Quantum speed limit for thermal states

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Quantum speed limits are rigorous estimates on how fast a state of a quantum system can depart from the initial state in the course of quantum evolution. Most known quantum speed limits, including the celebrated Mandelstam-Tamm and Margolus-Levitin ones, are general bounds applicable to arbitrary initial states. However, when applied to mixed states of many-body systems, they, as a rule, dramatically overestimate the speed of quantum evolution and fail to provide meaningful bounds in the thermodynamic limit. Here we derive a quantum speed limit for a closed system initially prepared in a thermal state and evolving under a time-dependent Hamiltonian. This quantum speed limit exploits the structure of the thermal state and, in particular, explicitly depends on the temperature. In a broad class of many-body setups it proves to be drastically stronger than general quantum speed limits.

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I. INTRODUCTION

Quantum speed limits (QSLs) are a family of fundamental results in quantum mechanics limiting the maximal possible speed of quantum evolution. The first QSL was derived by Mandelstam and Tamm in 1945 [1] in a successful attempt to put the time-energy uncertainty relation on a rigorous basis (see also [2]). Decades later, a quite different QSL was derived by Margolus and Levitin [3]. Further developments included generalizations to mixed states [4-10], time-dependent Hamiltonians [4,11-13], open quantum systems [8,14,15], etc., as reviewed, e.g., in [16-18]. The scope of QSL was broadened to optimal control theory [19], quantum resource theory [20], abstract quantum information theory [21], semiclassical and classical dynamics [22,23], etc. Apart from the foundational importance per se, quantum speed limits enjoy a diverse range of applications, from a deep interrelation between QSLs, orthogonality catastrophe, adiabatic conditions, and adiabatic quantum computation [24-29] to ultimate limits for performance of quantum gates [3,30-32], quantum heat machines [33,34], quantum transport [35], and even quantum batteries [36,37].

Quantum speed limits can be particularly useful in many-body systems—there the exact calculations of the timedependent state ρ_t is, in general, of prohibitive complexity, and one may hope that QSLs would deliver valuable information on the dynamics not accessible otherwise. It turns out, however, that both the Mandelstam-Tamm (MT) and Margolus-Levitin (ML) QSLs applied to many-body systems often prove to be notoriously loose [38].

Here we derive a QSL with a drastically improved manybody performance. It applies to a ubiquitous situation when a system is initially prepared in a thermal state of some Hamiltonian H_0 and then evolves under a different (possibly, time-dependent) Hamiltonian $H_0 + V_t$. For few-body systems such setup has been successfully studied before (see, e.g., Refs. [39,40] where an optimal driving protocol has been presented for the case of a quantum parametric oscillator initialized in a thermal state). However, as mentioned above, in the many-body case one typically faces significant difficulties. The derived QSL alleviates much of these difficulties, as summarized in Table I.

The rest of the paper is organized as follows. We first introduce a quantum quench with the system initialized in a thermal state with $V_t = V$ independent on time. Then we discuss figures of merit appropriate to distinguish many-body mixed states. After that we formulate our QSL for a quench, Eq. (8). Then we contrast the performance of our QSL to that of the MT and ML QSLs, as well as to a notable recent QSL by Mondal, Datta, and Sazim (MDS) [9]. We argue that our QSL has a dramatic advantage over these QSLs in broad classes of many-body setups, and demonstrate these advantages in two exemplary systems: a spin-boson model and a mobile impurity model. Then we generalize our QSL to time-dependent potentials [see Eq. (21)] and provide the proof thereof. Finally, we conclude the paper by summarizing the results.

II. QUENCHING A THERMAL STATE

Let us consider a closed quantum system with the Hamiltonian quenched from H_0 at $t \le 0$ to $H_0 + V$ at t > 0. Before the quench the system is in the thermal state

$$\rho_0 = e^{-\beta H_0} / Z_0, \quad Z_0 = \text{tr} e^{-\beta H_0}, \tag{1}$$

TABLE I. Merits of the thermal QSL (8) as compared to three other QSLs, Eqs. (10)–(13). Loose performance implies that the corresponding bound on $D_{tr}(\rho_0, \rho_t)$ diverges as \sqrt{N} or faster in the thermodynamic limit despite $D_{tr}(\rho_0, \rho_t)$ itself being finite. Tight performance implies the absence of such spurious divergence. The first two lines correspond to the trivial dynamics $\rho_t = \rho_0$. The last two lines correspond to nontrivial dynamics where the complexity of calculating ρ_t becomes prohibitive for large system sizes. The original form (12) of the MDS inequality is used in the first two lines, and the modified one, (13), in the last two lines.

