

The thermodynamic cost of quantum operations

This content has been downloaded from IOPscience. Please scroll down to see the full text.

2016 New J. Phys. 18 113050

(<http://iopscience.iop.org/1367-2630/18/11/113050>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 163.1.203.121

This content was downloaded on 08/12/2016 at 12:50

Please note that [terms and conditions apply](#).

You may also be interested in:

[Measures and applications of quantum correlations](#)

Gerardo Adesso, Thomas R Bromley and Marco Cianciaruso

[Distinguishability of countable quantum states and von Neumann lattice](#)

Ryûitirô Kawakubo and Tatsuhiko Koike

[Lively quantum walks on cycles](#)

Przemysław Sadowski, Jarosław Adam Miszczyk and Mateusz Ostaszewski

[Robustness of quantum correlations against linear noise](#)

Zhihua Guo, Huaixin Cao and Shixian Qu

[Optimal quantum networks and one-shot entropies](#)

Giulio Chiribella and Daniel Ebler

[Causal and causally separable processes](#)

Ognian Oreshkov and Christina Giarmatzi

[Thermodynamic and logical reversibilities revisited](#)

Takahiro Sagawa

[Quantum measurement and uncertainty relations in photon polarization](#)

Keiichi Edamatsu

[Equilibration of quantum gases](#)

Terry Farrelly



PAPER

The thermodynamic cost of quantum operations

D J Bedingham¹ and O J E Maroney

Faculty of Philosophy, University of Oxford, OX2 6GG, UK

¹ Author to whom any correspondence should be addressed.E-mail: daniel.bedingham@philosophy.ox.ac.uk and owen.maroney@philosophy.ox.ac.uk

Keywords: thermodynamics, information processing, quantum computing

OPEN ACCESS

RECEIVED
4 July 2016REVISED
21 October 2016ACCEPTED FOR PUBLICATION
24 October 2016PUBLISHED
24 November 2016Original content from this work may be used under the terms of the [Creative Commons Attribution 3.0 licence](https://creativecommons.org/licenses/by/3.0/).

Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.



Abstract

The amount of heat generated by computers is rapidly becoming one of the main problems for developing new generations of information technology. The thermodynamics of computation sets the ultimate physical bounds on heat generation. A lower bound is set by the Landauer limit, at which computation becomes thermodynamically reversible. For classical computation there is no physical principle which prevents this limit being reached, and approaches to it are already being experimentally tested. In this paper we show that for quantum computation with a set of signal states satisfying given conditions, there is an unavoidable excess heat generation that renders it inherently thermodynamically irreversible. The Landauer limit cannot, in general, be reached by quantum computers. We show the existence of a lower bound to the heat generated by quantum computing that exceeds that given by the Landauer limit, give the special conditions where this excess cost may be avoided, and provide a protocol for achieving the limiting heat cost when these conditions are met. We also show how classical computing falls within the special conditions.

1. Introduction

Information processing does not come for free. Physical systems are needed to store, transmit and process information, and these come with physical resource costs, in time, space and energy. The heat generated by information processing is becoming one of the most significant of these costs. Modern integrated circuits have power densities of the order 100 W cm^{-2} with operating temperatures near to their upper limit [1]. Thermal management is already the main constraint on the performance of modern electronics and advances in technology will increasingly need to test the fundamental limits of energy consumption.

For classical information processing, Landauer's principle [2–5] relates the change in information from a computation to a minimum thermodynamic cost in the form of heat generated in the environment. The information content of a source of signals is measured by the Shannon measure $H = -\sum_n p_n \log_2 p_n$, where p_n is the probability of signal n occurring. Landauer's principle states that the mean heat generated by an information processing device is given by

$$\Delta E_{\text{classical}} \geq -kT \ln 2 \Delta H, \quad (1)$$

where ΔH is the change in the Shannon information.

The limit cost, which corresponds to the condition of thermodynamic reversibility [6, 7], is defined purely in terms of the information processing operation itself: every physical system which performs the task must pay at least this cost [6, 8, 9]. Most importantly, it is a tight bound: while there are practical barriers to reaching the limit (finite size and time effects, single shot costs, etc [10, 11]) there is no physical principle that prevents their effects becoming arbitrarily small, with experimental tests increasingly pushing at this boundary [12–14]. This tight relationship between information theory and thermodynamics makes Landauer's principle the basis of our understanding of the thermodynamic cost of information processing.

However, both the theoretical studies and experimental tests of the Landauer limit have almost exclusively considered classical information processing. Quantum computing radically alters the nature of information, leading to many attempts to extend Landauer's principle to quantum theory [15–27].

Quantum information processing involves a quantum system S with non-orthogonal states $\rho_S^{n'}$ as signal states, undergoing a quantum operation Q , defined by its effect upon the signal states $\rho_S^n \rightarrow \rho_S^{n'} = Q(\rho_S^n)$. Given that the input ρ_S^n appears with probability p_n , the average input is $\rho_S = \sum_n p_n \rho_S^n$, and the average output is $\rho_S' = \sum_n p_n \rho_S^{n'}$.

The natural quantum generalisation of Shannon information to quantum theory is the Schumacher information measure $S(\rho_S) = -\text{Tr}[\rho_S \log_2 \rho_S]$ [28], which agrees with the Shannon information when the signal states are orthogonal. This suggests that equation (1) should be replaced by

$$\Delta E_Q \geq kT \ln 2 [S(\rho_S) - S(\rho_S')]. \quad (2)$$

While it is well known that equation (2) must hold, and that reaching the equality is required for thermodynamic reversibility [29, 30], we show that it fails as a tight bound due to the non-orthogonality of states in quantum information processing. There is an unavoidable excess heat generation in quantum computation that is not present in the classical case.

Summary of the theorem

For any given quantum operation Q there is non-negative quantity ϵ_Q , defined independently of how the quantum operation is physically implemented, such that the heat generated by the operation is bounded by:

$$\Delta E_Q \geq kT \ln 2 [S(\rho_S) - S(\rho_S')] + \epsilon_Q.$$

In general for quantum operations $\epsilon_Q > 0$. Barring exceptional symmetric cases, $\epsilon_Q = 0$ if, and only if, all the output signal states $Q(\rho_S^n)$ share a common diagonalised basis, and there exists a common left stochastic map from diagonal elements of the input states (in the diagonal basis of ρ_S) to eigenvalues of the output states. If these conditions do not hold, there is an excess, thermodynamically irreversible cost to any physical process that performs the quantum operation. For cases where these conditions do hold we provide a protocol for achieving the limiting heat cost.

This paper will define quantum operations, characterise the thermodynamics of implementing quantum operations, state the theorem, and then give examples of operations which meet, and operations which do not meet, the conditions for $\epsilon_Q = 0$.

2. Quantum operations

While classical information processing is built up from logical operations such as AND, OR and NOT gates, the fundamental element in quantum information processing is the quantum operation [31]. This acts upon one of a number of possible input states, each represented by a different quantum density matrix, $\{\rho_S^n\}$, and maps each one to a specific output state $\rho_S^n \rightarrow \rho_S^{n'}$.

Not all maps of the form $\rho_S^n \rightarrow \rho_S^{n'}$ are physically possible. A general quantum operation, Q_α , must be a completely positive linear map $Q_\alpha(\rho_S^n) = \sum_k Q_{\alpha,k} \rho_S^n Q_{\alpha,k}^\dagger$ with $\sum_k Q_{\alpha,k}^\dagger Q_{\alpha,k} \leq \mathbb{1}_S$. If the operation is trace-decreasing it involves the selection of an outcome, α , which occurs with probability $P(\alpha|n) = \text{Tr}[\sum_k Q_{\alpha,k} \rho_S^n Q_{\alpha,k}^\dagger] < 1$, and $\sum_\alpha P(\alpha|n) = 1$. For a thermodynamic analysis, all possible outcomes must be included, so we must use the non-selective operation $Q(\rho_S^n) = \sum_\alpha Q_\alpha(\rho_S^n)$, for which $\sum_{\alpha,k} Q_{\alpha,k}^\dagger Q_{\alpha,k} = \mathbb{1}_S$. If the operation Q_α is trace-preserving, then clearly $Q(\rho_S^n) = Q_\alpha(\rho_S^n)$.

