Fluctuations in Single-Shot $\epsilon$-Deterministic Work Extraction

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In the single-shot regime it is argued that the criterion for allowed state transitions ought to be more restricted than the second law of thermodynamics, and is given by a condition called thermo-majorisation. Hence to arrive at a fluctuation theorem for the single-shot scenario, such a restriction has to be taken into account. Here we formulate and prove a tighter fluctuation relation for the single-shot $\epsilon$-deterministic work extraction. The result links two areas of thermodynamics which have been of great interest recently, fluctuation relations for non-equilibrium processes and the $\epsilon$-deterministic work extractable from single microscopic non-equilibrium systems. Furthermore, in doing so, we unify the notions of fluctuation in $\epsilon$-deterministic work extraction and in fluctuation theorems.

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I. INTRODUCTION

Crooks Fluctuation Theorem is a powerful tool that can be utilised to study processes which occur far from equilibrium $^1$. It is significant in the microscopic regime where fluctuations of observed quantities can be of the same order as the quantities themselves. Crooks Fluctuation Theorem has been experimentally confirmed to a good degree in various set-ups.

Crooks Fluctuation Theorem relies on the standard assumptions in thermodynamics for allowed transitions. Standard thermodynamics has been developed for average quantities, i.e. where one has access to independent and identically prepared ensembles and measurements can be performed numerous times. In this framework the criterion for transition of a state to another is given by the second law of thermodynamics. Recently with the rise of quantum thermodynamics beyond i.i.d. we ask similar questions about single values of thermodynamic quantities with access to only a finite amount of resources. It has been shown that within this regime the allowed transitions are subject to more stringent conditions than given by the second law: they are determined by thermo-majorisation, and the transitions are achieved via so-called Thermal Operations $^8$ $^2$. Thus, we require a variation of Crooks Fluctuation Theorem, compatible with the assumptions of the single-shot scenario to make predictions about quantities such as work in the presence of fluctuations, in this regime, which is the aim of this paper.

The first law of thermodynamics distinguishes between an ordered form of energy, which we call work, and a disordered form of it, which we call heat. In the microscopic single-shot regime, however, the ‘work’ extracted via an ordinary work extraction protocol is very noisy, due to the presence of fluctuations on the order of the amount of work extracted. Thus, to have a notion of work akin to its ordered classical counterpart there is a need for the introduction of $\epsilon$-deterministic work $^2$ $^3$.

$\epsilon$-deterministic work extraction protocols guarantee a specific value of work to be extracted from a system with failure probability $\epsilon << 1$. This framework has its origin in single-shot information theory and variants of so-called min- and max-entropies $^1$. Horodecki-Oppenheim $^2$ and Åberg $^3$ independently quantified the amount of work that can be extracted from a system $\epsilon$-deterministically for a nontrivial Hamiltonian from an arbitrary initial, and thermal final state.

Note that in both paradigms – Crooks Fluctuation Theorem and single-shot $\epsilon$-deterministic work extraction – a concept of fluctuation is central. Nevertheless, a formal study of a possible relationship between the seemingly different notions of fluctuation is absent in the literature. Here we fill this existing gap by formulating and proving a fluctuation relation for single-shot $\epsilon$-deterministic work extraction, compatible with the assumption of thermo-majorisation.

Our set-up is compatible with the assumptions in the work of Horodecki-Oppenheim $^2$. In particular we do not restrict ourselves to thermal initial states. Our setup consists of a work system, a battery, and a thermal bath. The system, initially in an arbitrary block diagonal state $\rho_s$, is in contact with a thermal bath in state $\tau_{\text{bath}}$, and a work storage device, referred to as battery and initially in its ground state $|0\rangle \langle 0|$. The protocol extracts work $w$ by performing thermal operations on the system state and as a result lifts the battery to the excited state $|w\rangle \langle w|$. To gain the maximum amount of work, we choose a protocol such that the system’s final state will be the thermal state, $\tau_w$, of the Hamiltonian.

In this paper we obtain a fluctuation relation between the amount of work extracted $\epsilon$-deterministically in a forward protocol vs the amount of work cost in the reverse protocol in terms of the smooth min-relative entropy (Eq. $^10$). As a corollary of our result we obtain the lower bound of the extractable work found by Åberg $^9$.

