Letter

Adiabatic theorem for closed quantum systems initialized at finite temperature

Nikolai Il'in,[1] Anastasia Aristova,[1,3] and Oleg Lychkovskiy[1,2,3]

[1]*Skolkovo Institute of Science and Technology, Bolshoy Boulevard 30, bld. 1, Moscow 121205, Russia*

[2]*Department of Mathematical Methods for Quantum Technologies, Steklov Mathematical Institute of Russian Academy of Sciences, 8 Gubkina St., Moscow 119991, Russia*

[3]*Laboratory for the Physics of Complex Quantum Systems, Moscow Institute of Physics and Technology, Institutsky per. 9, Dolgoprudny, Moscow region 141700, Russia*

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The evolution of a driven quantum system is said to be adiabatic whenever the state of the system stays close to an instantaneous eigenstate of its time-dependent Hamiltonian. The celebrated quantum adiabatic theorem ensures that such *pure state adiabaticity* can be maintained with arbitrary accuracy, provided one chooses a small enough driving rate. Here, we extend the notion of quantum adiabaticity to closed quantum systems initially prepared at finite temperature. In this case adiabaticity implies that the (mixed) state of the system stays close to a quasi-Gibbs state diagonal in the basis of the instantaneous eigenstates of the Hamiltonian. We prove a sufficient condition for the finite temperature adiabaticity. Remarkably, it turns out that the finite temperature adiabaticity can be more robust than the pure state adiabaticity with respect to increasing the system size. This can be the case for one-body systems with large Hilbert spaces, such as a particle in a large box, as well as for certain many-body systems. In particular, we present an example of a driven many-body system where, in the thermodynamic limit, the finite temperature adiabaticity is maintained, while the pure state adiabaticity breaks down. On the other hand, for generic many-body systems the scaling of the finite temperature adiabatic condition with the system size is exponential, analogously to pure state adiabatic conditions.

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I. INTRODUCTION

A concept of quantum adiabatic evolution was introduced by Born and Fock in the early days of quantum mechanics [1,2]. The concept pertains to a driven closed quantum system described by a time-dependent Hamiltonian. The evolution of the system is called adiabatic as long as the state of the system stays close to the time-dependent instantaneous eigenstate of the Hamiltonian. The celebrated adiabatic theorem [2,3] states that adiabaticity can be maintained with any prescribed accuracy, provided the driving rate (i.e., the rate of change of the Hamiltonian) is chosen small enough. The adiabatic theorem enjoys a glorious history and a wide range of theoretical and practical applications, including dynamics of chemical reactions [4], population transfer between molecular vibrational levels [5,6], theory of quantum topological order [7], quantized charge transport [8], quantum memory [9], and quantum adiabatic computation [10–12].

Nowadays there is a wealth of experimental techniques available to manipulate large quantum systems consisting of cold atoms in optical lattices, ions in ion traps, arrays of superconducting qubits and quantum dots, *etc.* [13]. However, these systems are rarely prepared in pure states. Rather, they are typically initialized at some finite temperature determined by the preparation protocol. Therefore, the conventional concept of adiabaticity [1–3], which we refer to as *pure state adiabaticity* (PSA) in what follows, calls for extension to the case of finite temperature.

Here we introduce the *finite temperature adiabaticity* (FTA) as the property by which the state of a system initially prepared at finite temperature stays close to the quasi-Gibbs state in the course of the unitary quantum evolution. The time-dependent quasi-Gibbs state, defined by Eq. (12) below, is diagonal in the instantaneous eigenbasis of the Hamiltonian and has the same spectrum as the initial thermal state.

The central result of the present Letter is a finite temperature quantum adiabatic theorem with an explicit sufficient condition for FTA. Examining this condition, we discover that FTA can be more robust than PSA in certain cases, in particular, for locally perturbed single-body systems with large Hilbert spaces (such as a particle in a large box) and, sometimes, for isospectrally driven many-body systems. On the other hand, for generic many-body systems the scaling of the FTA condition with the system size is exponential, analogously to the PSA case.

The rest of the paper is organised as follows. We start from introducing required definitions and notions (most importantly, the notion of the quasi-Gibbs state). Then we state the adiabatic theorem for closed quantum systems prepared in thermal states. Then we discuss its scope and implications, with the emphasis on the scaling with system size. General considerations are illustrated by examples. We conclude the paper with the summary and outlook. Technical details are relegated to the Supplemental Material [14].

