

Quantum adiabatic theorem in light of the Marzlin-Sanders inconsistency

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A consensus that questions the perfunctory use of the quantum adiabatic theorem has emerged since Marzlin and Sanders [Phys. Rev. Lett. **93**, 160408 (2004)] showed the existence of an inconsistency in the applicability of the theorem. Further analysis proved that the inconsistency may arise from the existence of resonant terms in the Hamiltonian, but recent work indicates that the debate about the full extent of the problem remains open. Here, we first show that key premises required in the standard demonstration of the theorem do not hold for a dual Hamiltonian involved in the Marzlin-Sanders inconsistency. Also, we show that two simple conditions can identify systems for which the adiabatic approximation fails, in spite of satisfying traditional quantitative conditions that were believed to guarantee its validity. Finally, we prove that the inconsistency only arises for Hamiltonians that contain resonant terms whose amplitudes go asymptotically to zero.

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I. INTRODUCTION

A folk quantum adiabatic theorem (QAT) establishes that a system initially described by an eigenstate associated with an isolated eigenvalue of an instantaneous time-dependent Hamiltonian, $H(0)$, will be at further times in the corresponding eigenstate of $H(t)$ if H changes slowly enough. The rate at which the adiabatic limit is reached depends on the gap separating the eigenvalue of interest from the rest of the energy spectrum.

The theorem was initially proven by Born and Fock [1] for bounded Hamiltonians with discrete energy levels and extended later by Kato [2] who removed the assumption of spectral discreteness, provided the initial eigenstate corresponds to a discrete eigenvalue. On the other hand, Avron and Elgart [3] showed that an adiabatic theorem can be formulated for systems with no spectral gaps. In practice, when the Hamiltonian variation is not infinitely slow, the adiabatic theorem does not hold although, under certain conditions, the dynamics can be approximately adiabatic. Statements about these conditions constitute the so-called adiabatic approximation [4]. The present paper deals, somehow simultaneously, with the theorem and the approximation, but we emphasize that both concepts are not synonymous and must be clearly distinguished.

The publication in 2004 of a paper [5] pointing out an inconsistency in the theorem has resulted in a new consensus among an increasing number of physicists, which indicates that “extreme caution should be used when interpreting results based on the standard application of the theorem” [6]. The so-called Marzlin-Sanders inconsistency [5] can be presented in the following simple way due to Tong *et al.* [7]: If a system S_a evolves adiabatically under the dynamics generated by a Hamiltonian $H_a(t)$, a dual system S_b , described by the Hamiltonian $H_b(t) = -U_a(t,0)^\dagger H_a(t) U_a(t,0)$, where $U_a(t,0)$ is the exact evolution operator for system S_a , does not evolve adiabatically in general. However, both systems satisfy the same quantitative requirements

$$\left| \frac{\langle E_m(t) | \dot{E}_n(t) \rangle}{E_n(t) - E_m(t)} \right| \ll 1, \quad m \neq n, \quad \forall t, \quad (1)$$

that traditionally were considered to guarantee that a given Hamiltonian [with eigenpairs $E_n(t)$, $|E_n(t)\rangle$] evolves slowly enough.

Tong *et al.* [7] attributed the inconsistency to the insufficiency of Eq. (1). Comparat [8] argued that Eq. (1) is valid to detect adiabatic systems except when the Hamiltonian contains oscillatory terms. MacKenzie *et al.* [4] emphasized the differences between adiabatic approximation and adiabatic theorem and explained that the inadequacy of the quantitative conditions arises in situations where the approximation, but not the theorem, is invalid. Duki *et al.* [9] showed that the paradox results from the breakdown of the adiabatic approximation for the dual system. Similarly, Amin [10] showed that the inconsistency arises because the dual Hamiltonian contains resonant terms. Other authors [11,12] indicated that the dual Hamiltonian, H_b , present multiple time scales and for that reason adiabatic theorems do not apply to it. Finally, some works have denied the inconsistency [13,14].

The current consensus indicates that QAT has been rigorously proven beyond any doubt, and it is not in question. In fact, no problems have been reported so far in the derivations of the theorem. The dominant notion seems to be that the Marzlin-Sanders paradox is related to a failure or insufficiency of the conditions that assure that the adiabatic approximation is applicable to a particular system. Following this line of thought, large efforts have been dedicated to propose new adiabatic conditions [4,8,11,12,15–19]. Nonetheless, recent work [20,21] indicates that the debate about the full extent of the inconsistency remains open.

Here, by carefully examining the standard proof of QAT due to Messiah [22], we show in Sec. II that the theorem does not hold for the dual system because some key premises required in the demonstrations of the theorem are not satisfied by H_b . This confirms that only the adiabatic approximation is affected by the Marzlin-Sanders inconsistency, while the theorem is correct [4]. As a result of our analysis we show in Sec. III that two simple conditions can be used to determine if a system for which Eq. (1) holds satisfies the adiabatic approximation. We illustrate our findings in Sec. IV with an example. In Sec. V we discuss the full extent of the inconsistency, showing that it only arises when the Hamiltonian contains resonant oscillatory

terms whose amplitude goes to zero in the asymptotic limit. Finally, we give a summary and a general discussion in Sec. VI.

II. THE QUANTUM ADIABATIC THEOREM

A. Premises

The adiabatic theorem refers to the limit in which a time-dependent Hamiltonian $H_a(t)$ varies infinitely slowly. The theorem gives approximate solutions to the time-dependent Schrödinger equation in an interval $0 \leq t \leq \tau$, when $\tau \rightarrow \infty$ and the total change of $H_a(t)$ is finite [2]. Using a scaled time variable s defined by $t = \tau s$, $0 \leq s \leq 1$, the Schrödinger equation can be written

$$i\hbar \frac{d\phi(s)}{ds} = \tau H_a(s)\phi(s). \quad (2)$$

In the following, we assume that the energy spectrum is discrete at all times as the Marzlin-Sanders paradox arises in such a context. Hence, the following theorem

$$U_a(s)P_n^a(0) - P_n^a(s)U_a(s) = O(1/\tau), \quad \tau \rightarrow \infty, \forall n, \quad (3)$$

can be proven under the following additional premises [22]: (p1) the eigenvalues $E_n^a(s)$ are continuous functions of s , (p2) there are no eigenvalue crossings (i.e., $E_n^a(s) \neq E_m^a(s)$, $n \neq m$, $s \in [0, 1]$), and (p3) the derivatives of the eigenprojectors, $dP_n^a(s)/ds$ and $d^2P_n^a(s)/ds^2$, are well defined and are piecewise continuous in the interval $0 \leq s \leq 1$. For simplicity $H_a(s)$ is usually assumed to be independent of τ but the arguments leading to the adiabatic theorem apply similarly to the case in which H_a depends explicitly on τ , as far as premises (p1)–(p3) are uniformly fulfilled for $\tau \rightarrow \infty$ [2,23].

