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# Perturbative analysis of possible failures in the traditional adiabatic conditions

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**Abstract**

The breakdown of adiabatic approximation, demonstrated by Marzlin and Sanders [K.-P. Marzlin, B.C. Sanders, Phys. Rev. Lett. 93 (2004) 160408] and Tong et al. [D.M. Tong, et al., Phys. Rev. Lett. 95 (2005) 110407] for time-evolving "inverse" systems, is traced to the appearance of some nonzero terms in a perturbational treatment and is related to two time scales in the "inverse" systems' Hamiltonian. New adiabatic conditions of Ye et al. [M.-Y. Ye, et al., quant-ph/0509083] can restore the theoretical consistency.
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## 1. Introduction

The quantum adiabatic theorem is one of the oldest fundamental results in quantum physics [1]. It concerns development of systems where the nondegenerate Hamiltonian evolves slowly in time. In the limit when the change of Hamiltonian $H(t)$ is made infinitely slow the system, which started from one of the eigenstates of $H(0)$, passes through the corresponding instantaneous eigenstate of $H(t)$ [2–5]. The adiabatic theorem underlies the adiabatic approximation scheme, which states that if the Hamiltonian $H(t)$ evolves slowly enough by satisfying the adiabatic condition in time interval $t \in [0, T]$, then the evolving state of the system will remain close to its instantaneous eigenstate up to a multiplicative phase factor in the interval $[0, T]$. The adiabatic approximation has potential applications in several areas of physics such as the Landau–Zener transition in molecular physics [6], Gell-Mann–Low theorem in quantum field theory [7] or in the lore of Berry phase [8]. Recently, with the emergence of the new field of quantum information theory, new interest has arisen in the application of the quantum adiabatic theorem [9]. An alternative scheme appeared beside the usual quantum algorithms, based on an adiabatic time evolution of the state of the Hamiltonian where the final Hamiltonian encodes the solution for a given problem [10]. In another application, the Berry phase has been proposed to perform quantum information processing tasks [11]. Both of these concepts exploit the circumstance, that the adiabatically evolving ground state is very robust against decoherence and small perturbations [12]. It is thus important to explore the limits of the adiabatic conditions in order to understand better when the evolution of a quantum system can be considered adiabatic.

In a recent letter Marzlin and Sanders [13] demonstrated on a dual pair of systems (called a-system and b-system), that if the evolution operator of the b-system is the Hermitian conjugate of an adiabatically evolving a-system, then the application of the adiabatic approximation in the b-system can lead to contradiction. Tong et al. [14] explained this inconsistency by pointing out that the widely used traditional adiabatic conditions are not sufficient to guarantee adiabaticity.

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In the present Letter our aim is to find the common root of the problems by analyzing the time evolution of the dual systems in a perturbative manner. In a first order approximation we obtain certain non-vanishing terms in the regime where the traditional adiabatic conditions hold. We point out that these nonzero terms are responsible for the violation of the adiabatic approximation. We further argue that in this case the Hamiltonian of the b-system cannot be written in terms of $t/T$, where $T$ denotes the total evolution time. In addition, an explicit example is provided which on one hand illustrates our arguments, and, on the other hand, allows a new adiabatic condition of Ye et al. [16] to be tested on.

## 2. Analysis of dual pair of systems

### 2.1. Expansion of state

Consider a closed $N$-dimensional quantum system in a state $|\psi(t)\rangle$, which evolves through the time-dependent Schrödinger equation

$$i\frac{d}{dt}\big|\psi(t)\big\rangle = H(t)\big|\psi(t)\big\rangle, \tag{1}$$

where $H(t)$ denotes the time-dependent non-degenerate Hamiltonian of the system and we set $\hbar = 1$. Let us introduce the normalized time $s$ by the variable-transformation $t = sT$, $0 \leqslant s \leqslant 1$, and rewrite Eq. (1) as

$$i\frac{\partial}{\partial s}\big|\psi(s,T)\big\rangle = T\,H(s,T)\big|\psi(s,T)\big\rangle, \tag{2}$$

where $T$ denotes the total evolution time. The instantaneous eigenstates $|E_n(s,T)\rangle$ of the Hamiltonian $H(s,T)$ satisfy

$$H(s,T)\big|E_n(s,T)\big\rangle = E_n(s,T)\big|E_n(s,T)\big\rangle, \quad n = 1,\ldots,N, \tag{3}$$

and the elements of the non-adiabatic coupling matrix are defined by

$$\tau_{nk}(s,T) = \left\langle E_k(s,T)\left|\frac{\partial}{\partial s}E_n(s,T)\right.\right\rangle. \tag{4}$$

We now expand the state $|\psi(s,T)\rangle$ in the basis of the instantaneous eigenstates of $H(s,T)$,

$$\psi(s,T) = \sum_{n=1}^{N}\phi_n(s,T)\exp\left\{-iT\int_0^s E_n(s',T)\,ds'\right\}\big|E_n(s,T)\big\rangle. \tag{5}$$

(We shall frequently neglect in the text, but not in the formulae, the variables $(s,T)$ from the expressions following from Eqs. (2), (3), (4), and the possible $(s,T)$-dependence is understood without denoting it.)

### 2.2. Parallel transport

Let us now introduce the following local phase change for the $n$th instantaneous eigenstate

$$\big|\tilde{E}_n(s,T)\big\rangle = e^{i\Theta_n(s,T)}\big|E_n(s,T)\big\rangle, \quad n = 1,\ldots,N, \tag{6}$$

where $\Theta_n$ are real, $(s,T)$-dependent parameters. Plugging (6) into the definition (4) the transformation formula for the non-adiabatic coupling terms [17] reads

$$\tilde{\tau}_{nk}(s,T) = e^{i(\Theta_n(s,T)-\Theta_k(s,T))}\tau_{nk}(s,T) + i\frac{\partial\Theta_n(s,T)}{\partial s}\delta_{nk}. \tag{7}$$

This simple relation says that the diagonal element $\tilde{\tau}_{nn}$ is shifted with respect to $\tau_{nn}$ by $i\,\partial\Theta_n/\partial s$, while the non-diagonal elements of $\tilde{\tau}$ take up a phase with respect to those of $\tau$. If we choose the phase $\Theta_n(s,T) = i\int_0^s \tau_{nn}(s',T)\,ds'$, then under relation (7) $\tilde{\tau}_{nn}$ becomes zero, and by definition (4) the $n$th eigenstate satisfies the parallel transport law $\langle E_n(s,T)|\partial/\partial s|E_n(s,T)\rangle = 0$. Let us denote in this gauge the matrix elements of $\tau$ by $\tau^{\parallel}_{nk}$, then we get

$$\tau^{\parallel}_{nk}(s,T) = \exp\left\{\int_0^s \tau_{kk}(s',T) - \tau_{nn}(s',T)\,ds'\right\}\tau_{nk}(s,T), \tag{8}$$

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