II. PRELIMINARIES

We describe an isolated driven quantum system by means of a time-dependent Hamiltonian. To be more precise, we need a family of time-dependent Hamiltonians that traverse a

given path $\mathbf{r}(s)$ in a parameter space (where s is the dimensionless coordinate parametrizing the path) in different physical times t. The time scale is set by the driving rate ω:

$$s = \omega t. \tag{1}$$

It should be stressed that the parametrization of the path itself must not be linear, i.e., $|d\mathbf{r}/ds|$ must not be constant. We assume that the path along with its parametrization, $\mathbf{r}(s)$, is fixed, with H_s being the Hamiltonian in the point s. The adiabatic limit is defined as

$$\omega \to 0, \qquad t \to \infty, \qquad \omega t = \text{const} > 0. \tag{2}$$

Let E_s^n and Φ_s^n be, respectively, eigenenergies and eigenvectors of H_s,

$$H_s \Phi_s^n = E_s^n \Phi_s^n, \quad n = 1, 2, ..., d, \tag{3}$$

where d is the dimension of the Hilbert space. We assume that E_s^n and Φ_s^n are continuously differentiable in s.

Importantly, H_s can be represented as

$$H_s = U_s \widetilde{H}_s U_s^\dagger, \tag{4}$$

where U_s is a continuously differentiable unitary operator,[1] $U_0 = 1$ and $\widetilde{H}_s$ is an auxiliary operator with the same eigenvalues as H_s and the same eigenvectors as H_0,

$$\widetilde{H}_s = \sum_n E_s^n \, |n\rangle\langle n|, \tag{5}$$

where $|n\rangle \equiv \Phi_0^n$. Note that time dependence enters $\widetilde{H}_s$ only through E_s^n. An important object in our study is the *adiabatic gauge potential* (AGP) [15]

$$\mathcal{A}_s \equiv i(\partial_s U_s)\, U_s^\dagger. \tag{6}$$

To characterize the spectrum, we define

$$\frac{1}{\mu_s} = \max_n \left| \frac{E_0^{n+1} - E_0^n}{E_s^{n+1} - E_s^n} \right| \tag{7}$$

and

$$\nu_s = \max_n |\partial_s \ln \left(E_s^{n+1} - E_s^n\right)|. \tag{8}$$

If the spectrum of the driven Hamiltonian does not change with time, we refer to the driving as *isospectral*. In this case $\widetilde{H}_s = H_0$, $\mu_s = 1$, $\nu_s = 0$ and the AGP can often be easily obtained explicitly.

The state of the system ρ_t satisfies the von Neumann equation

$$i\partial_t \rho_t = [H_{\omega t}, \rho_t]. \tag{9}$$

We assume that at $t = 0$ the system is initialized in a thermal state,

$$\rho_0 = e^{-\beta H_0}/Z_0, \qquad Z_0 \equiv \operatorname{tr} e^{-\beta H_0}, \tag{10}$$

β being the inverse temperature.

To quantify the difference between two mixed quantum states we employ the trace distance

$$D_{\text{tr}}(\rho, \rho') \equiv (1/2)\operatorname{tr}|\rho' - \rho|, \tag{11}$$

which is known to have a straightforward operational meaning [16–20]. As a side remark, we note that the (more easily computable) Hilbert-Schmidt distance is unsuitable for fairly discriminating many-body states [19] and thus will not be used.

III. GENERALIZED GIBBS STATE

If the system were prepared in an eigenstate (in particular, in the ground state, i.e., "at zero temperature"), the adiabatic theorem [2,3,11] would imply that for any given s one can choose sufficiently small ω so that the state of the system at a (large) time $t = s/\omega$ is close (within a given error margin) to the corresponding instantaneous eigenstate. This is the exact meaning of PSA.

When we turn to the case of finite temperatures, the first question we have to address is what state one should compare the dynamical state ρ_t with. When the conditions for PSA are met for any eigenstate, then ρ_t stays close to the *quasi-Gibbs* state given by (see also Ref. [21])

$$\theta_t^\beta \equiv Z_0^{-1} \sum_n e^{-\beta E_0^n} |\Phi_{\omega t}^n\rangle\langle\Phi_{\omega t}^n|. \tag{12}$$

In fact, in some cases this happens under conditions less restrictive than those for PSA, as will be demonstrated in what follows. We define FTA as the closeness of ρ_t and θ_t^β in the course of quantum evolution.