As in $^2$, our results are derived in the time-independent Hamiltonian framework. This is not a loss

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II. PRELIMINARIES

The set-up for Crooks Fluctuation Theorem is that we prepare a system in thermal equilibrium with respect to an initial Hamiltonian. Then an energy measurement is performed on the system using projective operators in the eigenbasis of the initial Hamiltonian. The system is then driven to a new state by changing the Hamiltonian to the final energy levels and an energy measurement is performed in the energy eigenbasis of the final Hamiltonian. This defines the forward process, denoted \( \mathcal{P} \). Next, we define a reversed process, \( \mathcal{P}^{\text{rev}} \), by preparing the state in the thermal state of the final Hamiltonian of the forward process and performing an energy measurement. The system is then driven to a new state by changing the energy levels back to the initial Hamiltonian of the forward process, and the final energy measurement is performed. Crooks Fluctuation Theorem relates the work cost distribution, \( P(w, \mathcal{P}) \), in the forward process, given a process \( \mathcal{P} \), to that of the work gain of the same amount in the reversed process, \( P(-w, \mathcal{P}^{\text{rev}}) \), by

\[
\frac{P(w, \mathcal{P})}{P(-w, \mathcal{P}^{\text{rev}})} = e^{\beta(w - \Delta F)},
\]

where \( \beta = \frac{1}{RT} \) is the inverse temperature of the environment divided by the Boltzmann constant, \( w \) is the work cost of the process, and \( \Delta F \) is the free energy difference of the initial and final state. Notice that while each distribution depends on the process used, the ratio depends only on the difference between equilibrium free energies. The physical significance of this equality is that it implies that it is possible, however unlikely, to have fluctuations in work gain larger than \( \Delta F \). This is not in contrast to the second law of thermodynamics, as the law is a statement about average work, whereas here we are concerned with a single value of work.

To formulate a similar fluctuation theorem for single-shot \( \epsilon \)-deterministic work extraction we adopt the same assumptions as \( \mathcal{P}^{\text{rev}} \) on the bath, namely that

(i) the spectrum of the heat bath is continuous, i.e. for an energy of the heat bath \( E_R \) and two arbitrary energies of the system, \( E_S \) and \( E'_S \), there exists \( E'_R \), such that \( E_R + E_S = E'_R + E'_S \),

(ii) and around the energy \( E \) the degeneracies can be written as

\[
g(E + \Delta E) = e^{S(E + \Delta E)} = e^{S(E) + \Delta E \frac{\partial S(E)}{\partial E} + O(\Delta E^2)}
\]

where \( S(E) := \ln g(E) \) and \( \beta = \frac{\partial S(E)}{\partial E} \). Notice that for a large enough bath the second order and higher terms in Eq. (1) and (2) can be neglected, which is the assumption we adopt throughout this paper.

Initially, the total system consists of the system \( \rho_s \) from which we intend to extract work, a bath \( \tau_{\text{bath}} \) and a battery in its ground state. Extracting work, \( w \), by Thermal Operations amounts to lifting the battery state to the pure excited state \( \ket{w} \). Since the total energy has to be conserved, the change in the energy of the battery has to be compensated by a change in the work content of the rest of the system. A general final state would be \( \tau_{\text{bath}} \otimes \sigma_r \otimes \ket{w} \bra{w} \). This transition was shown to be possible, if and only if the initial state thermo-majorises the final \( \sigma_r \). A special case is when \( \sigma_r \) is the thermal state \( \tau_r \), which we choose in order to achieve maximum work. Denote with \( P(w, \mathcal{P}) \) the probability of transferring the energy value \( w \) from the system to the battery in a forward process \( \mathcal{P} \) and with \( P(-w, \mathcal{P}^{\text{rev}}) \) the probability of transferring the same energy value \( w \) from the battery back to the system in a reverse process \( \mathcal{P}^{\text{rev}} \). To begin with we consider the simple case of a process which extracts the amount of work \( w \) from the working system with probability one, i.e. with failure probability \( \epsilon = 0 \). For such a case, the following lemma holds. This does not give a fluctuation theorem directly. However, it is an important building block in proving the theorem in the next section.

