

A Sufficient Set of Experimentally Implementable Thermal Operations for Small Systems

Christopher Perry,¹ Piotr Ćwikliński,² Janet Anders,³ Michał Horodecki,² and Jonathan Oppenheim¹

¹*Department of Physics and Astronomy, University College London,
Gower Street, London WC1E 6BT, United Kingdom*

²*Faculty of Mathematics, Physics and Informatics, Institute of Theoretical Physics and Astrophysics,
University of Gdańsk, 80-952 Gdańsk, Poland
and National Quantum Information Centre of Gdańsk, 81-824 Sopot, Poland*

³*Department of Physics and Astronomy, University of Exeter,
Stocker Road, Exeter EX4 4QL, United Kingdom*

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Recent work using tools from quantum information theory has shown that for small systems where quantum effects become prevalent, there is not one thermodynamical second law but many. Derivations of these laws assume that an experimenter has very precise control of the system and heat bath. Here we show that these multitude of laws can be saturated using two very simple operations: changing the energy levels of the system and thermalizing over any two system energy levels. Using these two operations, one can distill the optimal amount of work from a system, as well as perform the reverse formation process. What is more, using only these two operations and one ancilla qubit in a thermal state, one can transform any state into any other state allowable by the second laws. We thus have the result that the second laws hold for fine-grained manipulation of system and bath, but can be achieved using very coarse control. This brings the full array of thermal operations towards a regime accessible by experiment, and establishes the physical relevance of these second laws, potentially opening a new direction of studies.

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I. INTRODUCTION

Thermodynamics and statistical physics are one of the most successful areas of physics, owing to their broad applicability. One can make statements which do not depend on the particulars of the dynamics, and such laws govern much of the world around us. Thermodynamics puts limitations on the efficiency of our cars' engines, determines the weather, can be used to predict many phenomena in particle accelerators, and even plays a central role in areas of fundamental physics, providing the only clue we have to a quantum theory of gravity through the laws of black hole thermodynamics. However, traditional thermodynamics, as derived from statistical mechanics, generally concerns itself with the average behavior of large systems, composed of many particles. Here the experimenter is only able to manipulate macroscopic quantities of the material such as its pressure and volume, and does not have access to the microscopic degrees of freedom (d.o.f.) of the system, much less the heat bath. The basic operations

are limited to very crude control of the system bath— isotherms, adiabats, isochors, etc.

However, as our abilities to manipulate and control small thermodynamical systems improve, we are able to control the microscopic d.o.f. of smaller and smaller systems [1–5]. It thus seems natural to consider the thermodynamical behavior of small, finite-sized systems or heat engines composed of just a few molecules.

For an n -level system interacting with a heat bath, one can imagine an experimenter manipulating the system, who has control over each of the levels and can interact the system in any way they want with the heat bath. From a practical point of view, needing to perform such arbitrary interactions is undesirable, as they require very precise control over and the ability to keep track of the entirety of the heat bath. Simpler interactions would be much more appealing. See Fig. 1 for a schematic of this comparison.

However, even if one allows for such fine-grained control, the most experimentally unfeasible scenario, the second law of thermodynamics still holds (provided one computes the entropy of the system in terms of its microstates rather than using a course-grained entropy). In fact, not only does the traditional second law hold, but additional second laws emerge for small systems, such as the so-called *thermomajorization* criteria [6,7], and those given by a family of generalized free energies [8,9]. These constrain

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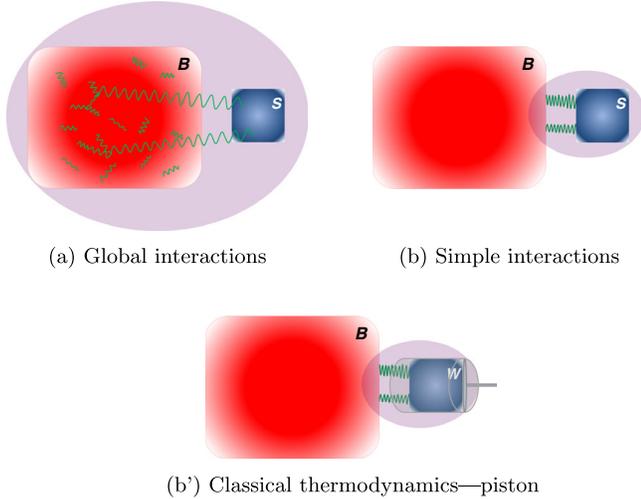


FIG. 1. Thermal operations versus crude operations versus classical operations. We consider a heat bath B together with a system S or working body W and illustrate the different levels of control an experimenter can have on the setup and interactions. (a) The most detailed, experimentally unfeasible control where the experimenter keeps a record of every microstate of the system and bath (the area contained within the purple oval) and controls interactions between the system and the entirety of the heat bath (illustrated by green stings). (b) The desired level of control where the experimenter keeps track of the system and a small portion of the bath (purple oval) and performs some simple interactions between these regions (green strings). (b') The previous case can be regarded as analogous to the setup in traditional thermodynamics where one has a working body W of which some parameters can be changed using simple processes such as moving a piston and weak couplings to the heat bath.

the set of states that it is possible to transition to from a given starting state and converge to the familiar second law in the thermodynamic limit [13].

However, such precise control will be impossible to implement as it could require accurately manipulating all of the 10^{20} molecules contained in a typical heat bath. As such, it may seem that what an experimenter can achieve without such incredibly fine-grained control must be very far from what is allowed by the second laws [14,15]. This contrasts sharply with traditional, macroscopic thermodynamics. There, those transformations allowed by the standard second law can easily be achieved by controlling macroscopic, coarse-grained parameters such as a system's volume or an external field. If the same level of control was needed macroscopically, as seems necessary for small systems, then running a car efficiently would require control of all of the molecules in the exploding fuel and cooler. Clearly this would be an undesirable feature—must it exist for small systems? The existence of a large gap between what is allowed by the most general class of operations and what is achievable without detailed control of the heat bath would make it hard to decide what the science of thermodynamics of microscopic systems should

actually be about and how applicable the recently derived second laws are.

Surprisingly, here we show that any state transformation permitted by the additional second laws can be achieved using three simple operations. These operations, which we term crude operations, are experimentally feasible for small systems and do not require fine control of bath d.o.f. to implement, only weak coupling to the bath. All allowed transformations can be implemented by applying thermalizations (assuming that the system can be thermalized), raising and lowering energy levels and rotations within energy subspaces to the system and a single thermal qubit taken from the heat bath. As a by-product, our simple operations can be viewed analogously to a universal gate set in quantum computing: they provide building blocks for the construction of more elaborate protocols.