B. Sketch of the standard proof of the theorem

Messiah's demonstration [22] is based on the use of a virtual evolution operator, $U_A(s)$, defined by Kato [2], that takes the system from a given eigenstate at the initial time to the corresponding eigenstate at future times. A purely geometric evolution is realized by [24]

$$U_A(s) = \sum_n |E_n^a(s)\rangle\langle E_n^a(0)|, \quad (4)$$

where the phases of the instantaneous eigenfunctions, $|E_n^a(s)\rangle$, are such that the parallel-transport condition $\langle E_n^a(s)|\dot{E}_n^a(s)\rangle = 0$ is satisfied. Operator U_A fulfills the so-called intertwining property

$$U_A(s)P_n^a(0) = P_n^a(s)U_A(s), \quad (5)$$

and therefore, QAT, Eq. (3), can be proven by showing that

$$\lim_{\tau \rightarrow \infty} U_A^\dagger(s)U_a(s) = \Phi_A(s)[1 + O(1/\tau)], \quad (6)$$

where the operator $\Phi_A(s)$ can be expanded in terms of the eigenprojectors at $s = 0$ multiplied by phase factors

$$\Phi_A(s) = \sum_n \exp\left[-i\tau/\hbar \int_0^s E_n^a(\sigma)d\sigma\right] P_n^a(0). \quad (7)$$

Messiah showed that the solution of the evolution equation for operator $\Omega_A \equiv U_A^\dagger U_a$ goes to Φ_A in the limit $\tau \rightarrow \infty$. For that, he made two unitary transformations over the evolution

equation in the Schrödinger representation. This procedure leads to the following Volterra integral evolution equation for operator $W_A \equiv \Phi_A^\dagger \Omega_A$:

$$W_A(s) = 1 + (i/\hbar) \int_0^s \bar{K}_a(\sigma)W_A(\sigma)d\sigma, \quad (8)$$

where the kernel,

$$\bar{K}_a(s) = \Phi_A^\dagger(s)U_A^\dagger(s)K_a(s)U_A(s)\Phi_A(s), \quad (9)$$

depends on the following operator:

$$K_a(s) = i\hbar \sum_n \dot{P}_n^a(s)P_n^a(s), \quad (10)$$

which is the generator of the virtual evolution given by U_A . The completion of the proof requires showing that the integral in the Volterra equation goes to zero when $\tau \rightarrow \infty$. If that is the case, Eq. (8) gives $W_A \rightarrow 1$, and from the definition of Ω_A results $\Omega_A \rightarrow \Phi_A$, and finally $U_a \rightarrow U_A \Phi_A$.

An estimate of the integral in Eq. (8) can be obtained by substituting in Eq. (9) the standard expansion $K_a = \sum_{nm} P_n(0)K_a P_m(0)$, and Eq. (7), which gives the following expression for the kernel:

$$\begin{aligned} \bar{K}_a(s) = i\hbar \sum_{m \neq n} \exp\left[(i\tau/\hbar) \int_0^s [E_m^a(\sigma) - E_n^a(\sigma)]d\sigma\right] \\ \times \langle E_m^a(s)|\dot{E}_n^a(s)\rangle |E_m^a(0)\rangle\langle E_n^a(0)|. \end{aligned} \quad (11)$$

Nondiagonal elements of the kernel contain exponential factors whose phases are never stationary because they oscillate at frequencies that increase with τ , as far as the differences $E_n^a(\sigma) - E_m^a(\sigma)$ are nonzero (i.e., if the eigenvalues are separated by gaps). Messiah showed that the integral in Eq. (8) can be expressed as a sum of two terms, which contain as a factor the operator

$$F_a(s) \equiv \int_0^s \bar{K}_a(\sigma)d\sigma. \quad (12)$$

Thus, if $F_a(s)$ goes to zero, the integral in the Volterra equation will go to zero, too. Due to the presence of oscillatory factors in the kernel, operator $F_a(s)$ approaches zero if the elements $\langle E_m^a(s)|\dot{E}_n^a(s)\rangle$ are continuous functions of s , and their derivatives remain finite for all s [22].

III. IDENTIFICATION OF SYSTEMS AFFECTED BY THE INCONSISTENCY

A. The dual system

Amin [10] showed, by taking into account the adiabaticity of S_a , that the dual Hamiltonian H_b can be expanded as

$$\begin{aligned} H_b(s, \tau) = - \sum_n E_n^a(s) |E_n^a(0)\rangle\langle E_n^a(0)| \\ - \frac{i\hbar}{\tau} \sum_{m \neq n} \exp\left[-i\tau/\hbar \int_0^s [E_n^a(\sigma) - E_m^a(\sigma)]d\sigma\right] \\ \times \langle E_m^a(s)|\dot{E}_n^a(s)\rangle |E_m^a(0)\rangle\langle E_n^a(0)|, \end{aligned} \quad (13)$$

where the expression given in Ref. [10] has been rewritten here as a function of scaled time.

Similarly, the eigenprojectors P_b can be written as

$$P_n^b(s, \tau) = P_n^a(0) - \frac{i\hbar}{\tau E_n^a(s)} \times \sum_m \exp \left[(-i\tau/\hbar) \int_0^s [E_n^a(\sigma) - E_m^a(\sigma)] d\sigma \right] \times \langle E_m^a(s) | \dot{E}_n^a(s) \rangle | E_m^a(0) \rangle \langle E_n^a(0) |, \quad (14)$$

which shows that the Hamiltonian and the eigenprojectors for the dual system depend explicitly on τ . This fact does not invalidate *a priori* the adiabatic theorem as far as premises (p1)–(p3) hold when $\tau \rightarrow \infty$.

Premises (p1) and (p2) depend only on the gaps between pairs of eigenvalues. Therefore, they are equally satisfied for H_a and H_b since $E_n^b(s) = -E_n^a(s)$. However, premise (p3) does not hold for H_b , since the operator-valued functions, dP_n^b/ds and $d^2P_n^b/ds^2$, are not defined when $\tau \rightarrow \infty$, because the argument of the exponential in Eq. (14) goes to infinity. The explicit τ dependence of the Hamiltonian, when premise (p3) does not hold, prevents the adiabatic limit for S_b from being reached when $\tau \rightarrow \infty$, unlike for S_a .

The adiabatic theorem holds for the dual system if the integral in the Volterra equation, Eq. (8), for S_b goes to zero in the $\tau \rightarrow \infty$ limit. As explained in Sec. II B such an integral goes to zero whenever (i) the eigenvalues are separated by gaps and (ii) the elements $\langle E_m^b(s) | \dot{E}_n^b(s) \rangle$ are continuous functions of s that remain finite along with their derivatives for all s . Thus, the adiabatic theorem would be satisfied for the dual system if (ii) holds since (i) is automatically guaranteed because $H_b(s)$ has the same spectral gaps as $H_a(s)$, which is adiabatic by hypothesis.

A wrong reasoning indicates that the integral in the Volterra equation should go to zero for system S_b as it does for S_a , since Eqs. (4)–(11) are apparently valid for S_b if subscript $A(a)$ is changed to $B(b)$. Then, the exact Ω_B would tend to an operator analogous to Eq. (7) and QAT would hold for S_b . From $E_n^b(s) = -E_n^a(s)$ and $P_n^a(0) = P_n^b(0)$, this operator is $\Phi_B = \Phi_A^\dagger$.