Arguably, the notion of FTA is the closest proxy of the notion of PSA one can imagine in the finite temperature setting. It is different from *thermodynamic* or *local* adiabaticity that is concerned not with the many-body state ρ_t itself, but rather with the expectation values of few-body observables such as total energy, spin polarization, etc. [22–31]. Since $D(\rho_t, \theta_t^\beta)$ constrains the difference between the expectation values of any bounded observable in the states ρ_t, θ_t^β [20], the finite temperature adiabaticity entails the thermodynamic adiabaticity. The reverse is not true; two many-body states can have close expectation values of, say, all single- and two-body observables, but be vastly different otherwise. We anticipate that the notion of the finite-temperature adiabaticity introduced here will gain significance in cases where the complete characterization of the many-body state ρ_t is important, such as quantum adiabatic computation, quantum annealing, and adiabatic preparation of many-body states for measurement-based quantum computation [32–43], while the thermodynamic adiabaticity will remain most appropriate in the field of quantum thermodynamics.

IV. ADIABATIC THEOREM FOR FINITE TEMPERATURES

Now we are in a position to state the following:

Theorem: The trace distance between the dynamical state of the system ρ_t [initialized in the Gibbs state (10) and evolving according to the von Neumann equation (9)] and the quasi-Gibbs state θ_t^β [defined by Eq. (12)] is bounded from

[1]Note that U_s is *not* an evolution operator.

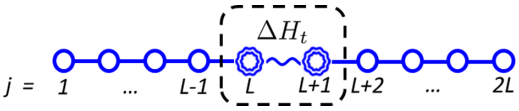

FIG. 1. A system of lattice fermions described by the Hamiltonian (14). The time-dependent part of the Hamiltonian, ΔH_t, acts only on the two middle sites of the lattice.

above by

$$D_{\rm tr}(\rho_t,\theta_t^\beta) \leqslant \sqrt{\sqrt{2}\omega\beta}\left(\frac{1}{\mu_{\omega t}}\|\mathcal{A}_{\omega t}\| + \int_0^{\omega t}\frac{1}{\mu_{s'}}\|\partial_{s'}\mathcal{A}_{s'}\|ds' + \int_0^{\omega t}\frac{\nu_{s'}}{\mu_{s'}}\|\mathcal{A}_{s'}\|ds' + \sqrt{2}\int_0^{\omega t}\frac{1}{\mu_{s'}}\|\mathcal{A}_{s'}\|^2 ds'\right)^{1/2}. \quad (13)$$

Here $\mathcal{A}_s$, μ_s and ν_s are defined in Eqs. (6), (7), and (8), respectively, and $\|\ldots\|$ refers to the operator norm.

This theorem implies that ρ_t converges to θ_t^β in the adiabatic limit (2), provided the term in brackets remains finite. The proof of the theorem can be found in the Supplemental Material [14].

The bound (13), which is the main result of the present Letter, is a sufficient condition for FTA. The following remarks on its merits are in order:

(1) The bound explicitly depends on temperature and vanishes in the limit of infinite temperature, $\beta = 0$. This is consistent with the simple fact that at the infinite temperature $\rho_t = \theta_t^{\beta=0} = \mathbb{1}/d$, and the evolution is trivially adiabatic for any driving rate.

(2) The system size can enter the bound through μ_s, ν_s and the norms $\|\mathcal{A}_s\|$, $\|\partial_s\mathcal{A}_s\|$.

(3) In practice, the application of the bound is greatly facilitated for an isospectral driving, where $\mu_s = 1$, $\nu_s = 0$ and, most importantly, the AGP $\mathcal{A}_s$ is often explicitly known, as will be exemplified in what follows.

(4) For a generic, nonisospectral driving in *many-body* systems the bound is less useful since the explicit form of AGP is usually unknown. Furthermore, the norm of nonisospectral many-body AGP generically diverges exponentially with the system size [44].[2] μ_s and ν_s will also typically diverge exponentially with the system size, however this divergence can be eliminated for chaotic many-body systems [45] by refining the bound, as discussed in the Supplemental Material [14].

To further elucidate the merits of the FTA condition (13), we analyze several examples below, focusing on the scaling of the bound with the system size.

V. LOCALLY DRIVEN LATTICE FERMIONS

Consider spinless fermions in a one-dimensional lattice with $2L$ sites described by the Hamiltonian (see Fig. 1)

$$H_s = H_{\rm hop} + H_{\rm int} + \Delta H_s, \quad (14)$$

where $H_{\rm hop} = (-1/2)(\sum_{j=1}^{L-1} + \sum_{j=L+1}^{2L-1})(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j)$ describes the nearest-neighbor hoppings in the left and the right halves of the lattice (but not between the two), $H_{\rm int} = \sum_{i<j} v_{ij} n_i n_j$ with $n_j \equiv c_j^\dagger c_j$ is the interaction term, v_{ij} being some interparticle potential, and ΔH_s is the time-dependent part acting on the two central cites of the lattice. The total number of fermions, $N = \sum_{j=1}^{2L} n_j$, is an integral of motion, and we can consider sectors with fixed N separately.