II. THERMAL OPERATIONS

The aforementioned thermomajorization constraints were derived [7] under the largest class of operations one is allowed to implement under thermodynamics—*thermal operations* [7,16,17]. These are presented in full detail in Sec. A1 of Supplemental Material (SM) [18] and aim to capture all energy preserving processes that can be performed on a system in the presence of a heat bath with fixed inverse temperature β . In particular, given a system in state ρ with Hamiltonian H_S , they allow for maps of the following form:

$$\rho \mapsto \text{tr}_B[U_{SB}(\rho \otimes \tau_B)U_{SB}^\dagger], \quad (1)$$

where $\tau_B = \{e^{-\beta H_B}/\text{tr}[e^{-\beta H_B}]\}$ for an arbitrary bath Hamiltonian H_B and U_{SB} is an energy conserving unitary applied to system and heat bath satisfying $[U, H_S + H_B] = 0$. If a state ρ can be transformed into a state σ using a map of the above form, we will denote this by $\rho \xrightarrow{\text{TO}} \sigma$.

Energy conservation does not pose an insurmountable constraint on what is allowed since it can be enforced by incorporating a work storage device into the system to account for any energy excess or deficit. Rather, imposing energy conservation allows us to account for all sources of energy as is necessary for thermodynamics in the micro-regime. Clearly, needing to apply all such unitaries to realize all possible transformations would require an enormous amount of control.

Analysis of such maps has led to investigations into constraints on state transformations [7,8,13,16,19–21], analysis of the third law of thermodynamics [22–24], the derivation of fluctuation theorems [25–28], and corrections to the Carnot efficiency [29,30]. The framework has also recently been extended to consider generalized Gibbs ensemble and scenarios where conserved charges do not commute [31–33]. Recent surveys on the field can be found in Refs. [34,35].

It is worth noting that thermal operations can also be used to incorporate processes in which the system Hamiltonian changes. This is covered in Sec. A3 of SM [18]. Furthermore, note that the paradigm of thermal operations is equivalent to many other methods of describing thermodynamics as the small scale. This is discussed in detail in Sec. VIII of the Supplemental Material of Ref. [13], where it is shown that both time-dependent system Hamiltonians and interaction Hamiltonians between system and bath can be realized within the thermal operations framework.

A. Thermomajorization

In the absence of a source of work, a state ρ with Hamiltonian H_1 can be transformed into a state σ with Hamiltonian H_2 under thermal operations only if the familiar second law of thermodynamics holds, namely,

$$F(\rho, H_1) \geq F(\sigma, H_2), \quad (2)$$

where $F(\rho, H) = \text{tr}[H\rho] - (1/\beta)S(\rho)$ is the free energy with $S(\rho) = -\text{tr}[\rho \log \rho]$. Furthermore, in the thermodynamic limit this constraint is the only one governing state transformations.

However, the above constraint is not sufficient for determining whether a state transformation is possible under thermal operations at the nanoscale. Instead, an additional set of criteria, the thermomajorization constraints, must be evaluated. These are best stated in terms of *thermomajorization curves*. Given a state ρ with n -level Hamiltonian $H_S = \sum_{i=1}^n E_i |i\rangle\langle i|$, the associated thermomajorization curve is constructed as follows.

- (1) Let $\eta_i = \text{tr}[\rho |i\rangle\langle i|]$; i.e., η_i denotes the occupation probability of energy level E_i .
- (2) β order the probabilities and energy levels so that $\eta_i e^{\beta E_i}$ is in nonincreasing order.
- (3) Plot the β -ordered points $\{(\sum_{i=1}^k e^{-\beta E_i}, \sum_{i=1}^k \eta_i)\}_{k=1}^n$ together with $(0,0)$ and connect them piecewise linearly to form a convex curve—the thermomajorization curve.

Given two states ρ and σ , we say that ρ *thermomajorizes* σ if the thermomajorization curve of ρ is never below that of σ . Examples of thermomajorization curves are given in Fig. 2.

The utility of thermomajorization curves to determining whether a state transformation is possible under thermal operations is given by the following theorem.

Theorem 1 (Ref. [7]).—Given two states ρ and σ of an n -level system with Hamiltonian H_S in contact with a heat bath with inverse temperature β :

- (1) If σ is block diagonal in the energy eigenbasis, then $\rho \xrightarrow{\text{TO}} \sigma$ if and only if ρ thermo-majorizes σ .
- (2) In general, $\rho \xrightarrow{\text{TO}} \sigma$ only if ρ thermomajorizes σ .

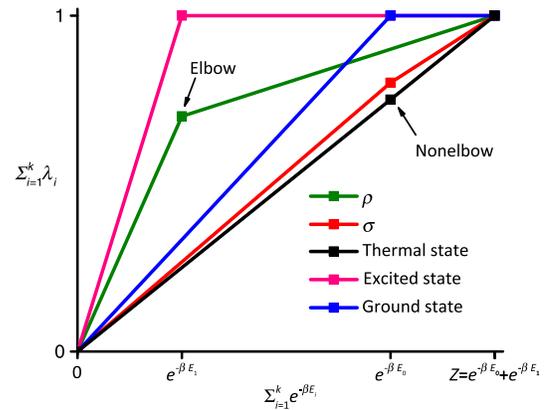


FIG. 2. Thermomajorization curves. Here we plot examples of thermomajorization curves for two-level systems. Observe that states associated with the same Hamiltonian may have different β orderings, as illustrated by ρ and σ here. We say that ρ *thermomajorizes* σ as the thermomajorization curve of ρ is never below the thermomajorization curve of σ . The thermomajorization curve of a Gibbs state is given by a straight line between $(0,0)$ and $(Z, 1)$. All other states thermomajorize it. The pure state corresponding to the highest energy level of an n -level system thermomajorizes all other states associated with that Hamiltonian. We call a point on a curve an *elbow*, if the gradient of the curve changes as it passes through the point. Otherwise, it is a *nonelbow*.

In the thermodynamic limit, the thermomajorization criteria collapses to the condition given by Eq. (2) [13]. However, for small systems diagonal in the energy eigenbasis (or if we have access to a source of coherence [13,21,36,37]), the above theorem shows that checking one constraint is not sufficient and instead it is necessary and sufficient to consider the entire thermomajorization curve. This was shown in Ref. [27] to correspond to checking $n - 1$ inequalities.

B. Deterministic work values

In general, if we want a transition from ρ to σ to be possible, work may have to be added. Alternatively, if a transition can be achieved with certainty, it can be possible to extract work. Typically, there are two figures of merit that can be used to quantify the amount of work that is expended or gained: *deterministic work* and *average work*.

The deterministic work cost introduced in Refs. [7,38,39] is defined to be the minimum amount of work that must be added for the transformation to be possible with certainty. This amount of work is used with certainty and is suitable for characterizing the work required when manipulating a single copy of a small system.

The average work cost is a meaningful quantity when work takes a distribution of values. This can occur when we consider transforming many copies of a system and hence can build up a set of statistics or if we have a weight system to store fluctuating work values, as in Refs. [28,40]. We are

interested in implementing thermal operations on single copies of a system when we do not have access to an additional weight system so we do not consider the average work cost in this paper.

For further elaboration on the differences between deterministic and average work for small systems, see Refs. [7,38,39].