In the following lemma we use Renyi relative entropy of order \( \alpha = 0 \) defined as \( D_{\alpha}(\rho_s \| \tau_r) := -\ln Tr[\rho_s^\alpha \tau_r] \), with \( \rho_s^\alpha \) being the support of the initial state and \( \tau_r \) the thermal state of the system. In the following lemma we adopt the same sign convention for work as used in \( \mathcal{P}^{\text{rev}} \).

Lemma 1. Consider the total system \( \tau_{\text{bath}} \otimes \rho_s \otimes \ket{0} \bra{0} \) consisting of a work system in some arbitrary state, diagonal in energy eigenbasis, \( \rho_s \), subject to a time-independent Hamiltonian, a thermal bath at temperature \( T \) in state \( \tau_{\text{bath}} \), and a two-level battery system in its pure ground state \( \ket{0} \bra{0} \). Furthermore, assume processes \( \mathcal{P} \) and \( \mathcal{P}^{\text{rev}} \) consisting of Thermal Operations only. Then

\[
\frac{P(w, \mathcal{P})}{P(-w, \mathcal{P}^{\text{rev}})} = e^{\beta w + D_{0}(\rho_s \| \tau_r)},
\]

where with \( w \) being the work extracted, and \( \beta = 1/kT \) where \( k \) is the Boltzmann constant.

Proof. In \( \mathcal{P}^{\text{rev}} \) it was shown that, for a fixed total energy \( E \) if the bath is very large compared to the system, the state \( \tau_{\text{bath}} \otimes \rho_s \otimes \ket{0} \bra{0} \) can be written as \( \bigoplus E_s \rho_s^{E_s} \otimes \Pi E_s \rho_s \Pi E_s \otimes \ket{0} \bra{0} \), where \( \rho_s^{E_s} := \frac{\rho_s}{g_R(E-E_s)} \), \( g_R(E-E_s) \) is the degeneracy of the bath, and the identity \( \Pi E_s \rho_s \Pi E_s \otimes \ket{0} \bra{0} \) is the thermal state of the final Hamiltonian of the forward process, denoted \( \mathcal{P} \).

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acts on a $g_R(E-E_s)$-dimensional space. Similarly, the final state can be written as $\bigoplus_{E_i} F_{E_i-w}^\dagger \Pi_{E_i} \tau_s \Pi_{E_i} \otimes |w\rangle \langle w|$. Since the total system is block diagonal in energy eigenbasis, we can treat the eigenvalues of it as probabilities. Denote the energy levels of initial and final state by $E_i$ and $E_j$, respectively. The eigenvalues of the initial and final state are $g(E_{i-j})$ and $g(E_{j-i})$, respectively. Denote the transition current, i.e. the number of eigenstates that go from $E_i$ to $E_j$ by $k_{i-j}$. Then occupation probabilities of the final state of the system are given by

$$P(E_j) = \sum_i k_{i-j} \frac{P(E_i)}{g(E-E_i)}. \quad (4)$$

Each summand on the RHS is the joint probability of the system initially occupying the $i$th energy level and ending up in the $j$th energy level in the final state. Since the protocol stores the energy difference between initial and final state, i.e. the work $w$, in the battery state the probability of a value of work $P(w, \mathcal{P})$ can be calculated by summing the RHS over $j$. Notice that the total number of eigenstates in initial energy level $E_i$ are

$$d_i = \sum_j k_{i-j} = g(E-E_i), \quad (5)$$

and that the total number of eigenstates in final energy level $E_j$ are

$$d_j = \sum_i k_{i-j} = g(E-E_j-w). \quad (6)$$

Furthermore, for the reversed process it is the case that

$$\sum_i k_{i-j}^{rev} = g(E-E_j-w). \quad (7)$$

Below, we calculate the ratio of the work cost probability to that of work gain probability for such a process.

$$\frac{P(w, \mathcal{P})}{P(-w, \mathcal{P}^{rev})} = \frac{\sum_{i,j} k_{i-j} \frac{P(E_i)}{g(E-E_i)}}{\sum_{i,j} k_{i-j}^{rev} \frac{P(E_i)}{g(E-E_i-w)}} = \frac{\sum_i g(E-E_i) \frac{P(E_i)}{g(E-E_i)}}{\sum_j g(E-E_j-w) \frac{P(E_i)}{g(E-E_i-w)}} = \frac{\sum_i g(E-E_i) \sum_j k_{i-j}^{rev} \frac{P(E_j)}{g(E-E_j-w)}}{\sum_j g(E-E_j-w) \frac{P(E_i)}{g(E-E_i-w)}} \quad (8)$$