B. Properties satisfied by the dual system in the $\tau \rightarrow \infty$ limit

The naivety of the previous argument is exposed by realizing that a virtual adiabatic operator for S_b is given, in general, as $U_B = U_A^\dagger U_A \Phi$. Note that a Volterra equation analogous to Eq. (8) is obtained *only* if U_B is a geometric evolution operator; that is, if it can be expanded like Eq. (4) in terms of eigenfunctions of H_b that satisfy $\langle E_n^b(s) | \dot{E}_n^b(s) \rangle = 0$. The following relationship between parallel-transport eigenfunctions of S_a and S_b :

$$|E_n^b(s, \tau)\rangle = \exp \left[(-i\tau/\hbar) \int_0^s E_n^a(\sigma) d\sigma \right] U_A^\dagger(s) |E_n^a(s)\rangle, \quad (15)$$

allows us to expand the virtual evolution operator U_B in terms of eigenfunctions of S_a , which satisfy $\langle E_n^a(s) | \dot{E}_n^a(s) \rangle = 0$, as

$$U_B(s, \tau) = \sum_n \exp \left[(-i\tau/\hbar) \int_0^s E_n^a(\sigma) d\sigma \right] \times U_a(s)^\dagger |E_n^a(s)\rangle \langle E_n^a(0)|. \quad (16)$$

On the other hand, the relation between the eigenprojectors of both systems

$$P_n^b(s, \tau) = U_a^\dagger(s) P_n^a(s) U_a(s), \quad (17)$$

gives $K_b(s) = U_a^\dagger(s) K_a(s) U_a(s)$, which can be substituted, along with $\Phi_B(s) = \Phi_A^\dagger(s)$, and Eq. (16), in the analogous equation to Eq. (9) appropriate for system S_b , to obtain

$$\bar{K}_b = \Phi_B^\dagger U_B^\dagger K_b U_B \Phi_B = \Phi_A \Phi_A^\dagger U_A^\dagger U_a U_a^\dagger K_a U_a U_a^\dagger U_A \Phi_A \Phi_A^\dagger, \quad (18)$$

where the s dependence has been omitted for simplicity. Finally, by using the equations for S_b analogous to Eqs. (4) and (10), \bar{K}_b can be expanded as

$$\bar{K}_b(s) = i\hbar \sum_{m \neq n} \langle E_m^a(s) | \dot{E}_n^a(s) \rangle |E_m^a(0)\rangle \langle E_n^a(0)|, \quad (19)$$

which does not contain oscillating functions. Hence,

$$F_b(s) \equiv \int_0^s \bar{K}_b(\sigma) d\sigma \rightarrow 0 \left(\frac{1}{\tau} \right), \quad (20)$$

which implies that the integral in the Volterra evolution equation does not go to zero. In other words,

$$\int_0^s \bar{K}_b(\sigma) W_B(\sigma) d\sigma \rightarrow 0 \left(\frac{1}{\tau} \right), \quad (21)$$

because

$$\begin{aligned} \lim_{\tau \rightarrow \infty} \int_0^s \exp \left\{ (i\tau/\hbar) \int_0^\sigma [E_m^b(\sigma') - E_n^b(\sigma')] d\sigma' \right\} \\ \times \langle E_m^b(\sigma) | \dot{E}_n^b(\sigma) \rangle d\sigma \\ = \int_0^s \langle E_m^a(\sigma) | \dot{E}_n^a(\sigma) \rangle d\sigma \rightarrow 0, \end{aligned} \quad (22)$$

due to the cancellation of the exponential factors.

The adiabatic theorem does not hold for system S_b because the mechanism that makes the integral in Eq. (8) approach zero for S_a fails for S_b in spite of the fact that both systems have the same spectral gaps. The reason is that the oscillations of the elements $\langle E_m^b(s) | \dot{E}_n^b(s) \rangle$ cancel the terms that arise from the gap condition. We emphasize that this does not imply an inconsistency in QAT since system H_b does not satisfy the hypotheses of the theorem. Here, we prove that systems for which the effects of the gap condition are canceled can be easily identified by simple conditions. Also, we will show that such conditions can be applied without modification to identify systems that do not satisfy the adiabatic approximation in spite of satisfying Eq. (1).

By substituting the relationship between the eigenprojectors of systems S_a and S_b , Eq. (17), into the intertwining property, Eq. (5), which U_A satisfies due to the adiabaticity of S_a , we get

$$[U_a^\dagger(s) U_A(s)] P_n^b(0) [U_A(s)^\dagger U_a(s)] = P_n^b(s, \tau). \quad (23)$$

By taking the $\tau \rightarrow \infty$ limit, and substituting Eq. (6) into the previous expression, we obtain

$$\lim_{\tau \rightarrow \infty} P_n^b(s, \tau) = P_n^b(0) [1 + O(1/\tau)]^2, \quad \forall n, s \in [0, 1], \quad (24)$$

which holds for systems affected by the Marzlin-Sanders inconsistency; that is, for systems that satisfy Eq. (1) but do

not evolve adiabatically. However, Eq. (24) is ambiguous and therefore is not a sufficient condition. In effect, a system S_c with Hamiltonian $-H_b$ has the same eigenprojectors but, being the Heisenberg representation of H_a , is trivially adiabatic. This ambiguity can be eliminated by finding some other property that holds for S_b but not for S_c . The kernel for $H_c = -H_b$ is

$$\bar{K}_c(s) = \Phi_A^\dagger \Phi_A^\dagger U_A^\dagger K_a U_A \Phi_A \Phi_A, \quad (25)$$

which shows that the phase cancellation that produces the inconsistency for system S_b does not occur for system S_c . The kernel expansion for S_c contains oscillatory factors that are related to those of S_a by

$$\begin{aligned} & \exp \left\{ (i\tau/\hbar) \int_0^\sigma [E_m^c(\sigma') - E_n^c(\sigma')] d\sigma' \right\} \langle E_m^c(\sigma) | \dot{E}_n^c(\sigma) \rangle \\ &= \exp \left\{ (2i\tau/\hbar) \int_0^\sigma [E_m^a(\sigma') - E_n^a(\sigma')] d\sigma' \right\} \langle E_m^a(\sigma) | \dot{E}_n^a(\sigma) \rangle, \end{aligned} \quad (26)$$

where the eigenvectors $|E_n^a\rangle, |E_n^c\rangle$ fulfill the parallel-transport condition. Since system S_a is adiabatic by hypothesis, the integral of the expression at the right-hand side of Eq. (26) goes to zero as $1/\tau$, which implies, for $\tau \rightarrow \infty$,

$$\begin{aligned} & \int_0^s \exp \left\{ (i\tau/\hbar) \int_0^\sigma [E_m^c(\sigma') - E_n^c(\sigma')] d\sigma' \right\} \\ & \times \langle E_m^c(\sigma) | \dot{E}_n^c(\sigma) \rangle d\sigma = O(1/\tau), \end{aligned} \quad (27)$$

while, as shown in Eq. (22), the analogous integral for system S_b does not go to zero.

In conclusion, if the eigenprojectors of a given Hamiltonian fulfill Eq. (24), the traditional adiabatic conditions, Eq. (1), are insufficient to determine the adiabaticity of the time evolution. In such a case, only if the integral in the left-hand side of Eq. (22) goes to zero, will the evolution be adiabatic.