More formally, within the thermal operations framework, the optimal amount of deterministic work that must be added or can be gained, the work of transition, can be quantified using (for example) the energy gap W of a two-level system, a *wit* [7], with zero energy state $|0\rangle$ and an additional state $|1\rangle$. The associated Hamiltonian is

$$H_W = W|1\rangle\langle 1|. \quad (3)$$

The deterministic work of transition, denoted $W_{\rho \rightarrow \sigma}$, is then defined to be the greatest value of W such that the following holds:

$$\rho \otimes |0\rangle\langle 0| \xrightarrow{\text{TO}} \sigma \otimes |1\rangle\langle 1|. \quad (4)$$

If $W_{\rho \rightarrow \sigma}$ is negative, to convert ρ into σ work has been taken from the work storage system to enable the transition to take place. On the other hand, if $W_{\rho \rightarrow \sigma}$ is positive, in converting ρ into σ it has been possible to store some extracted work in the work system.

Defining work in such a way enables the quantification of the worst-case work of a process. When $W_{\rho \rightarrow \sigma}$ is negative, it can be interpreted as the smallest amount of work that must be supplied to guarantee the transition. If it is positive, it is the largest amount of work we are guaranteed to extract in the process. As the work system is both initially and finally in a pure state, no entropy is stored in it and its energy change must be completely due to work being exchanged with the system.

III. CRUDE OPERATIONS

Implementing arbitrary transformations of the form given in Eq. (1) would require an unprecedented level of control. It is thus natural to ask whether the transformations that are possible under thermal operations can be achieved with much simpler operations. In this section, we introduce three such operations, which we call crude operations. These consist of (1) partial level thermalizations (PLTs), (2) level transformations (LTs), and (3) subspace rotations (SRs). In the following sections, we describe them each in turn in more detail before concluding the section by comparing them (and, in particular, the level of control they require) with other classes of operations that have been introduced in the literature. In Sec. IV, we show how applying protocols consisting of these operations to a system and a single thermal qubit (which is returned unchanged at the end of the protocol) is sufficient for

implementing any transformation to a block-diagonal state that is possible under thermal operations.

A. Partial level thermalizations

The first of our three basic operations is partial level thermalizations. A thermalization essentially changes the state of the system into a thermal state and is usually achieved by putting the system in thermal contact with the reservoir until it equilibrates or by swapping the system with one from the reservoir. Thermalizations have no work cost or gain associated with them. A partial thermalization generalizes this, allowing one to thermalize with some probability p , implementing

$$\rho \rightarrow p\rho + (1-p)\tau_S,$$

with τ_S being the thermal state of the system at inverse temperature β . The probability p can be determined by using the ambient heat bath as a source of noise or by putting the system in contact with it for a time shorter than the equilibration time.

With partial level thermalizations we go one step further and allow for the partial thermalization to act on any subset of energy levels. In order to implement them, one needs to be able to either perform the SWAP gate between any subset of energy levels of the system and of the thermal bath or to selectively put system energy levels in contact with the reservoir, e.g., by making use of an optical cavity or intermediate system which acts as a filter to restrict which energy levels are being addressed by the thermal contact. More precisely, a PLT is defined as

Definition 2 (Partial level thermalizations).—A partial level thermalization on an n -level system is parametrized by $\lambda \in [0, 1]$ and a subset $\mathcal{P} \subseteq \{1, \dots, n\}$ of the system's energy levels. We denote it by $\text{PLT}_{\mathcal{P}}(\lambda)$.

Given a diagonal state $\rho = \sum_{i=1}^n \eta_i |i\rangle\langle i|$ with associated Hamiltonian $H_S = \sum_{i=1}^n E_i |i\rangle\langle i|$ in contact with a heat bath at inverse temperature β , the action of $\text{PLT}_{\mathcal{P}}(\lambda)$ on ρ is given by

$$\rho \xrightarrow{\text{PLT}_{\mathcal{P}}(\lambda)} \rho', \quad (5)$$

where $\rho' = \sum_{i=1}^n \eta'_i |i\rangle\langle i|$ and the η'_i are such that

$$\eta'_i = \begin{cases} (1-\lambda)\eta_i + \frac{\lambda e^{-\beta E_i}}{\sum_{j \in \mathcal{P}} e^{-\beta E_j}} \sum_{j \in \mathcal{P}} \eta_j & \text{for } i \in \mathcal{P} \\ \eta_i & \text{for } i \notin \mathcal{P}. \end{cases} \quad (6)$$

The action of PLTs on a state is illustrated in terms of the thermomajorization curve in Fig. 3. Note that if we apply PLTs to energy levels that are adjacent with respect to the β ordering of ρ , the final states maintain this β order.

Finally, it has recently been proposed that such operations be incorporated into heat bath algorithmic cooling protocols to enhance their performance [41].

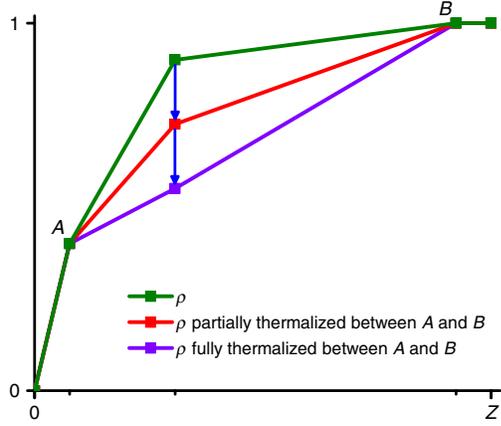


FIG. 3. Action of partial level thermalization. Here we illustrate the action of PLTs applied to a state four-level system with $\mathcal{P} = \{0, 1\}$. We take ρ to be block diagonal in the energy eigenbasis with occupation probabilities $p = (0.1, 0.5, 0.4, 0)$ and H_S and β to be such that $e^{-\beta E_1} = 0.4$, $e^{-\beta E_2} = 0.15$, and $e^{-\beta E_3} = e^{-\beta E_4} = 0.05$. For these choices, the affected portion of the thermomajorization curve lies between the points A and B and we show the impact of $\text{PLT}_{\{1,2\}}(\lambda = 0.5)$ (partial thermalization) and $\text{PLT}_{\{1,2\}}(\lambda = 1)$ (full thermalization) on ρ .

Such protocols are important for NMR-based quantum devices as they provide a route towards purifying qubits. As such, we expect the experimental implementation of PLTs to be developed.

B. Level transformation

Our second type of operation is level transformations, namely the raising and lowering of any subset of energy levels of the system's Hamiltonian. This type of transformation is common within thermodynamics and the work cost of implementing them is given by the change in energy of the level (when the level is populated). More formally,

Definition 3 (Level transformations).—A level transformation on an n -level system is parametrized by a set of real numbers $\mathcal{E} = \{h_i\}_{i=1}^n$ and denoted by $\text{LT}_{\mathcal{E}}$.

Given a state ρ with associated Hamiltonian $H_S = \sum_{i=1}^n E_i |i\rangle\langle i|$, the action of $\text{LT}_{\mathcal{E}}$ on (ρ, H_S) is

$$(\rho, H_S) \xrightarrow{\text{LT}_{\mathcal{E}}} (\rho, H'_S), \quad (7)$$

where $H'_S = \sum_{i=1}^n (E_i + h_i) |i\rangle\langle i|$.

Their effect on thermomajorization curves is shown in Fig. 4.