	Quantum Speed Limits			
	Mandelstam-Tamm	Margolus-Levitin	Mondal-Datta-Sazim	Thermal
Infinite temperature	Loose	Loose	Exact	Exact
Trivial perturbation	Loose	Loose	Exact	Exact
Local perturbation	Loose	Loose	Tight	Tight
Finitely disturbing nonlocal perturbation	Loose	Loose	Loose	Tight

 β being the inverse temperature. After the quench the state of the system ρ_t starts to evolve according to the von Neumann equation

$$i\partial_t \rho_t = [H_0 + V, \rho_t]. \tag{2}$$

We will refer to V as *perturbation*.¹

Our goal is to assess how far ρ_t can depart from ρ_0 . The difference between two arbitrary mixed quantum states, ρ_1 and ρ_2 , can be quantified by various distinguishability measures, two popular ones being the trace distance

$$D_{\rm tr}(\rho_1, \rho_2) \equiv (1/2) {\rm tr} |\rho_2 - \rho_1|$$
(3)

and the Bures angle

$$\mathcal{L}(\rho_1, \rho_2) \equiv \arccos \operatorname{tr} \sqrt{\sqrt{\rho_1} \rho_2 \sqrt{\rho_1}}.$$
 (4)

We will mostly employ the trace distance, which is known to have a well-defined operational meaning [41–44] and can be used for quantum state discrimination in the many-body case [45]. In addition, we will provide a QSL in terms of the Bures angle. To prove our QSL we will need a yet different distance, the quantum Hellinger distance [46] given by

$$D(\rho_1, \rho_2) \equiv 1 - \operatorname{tr}(\sqrt{\rho_1}\sqrt{\rho_2}).$$
(5)

In fact, the three distances introduced above are all mutually related by rather strong two-sided inequalities [42,46,47] and therefore can be used essentially interchangeably. The two particular inequalities we will use read [42]

$$D_{\rm tr}(\rho_1, \rho_2) \leqslant \sqrt{D(\rho_1, \rho_2)[2 - D(\rho_1, \rho_2)]}$$
$$\leqslant \sqrt{2D(\rho_1, \rho_2)} \tag{6}$$

and [47]

$$\mathcal{L}(\rho_1, \rho_2) \leqslant \arcsin \sqrt{D(\rho_1, \rho_2)[2 - D(\rho_1, \rho_2)]}$$
$$\leqslant \arcsin \sqrt{2D(\rho_1, \rho_2)}. \tag{7}$$

As a side remark, we note that the (more easily computable) Hilbert-Schmidt distance is unsuitable for fairly discriminating many-body states [45] and thus will not be used.

III. QSL FOR THERMAL STATES

The central result of the present paper is the quantum speed limit for thermal states (T-QSL). It reads as follows:

T-QSL:
$$D_{\rm tr}(\rho_0, \rho_t) \leqslant \sqrt{\beta t} \sqrt[4]{-2} \langle [H_0, V]^2 \rangle_{\beta}.$$
 (8)

Here and in what follows thermal averaging is understood with respect to ρ_0 , i.e., $\langle A \rangle_\beta \equiv \text{tr}(\rho_0 A)$ for an arbitrary operator *A*.

Essentially the same result can be cast in terms of the Bures angle:

$$\mathcal{L}(\rho_0, \rho_t) \leqslant \arcsin\left(\sqrt{\beta t} \sqrt[4]{-2\langle [H_0, V]^2 \rangle_\beta}\right).$$
(9)

Finally, the bound in terms of the Hellinger distance is given in Eq. (30).

The QSLs (8) and (9) follow from more general QSLs (21) and (22), respectively, that are reported and proven in what follows. However, before we turn to the proof, we elucidate the significance and merits of the T-QSL (8).