C. Properties satisfied by the dual system for finite τ

The adiabatic approximation, as mentioned in the Introduction, is the set of conditions under which the time evolution of a system that evolves during a finite time interval is still approximately adiabatic. A system for which the adiabatic theorem holds when $\tau \rightarrow \infty$ could fail to evolve adiabatically for a certain set of finite values of the parameter τ . However, if the adiabatic theorem does not hold when $\tau \rightarrow \infty$, the evolution cannot be approximately adiabatic for any finite τ . Since the dual system does not obey the adiabatic theorem it does not obey the adiabatic approximation either. However, the failure to obey premise (p3), which invalidates the theorem, refers to the strict adiabatic limit and cannot be used to determine whether the adiabatic approximation does not hold. Next, we show that there exist common conditions that apply to both the adiabatic theorem and the adiabatic approximation, from which we will obtain properties that can be used to determine the validity of Eq. (1).

Previous studies of the Marzlin-Sanders inconsistency have considered mainly the development of new criteria of validity for the adiabatic approximation [4,8,11,12,15,16]. In the following, we use directly the variable t for time instead of s , as it is traditional in the analysis of the adiabatic approximation. Appropriate criteria must identify

unambiguously if a Hamiltonian that acts during a finite time interval varies slowly enough for the state vector at time t to be approximated by the eigenstate $|E_n(t)\rangle$ except for a phase factor, if the state vector at initial time was $|E_n(0)\rangle$.

In the $\tau \rightarrow \infty$ limit, conditions, Eqs. (22) and (24) are sufficient to indicate if a given Hamiltonian H_b does not satisfy the adiabatic theorem. These same conditions can identify systems that satisfy Eq. (1) but that, however, do not satisfy the adiabatic approximation. In effect, if H_a satisfies the adiabatic approximation, we get

$$U_a(t) \approx U_a(t) \Phi_A(t). \quad (28)$$

Substituting this expression in Eq. (23), which approximately holds for finite but long enough τ , we obtain

$$P_n^b(t) \approx P_n^b(0), \quad \forall t. \quad (29)$$

On the other hand, Eq. (22) holds too, because the matrix elements $\langle E_m^b(t) | \dot{E}_n^b(t) \rangle$ cancel the exponentials arising from the gap condition for finite τ as in the $\tau \rightarrow \infty$ case. Finally, if the adiabatic approximation is obeyed, the integral in Eq. (27) will be small.

IV. EXAMPLE

The previous results can be illustrated by analyzing a model that has been extensively studied in relation to the Marzlin-Sanders inconsistency. This model consists of a spin-half particle in a rotating magnetic field whose Hamiltonian is [7]

$$H_a(t) = -\omega_0/2(\sigma_x \sin \theta \cos \omega t + \sigma_y \sin \theta \sin \omega t + \sigma_z \cos \theta), \quad (30)$$

where ω and ω_0 are constants, while the σ_i are Pauli matrices. The instantaneous eigenvalues are $E_1^a(t) = \omega_0/2$ and $E_2^a(t) = -\omega_0/2$, while the instantaneous eigenvectors are [7]

$$|\bar{E}_1^a(t)\rangle = \begin{pmatrix} e^{-i\omega t/2} \sin \frac{\theta}{2} \\ -e^{i\omega t/2} \cos \frac{\theta}{2} \end{pmatrix}, \quad (31)$$

and

$$|\bar{E}_2^a(t)\rangle = \begin{pmatrix} e^{-i\omega t/2} \cos \frac{\theta}{2} \\ e^{i\omega t/2} \sin \frac{\theta}{2} \end{pmatrix}, \quad (32)$$

which do not obey the parallel-transport phase condition.

The Hamiltonian (30) can be written as a function of scaled time $s = 2\pi t/\tau = \omega t$:

$$H_a(s) = -\omega_0/2(\sigma_x \sin \theta \cos s + \sigma_y \sin \theta \sin s + \sigma_z \cos \theta). \quad (33)$$

Eigenfunctions of $H_a(s)$ that obey the parallel-transport condition are given, after transforming Eqs. (31) and (32) to scaled time, by $|E_n\rangle = \exp(-\int_0^s \langle \bar{E}_n | \dot{\bar{E}}_n \rangle d\sigma) |\bar{E}_n\rangle$. Thus, we get

$$|E_1^a(s)\rangle = e^{-i(s/2)\cos \theta} \begin{pmatrix} e^{-is/2} \sin \frac{\theta}{2} \\ -e^{is/2} \cos \frac{\theta}{2} \end{pmatrix}, \quad (34)$$

and

$$|E_2^a(s)\rangle = e^{i(s/2)\cos \theta} \begin{pmatrix} e^{-is/2} \cos \frac{\theta}{2} \\ e^{is/2} \sin \frac{\theta}{2} \end{pmatrix}. \quad (35)$$

Finally, note that the adiabatic limit for $H_a(s)$ corresponds to $\tau \rightarrow \infty$, which is equivalent to $\omega \rightarrow 0$. Such a limit is not physically realizable, but that is not relevant for the illustration of the inconsistency.

A. The $\omega \rightarrow 0$ limit

We showed above that a dual Hamiltonian $H_b(s, \tau) = -U_a^\dagger(s, \tau)H_a(s)U_a(s, \tau)$ does not satisfy, in general, the

adiabatic theorem. Let us study the case corresponding to H_a given by Eq. (33). Hamiltonian H_b can be written as

$$H_b(s, \tau) = - \sum_n E_n^a P_n^b(s, \tau), \tag{36}$$

where the instantaneous eigenprojectors are given by $P_n^b = U_a^\dagger P_n^a U_a$. Transforming the expression for U_a given by Tong [7] to scaled time, we get

$$U_a(s, \tau) = \begin{pmatrix} \left(\cos \frac{\bar{\omega}s}{2\omega} + i \frac{\omega + \omega_0 \cos \theta}{\bar{\omega}} \sin \frac{\bar{\omega}s}{2\omega} \right) e^{-is/2} & i \frac{\omega_0 \sin \theta}{\bar{\omega}} \sin \frac{\bar{\omega}s}{2\omega} e^{-is/2} \\ i \frac{\omega_0 \sin \theta}{\bar{\omega}} \sin \frac{\bar{\omega}s}{2\omega} e^{is/2} & \left(\cos \frac{\bar{\omega}s}{2\omega} - i \frac{\omega + \omega_0 \cos \theta}{\bar{\omega}} \sin \frac{\bar{\omega}s}{2\omega} \right) e^{is/2} \end{pmatrix}, \tag{37}$$

where $\bar{\omega} = (\omega_0^2 + \omega^2 + 2\omega\omega_0 \cos \theta)^{1/2}$. On the other hand, the following matrix representation for P_1^a can be constructed from the instantaneous eigenvector, Eq. (34):

$$P_1^a(s) = \begin{pmatrix} \sin^2 \frac{\theta}{2} & -\sin \frac{\theta}{2} \cos \frac{\theta}{2} e^{-is} \\ -\sin \frac{\theta}{2} \cos \frac{\theta}{2} e^{is} & \cos^2 \frac{\theta}{2} \end{pmatrix}. \tag{38}$$