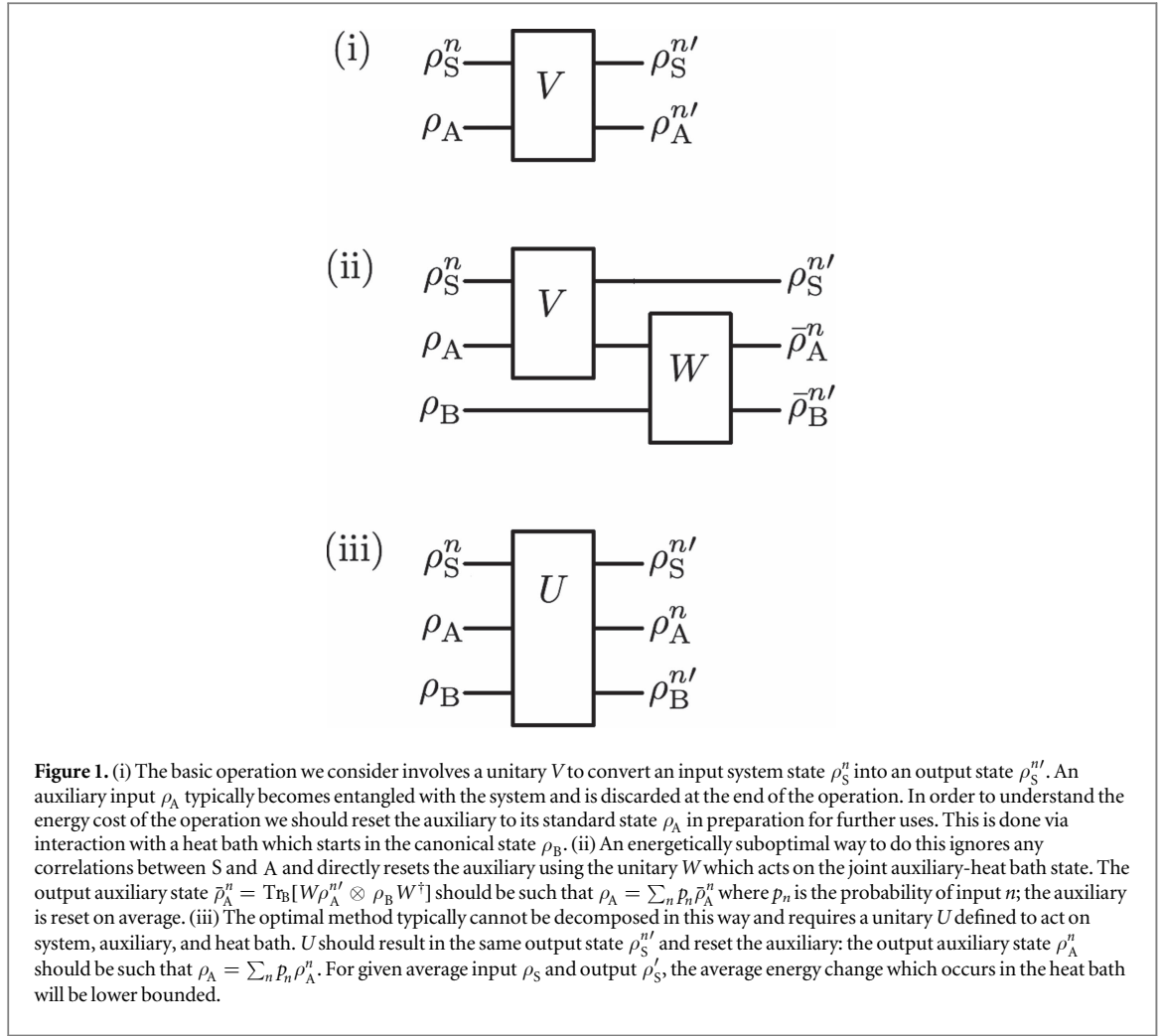
When it is not a pure unitary rotation, a quantum operation requires the use of an auxiliary system A , initially in a standard state, ρ_A . A joint unitary V acting on $\rho_S^n \otimes \rho_A \rightarrow \rho_{SA}^{n'} = V \rho_S^n \otimes \rho_A V^\dagger$ results in an entangled state of system and auxiliary (see figure 1). The reduced state of the system, $\rho_S^{n'} = \text{Tr}_A[V \rho_S^n \otimes \rho_A V^\dagger]$, is the output state (see [31] Chapter 8, for a textbook presentation).

3. Thermodynamics of quantum operations

It is essential, when quantifying the thermodynamic costs of operations, to keep track of the effects upon auxiliary systems. If an auxiliary is disregarded, then the quantum operation would appear to be performed without generating heat. However, this leaves the auxiliary in a state $\rho_A^{n'} = \text{Tr}_S[V \rho_S^n \otimes \rho_A V^\dagger]$. Simply discarding the auxiliary would, on average, change the entropy of the environment by $\ln 2 [S(\rho_A^{n'}) - S(\rho_A)]$

where $\rho_A^{n'} = \text{Tr}_S[V \rho_S \otimes \rho_A V^\dagger] = \sum_n p_n \rho_A^{n'}$.

The most straightforward way to deal with this is to reset the auxiliary to its original state ρ_A . To do this a thermal environment is introduced in the form of a heat bath in a canonical state ρ_B at temperature T . The reset can be performed by some unitary W acting on both the auxiliary and the heat bath such that



$\rho_A = \text{Tr}_B[W\rho_A^{n'} \otimes \rho_B W^\dagger]$ (see figure 1). This operation would transfer at least $kT \ln 2 [S(\rho_A') - S(\rho_A)]$ of heat to the heat bath [29]. Either way, the cost to the environment will generally be more than required by equation (2). A quantum operation typically leaves correlations between system and auxiliary, with a mutual information [18] of $S(\rho_S' : \rho_A') = [S(\rho_S') - S(\rho_S)] + [S(\rho_A') - S(\rho_A)] \geq 0$. A simple resetting (or discarding) of the auxiliary, as described above, is therefore paying $kT \ln 2 S(\rho_S' : \rho_A')$ as an excess cost over and above the cost of equation (2) unless there is no correlation: $V\rho_S \otimes \rho_A V^\dagger = \rho_S' \otimes \rho_A'$.

To find the minimum thermodynamic cost of the quantum operation, the auxiliary must be reset more efficiently, exploiting correlations with the system. The unitary V must be embedded in a larger unitary U which includes interactions between system, auxiliary, and heat bath. U must preserve the output of the computation

$$\text{Tr}_{AB}[U\rho_S^n \otimes \rho_A \otimes \rho_B U^\dagger] = \rho_S^{n'}, \quad \forall n; \quad (3)$$

while resetting the auxiliary

$$\text{Tr}_{SB}[U\rho_S \otimes \rho_A \otimes \rho_B U^\dagger] = \rho_A \quad (4)$$

(see figure 1, and appendix A for formal details on this set up). Standard calculations show that this implies equation (2) (see appendix B). If the quantum operation is only defined for a single signal state, then physical implementations are possible which can get arbitrarily close to the equality in (2) (appendix C).

In general, a quantum operation must produce the result $\rho_S^{n'} = \mathcal{Q}(\rho_S^n)$, for multiple signal states $\{\rho_S^n\}$. The same U must satisfy (3) for all n . Our principal result is to show this additional constraint forces a higher thermodynamic cost than equation (2). An operation which generates a quantity of heat, ϵ_Q , in excess of this bound will be thermodynamically irreversible, as any second operation which restores the original average state $\rho_S = \mathcal{Q}'(\rho_S')$ must necessarily leave a net heat gain in the heat bath of at least ϵ_Q over the complete cycle. Quantum computations cannot, in general, be performed in a thermodynamically reversible manner.

4. The theorem

Let $\rho_S^n \rightarrow \rho_S^{n'} = \text{Tr}_{AB}[U\rho_S^n \otimes \rho_A \otimes \rho_B U^\dagger]$ be a quantum operation Q where ρ_B is the state of a canonical heat bath at temperature T , and ρ_A is a standard state of an auxiliary which should be restored by the operation (see equation (4)).

The average system input state ρ_S can be expressed in terms of its diagonal basis vectors $\{|\phi_i\rangle\}$ as

$$\rho_S = \sum_n p_n \rho_S^n = \sum_i \lambda_i |\phi_i\rangle \langle \phi_i|.$$

Similarly the average system output state can be expressed in terms of its diagonal basis vectors $\{|\phi'_k\rangle\}$ as

$$\rho_S' = \sum_n p_n \rho_S^{n'} = \sum_k \lambda'_k |\phi'_k\rangle \langle \phi'_k|.$$

In terms of these basis vectors the individual inputs and outputs are represented by

$$\rho_S^n = \sum_{ij} \mu_{ij}^n |\phi_i\rangle \langle \phi_j| \quad \text{and} \quad \rho_S^{n'} = \sum_{kl} \mu_{kl}^{n'} |\phi'_k\rangle \langle \phi'_l|.$$

We now state the theorem:

Theorem 1. *If there exists a stochastic map, $P_Q(k|i)$ with*

$$\sum_k P_Q(k|i) = 1 \quad \text{and} \quad P_Q(k|i) \geq 0 \quad \forall i, k,$$

such that

$$\mu_{kl}^{n'} = \delta_{kl} \sum_i P_Q(k|i) \mu_{ii}^n, \quad (5)$$

for all n , then the minimum thermodynamic cost of the operation

$$\Delta E_Q \geq kT \ln 2 [S(\rho_S) - S(\rho_S')] + \epsilon_Q,$$

can approach $\epsilon_Q = 0$. Otherwise, provided there are no symmetries of the form $\lambda_i/\lambda_j = \lambda'_k/\lambda'_l$ where $i \neq j$ or $k \neq l$, then necessarily $\epsilon_Q > 0$.

Note that the set of properties $\{\{\lambda_i\}, \{\lambda'_k\}, \{\mu_{ij}^n\}, \{\mu_{kl}^{n'}\}\}$, used to state the theorem are defined solely in terms of the quantum operation, independently of the particular physical process used to implement it.