IV. COMPARISON WITH GENERAL QSLS

We would like to discuss the merits of the T-QSL (8) in comparison with three general (i.e., applicable to arbitrary, not necessarily thermal initial states) QSLs. The first two are the MT [1,2,4] and ML [3,5,48] QSLs which read

MT QSL:
$$D_{tr}(\rho_0, \rho_t) \leq \Delta E t$$
,
$$\Delta E \equiv \sqrt{\langle (H_0 + V)^2 \rangle_\beta - \langle H_0 + V \rangle_\beta^2}, \quad (10)$$

ML QSL:
$$D_{\rm tr}(\rho_0, \rho_t) \leqslant \sqrt{2\overline{E}t}, \quad \overline{E} \equiv \langle H_0 + V \rangle_\beta - E_{\rm gs}.$$
 (11)

Here ΔE is the quantum uncertainty of the Hamiltonian $H_0 + V$ in the thermal state (1), E_{gs} is the ground state energy of this Hamiltonian, and \overline{E} is the average energy relative to E_{gs} .

Both the MT and ML QSLs are saturated by a particular pure state [49]. However, this state is very special: it is a coherent, equally weighted superposition of two lowest eigenstates of the Hamiltonian.

When it comes to thermal states, both ΔE and \sqrt{E} scale as \sqrt{N} in the thermodynamic limit (N being the number of particles which grows with the particle density kept constant). Therefore, as noted in Ref. [38], the MT and ML QSLs misleadingly suggest that a state can always evolve into an (almost) orthogonal one in no time. We will see that, in fact,

¹Note that we do not imply that V is small or treated perturbatively.

this \sqrt{N} divergence is spurious for a broad class of perturbations, and MT and ML QSLs dramatically overestimate the speed of quantum evolution at a finite temperature.

The third QSL we have picked for comparison is the MDS QSL. In its original form it reads

$$D(\rho_0, \rho_t) \leqslant 2 \left[\sin\left(t \sqrt{-\operatorname{tr}[\sqrt{\rho_0}, V]^2}/2\right) \right]^2, \quad (12)$$

valid for times such that the argument of sin does not exceed $\pi/4$ [9]. However, the quantity tr $[\sqrt{\rho_0}, V]^2$, known as Wigner-Yanase skew information (with respect to the observable *V*) [50], is hardly computable in the many-body case. To obtain a practical bound, we employ the inequality $-\text{tr} [\sqrt{\rho_0}, V]^2 \leq 2\langle V^2 \rangle_{\beta}$. We also choose to get rid of the sine by using the inequality $(\sin x)^2 \leq x^2$ valid for any *x*. This way we obtain $D(\rho_0, \rho_t) \leq t^2 \langle V^2 \rangle_{\beta}$. Finally, we present this bound in terms of the trace distance with the help of the inequality (6):

MDS QSL:
$$D_{\rm tr}(\rho_0, \rho_t) \leq t \sqrt{2 \langle V^2 \rangle_{\beta}}.$$
 (13)

In what follows we will refer to this modified MDS bound simply as the MDS QSL.

At this point it is worth noting that all QSLs considered in the present paper [except the bound (12)] can be regarded as inequalities relating nonequilibrium dynamics (left-hand side) to an equilibrium expectation value of some physical observable or a function thereof (right-hand side). This type of QSLs is particularly useful in the many-body setting since the equilibrium expectation values are more easily accessible both theoretically and experimentally than the farfrom-equilibrium dynamics. Different types of QSLs (see, e.g., [10]) are not discussed here.

Now we are in a position to compare the general MT, ML, and MDS QSLs to the T-QSL. First we will consider limiting cases of infinite temperature and trivial perturbation, and then turn to nontrivial perturbations and specific examples.

Infinite temperature. Consider a system at the infinite temperature, $\beta = 0$ (here we assume that the Hilbert space is finite dimensional). Trivially $\rho_t = \rho_0 \sim 1$ and $D_{tr}(\rho_0, \rho_t) = 0$ in this case. This result is readily reproduced by T-QSL (8) as well as MDS QSL in its original form (12). However, both MT (10) and ML (11) QSLs provide loose $O(\sqrt{N})$ bounds.

