is given by the phase of  $\langle\psi(0)|\psi(t)\rangle = \langle\psi(0)|U(t)|\psi(0)\rangle$ . If we consider the case that the unitary operator is slightly perturbed by an operator  $P$ , one can show that for an open quantum system the associated corrections include terms of the forms  $\langle\psi(0)|U(t)P|\psi(0)\rangle$  and  $\langle\psi(0)|PU(t)|\psi(0)\rangle$  [16]. In order to calculate these corrections one needs, in particular, to find an expression for the state  $\langle\psi(0)|U(t) = (U^\dagger(t)|\psi(0))^\dagger$ . It is obvious that the inconsistency would then lead to a wrong result for the GP.

In general, a potential problem in the application of the AT could be the presence of small fluctuations in an experiment, even if the ideal case would not be affected by the inconsistency. The reason is that example (10) indicates that small changes can invalidate the predictions of the AT, even if they respect the adiabaticity criterion (2). In the two-level CE, the small terms proportional to  $\tilde{\mathbf{R}}$  in the Hamiltonian change a system where the AT is valid to one where it is maximally violated. Thus whenever adiabatic fluctuations are present in an experiment, it seems to be necessary to check the predictions of the AT. This could be done by checking the quantities  $\mathcal{F}_0$  and  $\mathcal{Q}$  for mixed states. To be more specific, we consider a system with fluctuations in the classical parameters that determine its Hamiltonian. Thus, in each run the system undergoes a unitary evolution, described by a Hamiltonian  $H^{(\alpha)}(t)$  which occurs with probability  $p_\alpha$ . Assuming that the system initially is always prepared in an eigenstate  $|E_\alpha(0)\rangle$ , the density matrix for the fluctuating system is given by  $\rho(t) = \sum_\alpha p_\alpha U_\alpha(t)P_{|E_\alpha(0)\rangle}U_\alpha^\dagger(t)$ , and one finds

$$\mathcal{F}_0 = \text{Tr} \sum_\alpha p_\alpha P_{|E_\alpha(0)\rangle} P_{|E_\alpha(t)\rangle}, \quad (18)$$

$$\mathcal{Q} = \text{Tr} \sum_\alpha p_\alpha P_{U_\alpha|E_\alpha(0)\rangle} P_{|E_\alpha(t)\rangle}. \quad (19)$$

For some index  $\alpha$ , the application of the AT may fail, but averaging over  $\alpha$  could mitigate the deleterious effects.

The exploration of the AT for fluctuating systems and mixed states [17] is an important future direction for ascertaining the validity and limits of the AT.

In conclusion, we have demonstrated an inconsistency implied by the standard statement of the AT and presented a counterexample of a two-level system. Both examples alert us to the fact that the AT must be applied with care. Further work will concern testing the AT for various systems, especially those that involve stochastic fluctuations and mixed states.

Since this work first appeared as a preprint [18], two subsequent preprints appeared that deal with our inconsistency. Sarandy *et al.* [19] have presented a simplified form of the inconsistency which they regard as a validation of the standard statement of the AT. We interpret their work as an alternative explanation of the cause of the inconsistency and a second demonstration that the standard statement of the AT, taken as it is, can lead to contradictory results. Pati and Rajagopal [20] consider a different form of inconsistency. Comments on their work and the present inconsistency have been made in Ref. [21].

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