The deterministic work cost of performing the level transformations $\text{LT}_{\mathcal{E}}$ is naturally given by $-\max h_i$, where the maximization is taken over all occupied energy levels. This captures the maximum (worst-case) amount of work that needs to be supplied to implement a transformation. Here, we are interested in realizing those transformations that can be implemented using thermal operations at zero deterministic work cost. As such, when performing

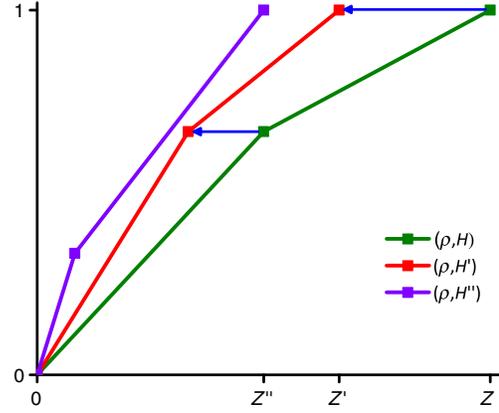


FIG. 4. Action of level transformations. Here we illustrate the action of LTs applied to a system with a thermodynamical configuration (ρ, H) . Note that LTs leave the occupation probabilities of ρ unchanged but may alter the β ordering as discussed in Supplemental Material [18].

transformations using crude operations, we will use only LTs that do not cost work to implement, i.e., $h_i \leq 0$ or $h_i \approx 0$, for all i . This will be done by combining them with partial level thermalizations to form a protocol akin to an isothermal process. We discuss this further in Sec. IV C 1.

C. Subspace rotation

Finally, we will sometimes need to implement an energy conserving unitary that acts upon system only [this is in contrast to the unitaries in Eq. (1) which act on both system and heat bath]. We call this operation a subspace rotation, and allowing such unitaries is desirable for two reasons.

Firstly, applying such a unitary at random will cause a system to decohere into the energy eigenbasis. This may be desirable if we begin with a state which contains coherence. As decoherence is a mechanism that occurs naturally, allowing for it does not require an unreasonable amount of control.

Secondly, in the special case where the system has degenerate energy levels, one may need to implement an energy conserving unitary acting within the degenerate subspace to rotate the state to be diagonal in a specific basis.

As we are predominantly interested in target states that are decoherent in energy, we can therefore take the initial and final states of any protocol to be diagonal in the energy eigenbasis. If necessary, we can always begin any protocol by decohering in the energy eigenbasis and then rotating the resulting state to be diagonal using a SR. At the end of the protocol we can apply a final SR to rotate within a degenerate energy subspace as required.

D. Comparison with other sets of operations

These operations are detailed with greater specificity in Sec. B of SM [18], where it is also shown that they are a subset of thermal operations. Having introduced them, here

we shall contrast them with operations that have appeared in other resource theoretic approaches to thermodynamics.

In Ref. [39] it was shown that full thermalizations and level transformations suffice for extracting the optimal amount of deterministic work from a given state under thermal operations as evaluated in Ref. [7]. Our crude operations are a larger set of operations and (as we see in the next section) enable any allowed transformation between block-diagonal states at the optimal work cost rather than just transformations to the thermal state.

In Ref. [39] it was shown that full thermalizations and level transformations suffice for extracting the optimal amount of deterministic work from a given state under thermal operations as evaluated in Ref. [7]. Our crude operations are a larger set of operations and (as we see in the next section) enable any allowed transformation between block-diagonal states at the optimal work cost rather than just transformations to the thermal state. A protocol is also given in Ref. [39] that uses full thermalizations and LTs to perform the conversion between two block-diagonal states at the optimal average work cost or gain. However, for most transformation at least one of the LTs performed will have a work cost (as defined after Definition 3). As such, this protocol is not suitable for implementing the transformations we are interested in where we demand that no work be expended.

A set of operations consisting of discrete unitary transformations (which allow for arbitrary unitaries to be applied to the system and arbitrary changes of Hamiltonian and hence contain level transformations as a special case) and discrete thermalizing transformations (which fully thermalize the system) was considered in Ref. [42]. These operations characterize processes that involve work and those that transfer heat, respectively. Using these primitives, isothermal transformations between states in thermal equilibrium can be performed at optimal heat exchange. However, they do not enable all transformations that are possible under thermal operations with zero deterministic work cost.

In Ref. [19] it was shown that for transitions between two block-diagonal states, perhaps with the expenditure or gain of deterministic work, it is enough to apply thermal operations on the bath and the system, and instead of the work system used in Ref. [7] use just level transformations. Still, however, the system-bath coupling term used in Ref. [19] requires being able to implement an arbitrary thermal operation (see Refs. [43,44], where it is shown that the operations used in Ref. [19] are a subset of thermal operations) and thus, in principle, requires a high degree of control.

A subset of thermal operations was considered in Ref. [40], which involved interacting with a designer heat bath which contained an arbitrarily large number of systems in a series of states that interpolated between the input state and the target state. Such a model allowed for achieving state transformations at the optimal average work

cost. Again, this would require an unfeasible amount of control in preparing the states of the heat bath. Note, however, that it was shown in Ref. [45] that the interactions themselves could be taken to be thermalizations and that these are robust to experimental imperfections.

In Ref. [14], corrections to the average amount of work that can be extracted were considered under various control restrictions. In particular, bounds on the accessible set of system Hamiltonians and restrictions on the allowed interactions with the heat bath were considered. Our crude operations also consider a restricted set of heat bath interactions, but we place no restriction on the allowed system Hamiltonians and consider single-shot transformations rather than the case of average work extraction.

A subclass of thermal operations was considered in Ref. [46], in which each operation could act on only two energy levels of the system at a time. While it was shown that such operations could be closely approximated in certain temperature regimes using a Jaynes-Cummings model, it was also shown that such a restricted set could not implement all of the transformations that are possible under thermal operations (a similar implication was also found in Ref. [47]). In contrast, we show that by applying PLTs that act on two energy levels (a subset of the aforementioned operations) and allowing in addition for level transformations and the use of a single thermal qubit, it is possible to reproduce the full set of transformations.

One can also consider simple operations for manipulating states that contain coherence. For example, in Ref. [48] a simple protocol for extracting the optimal amount of average work from a state with coherence that made use of non-energy-preserving unitary rotations, level transformations, and isothermal reversible processes was investigated. However, such unitary rotations are not contained within thermal operations and so we do not consider such protocols here. Furthermore, deterministic work extraction is not understood for this class of operations (see also Ref. [37] for a discussion on single-shot work extraction from coherent states using thermal operations in the presence of a reusable ancilla).

As we see in the next section, crude operations allow all transformations between block-diagonal states that are possible under thermal operations to be implemented without the need for unreasonable levels of control and at zero deterministic work cost.

IV. TRANSFORMATIONS USING CRUDE OPERATIONS

In this section, our goal is to show that any transformation to a block-diagonal state that is possible under thermal operations can also be achieved by applying crude operations to the system and a single thermal qubit. As Theorem 1 indicates that for such states $\rho \xrightarrow{\text{TO}} \sigma$ if and only if ρ thermomajorizes σ , we hence want to show that if ρ

thermomajorizes σ , then ρ can be converted into σ using crude operations without expending any work. If this is possible we will denote it by $\rho \xrightarrow{\text{CO}} \sigma$. The converse direction (that $\rho \xrightarrow{\text{CO}} \sigma$ implies that ρ thermomajorizes σ) also holds, and this follows from the fact that such crude operations are a subset of thermal operations.

