Macroscopic Thermodynamic Reversibility in Quantum Many-Body Systems

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The resource theory of thermal operations, an established model for small-scale thermodynamics, provides an extension of equilibrium thermodynamics to nonequilibrium situations. On a lattice of any dimension with any translation-invariant local Hamiltonian, we identify a large set of translation-invariant states that can be reversibly converted to and from the thermal state with thermal operations and a small amount of coherence. These are the spatially ergodic states, i.e., states that have sharp statistics for any translation-invariant observable, and mixtures of such states with the same thermodynamic potential. As an intermediate result, we show for a general state that if the min- and the max-relative entropy to the thermal state coincide approximately, this implies the approximately reversible interconvertibility to and from the thermal state with thermal operations and a small source of coherence. Our results provide a strong link between the abstract resource theory of thermodynamics and more realistic physical systems, as we achieve a robust and operational characterization of the emergence of a thermodynamic potential in translation-invariant lattice systems.

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Introduction.— The quantum information approach to thermodynamics has allowed thermodynamic concepts, such as work, to be successfully extended into regimes of small-scale systems that store and process quantum information [1]. Notably, formulating thermodynamics as a resource theory [2–5] allows for a precise characterization of the resources that are required in single-instance state transformations, for instance thermodynamic work [6–8] and quantum coherence [9–12]. This is done by establishing a set of natural rules such as energy conservation, characterizing which possible evolutions a quantum state can undergo under these rules, and studying which external resources allows the system to undergo otherwise forbidden state transformations. A simple such framework is the resource theory of *thermal operations*, where one allows any energy-conserving unitary interaction with a heat bath at a fixed background temperature [4, 8, 13], and can be extended to more general types of reservoirs [14–17]. This approach has strong connections with information-theoretic entropy measures and quantum Shannon theory [18, 19]. More generally, information-theoretic approaches have provided new descriptions of nonequilibrium states and dynamics in statistical mechanics and thermodynamics, both in the classical and quantum regimes [20–24]. The resource theory connects to standard macroscopic thermodynamics in several ways. This approach is equivalent [25–27] to an established abstract and axiomatic formulation of thermodynamics by Lieb and Yngvason [28–31]. Second, one recovers the usual laws of thermodynamics in regimes of many identically and independently distributed (i.i.d.) copies of a state, such as for an ideal gas, or if the states considered are quantum statistical ensembles [4, 8, 32–34].

The resource theory of thermodynamics extends equilibrium thermodynamics to non-equilibrium situations. In standard macroscopic thermodynamics, a system is defined to be in thermodynamic equilibrium if it no longer presents macroscopic changes or currents, and if it has lost memory of its initial, possibly non-equilibrium state [35]. The purpose of this definition is to ensure that the thermodynamic behavior of the system is entirely specified by a *thermodynamic potential*: The optimal work required to transform one equilibrium state into another by a reversible thermodynamic process is given by the difference of the potentials for the initial and final states, and does not depend on any further details of the process. In the resource theory, this can be verified directly: Is the amount of work required to transform a state A into a state B equal to the amount of work that can be extracted in the reverse process? If so, the resource theory is said to be *reversible.* Crucially, reversibility of a resource theory—i.e., the emergence of a thermodynamic potential—can happen for states that are not necessarily in thermodynamic equilibrium, as we show in this paper.

A natural question is whether the notion of resource-theoretic reversibility can be leveraged to show the emergence of a thermodynamic potential for new classes of states that are physically relevant, such as interacting particles on a lattice, which go beyond idealized macroscopic settings such as i.i.d. states.

Here, we show that on a translation-invariant lattice of any spatial dimension with a local Hamiltonian, all ergodic states—i.e., states for which macroscopic quantities have sharply peaked statistics—can be reversibly converted to and from the thermal state. Furthermore, mixtures of ergodic states with the same thermodynamic potential also have this property. This ensures the emergence of a thermodynamic potential for this class of states even if some of these states are far out of equilibrium.