Outline of proof

In appendix A we show that the implementation of the operation can be re-written in the form

$$\mu_{kl}^{n'} = \sum_{ij} q(kl|ij) \mu_{ij}^n, \quad (6)$$

where the complex coefficients $q(kl|ij)$ carry the effects of interaction with the environment. They have the properties $q(kk|ii) = q^*(kk|ii) \geq 0$, and $\sum_k q(kk|ij) = \delta_{ij}$. In appendix B we show that for a given physical implementation of the quantum operation where $\rho' = U\rho_S \otimes \rho_A \otimes \rho_B U^\dagger$, and $\rho_* = \rho_S' \otimes \rho_A \otimes \rho_B$,

$$\epsilon_Q \geq \frac{1}{2} kT \|\rho' - \rho_*\|_1^2. \quad (7)$$

Finally in appendix D we show that

$$\|\rho' - \rho_*\|_1 \geq \frac{|\lambda_j \lambda'_k - \lambda_i \lambda'_l|}{\lambda'_k + \lambda'_l} |q(kl|ij)|. \quad (8)$$

It follows that if there is a value of $|q(kl|ij)| > 0$ for which $\lambda_i/\lambda_j \neq \lambda'_k/\lambda'_l$, then the implementation has an excess thermodynamic cost.

The coefficients $q(kk|ii)$ imply no bound as $\lambda_i/\lambda_j = \lambda'_k/\lambda'_l$ automatically holds for them. If equation (5) holds, then $q(kk|ii) = P_Q(k|i)$ gives an implementation with no excess cost (see appendix F for an explicit construction of a suitable protocol). Otherwise, there must be some $|q(kl|ij)| > 0$ for $i \neq j$ or $k \neq l$. If $\lambda_i/\lambda_j \neq \lambda'_k/\lambda'_l$ for any of these $ijkl$ values, then there is an excess cost for that implementation. We can therefore use numerical optimisation techniques to find the coefficients satisfying (6) which minimise the largest value of (8), and equation (7) shows this gives a lower bound for ϵ_Q .

When the output states do not have a shared diagonalised basis, so that there is some $\mu_{kl}^{n'} > 0$ for $k \neq l$, there is also an analytical bound:

$$\epsilon_Q \geq \frac{1}{2} kT \max_{n,k,l \neq k} \left\{ \frac{|\mu_{kl}''|/(\lambda_k' + \lambda_l')}{\sum_{ij} |\mu_{ij}''|/|\lambda_j \lambda_k' - \lambda_i \lambda_l'|} \right\}^2. \quad (9)$$

For further details see appendix E.

This energy bound and others derived here will not in general be tight. It is an open problem to demonstrate a protocol which reaches ϵ_Q —our results only place a non-zero lower bound on the excess energy cost.

5. Examples of thermodynamically reversible operations

There are well known cases of quantum operations where $\epsilon_Q = 0$. We now show how they fit into our proof.

Pure unitary. In a pure unitary quantum operation, $\rho_S'' = U \rho_S' U^\dagger$. This does not involve an auxiliary or heat bath, and does not change the eigenvalues of any input signal states. Solutions with $q(kl|ij) = \delta_{ik} \delta_{jl}$ satisfy the operation, and the exceptional symmetry condition applies: the only terms which contribute to equation (6) are ones for which $\lambda_i/\lambda_j = \lambda_k'/\lambda_l'$.

Single input. When there is only one possible input $\rho_S'' = \rho_S$. As $\mu_{ij}'' = \delta_{ij} \lambda_i$ and $\mu_{kl}'' = \delta_{kl} \lambda_k'$, choosing $P_Q(k|i) = \lambda_k'/\lambda_i$ shows that equation (5) holds.

Single output. Resetting to a standard state is known to satisfy $\epsilon_Q = 0$ [16, 17]. In this case the output states for all inputs are of the form $\rho_S' = \sum_k \lambda_k' |\phi_k\rangle \langle \phi_k|$, so $\mu_{kl}'' = \delta_{kl} \lambda_k'$. Again, choosing $P_Q(k|i) = \lambda_k'$, shows that equation (5) holds.

Classical information processing. For classical information processing, where the signal states correspond to orthogonal quantum states, $\epsilon_Q = 0$ [6, 7, 32]. $\rho_S'' = |\phi_n\rangle \langle \phi_n|$, so $\mu_{ij}'' = \delta_{ij} \delta_{in}$. In general the outputs take the form $\rho_S'' = \sum_k P_Q(k|n) |\phi_k'\rangle \langle \phi_k'|$, representing a distribution of possible outputs $|\phi_k'\rangle$, so $\mu_{kl}'' = \delta_{kl} P_Q(k|n)$, and equation (5) holds. This generalises to signal states corresponding to overlapping classical probability distributions. The inputs are then mixed states of the form $\rho_S' = \sum_i P^n(i) |\phi_i\rangle \langle \phi_i|$, so $\mu_{ij}'' = \delta_{ij} P^n(i)$. In general the outputs take the form $\rho_S'' = \sum_{ik} P_Q(k|i) P^n(i) |\phi_k'\rangle \langle \phi_k'|$, and so μ_{kl}'' is precisely given by (5).

6. Case study of a thermodynamically irreversible operation

In general it will not be the case that $\epsilon_Q = 0$. Even the simplest quantum operations will fail to satisfy equation (5). As an example, we consider single qubit dephasing operations, which exhibit all the features of the theorem. Inputs of the form $\rho_S'' = |\nu_S''\rangle \langle \nu_S''|$ with $|\nu_S''\rangle = c_0''|0_S\rangle + c_1''|1_S\rangle$ give outputs

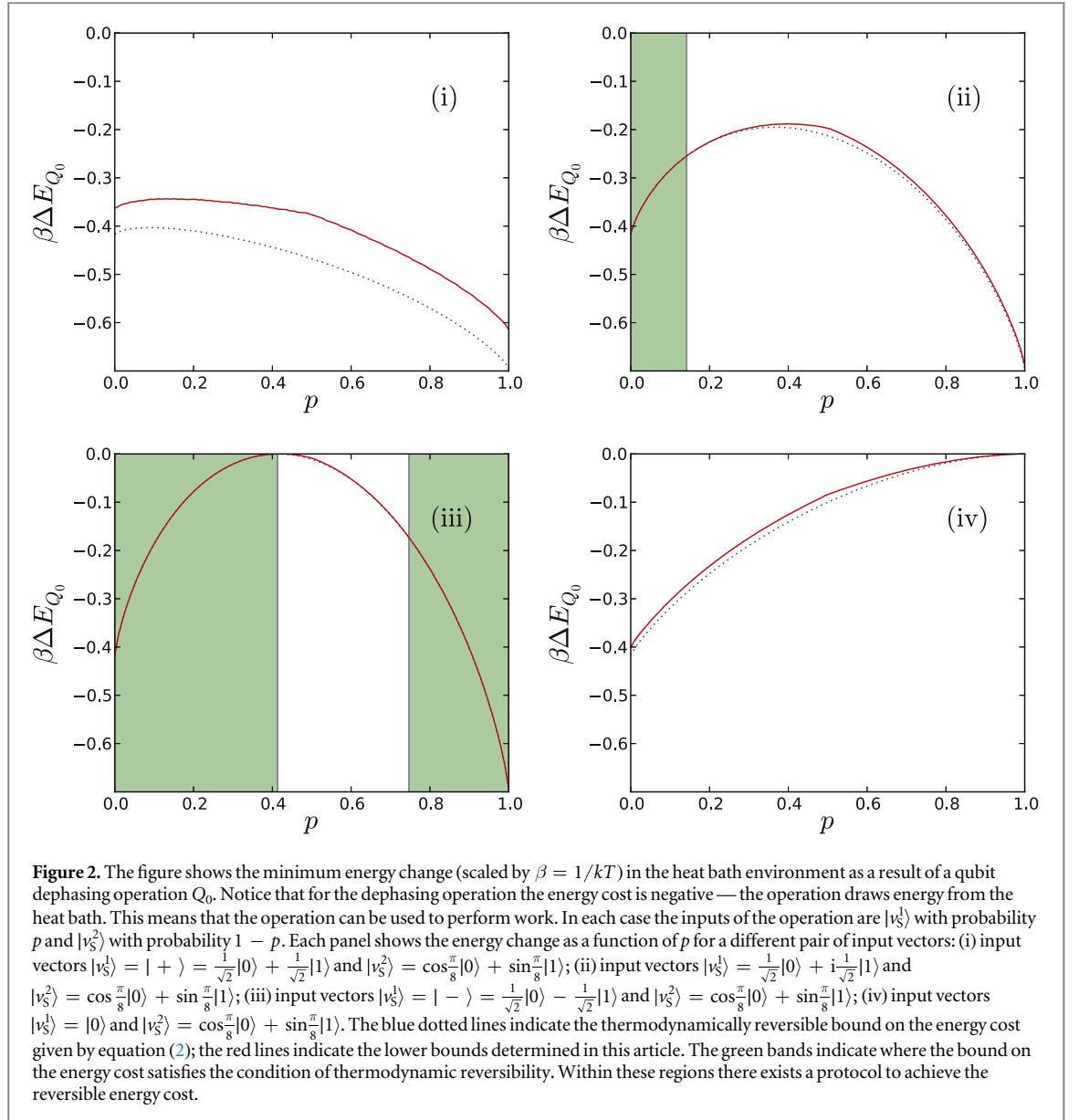
$\rho_S''(r) = r \rho_S'' + (1-r)[|c_0''|^2|0_S\rangle \langle 0_S| + |c_1''|^2|1_S\rangle \langle 1_S|]$. Each value of r defines a different quantum operation, $\rho_S''(r) = Q_r(\rho_S'')$, with Q_1 the identity, and Q_0 completely dephasing the qubit.