A. Trivial Hamiltonian

When the Hamiltonian of the system is trivial, $H_S = 0$, and the energy spectrum is completely degenerate, the thermomajorization criteria collapses to a criteria known as *majorization*. If ρ has eigenvalues $\{p_i\}_{i=1}^n$ and σ has eigenvalues $\{q_i\}_{i=1}^n$, where each set is written in non-increasing order, we say ρ majorizes σ if

$$\sum_{i=1}^k p_i \geq \sum_{i=1}^k q_i, \quad \forall k \in \{1, \dots, n\}. \quad (8)$$

If the system Hamiltonian is trivial, then ρ majorizes σ if and only if $\rho \xrightarrow{\text{TO}} \sigma$ [49].

It is well known for two probability distributions of n elements, that if p majorizes q , then p can be converted into q using at most $n - 1$ T transforms [50,51]. A T transform T is parametrized by $r, s \in \{1, \dots, d\}$ and $\lambda \in [0, 1]$ and acts on the probability distribution p via $p \xrightarrow{T_{r,s}(\lambda)} p'$. Here,

$$p'_i = \begin{cases} (1 - \lambda)p_i + \frac{\lambda}{2}(p_r + p_s) & \text{for } i \in \{r, s\} \\ p_i & \text{for } i \notin \{r, s\}. \end{cases} \quad (9)$$

This action of T transforms is illustrated in Fig. 5.

Equation (9) is highly reminiscent of the action of PLTs defined in Eq. (6). Indeed, for trivial Hamiltonians the thermal state is just the maximally mixed one and all unitaries are energy conserving, so we can assume that our states are diagonal. Hence, the action of a PLT on two energy levels is to perform a T transform on the corresponding eigenvalues. Combining this with the aforementioned result of Refs. [50,51] gives the following.

Theorem 4.—Let ρ and σ be two states of an n -level system with trivial Hamiltonian $H_S = 0$. Then $\rho \xrightarrow{\text{TO}} \sigma$ implies that $\rho \xrightarrow{\text{CO}} \sigma$. Furthermore, this transformation can be done by applying a sequence of $n - 1$ PLTs that each act on only two energy levels.

In Sec. F of SM [18] we give an example of this protocol using a physical setup involving a molecule in a box (a so-called Szilard engine). Furthermore, we show how to distill the optimal amount of work from a given state in this setup and also the reverse process of forming a state. These examples provide some physical insight into the crude operations we allow and the form protocols built from them take.

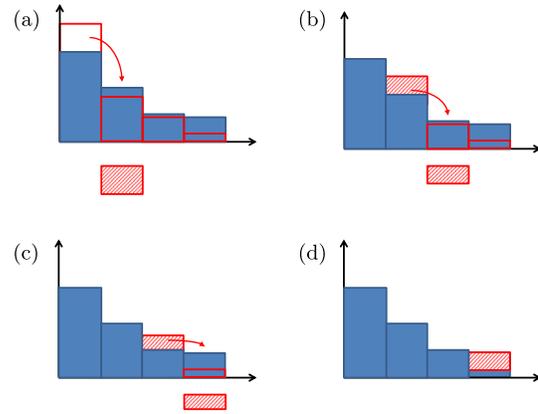


FIG. 5. The heights of each column are given by the probability of being in a particular eigenstate. The action of T transforms an initial state represented by red columns into the state represented by blue columns. The probabilities (column heights) of the red state majorize those of the blue state. We work our way from left to right, moving probability mass from the red histogram to the right until it matches the blue histogram. In each step we move some probability mass from a column of the histogram of the initial state and move it to the right either until it matches the probability required of the target state or until the left column of the initial state matches the right column of the final state. Red dashed rectangles represent the part of the column that is added to the next one due to the action of the T transform.

B. General Hamiltonian: States with the same β order

Transformations involving trivial Hamiltonian are straightforward because in this situation there is only one β order. In terms of thermomajorization curves, this means that the “elbows” of all states (see Fig. 2 for a definition) are vertically aligned. For general Hamiltonians, the same form of alignment arises if the states that we are attempting to convert between have the same β order. As PLTs are intuitively the generalization of T transforms to general Hamiltonians, the result of Refs. [50,51] can be generalized as follows.

Theorem 5.—Let ρ and σ be two states of an n -level system with Hamiltonian H_S such that ρ and σ have the same β order and σ is block diagonal in the energy eigenbasis. Then $\rho \xrightarrow{\text{TO}} \sigma$ implies that $\rho \xrightarrow{\text{CO}} \sigma$. Furthermore, this transformation can be done by applying a sequence of $n - 1$ PLTs.

Proof.—The full proof is given in Theorem 17 in Sec. C of SM [18], but we sketch the idea here. Firstly, by making use of appropriate subspace rotations we can assume that ρ and σ are in fact diagonal in the energy eigenbasis. As $\rho \xrightarrow{\text{TO}} \sigma$ is equivalent to ρ thermomajorizing σ , our task is to show that PLTs suffice for converting the thermomajorization curve of ρ into that of σ . The protocol for achieving this is illustrated in Fig. 6, which also serves as a simple, non-trivial example of how such a state transformation can be achieved. Roughly speaking, the aim is to use PLTs to

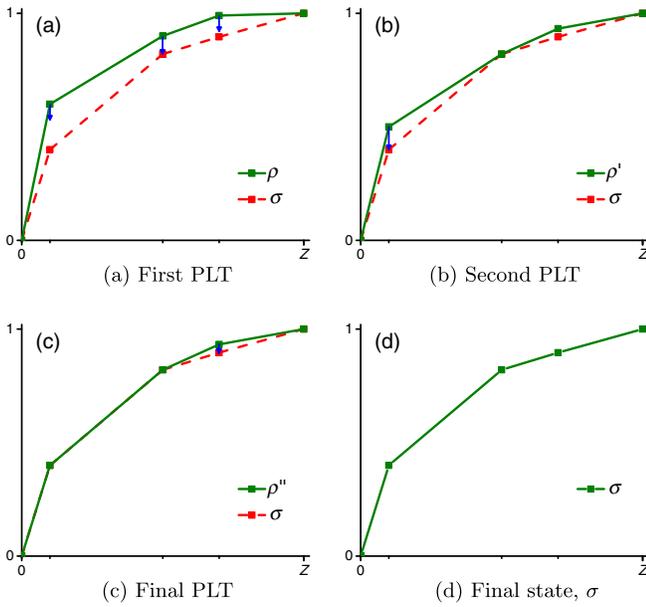


FIG. 6. Crude operations protocol for transforming between states with the same β order. If two states, ρ and σ , have the same β order and are such that ρ thermomajorizes σ , then ρ can be converted into σ using partial level thermalizations. First, a PLT is applied to ρ across the complete set of energy levels (a) lowering the thermomajorization curve of ρ until it meets that of σ (b). Next, a second PLT is applied to those energy levels to the left of this meeting point, again lowering the curve until it meets that of σ at a second point (c). By iterating this process, ρ is transformed into σ (d).

lower the elbows on the thermomajorization curve of ρ until one of these elbows meets an elbow of σ . This process is then repeated on subsets of energy levels that are adjacent in β order until the curves perfectly coincide. The level of thermalization required in each PLT is detailed in the full proof in Supplemental Material [18]. As the PLTs act only on adjacent energy levels, the β order never changes during the protocol. ■

Note that T transforms act only on two elements of a probability distribution while in the above theorem we have used PLTs that act on an arbitrary number of energy levels. It is thus natural to ask whether this result can be proved using only PLTs that act on two energy levels. In Sec. C, Theorem 18, of SM [18], we show that the answer is “yes” but present only the previous statement here as the associated protocol is easier to visualize on thermomajorization diagrams.