In the following, we first introduce the resource theory of thermodynamics and show that for general states, an equipartition property implies the emergence of a thermodynamic potential. We then consider translation-invariant lattices and explain our main result illustrated with an example of a 1-D Ising spin chain, before concluding with a discussion.

Resource theory of thermal operations.— In this resource theory, one is allowed to (i) bring in any ancilla systems in their thermal state, (ii) to carry out any energy-conserving unitaries, and (iii) to trace out any systems. We may then quantify the amount of work required to transform ρ into another state ρ' by including an explicit *battery system*, initialized in a pure energy eigenstate $|E\rangle$ and which we require to transition into another energy eigenstate $|E'\rangle$ at the end of the process. That is, if the transformation $\rho\otimes|E\rangle\langle E| \to \rho'\otimes|E'\rangle\langle E'|$ is possible with the operations (i)–(iii), then we define this process as consuming $E - E'$ work [8, 34, 36] (negative work consumption corresponds to work extraction).

We refer to the class of states which are block-diagonal in the energy eigenspaces as *semiclassical states*. For these states, transformations under thermal operations are fully characterized by *thermo-majorization* [8], a generalized notion of matrix majorization [37–39]. Let's consider two natural tasks associated with a semiclassical state ρ: *state formation* and *work distillation* (Fig. 1**a**). State formation consists in preparing the state ρ starting from the thermal state of the system, $\gamma = e^{-\beta H}/\operatorname{tr}(e^{-\beta H})$. The optimal amount of work that needs to be invested, if we allow an inaccuracy $\epsilon > 0$ in the final state and if ρ is semiclassical, is [7, 8]

$$W_{\mathrm{formation}}(\rho) = \beta^{-1} S^{\epsilon}_{\max}(\rho\,\|\,\gamma)\ , \tag{1}$$

with the *max-relative entropy* defined as $S^{\epsilon}_{\max}(\rho\,\|\,\sigma) = \min_{\tilde\rho\approx_\epsilon\rho} \ln \left\|\sigma^{-1/2}\,\tilde\rho\,\sigma^{-1/2}\right\|_\infty$ with the optimization ranging over all states $\tilde\rho$ that are ϵ-close to ρ in trace distance [40]. On the other hand, *work distillation* consists in extracting as much work as possible from a given state ρ, resulting in the thermal state γ on the system. The optimal amount of work that can be extracted from a semiclassical state ρ is [7, 8]

$$W_{\mathrm{distillable}}(\rho) = \beta^{-1} S^{\epsilon}_{\min}(\rho\,\|\,\gamma)\ , \tag{2}$$

with the *min-relative entropy* defined as $S^{\epsilon}_{\min}(\rho\,\|\,\sigma) = \max_{\tilde\rho\approx_\epsilon\rho} \left\{-\ln\operatorname{tr}\left(\Pi^{\tilde\rho}\,\sigma\right)\right\}$ where $\Pi^{\tilde\rho}$ is the projector onto the support of $\tilde\rho$ [40]. The min- and max-relative entropies are special cases of the Rényi relative entropies [41–43].