The operation Q_r can be implemented straightforwardly by a quantum CNOT gate and an auxiliary, making our theorem open to experimental investigation [33]. With the auxiliary initially prepared in the state $\alpha|0_A\rangle + \beta|1_A\rangle$ acting as the target, we have $r = (\alpha^* \beta + \alpha \beta^*)$.

Non-diagonalisable outputs. When $0 < r < 1$, the outputs, $\rho_S''(r)$, will not typically be simultaneously diagonalisable. Consider $r = \frac{1}{\sqrt{2}}$ with two possible inputs: $|0_S\rangle$ occurring with probability 0.3, and

$|+\rangle = \frac{1}{\sqrt{2}}|0_S\rangle + \frac{1}{\sqrt{2}}|1_S\rangle$ occurring with probability 0.7. After tracing away the auxiliary we find that the individual outputs are not simultaneously diagonalisable. There is enough information to calculate the lower bound on ϵ_Q from equation (9) and this is found to be $0.0007 \times kT$. This can be compared with the bound $kT \ln 2 [S(\rho_S) - S(\rho_S')] = -0.15 \times kT$. An overall negative value of ΔE_Q indicates that this operation may still be used to extract energy from the heat bath.

Diagonalisable outputs. For Q_0 , the outputs will be simultaneously diagonalised in the basis $\{|0_S\rangle, |1_S\rangle\}$. We choose two pure state inputs: ρ_S^1 with probability p , and ρ_S^2 with probability $1-p$. The average input density matrix is therefore $\rho_S = p \rho_S^1 + (1-p) \rho_S^2$. Figure 2 shows the minimum energy change in the heat bath with p for four different pairs of inputs. We see that for some combinations of inputs there are no values of p for which the operation can be thermodynamically reversible, and it necessarily requires an excess energy cost. For other inputs there are regions of p where there is no excess cost and regions where there is a minimum non-zero excess cost. Figure 3 shows, for a given ρ_S^1 , the regions of ρ_S^2 on the Bloch sphere where a zero excess cost is possible for various values of p . Further details of how to determine the minimum energy change in the heat bath can be found in appendix G.

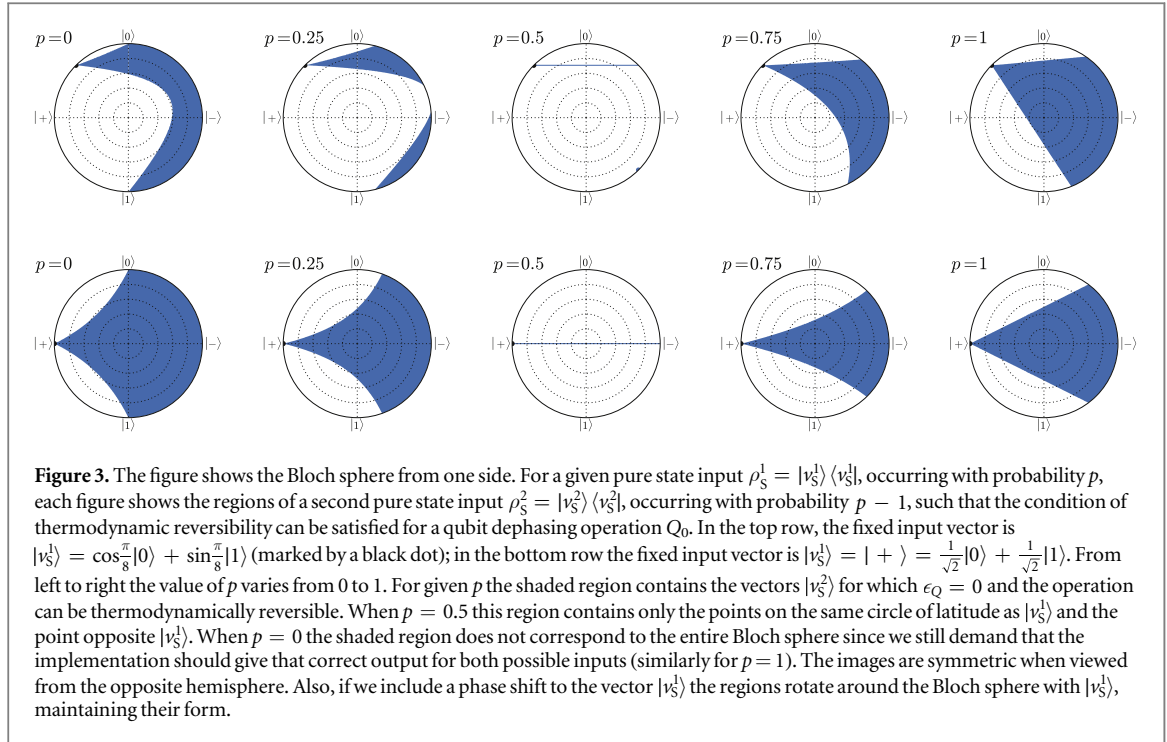


The qubit dephasing example shows, in particular, that $\epsilon_Q = 0$ is possible both with $\Delta E_Q < 0$ and with non-trivial non-orthogonal input states, and that $\epsilon_Q > 0$ is possible even when the output states share a common diagonalisation.

7. Discussion

The excess thermodynamic costs of quantum operations stem from the requirement that the operation should get the computation right for every individual input, and not just on average. For well known cases, including classical information processing, we have shown how thermodynamic reversibility can be reached as a special case. However, for general quantum operations, with non-orthogonal signal states, an excess thermodynamic cost must be paid.

This might seem counter intuitive, since quantum computations can always be represented as unitary operations, which can always be run in reverse. How can thermodynamic irreversibility arise with a reversible unitary operation? Simply running the overall unitary operation in reverse does not just tidy up the auxiliary, returning it to its initial state, but it also undoes the computation, converting the output back to the input. If we wish to retain the result of the computation, we cannot simply reverse the unitary operation. In the classical reversible computing model of Bennett [34], we save a copy of the output before reversing the computation. For quantum operations this is forbidden by the no-cloning theorem, and no quantum generalisation of Bennett's procedure is possible [35].



As long as we keep the results of the computation, we are left with the changes in the auxiliaries, representing spent resources and a cost to reset them to their initial states. This is the stage at which thermodynamic costs are incurred. We have shown that in general, for quantum operations this cost is necessarily in excess of the Landauer limit given in equation (2). Quantum computing requires a thermodynamically irreversible generation of heat.

Acknowledgments

We would like to thank Chris Timpson and Oscar Dahlsten for discussions. This work was funded by the Templeton World Charity Foundation.

Appendix A. Notation and formal set up

Given an input ρ_S^n and an output $Q(\rho_S^n) = \rho_S^{n'}$ of a quantum operation Q on a quantum system S we can describe the operation as

$$\rho_S^{n'} = \text{Tr}_{AB}[U\rho_S^n \otimes \rho_A \otimes \rho_B U^\dagger], \quad (\text{A.1})$$

where the subscript on the trace indicates which components have been traced over. The unitary U acts on an initial state $\rho_S^n \otimes \rho_A \otimes \rho_B$ which includes, besides the system, a thermal environment in the form of a canonical heat bath, ρ_B , and an auxiliary to be used as a catalyst ρ_A . Given that inputs ρ_S^n appear with probability p_n we can define an average system input state and an average system output state by

$$\rho_S = \sum_n p_n \rho_S^n \quad \text{and} \quad \rho_S' = \sum_n p_n \rho_S^{n'},$$

respectively.

The auxiliary is a resource which is spent by the operation. In order to account for this cost we demand that it must be returned to the same standard state ρ_A at the end of the computation

$$\text{Tr}_{SB}[U\rho_S \otimes \rho_A \otimes \rho_B U^\dagger] = \rho_A.$$

This ensures that the auxiliary can be reused in subsequent computations. We need only demand that the auxiliary is reset on average.

For convenience we define the following notation

$$\begin{aligned}\rho_{AB} &= \rho_A \otimes \rho_B, \\ \rho' &= U(\rho_S \otimes \rho_A \otimes \rho_B)U^\dagger, \\ \rho'_B &= \text{Tr}_{SA}[U(\rho_S \otimes \rho_A \otimes \rho_B)U^\dagger].\end{aligned}$$

Let us denote the basis states in which ρ_S is diagonal by $\{|\phi_i\rangle\}$. In general ρ'_S will not be diagonal in the same basis. Let us denote the basis in which ρ'_S is diagonal by $\{|\phi'_i\rangle\}$. We can write

$$\rho_S = \sum_i \lambda_i |\phi_i\rangle \langle \phi_i| \quad \text{and} \quad \rho'_S = \sum_i \lambda'_i |\phi'_i\rangle \langle \phi'_i|.$$

An individual input and output state can in general be expressed as

$$\rho_S^n = \sum_{ij} \mu_{ij}^n |\phi_i\rangle \langle \phi_j| \quad \text{and} \quad \rho_S^{n'} = \sum_{ij} \mu_{ij}^{n'} |\phi'_i\rangle \langle \phi'_j|. \quad (\text{A.2})$$

We define

$$A_{ij} = \langle \phi'_i | U | \phi_j \rangle,$$

so that we can express the unitary operator U as

$$U = \sum_{ij} |\phi'_i\rangle \langle \phi_j| \otimes A_{ij}. \quad (\text{A.3})$$