We will consider two types of ΔH_s. The first one is nonisospectral:

$$\Delta H_s^{\rm gen} = \varepsilon_s\left(c_j^\dagger c_j + c_{j+1}^\dagger c_{j+1}\right) - \left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j\right)/2. \quad (15)$$

Here only the first term depends on time through the on-site potential ε_s.

First let us discuss the one-body sector of the model, $N = 1$. In this sector we numerically verify that $\|\mathcal{A}_s\|$, $\|\partial_s\mathcal{A}_s\|$, μ_s and ν_s are finite in the limit of $L \to \infty$ [14]. This is consistent with Refs. [15,46] where a local approximation to AGP has been calculated (see the Supplemental Material for more details [14]). Therefore, for a fixed driving rate, the FTA remains robust in the large system size limit of $L \to \infty$.

In contrast, to maintain the PSA, one needs to polynomially scale down the driving rate with the system size (here and throughout the paper "polynomially" means "as a power law", not necessarily with an integer power). One can anticipate this already from spectral gaps that vanish polynomially in this limit. Alternatively, one can notice that restructuring of a dynamical pure state evolving according to the Schrodinger equation takes at least $O(L)$ time due to the locality of the driving and the finiteness of the Lieb-Robinson speed, therefore the driving rate should scale at least as $O(1/L)$ in order to catch up the instantaneous eigenstate. The latter reasoning closely follows that in Ref. [47]. In the Supplemental Material [14] we verify numerically that maintaining PSA with a prescribed accuracy requires driving rates that vanish with the system size.

Next, we turn to the many-body case with the fixed density $n \equiv N/L$. In this case $\|\mathcal{A}_s\|$ and $\|\partial_s\mathcal{A}_s\|$ diverge exponentially with the system size [44]. We therefore conclude that in the many-body sector the sufficient condition (13) for FTA performs essentially not better than known sufficient conditions for PSA,[3] indicating the exponential fragility of FTA in the thermodynamic limit.

The second ΔH_s we consider corresponds to the isospectral driving:

$$\Delta H_s^{\rm iso} = (-1/2)\left(e^{i\phi_s}c_j^\dagger c_{j+1} + e^{-i\phi_s}c_{j+1}^\dagger c_j\right). \quad (16)$$

Here ϕ_s is some smooth function of s with $\phi_0 = 1$. The corresponding unitary operator that takes H_0 to H_s reads

[2]This divergence has been established in Refs. [15,44] for a normalized Hilbert-Schmidt norm that does not exceed the operator norm.

[3]Here and in what follows we have in mind PSA conditions for an eigenstate whose energy corresponds to the inverse temperature β.

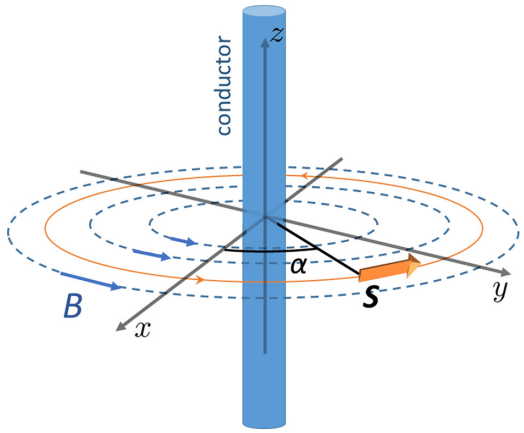

FIG. 2. A quantum spin is moved around a wire along a circular trajectory. Electrons in the wire are magnetically coupled to the spin due to fluctuations of the current. The many-body adiabaticity of the electron-spin system at finite temperature is robust with respect to increasing the length of the wire. In contract, the pure state adiabaticity breaks down at any finite driving rate.

$U_s = e^{i\phi_s N_{\rm L}}$, where $N_{\rm L} \equiv \sum_{j=1}^{L} n_j$ is the number of fermions in the left half of the chain.[4] The corresponding AGP is easily found to be $\mathcal{A} = -\partial_s\phi_s\, N_L$, and the bound (13) reads

$$D_{\rm tr}\big(\rho_t, \theta_t^{\beta}\big) \leqslant \sqrt{N}\sqrt{\sqrt{2}\omega\beta}\left(|\partial_s\phi_s| + \int_0^{\omega t} ds'|\partial_{s'}^2\phi_{s'}| + \sqrt{2}N\int_0^{\omega t} ds'|\partial_{s'}\phi_{s'}|^2\right)^{1/2}. \tag{17}$$

In the one-body sector the behavior of both FTA and PSA is analogous to that for the generic (nonisospectral) case. Indeed, for $N = 1$ the r.h.s. of the bound (17) does not depend on the system size L, and the FTA remains robust in the limit of $L \to \infty$. As for the PSA, it breaks down in this limit analogously to the nonisospectral case, as we verify numerically in the Supplemental Material [14].