C. General Hamiltonian: States with different β order

For general ρ and σ with σ block diagonal such that $\rho \xrightarrow{\text{TO}} \sigma$, the protocol described in the previous section will not work because, for states with different β orders, the associated elbows may not be perfectly aligned. The

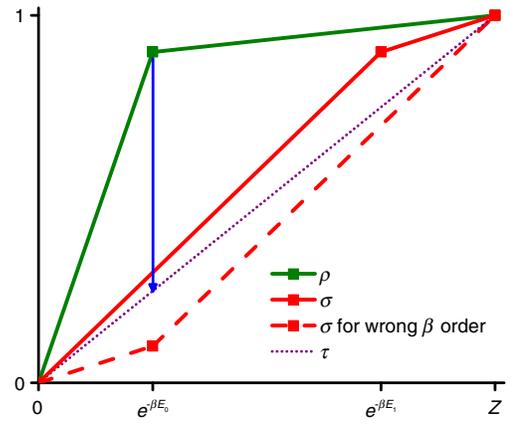


FIG. 7. Partial level thermalizations are not enough. Note that PLTs alone cannot implement all transitions possible under thermal operations. More specifically, they cannot implement changes of β order on qubits. In this above example, we see that a PLT cannot take the initial state ρ depicted in green to σ depicted in red, because it first passes through the thermal state before it reaches σ (which we have depicted in both its β -ordered and non- β -ordered form). Because of this, work is required to go from ρ to σ even though the optimal process does not require work.

essence of why this causes a problem can be seen in Fig. 7, where we consider a transformation on a two-level system where the initial and final state have different β orders. As we cannot write $\sigma = p\rho + (1-p)\tau_S$, a partial level thermalization cannot convert ρ into σ . Furthermore, we do not believe that a combination of PLTs and LTs acting on the system alone can achieve this without incurring a work cost.

However, if we are allowed to perform crude operations not just on the system but on the system and a single qubit τ_A from the thermal bath, then we will show that one can transform ρ into σ even if the β ordering is different. The effect of appending a thermal qubit on the thermomajorization curve of ρ is to introduce n additional “nonelbow” points (again, see Fig. 2 for an intuitive definition). The basic idea is to use a sequence of PLTs interlaced with LTs to convert this scenario into one where the states under consideration have the same β order. This is done by moving these new nonelbow points so that they are vertically aligned with the elbows of σ . If the sequence is performed sufficiently slowly, this can be done without expending any work.

In the next section, we describe this process before giving the full description of the protocol for dealing with states with different β orders.

1. Partial isothermal reversible processes and points flow

We now explain how to move nonelbow points without expending work or changing the shape of the thermomajorization curve. First, we show how to move a nonelbow

point within a line segment of the thermomajorization curve. Then, we explain how to transfer a nonelbow point that is close to the end of a segment to an adjacent segment. Combining these two processes we can freely move nonelbow points along the curve. A more detailed description can be found in Sec. B 3 of SM [18].

Partial isothermal reversible processes (PITRs): Moving nonelbows within a segment.—To gain intuition for how to move a nonelbow point within a segment, let us first consider the simpler case of converting a two-level system with Hamiltonian $H_S = \sum_{i=1}^2 E_i |i\rangle\langle i|$ that is initially in the Gibbs state $\tau_S = (e^{-\beta H_S}/Z_S)$ into a two-level system with Hamiltonian $H'_S = \sum_{i=1}^2 E'_i |i\rangle\langle i|$ in state $\tau'_S = (e^{-\beta H'_S}/Z'_S)$. When $Z_S = Z'_S$, the thermomajorization curves of both of these states are given by a straight line connecting $(0,0)$ to $(Z_S, 1)$ and both curves contain a nonelbow point which without loss of generality we can take to be at $(e^{-\beta E_1}, e^{-\beta E_1}/Z_S)$ and $(e^{-\beta E'_1}, e^{-\beta E'_1}/Z'_S)$, respectively. Thus, if we can perform $(\tau_S, H_S) \rightarrow (\tau'_S, H'_S)$ for any H'_S such that $Z'_S = Z_S$, we can effectively move the nonelbow point of τ_S to any position within the line segment.

It was shown in Ref. [39] that performing the transformation $(\tau_S, H_S) \rightarrow (\tau'_S, H'_S)$ can be done at a deterministic work cost (i.e., without work fluctuations) of $W = -(1/\beta) \log(Z_S/Z'_S)$ by alternating level transformations with full thermalizations of the system. The macroscopic equivalent of this process is the isothermal expansion of gas in a container and, hence, this process is called an isothermal reversible process.

Note that if $Z_S = Z'_S$, then no work is required to perform the above transformation. Thus, in this case, by keeping Z_S constant along the course of the protocol we can convert τ_S into τ'_S for free. To do this in t steps, we need to change the two energy levels in a special way. Namely, if we change the energy level labeled by 1 by $\Delta_1 = [(E'_1 - E_1)/t]$, we need to alter the energy level labeled by 2 by Δ_2 such that

$$e^{-\beta(E'_1 + \Delta_1)} + e^{-\beta(E'_2 + \Delta_2)} = Z, \quad (10)$$

where here E'_1 and E'_2 denote the energy levels of the system after the r th step of the protocol. This LT is then followed by a full thermalization and this sequence of LT followed by thermalization is repeated t times, resulting in (τ'_S, H'_S) . In the limit that t tends to infinity, it can be shown that the work cost of the transformation becomes deterministic and tends to zero [39].

A similar idea can be applied when (ρ, H_S) is such that ρ is not thermal but still contains a nonelbow. Note that a nonelbow implies that there are two energy levels E_i and E_j that are thermal with respect to one another, i.e.,

$$\eta_i = \alpha \frac{e^{-\beta E_i}}{e^{-\beta E_i} + e^{-\beta E_j}}, \quad \eta_j = \alpha \frac{e^{-\beta E_j}}{e^{-\beta E_i} + e^{-\beta E_j}}, \quad (11)$$

where $\alpha = \eta_i + \eta_j$. Moving this nonelbow along its associated line segment can then be achieved by applying LTs to E_i and E_j in such a way that

$$e^{-\beta(E_i + \Delta_i)} + e^{-\beta(E_j + \Delta_j)} = e^{-\beta E_i} + e^{-\beta E_j}, \quad (12)$$

and then applying the partial level thermalization $\text{PLT}_{\{i,j\}}(\lambda = 1)$ before repeating this sequence as necessary. In the limit that $\Delta_i \rightarrow 0$, this protocol again costs no work. We define the sequence of operations required to move a nonelbow along a line segment (which we call a partial isothermal reversible process in analogy to the above) more fully in Definition 13 in SM and prove [18] that it costs no work thereafter in Lemma 14. A description of a PITR is given in terms of thermomajorization diagrams in Fig. 8.