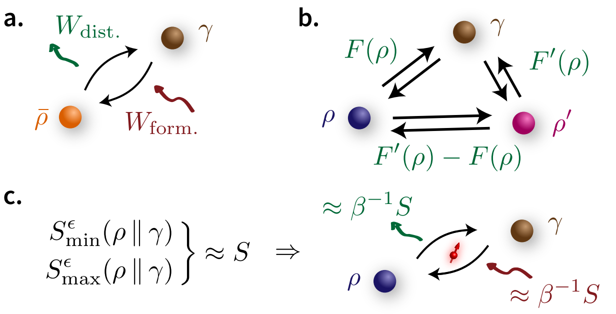

FIG. 1. A thermodynamic potential emerges when the underlying resource theory is reversible. **a.** For a state $\bar\rho$ that is block-diagonal in energy, the work that can be extracted is given by the min-relative entropy $W_{\mathrm{dist.}} = \beta^{-1}S^{\epsilon}_{\min}(\bar\rho\,\|\,\gamma)$, leaving the system in the thermal state $\gamma = e^{-\beta H}/\operatorname{tr}(e^{-\beta H})$. Conversely, the work required to prepare $\bar\rho$ from the thermal state is $W_{\mathrm{form.}} = \beta^{-1}S^{\epsilon}_{\max}(\bar\rho\,\|\,\gamma)$. **b.** Suppose a state ρ (respectively ρ') can be reversibly converted to and from the thermal state with work $F(\rho) - F(\gamma)$ (respectively $F(\rho') - F(\gamma)$). Then ρ and ρ' can be reversely interconverted. In this case the resource theory is said to be *reversible*, and the thermodynamic potential $F(\rho)$ fully characterizes the work required for state transformations. **c.** As an intermediate result, we show that if the min- and the max-relative entropies of any arbitrary quantum state ρ coincide approximately, then coherences in the state are suppressed, making it nearly block-diagonal in energy. The state is then approximately reversibly convertible to and from the thermal state with thermal operations and a small source of coherence.

There are no known necessary and sufficient conditions for transformations of arbitrary states under thermal operations. The reason is that thermal operations cannot generate any coherent superposition of energy levels, underscoring the role of time asymmetry in thermodynamics [9–12, 44–47]. It is thus necessary to account for coherence as a separate resource that enable operations that cannot be performed with thermal operations alone [48–52].

We resort to a very rudimentary way of accounting for coherence. We allow a system C with a bounded range of energy, which can be prepared in any pure state of our choosing and which we must dispose of in any state that is close to a pure state. This energy range is what we refer to as *amount of coherence* when such a system is used in a thermodynamic process. This crude approach is sufficient for our purposes, since our protocols only require such a system with an energy range that is negligibly small compared to the overall work cost of the transformation, thus forbidding any noticeable embezzling of work [13].

Emergence of a thermodynamic potential.— A resource theory is *reversible* for a class of states if the optimal work cost of any transition between two such states is equal to the optimal work extracted in the corresponding reverse process. This class of states then has a total order, and we can assign a "thermodynamic value" to each state—this is the thermodynamic potential. A sufficient condition for reversibility is to check whether the work required for state formation can fully be recovered in the reverse task of work distillation [8]; any transformation between two such states is then reversible (Fig. 1**b**). In well-behaved cases, such as in the i.i.d. regime [4] or for statistical ensembles [27], the thermodynamic potential is given by the Kullback-Leibler divergence or Umegaki relative entropy $S(\rho\,\|\,\gamma)$, defined as

$$S(\rho\,\|\,\sigma) = \operatorname{tr}\big(\rho(\ln\rho - \ln\sigma)\big)\ . \tag{3}$$

Equipartition implies reversibility with thermal operations.— We first present an intermediate result: If the min- and max-relative entropies coincide approximately, a condition which can be interpreted as a form of equipartition, then the state can approximately be reversibly converted to and from the thermal state (Fig. 1**c**). Our physical explanations are complemented by a fully rigorous proof that will be published elsewhere [53].

Theorem I. *For any ρ and for $\epsilon > 0$, suppose that*

$$S^{\epsilon}_{\mathrm{min}}(\rho\,\|\,\gamma) \geqslant S - \Delta\ ; \qquad S^{\epsilon}_{\mathrm{max}}(\rho\,\|\,\gamma) \leqslant S + \Delta\ ,$$

for some $S \in \mathbb{R}, \Delta > 0$. Then ρ can be approximately converted to and from the thermal state at a work cost (resp. work yield) of approximately $\beta^{-1}[S + O(\Delta)]$ (resp. $\beta^{-1}[S - O(\Delta)]$), with an amount of coherence of approximately $O(\Delta)$, and with arbitrarily good precision as $\epsilon \to 0$.

For a system of n particles, if we have $\Delta/n \to 0$ as $n \to \infty$, then the extractable work per system and the work of formation per system both converge to $s_\infty(\rho) := \lim_{n\to\infty} S/n$, and the amount of coherence used per copy goes to zero. In this case $s_\infty(\rho)$ becomes the thermodynamic potential in the thermodynamic limit $n \to \infty$.