These operators must satisfy

$$\langle \phi'_i | U U^\dagger | \phi'_j \rangle = \sum_k A_{ik} A_{jk}^\dagger = \delta_{ij} \mathbb{1}_{AB}, \quad (\text{A.4})$$

$$\langle \phi_i | U^\dagger U | \phi_j \rangle = \sum_k A_{ki}^\dagger A_{kj} = \delta_{ij} \mathbb{1}_{AB}. \quad (\text{A.5})$$

The unitary operation on the complete state results in

$$\langle \phi'_i | \rho' | \phi'_j \rangle = \sum_k \lambda_k A_{ik} \rho_{AB} A_{jk}^\dagger. \quad (\text{A.6})$$

It will also be useful to define the state $\rho_\star = \rho'_S \otimes \rho_{AB}$ which we can express as

$$\langle \phi'_i | \rho_\star | \phi'_j \rangle = \lambda'_i \delta_{ij} \rho_{AB}, \quad (\text{A.7})$$

and we denote

$$\langle \phi'_i | (\rho' - \rho_\star) | \phi'_j \rangle = \Delta_{ij}. \quad (\text{A.8})$$

The result of the quantum operation on individual inputs (A.1) can be written using (A.2) and (A.3) as

$$\mu_{kl}^{n'} = \sum_{ij} \mu_{ij}^n \text{Tr}[A_{ki} \rho_{AB} A_{lj}^\dagger]. \quad (\text{A.9})$$

We will also use the notation

$$q(kl|ij) = \text{Tr}[A_{ki} \rho_{AB} A_{lj}^\dagger]. \quad (\text{A.10})$$

Appendix B. Quantum thermodynamics

Lemma B.1. *The energy change in the heat bath as a result of a quantum operation Q on a system S implemented by some unitary $U \rho_S \otimes \rho_A \otimes \rho_B U^\dagger = \rho'$, involving a resetting of the auxiliary system A , is given by*

$$\frac{\Delta E_Q}{kT \ln 2} = [S(\rho_S) - S(\rho'_S)] + S(\rho' || \rho_\star), \quad (\text{B.1})$$

where $\rho_\star = \rho'_S \otimes \rho_A \otimes \rho_B$.

The Schumacher information measure is given by $S(\rho) = -\text{Tr}[\rho \log_2 \rho]$ and we use a definition of the relative entropy using log base 2

$$S(\rho || \sigma) = \text{Tr}[\rho \log_2 \rho] - \text{Tr}[\rho \log_2 \sigma].$$

Proof. The energy change in the bath is given by $\Delta E_Q = \text{Tr}[H_B(\rho'_B - \rho_B)]$ where H_B is the heat bath Hamiltonian. A standard result is that [29]

$$\frac{\Delta E_Q}{kT \ln 2} = S(\rho'_B) - S(\rho_B) + S(\rho'_B || \rho_B).$$

It follows that

$$\begin{aligned} \frac{\Delta E_Q}{kT \ln 2} &= S(\rho'_B) - [S(\rho) - S(\rho_S) - S(\rho_A)] + S(\rho'_B || \rho_B) \\ &= S(\rho'_B) - [S(\rho') - S(\rho_S) - S(\rho_A)] + S(\rho'_B || \rho_B) \\ &= [S(\rho_S) - S(\rho'_S)] + S(\rho'_B || \rho_B) + [S(\rho'_S) + S(\rho_A) + S(\rho'_B) - S(\rho')]. \end{aligned} \quad (\text{B.2})$$

Since the last term in square brackets in the last line must be positive by subadditivity and the relative entropy term must be positive as a result of Klein's inequality, we must have

$$\Delta E_Q \geq kT \ln 2 [S(\rho_S) - S(\rho'_S)]. \quad (\text{B.3})$$

The operation satisfies thermodynamic reversibility if the inequality is saturated. This can be seen by forming a second operation $\rho_S = \mathcal{Q}'(\rho'_S)$ which restores the original average state. There must be a net heat gain in the heat bath if, for any part of the cycle, the equality in (B.3) does not hold.

Write $\rho_* = \rho'_S \otimes \rho_A \otimes \rho_B$. As a result of the fact that ρ_* factorises we find that

$$\begin{aligned} S(\rho' || \rho_*) &= \text{Tr}[\rho' \log_2 \rho'] - \text{Tr}[\rho' (\log_2 \rho'_S \otimes \mathbb{1}_A \otimes \mathbb{1}_B)] - \text{Tr}[\rho' (\mathbb{1}_S \otimes \log_2 \rho_A \otimes \mathbb{1}_B)] \\ &\quad - \text{Tr}[\rho' (\mathbb{1}_S \otimes \mathbb{1}_A \otimes \log_2 \rho_B)] \\ &= \text{Tr}[\rho' \log_2 \rho'] - \text{Tr}[\rho'_S \log_2 \rho'_S] - \text{Tr}[\rho_A \log_2 \rho_A] - \text{Tr}[\rho'_B \log_2 \rho_B] \\ &= S(\rho'_B || \rho_B) + [S(\rho'_S) + S(\rho_A) + S(\rho'_B) - S(\rho')], \end{aligned} \quad (\text{B.4})$$

so that from (B.2)

$$\frac{\Delta E_Q}{kT \ln 2} = [S(\rho_S) - S(\rho'_S)] + S(\rho' || \rho_*).$$

The quantity $S(\rho' || \rho_*) \geq 0$ therefore encodes the extent to which the thermodynamic bound on the energy change (B.3) is breached. \square

Related results found using the same techniques can be found in [11] and [36].

The demand for $S(\rho' || \rho_*) = 0$ requires from (B.4) that both $S(\rho') = S(\rho'_S) + S(\rho_A) + S(\rho'_B)$ and $S(\rho'_B || \rho_B) = 0$. In particular the second of these conditions suggests an output state with $\rho'_B = \rho_B$ and therefore no energy change in the heat bath. In fact, in the limit where the dimension of the heat bath becomes large, it is possible to have ρ'_B sufficiently close to ρ_B such that $S(\rho'_B || \rho_B) < s$ for some arbitrarily small s while at the same time the energy change in the heat bath ΔE_Q need not be arbitrarily small. To see this we write $\rho'_B = \rho_B + \varepsilon \Delta$ where Δ is a fixed traceless matrix and ε is a small parameter. The change in energy of the heat bath is given by

$$\Delta E_Q = \text{Tr}[H_B(\rho'_B - \rho_B)] = \varepsilon \text{Tr}[H_B \Delta],$$

where $\text{Tr}[H_B \Delta]$ need not be zero. Now suppose that we have N identical independent copies of the same heat bath (this will also be a canonical state). If we further suppose that each copy undergoes the same uncorrelated change $\rho'_B = \rho_B + \varepsilon \Delta$, then to lowest order, the energy change of the N -copy heat bath is

$$\Delta E_Q^{(N)} = N \Delta E_Q.$$

This means that we can take $\varepsilon \propto 1/N$ and as N becomes large, $\Delta E_Q^{(N)}$ remains fixed with value of order $\text{Tr}[H_B \Delta]$.

Now consider the relative entropy between ρ_B and ρ'_B

$$\begin{aligned} S(\rho'_B || \rho_B) &= \varepsilon \frac{d}{d\varepsilon} S(\rho_B + \varepsilon \Delta || \rho_B) |_{\varepsilon=0} + \mathcal{O}(\varepsilon^2) \\ &= \varepsilon \text{Tr} \left[\frac{\Delta}{\ln 2} + \Delta \log_2 \rho_B - \Delta \log_2 \rho_B \right] + \mathcal{O}(\varepsilon^2) \\ &= \mathcal{O}(\varepsilon^2). \end{aligned}$$

The correction to the relative entropy is at least quadratic in ε . The relative entropy for the N -copy heat bath is

$$S(\rho'^{\otimes N}_B || \rho^{\otimes N}_B) = N S(\rho'_B || \rho_B).$$

Therefore, in the limit that N becomes large and $\varepsilon \propto 1/N$ tends to zero, the relative entropy for the N -copy heat bath tends to zero. This means that the N -copy heat bath satisfies the requirement that the relative entropy between initial and final states tends to zero while the energy change in the heat bath remains non zero.

Corollary B.1. *The energy change in the heat bath is bounded by*

$$\Delta E_Q \geq kT \ln 2 [S(\rho_S) - S(\rho'_S)] + \frac{1}{2} kT \|\rho' - \rho_S\|_1^2. \quad (\text{B.5})$$

Proof. We use [37, 38]

$$S(\rho \parallel \sigma) \geq \frac{1}{2 \ln 2} \|\rho - \sigma\|_1^2.$$

The result follows from equation (B.1). □

Appendix C. Standard thermodynamically reversible protocol

There is a standard protocol for reaching the bound given in equation (B.3), appearing in various forms in the literature ([18, 30] for examples), when the quantum operation is defined only to act upon an individual density matrix $\rho'_S = Q(\rho_S)$ of a system S (see also [11, 39, 40] for alternative protocols to reach the bound). Note that these protocols do not require that either the initial or final states are in thermal equilibrium.