Rewriting the term in the enumerator as follows

$$\sum_j k_{j-i}^{rev} \frac{P(E_j)}{g(E-E_j-w)} = \sum_j k_{j-i}^{rev} \frac{1}{g(E-w)} \frac{g(E-E_i)}{Z} = \frac{g(E-E_i)}{g(E-w)Z} \quad (9)$$

where $Z$ is the partition function of the Gibbs state, and using the fact that the system ends up in the Gibbs state, together with the assumption on the bath in Eq. 2 that $g(E-E_j) = g(E)e^{-\beta E_j}$ we find, simplifying the fraction,

$$\frac{P(w, \mathcal{P})}{P(-w, \mathcal{P}^{rev})} = \frac{\sum_i g(E-E_i)}{\sum_j g(E-E_j-w)} \quad (10)$$

We observe that the index $i$ runs over the support of $\rho$ and $j$ runs over all final states and

$$D_0(\rho_s||\tau_s) = \ln \sum_i e^{-\beta E_i} - \ln \sum_j e^{-\beta E_j}. \quad (11)$$

Hence using the equations $g(E-E_j-w) = g(E)e^{-\beta E_j}e^{-\beta w}$ and $g(E-E_i) = g(E)e^{-\beta E_i}$, we arrive at

$$\frac{P(w, \mathcal{P})}{P(-w, \mathcal{P}^{rev})} = \exp\{\beta w + D_0(\rho_s||\tau_s)\}. \quad (12)$$

Notice that each of these probabilities are equal to one, i.e.

$$\sum_{i,j} k_{i-j} \frac{P(E_i)}{g(E-E_i)} = \sum_i g(E-E_i) \frac{P(E_i)}{g(E-E_i)} = 1, \quad (13)$$

since the sum of probabilities of the initial energy levels has to be equal to one. Therefore, the fully deterministic work extraction has only a trivial distribution of one value of extracted work and zero everywhere else. For a fluctuation theorem to say something about the work probability, it has to have a width. Below we extend the relation for the $\epsilon$-deterministic case.

### III. $\epsilon$-DETERMINISTIC WORK EXTRACTION

In the case of $\epsilon$-deterministic work extraction we may not lift the battery state to a pure state $|w\rangle\langle w|$ with certainty. This means that the work distribution has a finite width and the final state of the battery, $\rho_s^w$ is only $\epsilon$-close to the desired work state $|w\rangle\langle w|$. That is, the final state of the battery is given by

$$\rho_s^w = (1-\epsilon)|w\rangle\langle w| + \epsilon \rho_{\perp w}, \quad (14)$$

where $\rho_{\perp w}$ is a mixed state orthogonal to $|w\rangle\langle w|$. We now state the result on the ratio between the probability of extracting work $w$ in an $\epsilon$-deterministic forward process and the probability of putting work $w$ back into the system in a $\delta$-deterministic backward process.

**Theorem 1.** Consider a system $\tau_{\text{bath}} \otimes \rho_s \otimes |0\rangle\langle 0|$ consisting of a work system in some arbitrary state, diagonal in energy eigenbasis, $\rho_s$ subject to a time-independent
Hamiltonian, a thermal bath at temperature $T$ in state $\tau_{\text{bath}}$, and a many-level battery system in its pure ground state $|0\rangle\langle 0|$. Furthermore, assume $\epsilon$-deterministic forward process $P$ and $\delta$-deterministic reverse process $P^{\text{rev}}$ consisting of Thermal Operations only. Then the ratio of work extraction probability, $P(w, P^\epsilon)$, to work cost probability, $P(-w, P^{\delta, \text{rev}})$, is given by

$$
P(w, P^\epsilon) = \frac{e^{\beta w - \ln(1-\delta) + D_0^b(\rho_s||\tau_s)}}{P(-w, P^{\delta, \text{rev}})},$$

where $w$ is the work extracted, multiplied by $\beta = 1/kT$, where $k$ the Boltzmann constant and $T$ the temperature. $D_0^b(\rho_s||\tau_s)$ is the smooth version of Renyi divergence of order $\alpha = 0$.