To prove Theorem I, we first show that a state ρ for which the min-entropy and the max-entropy differ by at most $O(\Delta)$ have off-diagonal elements $\langle E_k\,|\,\rho\,|\,E_{k'}\rangle$ that are exponentially suppressed in $\beta|E_k - E_{k'}|$ if $\beta|E_k - E_{k'}| \gtrsim O(\Delta)$. In this sense, such a state may not harbor a large amount of coherence. Theorem I is then proven by exhibiting protocols for work distillation and state formation with the claimed properties. For both protocols, we first replace the Hamiltonian by one where the energy levels are integer multiples of some elementary spacing $O(\Delta)$, which can be done by investing an amount of coherence of order $O(\Delta)$. The work distillation protocol is then executed as follows. One dephases ρ in the new energy basis. Then we apply the known protocol for work extraction of semiclassical states. Because ρ has little coherence, the work that was wasted by the dephasing is small and the min-entropy does not change by much, so we can still recover $S - O(\Delta)$ work.

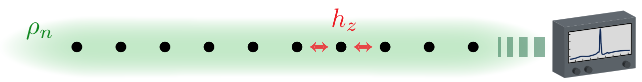

FIG. 2. Ergodic state on a lattice. An ergodic state is one that is translation-invariant and that produces sharp statistics for any translation-invariant observable. Our main result is to show that any two ergodic states can be reversibly interconverted with thermal operations and a sublinear amount of coherence, with the reversible work cost deriving from a thermodynamic potential given by the Kullback-Leibler divergence. Furthermore, a translation-invariant state has a thermodynamic potential if and only if it is a mixture of ergodic states of equal potential, providing a robust and operational understanding of the emergence of a thermodynamic potential in lattice systems.

For the second protocol, we use the notion of an *internal reference frame*: The state ρ is equivalently described by a completely incoherent state $\tilde\rho = \mathcal{D}[\rho\otimes\eta]$, where η is a special state called a *reference frame*, and where $\mathcal{D}[\cdot]$ is the joint dephasing operation on the system and the reference frame [54, 55]. Because ρ has only little coherence, a small reference frame η suffices to achieve an accurate description of ρ. Our protocol consists in first preparing the incoherent state $\tilde\rho$ using the known protocol for semiclassical states, and then "shifting" the coherence from η to ρ, a process known as "externalizing" the reference frame [55].

Ergodic states on a lattice.— We now consider a d-dimensional square lattice with a local Hamiltonian that is translation-invariant:

$$H = \sum_{\boldsymbol{z}\in\mathbb{Z}^d} h_{\boldsymbol{z}}\ , \tag{4}$$

where each term $h_{\boldsymbol{z}}$ is a lattice-translated version of a term $h_{\boldsymbol{0}}$ that acts on a constant number of sites neighboring the origin. Each site is a quantum system of some finite dimension. Our calculations will be performed for finite lattice sizes, where the total number of sites is denoted by n. For finite n, the Hamiltonian is truncated at the boundary by ignoring any terms that have support outside of the finite region considered.

In statistical mechanics, thermodynamic behavior is often captured in the notion of *ergodicity* (Fig. 2). Ergodic states are defined on the infinite lattice in two equivalent ways [56–60]. First, they are exactly those states that self-average over space translations. I.e., an ergodic state ρ satisfies the following property: For any local observable $a_{\boldsymbol{0}}$, we have $\mathrm{Var}_\rho\big(\frac{1}{n}\sum a_{\boldsymbol{z}}\big) \to 0$ as $n \to \infty$. Equivalently, ergodic states are the extremal points of the set of states that are translation-invariant on the infinite lattice. Consequently, any translation-invariant state can be written as a mixture of ergodic states.