The density matrix is initially in the state

$$\rho_S = \sum_i \lambda_i |\phi_i\rangle \langle \phi_i|,$$

where $\{|\phi_i\rangle\}$ are orthonormal eigenstates. The result of the operation Q is a state

$$\rho'_S = \sum_i \lambda'_i |\phi'_i\rangle \langle \phi'_i|,$$

for a possibly different set of orthonormal eigenstates $\{|\phi'_i\rangle\}$. We assume that both the initial and final sets of eigenstates are fully degenerate in energy with energy level zero. This avoids the complication of the system being used as a source or sink of energy.

Step 1. Starting with ρ_S , manipulate the energy levels E_i of each eigenstate $|\phi_i\rangle$ until

$$\lambda_i = \frac{e^{-\beta E_i}}{\sum_j e^{-\beta E_j}},$$

where $\beta = 1/kT$. This has a mean cost $\Delta E_1 = \sum_i \lambda_i E_i$. The new density matrix will now be canonically distributed at temperature T .

Step 2. Bring the system into contact with a heat bath at temperature T .

Step 3. Slowly, isothermally, change the energy eigenstates until they satisfy

$$\lambda'_i = \frac{e^{-\beta E'_i}}{\sum_j e^{-\beta E'_j}}.$$

The energy requirement for this is $\Delta E_2 = kT \ln \sum_j e^{-\beta E_j} - kT \ln \sum_j e^{-\beta E'_j}$. The density matrix is now canonically distributed at temperature T , with eigenvalues $\{\lambda'_i\}$.

Step 4. Remove the system from contact with the heat bath.

Step 5. Change the energy levels of the eigenstates back to zero, with a mean cost $\Delta E_3 = -\sum_i \lambda'_i E'_i$.

Step 6. Perform a unitary rotation to the final eigenstates $|\phi_i\rangle \rightarrow |\phi'_i\rangle$.

The operation is complete with a cost of

$$\Delta E_1 + \Delta E_2 + \Delta E_3 = kT \ln 2 [S(\rho_S) - S(\rho'_S)].$$

It is worth noting that this protocol works even when the system is a joint system with non-trivial correlations or entanglement between subsystems [18].

During the stages in which we manipulate the energy levels of the system we are assuming a time-dependent Hamiltonian $H(t)$ for the system and a standard definition of the mean rate of work given by $\text{Tr}[\rho \partial H / \partial t]$. This presupposes some idealised work reservoir, capable of doing work on (or taking work from) the system by manipulation of the Hamiltonian.

We will denote this operation $T_{\rho_S \rightarrow \rho'_S}$. As shown in [11], the theoretical energy cost can only be achieved in an asymptotic limit. Nevertheless, there is no physical principle which prevents us from getting arbitrarily close to this value.

Appendix D. Some useful results

Lemma D.1. *The following relation holds*

$$(\lambda_j \lambda'_k - \lambda_i \lambda'_l) q(kl|ij) = \sum_m (\lambda'_k \text{Tr}[A_{ki} A_{mj}^\dagger \Delta_{ml}] - \lambda'_l \text{Tr}[A_{mi} A_{ij}^\dagger \Delta_{km}]). \quad (\text{D.1})$$

Proof. In order to prove this relation use equations (A.6)–(A.8) to substitute for Δ_{ij} . Then use the identity (A.5) along with the cyclic property of the trace. The coefficients $q(kl|ij)$ are given in (A.10). \square

Lemma D.2. *The following bound can be placed on the output state ρ' :*

$$\|\rho' - \rho_\star\|_1 \geq \frac{|\lambda_j \lambda'_k - \lambda_i \lambda'_l|}{\lambda'_k + \lambda'_l} |q(kl|ij)|. \quad (\text{D.2})$$

Proof. We start by defining operators acting on the complete state of system, auxiliary, and heat bath

$$F_{ijklm} = |\phi'_l\rangle \langle \phi'_m| \otimes A_{ki} A_{mj}^\dagger,$$

in terms of which we define

$$G_{ijkl}^L = \sum_m F_{ijklm}; \quad G_{ijkl}^R = \sum_m F_{jiklm}^\dagger.$$

We can then express (D.1) as

$$(\lambda_j \lambda'_k - \lambda_i \lambda'_l) q(kl|ij) = (\lambda'_k \text{Tr}[G_{ijkl}^L(\rho' - \rho_\star)] - \lambda'_l \text{Tr}[G_{ijkl}^R(\rho' - \rho_\star)]). \quad (\text{D.3})$$

Let us define some arbitrary basis states $\{|\psi_x\rangle\}$ for the complete system, auxiliary, and heat bath. We can write

$$\begin{aligned} G_{ijkl}^{L/R} &= \sum_{xy} g_{xy}^{L/R} |\psi_x\rangle \langle \psi_y|, \\ (\rho' - \rho_\star) &= \sum_{xy} r_{xy} |\psi_x\rangle \langle \psi_y|. \end{aligned}$$

Then

$$\begin{aligned} |\text{Tr}[G_{ijkl}^L(\rho' - \rho_\star)]| &= \left| \sum_{xy} g_{xy}^L r_{yx} \right| \\ &\leq \sum_x \left| \sum_y g_{xy}^L r_{yx} \right| \\ &\leq \sum_x \left(\sum_y |g_{xy}^L|^2 \right)^{\frac{1}{2}} \left(\sum_z |r_{zx}|^2 \right)^{\frac{1}{2}}, \end{aligned} \quad (\text{D.4})$$

where the second line follows from the triangle inequality and the third line follows from the Cauchy–Schwartz inequality. Similarly

$$|\text{Tr}[G_{ijkl}^R(\rho' - \rho_\star)]| \leq \sum_x \left(\sum_y |g_{yx}^R|^2 \right)^{\frac{1}{2}} \left(\sum_z |r_{xz}|^2 \right)^{\frac{1}{2}}. \quad (\text{D.5})$$

Next we show that

$$\langle \psi_x | G_{ijkl}^L G_{ijkl}^{L\dagger} | \psi_x \rangle = \sum_y |g_{xy}^L|^2 \leq 1, \quad (\text{D.6})$$

and

$$\langle \psi_x | G_{ijkl}^{R\dagger} G_{ijkl}^R | \psi_x \rangle = \sum_y |g_{yx}^R|^2 \leq 1. \quad (\text{D.7})$$

The operator products can be written as

$$\begin{aligned} G_{ijkl}^L G_{ijkl}^{L\dagger} &= \sum_m F_{ijklm} F_{ijklm}^\dagger, \\ G_{ijkl}^{R\dagger} G_{ijkl}^R &= \sum_m F_{jiklm}^\dagger F_{jiklm}. \end{aligned}$$

We also have

$$\delta_{ij'}\delta_{kk'}\mathbb{1} = \sum_{ilm} F_{ijklm} F_{ij'k'lm}^\dagger,$$

which follows from (A.4) and (A.5). Since the identity is expressed as a sum of positive operators and since $G_{ijkl}^L G_{ijkl}^{L\dagger}$ is a sum of a subset of these positive operators, it must be the case that the diagonal elements of $G_{ijkl}^L G_{ijkl}^{L\dagger}$ in the arbitrary basis $\{|\psi_x\rangle\}$ must belong to the range $[0, 1]$ from which (D.6) follows. Similarly for (D.7). We can therefore write, from (D.4) and (D.5),

$$\begin{aligned} |\text{Tr}[G_{ijkl}^L(\rho' - \rho_\star)]| &\leq \sum_x \left(\sum_z |r_{zx}|^2 \right)^{\frac{1}{2}}, \\ |\text{Tr}[G_{ijkl}^R(\rho' - \rho_\star)]| &\leq \sum_x \left(\sum_z |r_{xz}|^2 \right)^{\frac{1}{2}}. \end{aligned}$$

If we choose the basis states $\{|\psi_x\rangle\}$ such that $(\rho' - \rho_\star)$ is diagonal we have

$$|\text{Tr}[G_{ijkl}^{L/R}(\rho' - \rho_\star)]| \leq \|\rho' - \rho_\star\|_1.$$

Finally from (D.3), using the triangle inequality

$$\begin{aligned} |\lambda_j \lambda'_k - \lambda_i \lambda'_l| |q(kl|ij)| &\leq \lambda'_k |\text{Tr}[G_{ijkl}^R(\rho' - \rho_\star)]| + \lambda'_l |\text{Tr}[G_{ijkl}^L(\rho' - \rho_\star)]| \\ &\leq (\lambda'_k + \lambda'_l) \|\rho' - \rho_\star\|_1, \end{aligned}$$

which completes the proof. \square

Lemma D.3 Special case when dimension $d = 2$. When the dimension of the system space $d = 2$, the following bound can be placed on the output state ρ' for $i \neq j$:

$$\|\rho' - \rho_\star\|_1 \geq |\lambda_i - \lambda_j| |q(kk|ij)|.$$

Proof. When $k = l$ equation (D.1) reduces to

$$(\lambda_i - \lambda_j) q(kk|ij) = \sum_{m \neq k} (\text{Tr}[A_{mi} A_{kj}^\dagger \Delta_{km}] - \text{Tr}[A_{ki} A_{mj}^\dagger \Delta_{mk}]). \quad (\text{D.8})$$