Trivial perturbation. The perturbation is called *trivial* if $[H_0, V] = 0$. For a trivial perturbation the dynamics is also trivial, $\rho_t = \rho_0$, and the performance of QSLs is absolutely analogous to the infinite temperature case.

Local perturbation. We refer to V as a *local* perturbation whenever $\langle V^2 \rangle_{\beta}$ is finite in the thermodynamic limit. If the perturbation is local, the MDS bound (13) is finite in the thermodynamic limit.

Finitely disturbing perturbation. We refer to V as a finitely disturbing perturbation whenever $\langle [H_0, V]^2 \rangle_\beta$ is finite in the thermodynamic limit. The T-QSL (8) is finite in the thermodynamic limit whenever the perturbation is finitely disturbing.

For most physical Hamiltonians H_0 (in particular, for lattice Hamiltonians with short-range interactions) a local perturbation is also a finitely disturbing one. The opposite, however, is not necessarily true, as will be shown in an example below. Therefore a T-QSL is expected to outperform the MDS QSL whenever the perturbation is finitely disturbing but not local.

V. SPIN-BOSON MODEL

As an explicit but still quite general example, we consider a spin-boson model

$$H_0 = \Omega \sigma^z + \frac{1}{\sqrt{N}} \sigma^x \sum_k g_k (a_k^{\dagger} + a_k) + \sum_k \omega_k a_k^{\dagger} a_k.$$
(14)

Here $\sigma^{x,z}$ are Pauli matrices of a two-level system that is coupled to *N* bosonic modes (oscillators) a_k . With the appropriate choices of the energies Ω , ω_k and coupling constants g_k , this Hamiltonian describes a multitude of many-body systems [51]. Note that a prefactor $1/\sqrt{N}$ in the interaction term has been explicitly singled out, so that coupling constants g_k remain independent on the system size [51].

We will consider two types of perturbations in the spinboson model. The first one is local and affects the spin degree of freedom with $V = \varepsilon \sigma^x$. Both ΔE and \sqrt{E} are dominated by the last term in the Hamiltonian (14) and diverge as \sqrt{N} , the same divergence plaguing the MT and ML QSLs, in accordance with the general considerations (the same is true for another perturbation considered below). The MDS bound (13) reads $D_{tr}(\rho_0, \rho_t) \leq \sqrt{2\varepsilon t}$. The T-QSL produces a somewhat different bound, $D_{tr}(\rho_0, \rho_t) \leq \sqrt{2\sqrt{2\varepsilon}\Omega\beta t}$. Both the MDS QSL and T-QSL avoid a spurious divergence in the thermodynamic limit.

Another perturbation we consider shifts the energies of oscillators:

$$V = \sum_{k} \delta \omega a_{k}^{\dagger} a_{k}.$$
⁽¹⁵⁾

This perturbation is finitely disturbing, but not local. The MDS bound (13) now diverges as *N*, namely, $D_{\rm tr}(\rho_0, \rho_t) \leq \sqrt{2}\delta\omega t \bar{n}_{\beta}N$, where $\bar{n}_{\beta} \equiv \sum_k \langle a_k^{\dagger} a_k \rangle_{\beta} / N$ is the average number of excitations per mode, with $\langle a_k^{\dagger} a_k \rangle_{\beta} = 1/(e^{\beta\omega_k} - 1)$ being the Bose-Einstein distribution (here and in what follows the subleading in *N* terms are omitted from the bounds). However, this divergence is spurious: the T-QSL provides a finite bound

$$D_{\rm tr}(\rho_0, \rho_t) \leqslant \sqrt{\delta \omega \widetilde{g} \beta t} \sqrt[4]{2(1+2\widetilde{n}_\beta)}, \tag{16}$$

where $\tilde{g}^2 \equiv \sum_k g_k^2/N$ and $\tilde{n}_\beta \equiv \sum_k g_k^2 \langle a_k^{\dagger} a_k \rangle_{\beta} / \sum_k g_k^2$ are finite in the thermodynamic limit. Thus, the T-QSL is the only reasonable bound in this case.