Ergodic states are the natural quantum analogue of classically ergodic probability distributions [61, 62] for spatial translations instead of time evolution. Examples of ergodic states include Gibbs states of a local Hamiltonian at sufficiently high temperature, where the correlation functions of local observables decay exponentially in space (see for example Ref. [63] and references therein). Also, any i.i.d. state is ergodic, being the Gibbs state of a noninteracting Hamiltonian. In contrast, a mixed state of macroscopically different sectors (e.g., different magnetization sectors in a symmetry-broken phase) is not ergodic, as spatial fluctuations do not vanish.

Ergodicity and reversibility under thermal operations.— Our main contribution is to prove that on a lattice of any dimension with a translation-invariant local Hamiltonian, all ergodic states fall into the setting of Theorem I and are thus reversibly interconvertible:

Theorem II. *In the thermodynamic limit $n \to \infty$, any two ergodic states can be reversibly converted into one another using thermal operations and a sublinear amount of coherence, and the corresponding reversible work cost rate is given by the thermodynamic potential*

$$s(\rho) = \lim_{n\to\infty} \frac{1}{n} S(\rho_n \,\|\, \gamma_n) \ , \tag{5}$$

where ρ_n is the reduced state of ρ on a finite sublattice of size n and $\gamma_n = e^{-\beta H_n}/\operatorname{tr}(e^{-\beta H_n})$ is the Gibbs state with the truncated Hamiltonian H_n on the sublattice.

The proof of Theorem II proceeds via the *hypothesis testing relative entropy* [64–69], which interpolates between the min- and max-relative entropies [69] and can be formulated as a semidefinite program [70]. Inspired by the proof techniques of [59, 60, 71–73], we construct a quantum relative typical projector for an ergodic state relative to a Gibbs state associated with a truncated local Hamiltonian. This allows us to prove a generalized version of Stein's lemma for hypothesis testing [59, 71, 74–76] from which it follows that the min- and max-relative entropies must coincide up to sublinear terms in n, and where the limiting value converges to $s(\rho)$. We are then in the setting of Theorem I: Any ergodic state can be reversibly converted to and from the thermal state with the reversible work deriving from the thermodynamic potential $s(\rho)$. A rigorous proof will be published elsewhere [53].

Translation-invariant states and reversibility.— We can further ask, is there a larger class of translation-invariant states on a lattice that can be reversibly converted to and from the thermal state? We provide an answer to this question as follows:

Theorem III. *A translation-invariant state ρ that is a mixture of a finite number of ergodic states is reversibly convertible to and from the thermal state if and only if all ergodic states in the mixture are of equal potential, i.e., $\rho = \sum p_k \rho^{(k)}$ with $s(\rho^{(1)}) = s(\rho^{(2)}) = \cdots$.*

To prove the above theorem, we note the following property of the min- and max-relative entropy for a mixture $\rho = \sum p_k \rho^{(k)}$:

$$S^{\epsilon}_{\min}(\rho_n \,\|\, \gamma_n) \approx \min_k S^{\epsilon'}_{\min}(\rho^{(k)}_n \,\|\, \gamma_n) \ ; \tag{6a}$$

$$S^{\epsilon}_{\max}(\rho_n \,\|\, \gamma_n) \approx \max_k S^{\epsilon'}_{\max}(\rho^{(k)}_n \,\|\, \gamma_n) \ , \tag{6b}$$

with the approximation holding up to terms that do not scale with n and up to an adjustment of the smoothing parameter ϵ that does not depend on n. If all the $\rho^{(k)}$ in the decomposition have the same potential, $S(\rho^{(1)}) = S(\rho^{(2)}) = \cdots$, then $S^{\epsilon}_{\min}(\rho_n \,\|\, \gamma_n) \approx S^{\epsilon}_{\max}(\rho_n \,\|\, \gamma_n)$ with equality in the thermodynamic limit, and we can apply Theorem I. Conversely, if the $\rho^{(k)}$ do not all have the same potential, then the min- and max-relative entropies differ even in the thermodynamic limit. This implies that ρ cannot be reversibly convertible to and from the thermal state, because the min- and max-relative entropies are monotones under thermal operations.