Theorem 1 says that if a quantum system is transformed to a thermal state via Thermal Operations only, thereby giving work, the probability of the work extracted is generally not the same as the probability of the work done to transform the system back to its initial state. This is quantified by the term in the exponent and implies an intrinsic irreversibility in the finite-run behaviour of microscopic system, in the single-shot regime. Note, that $-\ln(1-\delta)$ is the maximum work content of an equilibrium distribution in a $\delta$-deterministic process.\[3\]

For the proof of Theorem 1 we use the technique of $\beta$-ordering as introduced in Supplementary Note 4 of [2] and as illustrated in Fig. 4. The graph plots $P(E_i)e^{\beta E_i}$ vs $\sum_i e^{-\beta E_i}$ for each $E_i$, arranging states in decreasing order of their value $P(E_i)e^{\beta E_i}$. In this piecewise linear staircase function, the width of each rectangle equals the weight of the state $P(E_i)$, and the total width is equal to $Z$, the probability of the state. Removing the maximum number of states with the minimum total probability then corresponds to removing states from the right side of the $\beta$-ordered spectrum. This procedure is also called smoothing.

**Proof.** We wish to express the LHS of Eq. 10 in terms of the work extracted from the system. Starting with the $\epsilon$-deterministic forward process we need to find a minimal set of eigenstates such that their total weight is at least $1 - \epsilon$. Removing an $\epsilon$ weight of the initial state amounts to smoothing.

To achieve this we $\beta$-order the eigenstates of the initial state as explained above. Then we remove as many eigenstates from the low weight end of the spectrum as possible while staying within the $1 - \epsilon$ limit. This is done by choosing an index $l$, such that

$$1 - \epsilon \geq \sum_{i=1}^{l} g(E - E_i) \frac{P(E_i)}{g(E - E_i)} \quad (11)$$

and

$$1 - \epsilon \leq \sum_{i=1}^{l+1} g(E - E_i) \frac{P(E_i)}{g(E - E_i)}. \quad (12)$$

**FIG. 1:** A weight $\epsilon$ is being taken out after $\beta$-ordering. $\beta$-ordering refers to rearranging the eigenstates’ energies in decreasing order of their value $P(E_i)e^{\beta E_i}$. In this piecewise linear staircase function, the width of each rectangle equals the weight of the state $P(E_i)$, and the total width is equal to $Z$, the probability of the state. Removing the maximum number of states with the minimum total probability then corresponds to removing states from the right side of the $\beta$-ordered spectrum. This procedure is also called smoothing.

Now we map these eigenvalues of weight $1 - \epsilon$ to $w$. For such a mapping, the ratio of the work gain distribution to its work cost counterpart is
\[
P(w, P^\epsilon) = \frac{\sum_j \left( \sum_{i=1}^l k_{i\rightarrow j} P(E_i)_{g(E-E_i)} + \frac{\delta_{\beta}}{g(E-E_{i+1})} \right)}{\sum_{i,j} \sum_{l} k_{j\rightarrow i} P(E_j)_{g(E-E_{i+1}-w)}} \]
\[
= \sum_{i=1}^l g(E-E_i) \frac{P(E_i)_{g(E-E_i)}}{g(E-E_{i+1})} + \frac{1-\epsilon}{\sum_{i,j} k_{j\rightarrow i} P(E_j)_{g(E-E_{i+1}-w)}} \sum_{i,j} k_{j\rightarrow i} P(E_j)_{g(E-E_{i+1}-w)} \]
\[
= \sum_{i=1}^l g(E-E_i) \sum_{j} k_{j\rightarrow i} P(E_j)_{g(E-E_{i+1}-w)} + \frac{1-\epsilon}{\sum_{i,j} k_{j\rightarrow i} P(E_j)_{g(E-E_{i+1}-w)}} \sum_{i,j} k_{j\rightarrow i} P(E_j)_{g(E-E_{i+1}-w)} \]
\[
= \sum_{i=1}^l g(E-E_i) + \frac{1-\epsilon}{\sum_{i,j} g(E-E_{i+1})} \sum_{j} g(E-E_j - W^\delta) \]
\[
= \exp{\beta W^\delta + D_0^\epsilon(\rho_s||\tau_s)} \]
\]