If $i = j$ both sides of this equation are zero. If $i \neq j$ we can define operators acting on the complete system, auxiliary, and heat bath

$$H_{ijkm} = |\phi'_m\rangle \langle \phi'_k| \otimes A_{mi} A_{kj}^\dagger - |\phi'_k\rangle \langle \phi'_m| \otimes A_{ki} A_{mj}^\dagger,$$

and then express (D.8) as

$$(\lambda_i - \lambda_j) q(kk|ij) = \sum_{m \neq k} \text{Tr}[H_{ijkm}(\rho' - \rho_\star)]. \quad (\text{D.9})$$

Define arbitrary basis states $\{|\psi_x\rangle\}$ for the complete system, auxiliary, and heat bath. We can write

$$\begin{aligned} H_{ijkm} &= \sum_{xy} h_{xy} |\psi_x\rangle \langle \psi_y|, \\ (\rho' - \rho_\star) &= \sum_{xy} r_{xy} |\psi_x\rangle \langle \psi_y|. \end{aligned}$$

Then

$$\begin{aligned} |\text{Tr}[H_{ijkm}(\rho' - \rho_\star)]| &= \left| \sum_{xy} h_{xy} r_{yx} \right| \\ &\leq \sum_x \left| \sum_y h_{xy} r_{yx} \right| \\ &\leq \sum_x \left(\sum_y |h_{xy}|^2 \right)^{\frac{1}{2}} \left(\sum_z |r_{zx}|^2 \right)^{\frac{1}{2}}. \end{aligned} \quad (\text{D.10})$$

Next we show that

$$\langle \psi_x | H_{ijkm} H_{ijkm}^\dagger | \psi_x \rangle = \sum_y |h_{xy}|^2 \leq 1. \quad (\text{D.11})$$

The operator product can be written

$$H_{ijkm}H_{ijkm}^\dagger = F_{ijmmk}F_{ijmmk}^\dagger + F_{ijkkm}F_{ijkkm}^\dagger. \quad (\text{D.12})$$

We also have

$$\delta_{ij'}\mathbf{1} = \sum_{ikm} F_{ijkkm}F_{ij'kkm}^\dagger. \quad (\text{D.13})$$

Since (D.12) is the sum of two constituent positive terms of the sum of positive operators (D.13) then the same argument as that used in lemma D.2 can be used to show that (D.11) holds. It follows from (D.10) that

$$|\text{Tr}[H_{ijkm}(\rho' - \rho_\star)]| \leq \sum_x \left(\sum_z |r_{zx}|^2 \right)^{\frac{1}{2}},$$

and if we choose the basis states $\{|\psi_x\rangle\}$ such that $(\rho' - \rho_\star)$ is diagonal we have

$$|\text{Tr}[H_{ijkm}(\rho' - \rho_\star)]| \leq \|\rho' - \rho_\star\|_1.$$

Inserting into (D.9) we have

$$\begin{aligned} |\lambda_i - \lambda_j| |q(kk|ij)| &\leq \sum_{m \neq k} |\text{Tr}[H_{ijkm}(\rho' - \rho_\star)]| \\ &\leq (d-1) \|\rho' - \rho_\star\|_1, \end{aligned}$$

and choosing $d = 2$ completes the proof. \square

Note that lemma D.2 can also be applied to the case of $k = l$ and $i \neq j$ for general d with the result

$$\|\rho' - \rho_\star\|_1 \geq \frac{|\lambda_i - \lambda_j|}{2} |q(kk|ij)|,$$

which is half the size of the bound of lemma D.3 in the case of $d = 2$.

Appendix E. Proof of theorem 1

Theorem 1 is stated in the main text. We repeat it here for convenience

Theorem 1. *If there exists a stochastic map, $P_Q(k|i)$ with*

$$\sum_k P_Q(k|i) = 1 \quad \text{and} \quad P_Q(k|i) \geq 0 \quad \forall i, k,$$

such that

$$\mu_{kl}^{n'} = \delta_{kl} \sum_i P_Q(k|i) \mu_{ii}^n, \quad (\text{E.1})$$

for all n , then the minimum thermodynamic cost of the operation

$$\Delta E_Q \geq kT \ln 2 [S(\rho_S) - S(\rho'_S)] + \epsilon_Q,$$

can approach $\epsilon_Q = 0$. Otherwise, provided there are no symmetries of the form $\lambda_i/\lambda_j = \lambda'_k/\lambda'_l$ where $i \neq j$ or $k \neq l$, then necessarily $\epsilon_Q > 0$.

Proof. In general the output state of the quantum operation is given by (A.9)

$$\mu_{kl}^{n'} = \sum_{ij} \mu_{ij}^n q(kl|ij). \quad (\text{E.2})$$

By corollary B.1 the thermodynamic bound requires that $\|\rho' - \rho_\star\|_1 = 0$. By lemma D.2 this requires that if $|\lambda_j \lambda'_k - \lambda_i \lambda'_l|$ is non zero then

$$q(kl|ij) = 0.$$

It is helpful to separate equation (E.2) into three terms:

$$\mu_{kl}^{n'} = \delta_{kl} \sum_i q(kk|ii) \mu_{ii}^n + \delta_{kl} \sum_{i,j \neq i} q(kk|ij) \mu_{ij}^n + (1 - \delta_{kl}) \sum_{ij} q(kl|ij) \mu_{ij}^n. \quad (\text{E.3})$$

The first and second terms only deal with the diagonal elements of the output signal states in the basis of the average output density matrix. The third term deals with the off-diagonal elements.

By lemma D.2, the first sum implies only $\|\rho' - \rho_\star\|_1 \geq 0$, as $\lambda_i \lambda'_k - \lambda_i \lambda'_k = 0$ for $q(kk|ii)$. If equation (E.1) holds then $P_Q(k|i) = q(kk|ii)$ gives an implementation in which all other terms are zero, and there is no excess cost. The numbers $q(kk|ii)$ are real, non-negative and satisfy

$$\sum_k q(kk|ii) = \sum_k \text{Tr}[A_{ki}^\dagger A_{ki} \rho_{AB}] = 1,$$

by equation (A.5).

If equation (E.1) does not hold, then some values of $q(kl|ij)$ with $i \neq j$ or $k \neq l$ must be non-zero, in any implementation. For a given implementation, the largest value of the lower bound of equation (D.2) across all $ijkl$ determines an excess thermodynamic cost. If there are no symmetries of the form $\lambda_i/\lambda_j = \lambda'_k/\lambda'_l$ with $i \neq j$ or $k \neq l$, then this lower bound must be greater than zero. The minimum such value across all possible implementations gives a lower bound for $\epsilon_Q > 0$. \square

It should be noted that the existence of some values of $ijkl$ for which $\lambda_i/\lambda_j = \lambda'_k/\lambda'_l$ holds is not sufficient for $\epsilon_Q = 0$. To avoid an excess cost from our theorem through the exceptional symmetry condition, it must be possible to implement the operation in such a way that $q(kl|ij) = 0$ for every $ijkl$ value for which $\lambda_i/\lambda_j \neq \lambda'_k/\lambda'_l$.

When the output signal states do not share a common diagonalisation, we can give a general lower bound for ϵ_Q . The third sum in equation (E.3) is non-zero whenever there exists $k \neq l$ for which $\mu_{kl}^{n'} > 0$. For these cases, from equation (E.2), using the triangle inequality

$$|\mu_{kl}^{n'}| \leq \sum_{ij} |q(kl|ij)| |\mu_{ij}^n|.$$

From equation (D.2) this implies

$$\|\rho' - \rho_*\|_1 \geq \max_{n,k,l \neq k} \left\{ \frac{|\mu_{kl}^{n'}|/(\lambda'_k + \lambda'_l)}{\sum_{ij} |\mu_{ij}^n|/|\lambda_j \lambda'_k - \lambda_i \lambda'_l|} \right\} > 0,$$

where the maximum is taken across all k and l such that $k \neq l$, and across all inputs n . As the right hand side only involves terms independent of the specific implementation, then this bound must hold for all implementations and so by corollary B.1,

$$\epsilon_Q \geq \frac{1}{2} kT \max_{n,k,l \neq k} \left\{ \frac{|\mu_{kl}^{n'}|/(\lambda'_k + \lambda'_l)}{\sum_{ij} |\mu_{ij}^n|/|\lambda_j \lambda'_k - \lambda_i \lambda'_l|} \right\}^2.$$

If all $\mu_{kl}^{n'} = 0$, with $k \neq l$, but equation (E.1) does not hold, then

$$\mu_{kl}^{n'} = \delta_{kl} \sum_i q(kk|ii) \mu_{ii}^n + \delta_{kl} \sum_{i,j \neq i} q(kk|ij) \mu_{ij}^n, \quad (\text{E.4})$$

and any implementation must have values of $|q(kk|ij)| > 0$ with $i \neq j$. We can find complex coefficients $q(kk|ij)$, which satisfy equation (E.4), while minimising the largest value of the lower bound of (D.2), $\frac{1}{2} |\lambda_i - \lambda_j| |q(kk|ij)|$. This must be done using numerical optimisation techniques on a case-by-case basis. Given the set $\{\{\lambda_i\}, \{\lambda'_k\}, \{\mu_{ij}^n\}, \{\mu_{kl}^{n'}\}\}$, this establishes a minimum value for $\|\rho' - \rho_*\|_1$ and therefore, by corollary B.1, a minimum excess cost across all possible implementations, so again $\epsilon_Q > 0$.