In the many-body sector the bound (17) implies that to maintain the FTA in the thermodynamic limit it is sufficient to scale the driving rate as $\omega \sim 1/L^2$. Remarkably, the condition for PSA in the isospectral case is also polynomial in L, despite the exponentially small energy gaps, as discussed in the Supplemental Material [14] (see also Refs. [50,51]).

VI. SPIN COUPLED TO A COLLECTIVE COORDINATE

Consider a thin straight wire with N electrons and a quantum spin S that is moved around the wire, see Fig. 2. The spin has a magnetic moment $\mu_{\rm magn}$ [not to be confused with μ_s defined in Eq. (7)]. The interaction between the spin and the electrons is mediated by the magnetic field produced by the electron motion. In equilibrium the net current of electrons is zero, but the interaction persists due to fluctuations of the current, both classical and quantum. The Hamiltonian of the system reads

$$H_s = H^e + H^{Se}_{\alpha_s}, \tag{18}$$

where H_e is the Hamiltonian of electrons (its explicit form is not required), and

$$H^{Se}_{\alpha_s} = -\frac{\mu_{\rm magn}}{2\pi r}\,\mathcal{J}(-\sin\alpha_s\, S_x + \cos\alpha_s\, S_y) \tag{19}$$

is the Hamiltonian of the magnetic field-mediated interaction between electrons and the spin. Here (S_x, S_y, S_z) are the components of the spin operator, $\mathcal{J}$ is the operator of the electron current, r is the distance from the spin to the wire, and α_s is the time-dependent polar angle determining the position of the spin, see Fig. 2.

We further assume that the spin is moved along a circular trajectory around the wire with $r = \text{const}$, which amounts to the isospectral driving. The AGP is then given by $\mathcal{A}_s = (\partial_s\alpha_s)\, S_z$. Plugging this to Eq. (13), one gets a sufficient condition for FTA. Its explicit form is similar to Eq. (17) and can be obtained from the latter by replacing $\partial_s\phi_s$ by $\partial_s\alpha_s\sqrt{S(S+1)}$ and N by 1.

Remarkably, the number of electrons does not enter the sufficient condition for FTA. Consequently, one can increase the length of the wire indefinitely and still maintain the FTA with a given accuracy and a fixed driving rate. In contrast, the PSA breaks down in this limit (see [14]).[5]

VII. SUMMARY AND OUTLOOK

To summarize, we have introduced a notion of finite temperature adiabaticity (FTA) of an isolated quantum system and proved a finite temperature adiabatic theorem. To be more precise, we have proven a sufficient condition (13) for maintaining the FTA with a given accuracy. The system size enters the condition mainly through the norms of the adiabatic gauge potential and its derivative. The condition becomes particular tractable and useful for the isospectral driving, where the adiabatic gauge potential is often explicitly known.

We have analyzed in detail the scaling of the adiabatic condition (13) with the system size. While in a generic many-body case the FTA shares with the PSA the unfavorable exponential scaling, in certain special cases the former is dramatically more robust than the latter.[6] We have demonstrated this robustness for locally driven one-body models with large Hilbert spaces. We have also presented an example of an isospectrally and locally driven many-body model where the FTA survives the thermodynamic limit while the PSA breaks down.

Yet another class of many-body systems where the FTA might be more robust than the PSA are driven systems with

[4]Note that while the driving term is local, the AGP is extensive in the system size. This is a generic behavior [15]. Another interesting model with a local driving and an explicit AGP can be found in Refs. [48,49]. One can perform an analogous analysis of adiabaticity in this model, with the same qualitative conclusions.

[5]Note that there are examples of isospectrally and locally driven many-body systems where PSA is as robust as the FTA [50].

[6]This is consistent with earlier numerical observations that microcanonical mixed states are more robust to adiabaticity breaking than pure states [52].

integrable instantaneous Hamiltonians. This follows from the finding of Ref. [44] where the scaling of the normalized Hilbert-Schmidt norm for such a system has been demonstrated to be polynomial instead of exponential. One way to connect our work to this result would be to refine the FTA condition (13) by replacing operator norms by thermal averages. In fact, this can be done for three out of four terms in Eq. (13), as discussed in the Supplemental Material [14]. However, at the moment we are not able to avoid the operator norms altogether, and leave the improvement of the bound (13) for further work.

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