In Eq. (13), we use Eqs. (11) and (12) to count the number of states with their specific weights that are mapped to the work extracted. In Eq. (14), the probability of the system being in energy state \(E_{i+1}\) is re-written in terms of the final probabilities and the backward process. In the backward process the work \(w\) is returned from the battery to the system via a \(\delta\)-deterministic process. It was shown in [3] that for \(\delta\)-deterministic processes, the thermal distribution has a maximum work content of \(-\frac{1}{\beta} \ln(1-\delta)\) which has to be added to the work content of the battery when calculating the total number of states in the backward process in order to conserve the total energy. Hence, defining \(W^\delta = w - \frac{1}{\beta} \ln(1-\delta)\) we have

\[
\sum_j k_{j\rightarrow i}^{rev} = g(E-E_j - W^\delta),
\]

which gives the denominator in Eq. (15). Eq. (16) follows from a similar argument to Eq (9), albeit with a smoothing parameter. The \(D_0^\epsilon(\rho||\tau)\) admits the exact definition used in [2].

One might question whether the \(-kT \ln(1-\delta)\) work content is relevant to our setup. Whilst the result in [3] is sufficiently general, one can confirm the relevance by re-deriving it utilising our techniques. Using our framework, one should \(\beta\)-order the thermal state and remove a weight \(\delta\), similar to the case for our initial state of the forward process in Fig. (1), then driving the system to a fully thermal state. It is, then, straightforward to see that the \(-kT \ln(1-\delta)\) work content holds for our setting as well.

In the following corollary we shall observe how a known bound of work extraction follows from our result.

**Corollary 1.** The work that can be extracted from a system out of equilibrium by \(\epsilon\)-deterministic Thermal Operations is bounded from below as

\[
-kT D_0^\epsilon(\rho_s||\tau_s) + kT \ln(1-\epsilon) \leq w.
\]

To see this, we multiply both sides of the Eq. (10) by \(P(-w, P^{\delta,rev})\). From the fact that \(P(w, P^\epsilon) \geq 1-\epsilon\) and the \(\delta\) smoothing contribution to the work cancels out the backward probability, the statement in the corollary follows. This is the same lower bound for work extraction, given by Åberg [3].

**IV. DISCUSSION AND CONCLUSION**

In the discussion section of Ref. [3], Åberg leaves the question of the link between the fluctuations of the \(\epsilon\)-deterministic work extraction paradigm to that of the fluctuation theorems paradigm open. Theorem 1 above has answered this question. We have seen that (as it is the case in Lemma 1) in the absence of any fluctuations of the former type the distributions become trivial and there will be no fluctuations of the latter type. It is only through the introduction of the \(\epsilon\)- and \(\delta\)-uncertainties that we obtain a fluctuation theorem, and hence demonstrating the direct connection between the two. The relation in Theorem 1 quantifies the ratio of the probability of work extraction in a process to that of work cost in its backward process, in terms of the smooth Renyi divergence of order \(\alpha = 0\), whose corollary gives the known bounds of work extraction protocols. Another reason for formulating and proving this fluctuation theorem is the need for having such a relation for the single-shot regime where the allowed transitions are more restricted than the ones given by the second law of thermodynamics. There, the criterion is thermo-majorisation and the set of operations are the Thermal Operations. Thus we adopt the same restriction in our setting. In this paper we have focused on the notion of \(\epsilon\)-deterministic work. Nevertheless, probabilistic work in the single-shot scenario is also
an interesting concept and has been recently studied \[6\]. There has been a previous work on the direction of uni-
fication of single-shot scenarios and fluctuation theorems \[7\]. Our work is different in many respects. For instance, Halpern et al. assume Crooks relation and take its as-
sumptions. Also our result is in terms of the divergence of states, as opposed to the work distributions only, which connects more directly to the existing single-shot results. Note added: Similar results were obtained independently by Dahlsten et al, using a different set-up and different starting assumptions, in Equality for worst-case work at any protocol speed.

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[8] Thermal Operations are the set of allowed maps compatible with the assumption of thermo-majorisation \[2, 5, 6\]. They are characterised by the following rules i) a system with any Hamiltonian in the Gibbs state of that Hamiltonian can be added, ii) any subsystem can be discarded through tracing out and iii) any energy-conserving unitary, i.e. those unitaries that commute with the total Hamiltonian, can be applied to the global system.