Example: 1D Ising spin chain.— This toy example illustrates how a thermodynamic potential can emerge for states that are not in thermodynamic equilibrium. Consider a 1D chain of spin-1/2 particles with an Ising nearest-neighbor (n.n.) coupling and an external field h:

$$H = -J \sum_{i,j \text{ n.n.}} \sigma_z^i \sigma_z^j + h \sum_i \sigma_z^i \ , \tag{7}$$

where $\sigma_z = |{\uparrow}\rangle\langle{\uparrow}| - |{\downarrow}\rangle\langle{\downarrow}|$. Since i.i.d. states are ergodic, our results imply that two pure states of the form $|\psi\rangle^{\otimes n}, |\psi'\rangle^{\otimes n}$ can be converted into one another with thermal operations and an asymptotically negligible source of coherence at a reversible work cost of $F_\psi - F_{\psi'}$ per copy, where the thermodynamic potential is $F_\psi = \beta^{-1} \lim_{n\to\infty} S(\psi^{\otimes n} \,\|\, \gamma_n)/n$, which is the free energy per site up to an unimportant additive constant. The thermodynamic potential is well defined on an operational level even for states $\psi^{\otimes n}$ that are not in macroscopic equilibrium. Consider for instance the state $|\psi\rangle = |+\rangle = [|{\uparrow}\rangle + |{\downarrow}\rangle]/\sqrt{2}$. For $h \gg J$, the state $\psi^{\otimes n}$ presents macroscopic changes in the total spin along the X axis under time evolution according to H, but this does not prevent it from being reversibly convertible to and from another state $|\psi'\rangle^{\otimes n}$.

Discussion.— Our results provide a direct link between the abstract theory of thermodynamics at the small scale formulated in terms of a resource theory, and realistic many-body systems that are commonly studied in statistical mechanics. In statistical mechanics, an ergodic state physically corresponds to a definite macroscopic state; it describes a pure thermodynamic phase without phase coexistence [56]. We endow these ergodic states with a stronger notion of thermodynamic behavior: The notion of reversibility associated with the resource theory—which extends the concept in equilibrium thermodynamics to nonequilibrium situations—is tightly related to the notion of ergodicity. Furthermore, our analysis underscores how reversibility in the resource theory does not imply equilibrium. Indeed, spatially ergodic states, as considered here, can evolve nontrivially in time as illustrated in the toy example above.

Our rigorous proof [53] makes use of advanced information-theoretic techniques, including the information spectrum [77–83], hypothesis testing and quantum Stein's lemma [68, 69, 74, 75], as well as quantum typical projectors [59, 60, 71, 84]. Our results can be seen as an extension of the ergodic theorems of Refs. [59, 60]. We also use Ref. [85] to show that if we consider the reduced state of the infinite-dimensional Gibbs state instead of truncating the Hamiltonian for finite sublattices, then our results persist for sufficiently high temperatures where there is a unique KMS state.

Curiously, it is possible to construct toy situations in which the thermodynamic potential is not given by the Kullback-Leibler divergence [53]. While this does not happen in the setting considered in the present paper, it shows that the Kullback-Leibler divergence is not universally the correct expression of the emergent thermodynamic potential as defined via Theorem I when the min- and max-relative entropies converge to the same value. Whether this observation is relevant in physically interesting systems is an open question.

It seems plausible that our results could be robust to slight violations of translation invariance. For example, slight spatial inhomoginuity in a hydrodynamic mode could be allowed. Also, ergodic states exhibit some similarities with states obeying the eigenstate thermalization hypothesis [86–88], such as exponential decay of off-diagonal entries of the density matrix [53], suggesting that our techniques could be extended to such settings. Furthermore, a characterization of infinite or continuous mixtures of ergodic states is lacking, as opposed to the finite mixture considered in Theorem III. Finally, one might hope that our methods can be extended to models exhibiting disorder, where a gap between the min- and max-relative entropies would characterize the irreversibility of conversions between many-body-localized states.

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