VI. MOBILE IMPURITY MODEL

As a second example, we consider a model describing a single mobile impurity particle with mass m immersed in a fluid. The Hamiltonian reads

$$H_0 = H_{\rm f} + P^2 / (2m) + H_{\rm imp-f}, \tag{17}$$

where $H_{\rm f}$ is the Hamiltonian of the fluid, *P* is the momentum of the impurity, and $H_{\rm imp-f}$ describes the interaction between the impurity and the fluid. For ease of notation, we consider a one-dimensional case. The fluid and the impurity are in a box with the size *L*, the number of the particles of the fluid is *N*, and the particle density n = N/L is kept constant in the thermodynamic limit $N, L \rightarrow \infty$. The perturbation reads

$$V = FX, \tag{18}$$

where $X \in [0, L]$ is the coordinate of the impurity. This perturbation describes a force *F* applied to the impurity at time t = 0. This or similar setups are actively studied theoretically [52–61] and experimentally [62–64].

Again, the MT and ML bounds produce a spurious \sqrt{N} divergence. An even worse divergence plagues the MDS bound (13) which reads $D_{tr}(\rho_0, \rho_t) \leq \sqrt{2/3}NFt/n$. In contrast, the T-QSL (8) is finite in the thermodynamic limit:

$$D_{\rm tr}(\rho_0, \rho_t) \leqslant \sqrt{\beta t} \sqrt{(F/m)} \sqrt{2 \langle P^2 \rangle_{\beta}}.$$
 (19)

Here the thermal average $\langle P^2 \rangle_{\beta}$ depends on the explicit form of $H_{\rm f}$ and $H_{\rm imp-f}$ and in each particular case can be calculated approximately or, for an integrable H_0 , exactly (see, e.g., [65,66]).²

VII. T-QSL FOR A GENERAL DRIVING

Finally, let us state and prove a quantum speed limit for a Hamiltonian with an arbitrary time dependence. Namely, we consider a state ρ_t initialized in the thermal state (1) and evolving according to the von Neumann equation

$$i\partial_t \rho_t = [H_0 + V_t, \rho_t], \tag{20}$$

where V_t is an arbitrary time-dependent perturbation. Then the thermal QSL reads

$$D_{\rm tr}(\rho_0,\rho_t) \leqslant \sqrt{\beta \int_0^t dt' \sqrt{-2 \langle [H_0,V_{t'}]^2 \rangle_\beta}}.$$
 (21)

Essentially the same result cast in terms of the Bures angle reads

$$\mathcal{L}(\rho_0, \rho_t) \leqslant \arcsin \sqrt{\beta} \int_0^t dt' \sqrt{-2\langle [H_0, V_{t'}]^2 \rangle_\beta}.$$
 (22)

In the particular case of time-independent $V_t = V$ the inequalities (21) and (22) entail the inequalities (8) and (9), respectively.

Proof. The proof of Eqs. (21) and (22) goes as follows. We will first bound the Hellinger distance

$$D_t \equiv D(\rho_0, \rho_t) \tag{23}$$

defined in Eq. (5). Note that $\sqrt{\rho_t}$ also satisfies the von Neumann equation, $i\partial_t \sqrt{\rho_t} = [H_0 + V_t, \sqrt{\rho_t}]$. Therefore

$$\partial_t D_t = i \operatorname{tr}([\sqrt{\rho_0}, V_t] \sqrt{\rho_t}).$$
(24)

We rewrite this equality in the eigenbasis of H_0 :

$$\partial_t D_t = \frac{i\beta}{2\sqrt{Z_0}} \sum_{n,k} f^{\beta}_{E_n E_k} \langle n | V_t | k \rangle (E_n - E_k) \langle k | \sqrt{\rho_t} | n \rangle.$$
(25)

Here $|n\rangle$, $|k\rangle$ are eigenstates of H_0 , E_n and E_k are corresponding eigenenergies, and we have defined the function of three

variables

$$f_{EE'}^{\beta} = \frac{e^{-(\beta/2)E} - e^{-(\beta/2)E'}}{\beta(E - E')/2}.$$
(26)