The matrix representation for the instantaneous eigenprojector $P_1^b(s)$ can be calculated from the previous two equations and has a complicated form. For example, one of its matrix elements is

$$\begin{aligned} [P_1^b(s, \tau)]_{12} &= \sin^2 \left(\frac{\bar{\omega}}{2\omega} s \right) \left[\frac{\omega_0(\omega + \omega_0 \cos \theta)}{\bar{\omega}^2} \sin \theta \sin^2 \frac{\theta}{2} - \left(\frac{\omega_0 \sin \theta}{\bar{\omega}} \right)^2 \sin \frac{\theta}{2} \cos \frac{\theta}{2} \right. \\ &\quad \left. + \left(\frac{\omega + \omega_0 \cos \theta}{\bar{\omega}} \right)^2 \sin \frac{\theta}{2} \cos \frac{\theta}{2} - \frac{\omega_0 \sin \theta (\omega + \omega_0 \cos \theta)}{\bar{\omega}^2} \cos^2 \frac{\theta}{2} \right] \\ &\quad - \cos^2 \left(\frac{\bar{\omega}}{2\omega} s \right) \sin \frac{\theta}{2} \cos \frac{\theta}{2} + i \sin \left(\frac{\bar{\omega}}{2\omega} s \right) \cos \left(\frac{\bar{\omega}}{2\omega} s \right) \\ &\quad \times \left[\frac{\omega_0}{\bar{\omega}} \sin \theta \sin^2 \frac{\theta}{2} + 2 \frac{\omega + \omega_0 \cos \theta}{\bar{\omega}} \sin \frac{\theta}{2} \cos \frac{\theta}{2} - \frac{\omega_0}{\bar{\omega}} \sin \theta \cos^2 \frac{\theta}{2} \right]. \end{aligned} \tag{39}$$

We showed in Eq. (14) that the eigenprojectors of the dual system contain terms that, although they oscillate infinitely fast, go to zero in the $\tau \rightarrow \infty$ limit. Apparently, this is not the case for $[P_1^b]_{12}$. However, Eq. (39) can be written by using well-known trigonometric identities such as

$$\begin{aligned} [P_1^b(s, \tau)]_{12} &= \sin^2 \left(\frac{\bar{\omega}}{2\omega} s \right) \left[- \left(\frac{\omega_0}{\bar{\omega}} \right)^2 \sin \frac{\theta}{2} \cos \frac{\theta}{2} + \left(\frac{\omega}{\bar{\omega}} \right)^2 \sin \frac{\theta}{2} \cos \frac{\theta}{2} \right] \\ &\quad - \cos^2 \left(\frac{\bar{\omega}}{2\omega} s \right) \sin \frac{\theta}{2} \cos \frac{\theta}{2} + 2i \sin \left(\frac{\bar{\omega}}{2\omega} s \right) \cos \left(\frac{\bar{\omega}}{2\omega} s \right) \frac{\omega}{\bar{\omega}} \sin \frac{\theta}{2} \cos \frac{\theta}{2}. \end{aligned} \tag{40}$$

By taking into account that $\omega \rightarrow 0$ implies $\bar{\omega} \rightarrow \omega_0$, we get

$$\begin{aligned} \lim_{\omega \rightarrow 0} [P_1^b(s, \tau)]_{12} &= -\sin \frac{\theta}{2} \cos \frac{\theta}{2} \left[1 - \sin^2 \left(\frac{\bar{\omega}}{2\omega} s \right) \left(\frac{\omega}{\bar{\omega}} \right)^2 + 2i \sin \left(\frac{\bar{\omega}}{2\omega} s \right) \cos \left(\frac{\bar{\omega}}{2\omega} s \right) \frac{\omega}{\bar{\omega}} \right] \\ &= [P_1^b(0)]_{12} [1 + O(\omega) + O(\omega^2)]. \end{aligned} \tag{41}$$

Following the same procedure for the other elements of the eigenprojector matrix we obtain

$$\lim_{\omega \rightarrow 0} P_1^b(s, \tau) = \begin{pmatrix} \sin^2 \frac{\theta}{2} & -\sin \frac{\theta}{2} \cos \frac{\theta}{2} \\ -\sin \frac{\theta}{2} \cos \frac{\theta}{2} & \cos^2 \frac{\theta}{2} \end{pmatrix} \left[1 + O(\omega)M \left(\frac{\bar{\omega}}{2\omega} s \right) + O(\omega^2)N \left(\frac{\bar{\omega}}{2\omega} s \right) \right], \tag{42}$$

where M and N represent matrices whose elements are functions that oscillate infinitely fast. However, they are multiplied by terms that go to zero in the $\omega \rightarrow 0$ limit. Equation (42) shows that $P_1^b(s)$ [and $P_2^b(s)$, which is not given here], in the $\omega \rightarrow 0$ limit, tend to $P_1^b(0)$ [and $P_2^b(0)$]. Note

also that the instantaneous eigenprojectors do not contain several independent time scales. The time dependence has the form $\bar{\omega}s/(2\omega)$, which suggests the use of a new scaled variable $s' = \bar{\omega}s/(2\omega)$. Also, the eigenvalues are constant for this particular example and consequently the Hamiltonian can

be written as a function of s' , too. This shows that the adiabatic limit for H_b , for which QAT would hold, requires $\bar{\omega}/(2\omega) \rightarrow 0$ in addition to $\omega \rightarrow 0$. This limit is physically meaningless.

As explained above, Hamiltonian $H_c = -H_b$ has the same eigenprojectors as H_b but is adiabatic. Both systems can be distinguished by evaluating

$$\int_0^s \exp \left\{ (i/\omega) \int_0^\sigma [E_1(\sigma') - E_2(\sigma')] d\sigma' \right\} \langle E_1(\sigma) | \dot{E}_2(\sigma) \rangle d\sigma, \quad (43)$$

where $E_n(s) = -E_n^a(s)$ for H_b and $E_n(s) = E_n^a(s)$ for H_c . From the relationship between the eigenfunctions of both systems and those of H_a we have

$$\langle E_1(\sigma) | \dot{E}_2(\sigma) \rangle = \exp \left\{ (i/\omega) \int_0^\sigma [E_1^a(\sigma') - E_2^a(\sigma')] d\sigma' \right\} \times \langle E_1^a(\sigma) | \dot{E}_2^a(\sigma) \rangle, \quad (44)$$

and taking into account

$$\langle E_1^a(s) | \dot{E}_2^a(s) \rangle = -\frac{i}{2} \sin \theta e^{is \cos \theta}, \quad (45)$$

Eq. (43) becomes for H_b

$$\begin{aligned} & \int_0^s \exp \left\{ (i/\omega) \int_0^\sigma [E_1^b(\sigma') - E_2^b(\sigma')] d\sigma' \right\} \langle E_1^b(\sigma) | \dot{E}_2^b(\sigma) \rangle d\sigma \\ &= \int_0^s \langle E_1^a(\sigma) | \dot{E}_2^a(\sigma) \rangle d\sigma = \frac{1}{2} (1 - e^{is \cos \theta}) \tan \theta, \end{aligned} \quad (46)$$

which shows that S_b is not adiabatic unless $\theta = 0, \text{mod } \pi$. However, for H_c , we have

$$\begin{aligned} & \int_0^s \exp \left\{ (i/\omega) \int_0^\sigma [E_1^c(\sigma') - E_2^c(\sigma')] d\sigma' \right\} \langle E_1^c(\sigma) | \dot{E}_2^c(\sigma) \rangle d\sigma \\ &= \int_0^s \exp \left\{ (2i/\omega) \int_0^\sigma [E_1^a(\sigma') - E_2^a(\sigma')] d\sigma' \right\} \\ & \quad \times \langle E_1^a(\sigma) | \dot{E}_2^a(\sigma) \rangle d\sigma \\ &= -\frac{i}{2} \sin \theta \int_0^s e^{i(\frac{2\omega_0}{\omega} + \cos \theta)\sigma} d\sigma \\ &= \frac{\omega \sin \theta \{1 - \exp[\frac{is(2\omega_0 + \omega \cos \theta)}{\omega}]\}}{4(\omega_0 + 2\omega \cos \theta)}, \end{aligned} \quad (47)$$

which goes to zero in the limit $\omega \rightarrow 0$, indicating that the adiabatic theorem holds for system S_c , like for system S_a , regardless of the values of the parameters ω_0 and θ . This example shows the validity of Eqs. (22) and (24) to identify if a Hamiltonian H_b is related to an adiabatic Hamiltonian H_a through $H_b = -U_a^\dagger H_a U_a$.