We note here, that to the best of our knowledge, such a thermodynamical state transformation has never been performed in the lab, and we hope that our work will stimulate experimentalists to implement it.

Points flow: Transferring nonelbows between segments.—Suppose that by using a PITR we have moved a nonelbow very close to the elbow defining the end of the line segment. We shall now explain how to move it to a neighboring segment.

Let the nonelbow be associated with energy levels E_i and E_j . As it is close to the end of the line segment, one of these energy levels (without loss of generality, let it be E_i) must be much larger than all other energy levels of the

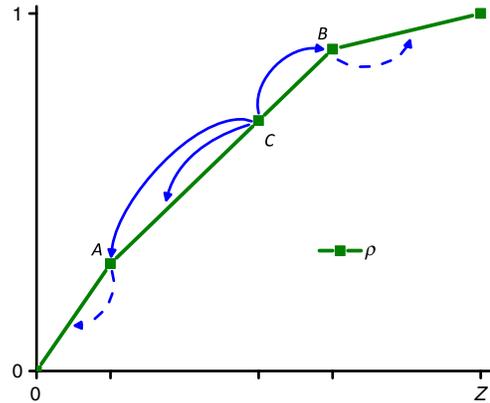


FIG. 8. Action of partial isothermal reversible processes. Here we illustrate the action of alternating level transformations and partial level thermalizations (so-called PITRs) applied to a system with state-Hamiltonian pair (ρ, H) . Using PITRs, the point at C can be moved such that it lies anywhere on the line segment between A and B and without changing the shape of the overall thermomajorization curve. By performing this process sufficiently slowly, this can be done with no deterministic work cost. If one moves the point C to coincide with point A (B), one can then use a second PITR to move point A (B) as illustrated by the dashed arrows. Again, this does not alter the shape of the thermomajorization curve.

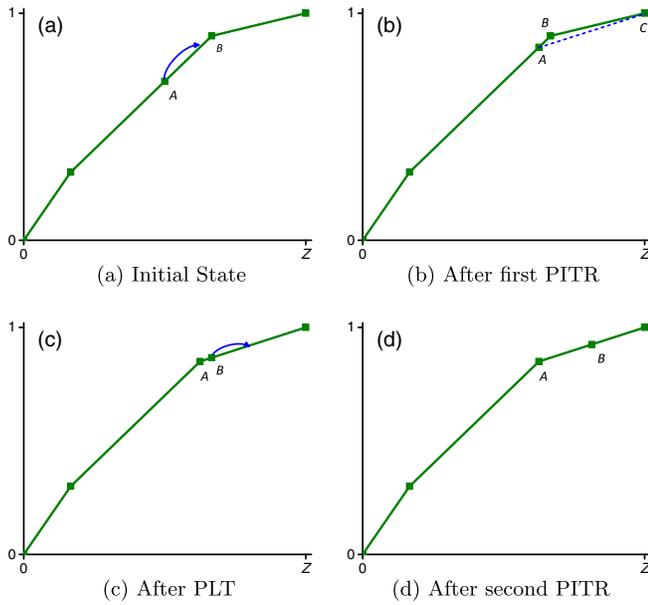


FIG. 9. Approximate points flow. Here we illustrate the protocol of approximate points flow using thermomajorization diagrams. Initially the system is as per (a). Using a PITR, the nonelbow point A is moved towards the elbow at point B . This results in (b). Next, a PLT is applied between points A and C , leading to (c). Point B is now a nonelbow and can be moved using a PITR, giving (d).

system. Indeed, as $E_i \rightarrow \infty$ the nonelbow becomes arbitrarily close to the end of the line segment. Let E_k denote the energy level associated with the line segment we wish to move our nonelbow to. To do this, we apply the partial level thermalization $\text{PLT}_{\{i,k\}}(\lambda = 1)$. This turns the nonelbow into an elbow and the elbow at the end of the line segment into a nonelbow that we can continue to move. The whole process is depicted in Fig. 9 and described more carefully in Definition 16 in Sec. B 3 of SM [18].

Note that the process described does not leave the thermomajorization curve completely unchanged. However, the closer the nonelbow initially was to the end of the line segment, the lesser the change. If we wish to transfer a nonelbow without altering the thermomajorization curve at all, we can do so if we are able to raise an energy level to infinity. This results in a simpler protocol, which we describe in Definition 15 and Fig. 15 in Sec. B 3 of SM [18].

2. Full protocol

With these concepts in place, we are now in a position to prove our main result.

Theorem 6.—Let ρ and σ be two states of an n -level system with Hamiltonian H_S such that σ is block diagonal in the energy eigenbasis. Then $\rho \xrightarrow{\text{TO}} \sigma$ implies that $\rho \xrightarrow{\text{CO}} \sigma$ without expending any work.

Proof.—The full proof can be found in the proof of Theorem 19 of Sec. D of SM [18] and we sketch it here.

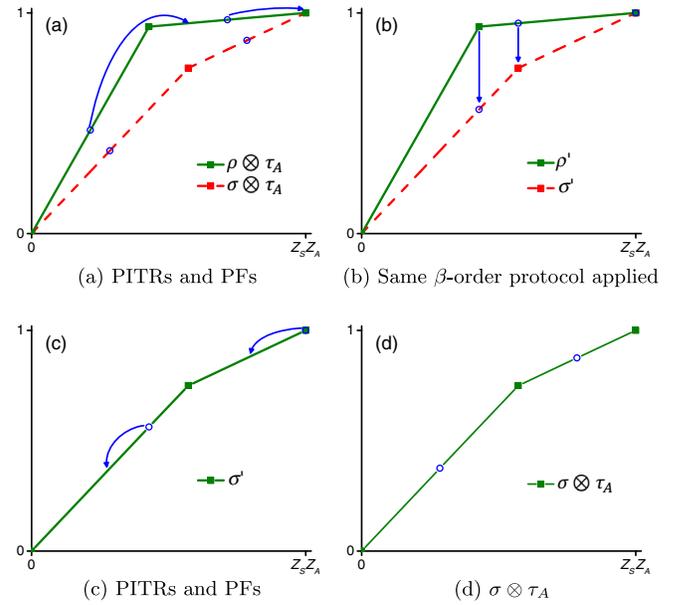


FIG. 10. Crude operations protocol for transforming between states with different β orders. If ρ thermomajorizes σ , then it is possible to transform ρ into σ using crude operations. First, a thermal qubit τ_A with known Hamiltonian is appended (a). Using partial isothermal reversible processes the blue circles on the thermomajorization curve of $\rho \otimes \tau_A$ can be moved to be vertically aligned with the “elbows” on the curve for $\sigma \otimes \tau_A$. This forms the state ρ' (b) that has a thermomajorization curve overlapping that of $\rho \otimes \tau_A$. Using the previously defined protocol for states with the same β order, ρ' can be converted into σ' (c) that has a thermomajorization curve overlapping that of $\sigma \otimes \tau_A$. A final round of PITRs converts σ' into $\sigma \otimes \tau_A$ (d), and upon discarding τ_A we obtain σ .