Notice that $\langle n|V_{t'}|k\rangle(E_n - E_k) = \langle n|[H_0, V_{t'}]|k\rangle$. Taking this into account and applying the Cauchy-Bunyakovsky-Schwarz inequality to Eq. (25) we obtain

$$\begin{aligned} |\partial_t D_t| &\leq \frac{\beta}{2} \left(\sum_{n,k} Z_0^{-1} \left(f_{E_n E_k}^{\beta} \right)^2 \Big| \langle n | [H_0, V_t] | k \rangle \Big|^2 \right)^{1/2} \\ &\times \left(\sum_{n,k} \Big| \langle k | \sqrt{\rho_{t'}} | n \rangle \Big|^2 \right)^{1/2}. \end{aligned}$$
(27)

The term in the second set of brackets reduces to $tr \rho_{t'} = 1$. The term within the first set of brackets can be estimated by using the inequality [67]

$$\left(f_{EE'}^{\beta}\right)^2 \leqslant e^{-\beta E} + e^{-\beta E'} \tag{28}$$

valid for any real E, E', and β . After some basic algebra we obtain

$$|\partial_t D_t| \leqslant \frac{\beta}{2} \sqrt{-2\langle [H_0, V_{t'}]^2 \rangle_{\beta}}.$$
(29)

Finally, using the fact that $|D_t - D_0| \leq \int_0^t |\partial_{t'} D_{t'}| dt'$, we obtain the QSL for the Hellinger distance:

$$D_t \leqslant \frac{\beta}{2} \int_0^t dt' \sqrt{-2\langle [H_0, V_{t'}]^2 \rangle_\beta}.$$
 (30)

Combining this bound with (the looser versions of) inequalities (6) and (7) concludes the proof.

Note that in the course of the proof we have also obtained the bound (29) on the time derivative of the Hellinger distance.

As is clear from the proof, the bounds (21) and (22) can be improved: one can, first, use the tighter versions of inequalities (6) and (7), and, second, exploit the fact that $f_{E_nE_n}^{\beta}$ (observe identical subscripts) can be substituted by zero. These straightforward but somewhat bulky improvements make the bound more tight quantitatively but, as far as we can see, do not bring new qualitative insights.

One can also attempt to optimize the obtained QSLs by applying a time-dependent gauge transformation to the Hamiltonian [16,68–70] prior to using the inequalities (21) and (22). We leave this interesting research direction for future work.

We note that the definitions of trivial, local and finitely disturbing perturbations extend to the time-dependent V_t without alterations, as well as the conclusions regarding the corresponding performance of QSLs.

VIII. SUMMARY

To summarize, we have proven a quantum speed limit (21) for a system prepared in a thermal state of an initial Hamiltonian H_0 and evolving under a different, possibly time-dependent Hamiltonian $H_0 + V_t$. By narrowing the set of initial states to thermal states only, we have enhanced the performance of this quantum speed limit (referred to as T-QSL) as compared to QSLs valid universally. We have compared the T-QSL to three other QSLs, including the paradigmatic Mandelstam-Tamm and Margolus-Levitin ones, with the results summarized in Table I. The superiority of the T-QSL is most spectacularly manifested for a class of nonlocal but

²Let us emphasize here that in the latter case $H_0 + V$ is still nonintegrable and the calculation of ρ_t is unfeasible.

locally disturbing perturbations V_t : To the best of our knowledge, in this class the T-QSL is the only QSL providing a reasonable bound that avoids a spurious divergence in the thermodynamic limit. We have demonstrated this advantage explicitly for two exemplary systems—a spin-boson and a mobile impurity model.

As a final remark, we stress that the T-QSL is capable of meaningfully bounding the distance between *many-body* mixed states ρ_t and ρ_0 . This should be distinguished from the open system setup where one is interested in a *reduced* state of a few-level system (e.g., a qubit) coupled to a thermal bath (see, e.g., [8,15,71,72]). Since the trace distance is contractive with respect to taking partial trace, the T-QSL implies a bound on the distance between the reduced states, but not vice versa.

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For example, in the spin-boson model the right-hand side of the inequality (16) bounds also $D_{tr}(\rho_0^s, \rho_t^s)$, where ρ_t^s is the reduced density matrix of the spin.

Note added. Recently, a quantum speed limit for projections on linear subspaces has been reported [73]. This result can be applied to microcanonical thermal states, which nicely complements our results on the canonical thermal states.

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