B. The case of finite ω

System S_a satisfies the adiabatic approximation if ω is small compared to ω_0 , which implies $\bar{\omega} \approx \omega_0$. If we employ this approximation in the expression for the matrix element of the eigenprojector $P_1^b(t)$, which can be obtained writing Eq. (39)

as a function of t , we get

$$\begin{aligned} [P_1^b(t)]_{12} &\approx -\sin \frac{\theta}{2} \cos \frac{\theta}{2} \left[\sin^2 \left(\frac{\omega_0}{2} t \right) + \cos^2 \left(\frac{\omega_0}{2} t \right) \right] \\ & \quad + i \sin \left(\frac{\omega_0}{2} t \right) \cos \left(\frac{\omega_0}{2} t \right) \times 0 \\ &= -\sin \frac{\theta}{2} \cos \frac{\theta}{2}. \end{aligned} \quad (48)$$

The other matrix elements can be simplified in the same way, so we finally obtain $P_1^b(t) \approx P_1^b(0)$, which proves that Eq. (29) holds for this system.

On the other hand, for finite ω (i.e., for finite τ), Eq. (46) becomes

$$\int_0^t \langle E_1^a(\sigma) | \dot{E}_2^a(\sigma) \rangle d\sigma = \frac{1}{2} (1 - e^{i\omega t \cos \theta}) \tan \theta, \quad (49)$$

which indicates that system S_b satisfies the adiabatic approximation only for $\theta = 0, \text{mod } \pi$, while the integral in Eq. (47) is

$$\begin{aligned} & \int_0^t \exp \left\{ 2i \int_0^\sigma [E_1^a(\sigma') - E_2^a(\sigma')] d\sigma' \right\} \langle E_1^a(\sigma) | \dot{E}_2^a(\sigma) \rangle d\sigma \\ &= \frac{\omega \sin \theta \{1 - \exp[it(2\omega_0 + \omega \cos \theta)]\}}{4(\omega_0 + 2\omega \cos \theta)}, \end{aligned} \quad (50)$$

which is small for $\omega_0 \gg \omega$; that is, system S_c satisfies the adiabatic approximation under the same conditions as system S_a , while S_b does not.

V. FULL EXTENT OF THE MARZLIN-SANDERS INCONSISTENCY

Traditional adiabatic conditions, given by Eq. (1), hold for the dual Hamiltonian defined by Tong [7]. However, the time evolution driven by H_b is not adiabatic. We have proven that the ultimate reason behind this inconsistency is the existence in the Hamiltonian of resonant terms that go asymptotically to zero. This makes the gap condition, usually invoked to guarantee adiabatic behavior in the $\tau \rightarrow \infty$ limit, become irrelevant. These peculiarities of Tong's dual Hamiltonian H_b are due to its special relationship with an adiabatic Hamiltonian H_a . In effect, both Hamiltonians are connected by a unitary transformation and a sign change. The transforming unitary operator is the exact time-evolution operator U_a for the adiabatic Hamiltonian. It seems pertinent to investigate the status of the inconsistency for Hamiltonians H_x that are related to an adiabatic Hamiltonian \tilde{H}_a through a more general unitary transformation, with or without a sign change (i.e., $H_x = \pm U_x^\dagger \tilde{H}_a U_x$, where $U_x \neq U_a$).

A. The family H_x is generic

At first sight it may seem that H_x is affected by a fundamental restriction, since its eigenvalues must satisfy $E_n^x = \pm E_n^a$. However, we argue here that all possible cases of interest can be studied within this approach. Specifically, H_x can contain generic oscillatory terms, as can be seen by turning upside down the previous argument relating H_x and \tilde{H}_a . In other words, instead of arguing that generic oscillatory Hamiltonians can be obtained by unitary transformation of a particular

adiabatic Hamiltonian, it can be argued that, for a given Hamiltonian H_x that by hypothesis is generic, appropriate unitary transformations lead to an adiabatic Hamiltonian. These unitary transformations are nonperturbative (i.e., they are not close to the identity). The resulting adiabatic Hamiltonian can be understood as an effective Hamiltonian that contains the effect of resonances [25].

Therefore, given a Hamiltonian $H_x(s, \tau)$ that is generic, in the sense that it may contain strong oscillatory terms (instead of the weak resonances that appear in the dual Hamiltonian used in the Marzlin-Sanders inconsistency), there exists a unitary operator $U_x(s, \tau)$ that depends explicitly on τ such that the transformed Hamiltonian $\pm U_x(s, \tau)H_x(s, \tau)U_x^\dagger(s, \tau) = \tilde{H}_a(s)$ is adiabatic. Note that \tilde{H}_a is not necessarily the same adiabatic Hamiltonian H_a studied in previous sections, since $H_x \neq H_b$. Note also that the unitary operator $U_x(s, \tau)$ is *not* the evolution operator for systems \tilde{S}_a . Thus, this procedure does not impose *a priori* any restriction on H_x . However, the unitary operator U_x is somehow restricted, because it must transform the generic H_x into an adiabatic Hamiltonian. This transformation can be very complicated but it is always possible for Hermitian matrices because they can be diagonalized. Thus, for a given H_x , there is always a similarity transformation with a unitary operator, $U_x = U_D$, that converts H_x into a diagonal matrix D . The time evolution driven by H_x , for an initial function Φ , can be expressed in terms of U_D as [26]

$$i\hbar \frac{\partial}{\partial s} \Psi(s) = \tau D(s) \Psi(s) - i\hbar U_D^\dagger(s, \tau) \frac{\partial U_D(s, \tau)}{\partial s} \Psi(s), \quad (51)$$

where $\Psi = U_D^\dagger \Phi$. When H_x contains strong oscillatory terms the derivative of U_D will be large and the time evolution is not adiabatic. However, the evolution driven by Hamiltonian D is

$$i\hbar \frac{\partial}{\partial s} \Psi(s) = \tau D(s) \Psi(s), \quad (52)$$

which is adiabatic since D does not contain off-diagonal couplings. This proves that a generic H_x can be related by a unitary transformation to an adiabatic Hamiltonian \tilde{H}_a . Strictly, the proof implies that, at least for $U_x = U_D$ and $\tilde{H}_a = D$, the transformation exists. However, it is clear that other adiabatic Hamiltonians can be generated from the same H_x by using less restrictive U_x operators.