We again note that for σ block diagonal, $\rho \xrightarrow{\text{TO}} \sigma$ implies that ρ thermomajorizes σ . Our aim is therefore to construct a sequence of crude operations that transform the thermomajorization curve of ρ into that of σ . The protocol for doing this is shown in Fig. 10. First a thermal qubit τ_A is appended. The thermomajorization curve of $\rho \otimes \tau_A$ has the same shape as ρ but contains n additional nonelbows. Using the PITR and point flow protocols introduced in the previous section, these nonelbows can be moved so that they are vertically aligned with the elbows of $\sigma \otimes \tau_A$. Using the PLT protocol introduced in Theorem 5, this can be converted into a state which has the same thermomajorization curve as $\sigma \otimes \tau_A$ but potentially with nonelbows in the wrong position. A final round of PITR and point flow protocols corrects this, leading to $\sigma \otimes \tau_A$, and upon discarding τ_A , we obtain σ . ■

The protocol described above assumes that we can implement points flow exactly; i.e., it is possible to raise energy levels to infinity. If this is not possible and we instead must perform them approximately, the above transformation is still possible but with a small caveat. The statement and proof of this is given in Theorem 20 in Sec. D of SM [18].

D. Deterministic work values with crude operations

Crude operations can also be used to construct protocols that achieve the optimal deterministic work values under thermal operations as determined through Eq. (4). Rather than using a wit to measure such a quantity, one can instead consider the work value of the level transformations used during the protocol. This is explored in more detail (including the ϵ -error case) in Sec. E of SM [18], but here we describe the optimal, zero-error protocols for both extracting work from a state and forming an incoherent state from a thermal state.

The maximum amount of work that can be deterministically extracted from a state ρ under thermal operations is given by [7,39]

$$W_{\text{distil}}(\rho) = W_{\rho \rightarrow \tau_S} = \frac{1}{\beta} \ln \left(\frac{Z_S}{\sum_{i:\eta_i > 0} e^{-\beta E_i}} \right). \quad (13)$$

The protocol for achieving this under crude operations is identical to that given in Ref. [39]. First, a level transformation is used to raise the unoccupied energy levels (those such that $\eta_i = 0$) to infinity. As the energy levels are unoccupied, this does not cost any work. Next, the state is completely thermalized. These two steps result in a thermal state τ'_S of Hamiltonian H'_S such that $Z'_S = \sum_{i:\eta_i > 0} e^{-\beta E_i}$. A round of partial isothermal reversible processes can now be applied (at no work cost) to convert this to a state-Hamiltonian pair (τ_S, H''_S) , where τ_S is the thermal state of both H''_S and H_S and $Z''_S = Z'_S$. Finally, the level transformation $\text{LT}_{\mathcal{E}}$, where $\mathcal{E} = \{h_i = -(1/\beta) \ln[Z_S / (\sum_{i:\eta_i > 0} e^{-\beta E_i})]\}_{i=1}^n$, is performed to convert (τ_S, H''_S) into (τ_S, H_S) while extracting the amount of deterministic work given in Eq. (13).

The reverse process to work distillation is that of formation. There, one starts with the thermal state τ_S and uses work to form the state ρ . For the case where ρ does not contain coherences, we can construct a process to do this using crude operations achieving

$$W_{\text{form}}(\rho) = W_{\tau_S \rightarrow \rho} = -\frac{1}{\beta} [\ln(\eta_1 e^{\beta E_1}) + \ln Z_S], \quad (14)$$

where we emphasize that the occupation probabilities and energy levels of ρ have been β ordered. This is the optimal value achievable under thermal operations [7]. The protocol for achieving this runs as follows. First, a round of partial isothermal reversible processes is applied to convert (τ_S, H_S) into (ρ, \tilde{H}_S) , where ρ is the thermal state of \tilde{H}_S and $Z_S = \tilde{Z}_S$. As the partition function does not change, this does not cost work. Next, the level transformation $\text{LT}_{\mathcal{E}}$, where $\mathcal{E} = \{h_i = E_i - \tilde{E}_i\}_{i=1}^n$, is performed to convert (ρ, \tilde{H}_S) into (ρ, H_S) . It can be shown that the deterministic work cost of this, $\text{LT} -\max_i h_i$, matches the expression given in Eq. (14) (see Supplemental Material [18]).

V. CONCLUSION

We show that thermal operations can be simulated by crude operations, a class of physical operations closer to that which can be implemented in the laboratory using current technology. This ought to bring thermodynamics of microscopic systems further into the experimental domain, and make the exploration of some of the results in the field [7,8,14,27,29,38–40,42,49,52–66] more feasible.

From a conceptual point of view, our results show that the paradigm of thermodynamics, which allows for the maximum amount of control of the system and bath, is in some sense equivalent to one which allows only very crude control of the system and bath. The second laws of thermodynamics, since they are fundamental limitations on state transitions, need to be derived assuming the experimenter has as much control and technology as would be allowed by nature (i.e., thermal operations). Yet remarkably, the fundamental limitations captured by thermomajorization and the generalized free energies, which are derived assuming such control, can be achieved with very little control, namely by crude operations. Control over bath d.o.f., with the exception of one qubit, is not needed.

There are additional second laws, which place constraints not only on the occupation probabilities of a state, but also place restrictions on the coherences over energy levels [8,20,21,37]. While we conjecture that crude operations are also sufficient for the control of quantum coherences, as we do not yet know what the necessary conditions are for coherence manipulation under thermal operations, this cannot yet be verified. Determining the allowed transformations between states that contain coherence remains an important open question in the resource theoretic approach to quantum thermodynamics. The progress that has been made on this question has considered thermal operations in the presence of a reusable source of coherence that typically takes the form of a high-dimensional quantum system [36,37]. However, even in these papers the extraction of deterministic work is not fully understood.

To achieve the state transformations that are possible under thermal operations using crude operations, we required the use of a single thermal qubit as an ancilla. It would be interesting to investigate the extent to which this is required. In other words, what state transformations can be performed using crude operations applied to the system alone?

Finally, with regards to the experimental applicability of our crude operations, we note that our operation of partial level thermalization has been proposed to be used in protocols for heat bath algorithmic cooling [41]. There they have been used to break previous cooling bounds which are important for quantum information processing on NMR systems. Hence, it would be interesting to investigate whether allowing for the full power of crude operations can be used to enhance these protocols still further. In another direction, perhaps NMR systems can

provide a useful test bed for the experimental study of crude operations and quantum and nanoscale thermodynamics in general.

The data that support the findings of this study are available from the corresponding author (j.oppenheim@ucl.ac.uk) upon reasonable request.

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