B. General relations between H_x and \tilde{H}_a

A generic unitary operator U_x is *always* the evolution operator for an unknown Hamiltonian $\tilde{H} \neq \tilde{H}_a$:

$$i\hbar \frac{dU_x(s, \tau)}{ds} = \tau \tilde{H}(s, \tau) U_x(s, \tau). \quad (53)$$

Parallel-transport eigenfunctions $|E_n^x\rangle$ for H_x can be obtained from eigenfunctions with arbitrary phase $|\bar{E}_n^x\rangle$ as follows:

$$|E_n^x\rangle = \exp \left[- \int_0^s \langle \bar{E}_n^x | \dot{\bar{E}}_n^x \rangle d\sigma \right] |\bar{E}_n^x\rangle. \quad (54)$$

Since we can choose $|\bar{E}_n^x\rangle = U_x^\dagger |\tilde{E}_n^a\rangle$, we get, by using Eq. (53),

$$|E_n^x(s, \tau)\rangle = \exp \left[(-i\tau/\hbar) \int_0^s \langle \tilde{E}_n^a(\sigma) | \tilde{H}(\sigma, \tau) | \tilde{E}_n^a(\sigma) \rangle d\sigma \right] \times U_x^\dagger(s, \tau) |\tilde{E}_n^a(s)\rangle. \quad (55)$$

Thus, for $n \neq m$,

$$\begin{aligned} \langle E_m^x(s, \tau) | \dot{E}_n^x(s, \tau) \rangle &= [(i\tau/\hbar) \langle \tilde{E}_m^a(s) | \tilde{H}(s, \tau) | \tilde{E}_n^a(s) \rangle + \langle \tilde{E}_m^a(s) | \dot{\tilde{E}}_n^a(s) \rangle] \\ &\times \exp \left\{ (i\tau/\hbar) \int_0^s [\langle \tilde{E}_m^a(\sigma) | \tilde{H}(\sigma, \tau) | \tilde{E}_m^a(\sigma) \rangle \right. \\ &\left. - \langle \tilde{E}_n^a(\sigma) | \tilde{H}(\sigma, \tau) | \tilde{E}_n^a(\sigma) \rangle] d\sigma \right\}. \end{aligned} \quad (56)$$

The relation between geometric evolution operators for S_x and \tilde{S}_a contains, in general, an additional phase factor Φ (i.e., $U_X = U_x^\dagger \tilde{U}_A \Phi$). Thus, the kernel, Eq. (9), for S_x is

$$\bar{K}_x = \Phi_X^\dagger \Phi_A^\dagger \tilde{U}_A^\dagger U_x K_x U_x^\dagger \tilde{U}_A \Phi \Phi_X, \quad (57)$$

where $\Phi_X = \tilde{\Phi}_A^\dagger$ if $\tilde{H}_a = -U_x H_x U_x^\dagger$ or $\Phi_X = \tilde{\Phi}_A$ if $\tilde{H}_a = U_x H_x U_x^\dagger$. Operator Φ_X gets canceled in the kernel if $\Phi = \tilde{\Phi}_A$ or $\Phi = \tilde{\Phi}_A^\dagger$, depending on the sign of the transformation connecting H_x and \tilde{H}_a . In both cases, the resulting U_X is not a geometric operator, except in special cases, because the parallel-transport phase fixing condition is not satisfied for eigenfunctions $|E_n^x\rangle = U_x^\dagger \tilde{\Phi}_A |\tilde{E}_n^a\rangle$ or $|E_n^x\rangle = U_x^\dagger \tilde{\Phi}_A^\dagger |\tilde{E}_n^a\rangle$. Hence, the kernel for a generic S_x contains oscillatory terms. Also, Eq. (57) depends on the sign of the transformation that relates H_x to \tilde{H}_a :

$$\begin{aligned} \bar{K}_x(s, \tau) &= -\tau \sum_{m \neq n} \langle \tilde{E}_m^a(s) | \tilde{H}(s, \tau) + (i\hbar/\tau)(d/ds) | \tilde{E}_n^a(s) \rangle \\ &\times |\tilde{E}_m^a(0)\rangle \langle \tilde{E}_n^a(0)| \\ &\times \exp \left\{ (i\tau/\hbar) \int_0^s [\langle \tilde{E}_m^a(\sigma) | \tilde{H}(\sigma, \tau) \pm \tilde{H}_a(\sigma) | \tilde{E}_m^a(\sigma) \rangle \right. \\ &\left. - \langle \tilde{E}_n^a(\sigma) | \tilde{H}(\sigma, \tau) \pm \tilde{H}_a(\sigma) | \tilde{E}_n^a(\sigma) \rangle] d\sigma \right\}. \end{aligned} \quad (58)$$

We will use these relations to study the adiabaticity of S_x based on the characteristics of U_x . Then, we will compare the results with the left-hand side of Eq. (1) for S_x . For that, it is necessary to write Eq. (56) as a function of usual time t instead of s , which gives

$$\left| \frac{\langle E_m^x(t) | \dot{E}_n^x(t) \rangle}{E_n^x(t) - E_m^x(t)} \right| = \left| \frac{(i/\hbar) \langle \tilde{E}_m^a(t) | \tilde{H}(t) | \tilde{E}_n^a(t) \rangle + \langle \tilde{E}_m^a(t) | \dot{\tilde{E}}_n^a(t) \rangle}{\tilde{E}_n^a(t) - \tilde{E}_m^a(t)} \right|. \quad (59)$$

We present, in the following, heuristic arguments instead of rigorous theorems. Thus, this analysis should be seen only as a sketch for future developments of the present work, whose core is the material contained in Sec. III.

C. Status of the inconsistency for various cases

1. H_x does not contain oscillatory terms

As H_x has, by hypothesis, spectral gaps, if it does not contain oscillatory terms, premises (p1)–(p3) in Sec. II hold. Then, in the $\tau \rightarrow \infty$ limit, the evolution is adiabatic. Comparat [8] showed that, in this case, Eq. (1) holds. Thus, no inconsistency *à la* Marzlin-Sanders takes place. In effect, adiabaticity for H_x implies that

$$\int_0^s \overline{K}_x(\sigma) d\sigma \rightarrow O(1/\tau), \quad (60)$$

which, in turn, implies that the kernel cannot contain terms that depend linearly on τ . This means that matrix elements $\langle \tilde{E}_m^a(s) | \tilde{H}(s, \tau) | \tilde{E}_n^a(s) \rangle \approx 0$. Thus, \tilde{H} must be close to \tilde{H}_a or it must be a constant with small time-dependent terms that vary slowly. The first case leads to a contradiction, since then the arguments of the exponentials get canceled and the system will not be adiabatic. Therefore, \tilde{H} must be given by a nearly constant term. Hence, Eq. (59) gives

$$\left| \frac{\langle E_m^x(t) | \dot{E}_n^x(t) \rangle}{E_n^x(t) - E_m^x(t)} \right| \approx \left| \frac{\langle \tilde{E}_m^a(t) | \dot{\tilde{E}}_n^a(t) \rangle}{\tilde{E}_m^a(t) - \tilde{E}_n^a(t)} \right| \ll 1 \quad \forall n, m; \forall t, \quad (61)$$

and no inconsistency results.

2. H_x contains strong resonant oscillatory terms

Previous studies [9,10] have related the Marzlin-Sanders inconsistency to the existence of resonances but have not discriminated between weak and strong perturbations. These previous works did not consider either the $\tau \rightarrow \infty$ limit. Thus, the full extent of the inconsistency and its relation to the standard proof of the adiabatic theorem was not analyzed before.

It is well known that the existence of exact resonances precludes adiabatic behavior [8–10,27]. Thus, we have

$$\int_0^s \overline{K}_x(\sigma) d\sigma \not\rightarrow O(1/\tau). \quad (62)$$

On the other hand, U_x contains strong oscillatory nondiagonal terms, since it relates an adiabatic Hamiltonian to a Hamiltonian with strong oscillatory terms. Thus, $\tilde{H} = i\hbar \dot{U}_x U_x^\dagger$ will contain strong oscillatory terms too and will be very different from H_a . In spite of the fact that the arguments of the exponentials in the kernel, Eq. (58), are not canceled, the kernel integral does not go to zero because the matrix elements $\langle \tilde{E}_m^a(s) | \tilde{H}(s, \tau) | \tilde{E}_n^a(s) \rangle$ are nonmonotonic functions that depend on τ .

The question at stake here is if Eq. (1) holds under these circumstances. If it does, there will be an inconsistency. Note the difference with Tong’s dual system, for which $U_x = U_a$, $\tilde{H} = H_a$, and the matrix elements $\langle \tilde{E}_m^a(t) | \tilde{H} | \tilde{E}_n^a(t) \rangle = 0$. Instead, when the resonances are strong these matrix elements will not be small. Then the matrix elements $\langle E_m^x(t) | \dot{E}_n^x(t) \rangle$ will not be small either. Therefore, the condition, Eq. (1), will not be satisfied, and no inconsistency results.

3. H_x contains strong nonresonant oscillatory terms

Nonresonant oscillatory terms can be safely averaged out, and therefore the exact time evolution is driven by the average Hamiltonian, which does not contain oscillating terms anymore. Thus, in the $\tau \rightarrow \infty$ limit the average Hamiltonian will be adiabatic. Numerous cases exist in the bibliography showing the adequacy of this approach. A well-known example is the time evolution of the molecular alignment that takes place when a molecule interacts via its polarizability with a strong nonresonant laser pulse. This interaction depends on the square of the electric field. The time evolution of the rotational wave functions can be faithfully studied by taking into account only the laser envelope after averaging out the rapid oscillatory terms $\cos^2(\omega t)$, where ω is the nonresonant laser frequency [28]. Thus, if the laser pulse is long enough the evolution is adiabatic, and Sec. V C1 applies.

Summarizing, the Marzlin-Sanders inconsistency takes place for a system S_x *only* if the kernel of the Volterra evolution equation does not oscillate at frequencies that increase with τ and does not contain terms that vary nonmonotonically. The kernel, Eq. (58), fulfills these two conditions if $\tilde{H} \pm H_a = 0$. The case $\tilde{H} = H_a$ implies, from Eq. (53), $U_x = U_a$, and the resulting H_x is precisely the dual Hamiltonian used by Tong [7] (i.e., $H_x = H_b = -U_a^\dagger H_a U_a$). Contrarily, for the positive sign choice in the transformation that relates H_x and H_a , the kernel satisfies the two conditions if $\tilde{H} = -H_a$. In this case, U_x is the exact evolution operator ($\approx U_A^*$) for the reversed Hamiltonian $-H_a$. In rigour, the kernel fulfills the two cited conditions not only if $\tilde{H} = \pm H_a$ but also if \tilde{H} admits a full asymptotic expansion, in powers of τ^{-1} , in which the zero-order term is given by $\pm H_a$ [i.e., if $\tilde{H}(s, \tau) = \pm H_a(s) + \sum_j (i\hbar/\tau)^j H^j(s)$], so the properties derived in Sec. III are approximately valid.

VI. DISCUSSION

The so-called Marzlin-Sanders inconsistency can be described as follows: If Eq. (1) is satisfied for a Hamiltonian H_a for which the adiabatic approximation holds, it will be satisfied too for the Hamiltonian $H_b = -U_a^\dagger H_a U_a$, where U_a is the exact evolution operator for H_a . However, in general, H_b does not satisfy the adiabatic approximation [7]. This implies that Eq. (1) is not a sufficient condition for a system to hold the adiabatic approximation.

The full extent of the inconsistency has been much debated and doubts about the consistency of the own adiabatic theorem have been raised. Here, we have proven that these doubts cannot be sustained. Given a Hamiltonian $H_a(s = t/\tau)$ for which an adiabatic theorem holds in the $\tau \rightarrow \infty$ limit, the dual Hamiltonian $H_b(s, \tau) = -U_a^\dagger(s, \tau) H_a(s) U_a(s, \tau)$ does not satisfy the theorem because H_b contains resonant terms that oscillate infinitely fast although their amplitude go asymptotically to zero. Due to these terms the dual Hamiltonian does not vary infinitely slowly when $\tau \rightarrow \infty$. Also, the derivatives of the eigenprojectors are not defined. Thus, no inconsistency affects the quantum adiabatic theorem because the dual Hamiltonian does not satisfy key premises required in the proofs of the theorem.

In Sec. II A, we showed that premises (p1)–(p3) were imposed to guarantee that some oscillatory integrals that arise in the evolution equations, due to the existence of spectral gaps, go to zero in the adiabatic limit. Therefore, they only make strict sense in such a limit and cannot be used to determine the validity of the adiabatic approximation. However, the adiabatic approximation does not hold for the dual system because the same integrals that do not go to zero in the adiabatic limit are not small for finite τ . On the other hand, the conditions Eq. (1) hold for the dual Hamiltonian because the matrix elements $\langle E_m^b(s) | \dot{E}_n^b(s) \rangle$, although they oscillate fast, have a small magnitude.

Systems affected by the inconsistency can be easily identified because the instantaneous eigenprojectors of the dual Hamiltonian oscillate with negligible amplitude, with respect to a baseline, at frequencies resonant with the energy levels of the system. This baseline is defined by the eigenprojectors at the initial time. As a consequence, the instantaneous eigenprojectors change very little with time. However, the condition, Eq. (24), is necessary but not sufficient for the inconsistency to occur, because it is equally satisfied by the Hamiltonian $-H_b$, which is adiabatic.

On the other hand, the presence of fast oscillations of very small amplitude does not invalidate the adiabatic approximation unless they cancel the oscillatory factors arising from the gap condition (i.e., unless they are resonant). Thus, resonant terms, even if very small, make the gap condition irrelevant.

Also, we have proven, by using an approach different to that of Comparat [8], that the adiabatic approximation does not

hold for Hamiltonians with strong oscillatory terms (resonant or nonresonant). In addition, our analysis indicates that, in this case, Eq. (1) is not satisfied. Hence, we conclude that Eq. (1) is a necessary and sufficient condition for a system to satisfy the adiabatic approximation unless the time-dependent part of the Hamiltonian contains resonant terms of very small magnitude.

In cases for which an analytical expression is known for a particular Hamiltonian, it should be clear, due to the obvious presence of oscillatory terms, that the system does not satisfy the adiabatic approximation even if Eq. (1) holds. Contrarily, when no such analytical expression is known, the inconsistency may be more relevant. This case occurs when the Hamiltonian is known only through experimental information on its energy levels and eigenstates.

In conclusion, the present work eliminates the mystery that has surrounded the adiabatic theorem since the publication of Ref. [5]. Although it is expected that only a few systems will be affected by the inconsistency the condition Eqs. (22) and (24) must supplement the quantitative conditions Eq. (1) whenever the validity of the adiabatic theorem and/or adiabatic approximation are investigated.

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