Appendix F. Thermodynamically reversible protocol for special cases

We now demonstrate a protocol which can achieve $\epsilon_Q = 0$ for the special class of quantum operations which satisfy equation (E.1). For these operations there exists a stochastic map $P_Q(k|i)$ such that the input and output states of a quantum operation are related by $\mu_{kl}^{n'} = \delta_{kl} \sum_i P_Q(k|i) \mu_{ii}^n$.

Let the initial state of the auxiliary be $|0_A\rangle \langle 0_A|$, so the combined system and auxiliary is initially

$$\rho_S^n \otimes \rho_A = \sum_{ij} \mu_{ij}^n |\phi_i\rangle \langle \phi_j| \otimes |0_A\rangle \langle 0_A|.$$

Step 1. Use the auxiliary to measure the input system in the basis of the average input density matrix. Correlate the auxiliary to the system using a unitary with $|\phi_i\rangle |0_A\rangle \rightarrow |\phi_i\rangle |i_A\rangle$. The joint state is now

$$\sum_{ij} \mu_{ij}^n |\phi_i\rangle \langle \phi_j| \otimes |i_A\rangle \langle j_A|.$$

Step 2. The operation $T_{|\phi_i\rangle \langle \phi_i| \rightarrow \rho_S^{(i)}}$ (see appendix C) performs a thermodynamically optimal conversion of $|\phi_i\rangle \langle \phi_i|$ to $\rho_S^{(i)} = \sum_k P_Q(k|i) |\phi_k\rangle \langle \phi_k|$. The conditional operation $\sum_i T_{|\phi_i\rangle \langle \phi_i| \rightarrow \rho_S^{(i)}} \otimes |i_A\rangle \langle i_A|$ puts the joint system in the state

$$\sum_{ki} P_Q(k|i) \mu_{ii}^n |\phi_k\rangle \langle \phi_k| \otimes |i_A\rangle \langle i_A|,$$

transferring mean heat to the heat bath $\Delta E_1 = -kT \ln 2 \sum_{ni} p_n \mu_{ii}^n S(\rho_S^{(i)})$. The average state takes the form

$$\sum_{ki} P_Q(k|i) \lambda_i |\phi_k\rangle \langle \phi_k| \otimes |i_A\rangle \langle i_A|.$$

Step 3. We now exploit the correlations between system and auxiliary to optimally reset the auxiliary. The operation $T_{\rho_A^{(k)} \rightarrow |0_A\rangle \langle 0_A|}$ performs an optimal conversion of $\rho_A^{(k)} = \sum_i P_Q(k|i) \lambda_i / (\sum_j P_Q(k|j) \lambda_j) |i_A\rangle \langle i_A|$ to $|0_A\rangle \langle 0_A|$, where $P_Q(k|i) \lambda_i / (\sum_j P_Q(k|j) \lambda_j)$ is the mean conditional probability of the auxiliary state being $|i_A\rangle$ given that the system state is $|\phi_k\rangle$. The conditional operation $\sum_k |\phi_k\rangle \langle \phi_k| \otimes T_{\rho_A^{(k)} \rightarrow |0_A\rangle \langle 0_A|}$ resets the auxiliary to $|0_A\rangle \langle 0_A|$ while transferring mean heat $\Delta E_2 = kT \ln 2 \sum_{ki} P_Q(k|i) \lambda_i S(\rho_A^{(k)})$.

The joint state is now

$$\sum_{ki} P_Q(k|i) \mu_{ii}^n |\phi_k\rangle \langle \phi_k| \otimes |0_A\rangle \langle 0_A|,$$

and provided the conditions of the theorem hold, the system is in the correct output state, up to a unitary. The average heat production is readily confirmed to be $\Delta E_Q = \Delta E_1 + \Delta E_2 = kT \ln 2 [S(\rho_S) - S(\rho_S')]_{\text{thus proving that } \epsilon_Q = 0}$. It is important to note that, if the conditions of the theorem do not apply, this protocol not only fails to be optimal, but fails to correctly implement the operation at all, i.e. ρ_S^n is not mapped to the correct $\rho_S^{n'}$.

Appendix G. Qubit dephasing example

We analyse the specific example of a qubit dephasing operation. This can be implemented using a CNOT. For this operation an input of the form $\rho_S^n = |\nu_S^n\rangle \langle \nu_S^n|$ with $|\nu_S^n\rangle = c_0^n |0\rangle + c_1^n |1\rangle$ gives the output $\rho_S^{n'} = |c_0^n|^2 |0\rangle \langle 0| + |c_1^n|^2 |1\rangle \langle 1|$. All outputs are simultaneously diagonalisable in the $\{|0\rangle, |1\rangle\}$ basis. We choose two pure state inputs ρ_S^1 and ρ_S^2 such that the average input state is $\rho_S = p \rho_S^1 + (1-p) \rho_S^2$ for some probability p .

All of the elements $\mu_{ij}^1, \mu_{ij}^2, \mu_{ij}^{1'}, \mu_{ij}^{2'}$ are specified by the operation together with the form and relative frequency of the inputs. To find μ_{ij}^1, μ_{ij}^2 we determine the diagonal basis of ρ_S and express the individual inputs in this basis

$$\begin{aligned} \rho_S^1 &= \mu_{11}^1 |\phi_1\rangle \langle \phi_1| + \mu_{12}^1 |\phi_1\rangle \langle \phi_2| + \mu_{21}^1 |\phi_2\rangle \langle \phi_1| + \mu_{22}^1 |\phi_2\rangle \langle \phi_2|, \\ \rho_S^2 &= \mu_{11}^2 |\phi_1\rangle \langle \phi_1| + \mu_{12}^2 |\phi_1\rangle \langle \phi_2| + \mu_{21}^2 |\phi_2\rangle \langle \phi_1| + \mu_{22}^2 |\phi_2\rangle \langle \phi_2|. \end{aligned}$$

The output elements are

$$\begin{aligned} \mu_{11}^{n'} &= |c_0^n|^2, \\ \mu_{22}^{n'} &= |c_1^n|^2, \\ \mu_{kl}^{n'} &= 0 \text{ for } k \neq l. \end{aligned}$$

The elements must satisfy equation (E.2) for some set of coefficients $q(kl|ij)$. The off-diagonal elements of the outputs can be solved by choosing $q(kl|ij) = 0$ for $k \neq l$, implying no constraint on excess heat cost by lemma D.2. For the diagonal elements of the outputs we denote $q(kk|ii) = q_{ki}$, and $q(11|12) = w = -q(22|12)$, $q(11|21) = w^* = -q(22|21)$, so that from equation (E.2) we can write

$$\begin{aligned} \mu_{11}^{1'} &= |c_0^1|^2 = \mu_{11}^1 q_{11} + \mu_{12}^1 w + \mu_{21}^1 w^* + \mu_{22}^1 q_{12}, \\ \mu_{11}^{2'} &= |c_0^2|^2 = \mu_{11}^2 q_{11} + \mu_{12}^2 w + \mu_{21}^2 w^* + \mu_{22}^2 q_{12}, \end{aligned}$$

and

$$\begin{aligned} \mu_{22}^{1'} &= |c_1^1|^2 = \mu_{11}^1 q_{21} - \mu_{12}^1 w - \mu_{21}^1 w^* + \mu_{22}^1 q_{22}, \\ \mu_{22}^{2'} &= |c_1^2|^2 = \mu_{11}^2 q_{21} - \mu_{12}^2 w - \mu_{21}^2 w^* + \mu_{22}^2 q_{22}. \end{aligned}$$

Since $|c_0^n|^2 + |c_1^n|^2 = 1$, $\mu_{11}^n + \mu_{22}^n = 1$, and $q_{1k} + q_{2k} = 1$, these pairs of equations are equivalent, so we focus on the first pair. The remaining numerical problem is to find the w with the smallest magnitude which can solve this pair of equations with $0 \leq q_{11}, q_{12} \leq 1$. This is done by scanning complex values of w of increasing magnitude and solving for q_{11} and q_{12} until they both fit within the required range. Once we have found $|w|_{\min}$ we can use lemma D.3 to bound $\|\rho' - \rho_\star\|_1$:

$$\|\rho' - \rho_\star\|_1 \geq |\lambda_1 - \lambda_2| |w|_{\min},$$

where λ_i are the eigenvalues of ρ_S . Finally we can use equation (B.5) to bound the energy cost:

$$\Delta E_{Q_0} \geq kT \ln 2 [S(\rho_S) - S(\rho'_S)] + \frac{1}{2} kT (\lambda_1 - \lambda_2)^2 |w|_{\min}^2.$$

Examples are given in figure 2.

References

- [1] Vassighi A and Sachdev M 2006 *Thermal and Power Management of Integrated Circuits* (Berlin: Springer)
- [2] Landauer R 1961 *IBM J. Res. Dev.* **5** 148
- [3] Bennett C H 1982 *Int. J. Theor. Phys.* **21** 905
- [4] Leff H S and Rex A F 2003 *Maxwell's Demon 2 Entropy, Classical and Quantum Information, Computing* (Bristol: IOP)
- [5] Maroney O J E 2009 Information processing and thermodynamic entropy *The Stanford Encyclopedia of Philosophy* ed E N Zalta (<http://plato.stanford.edu/archives/fall2009/entries/information-entropy/>)
- [6] Maroney O J E 2009 *Phys. Rev. E* **79** 031105
- [7] Sagawa T 2014 *J. Stat. Mech.* **2014** 03025
- [8] Piechocinska B 2000 *Phys. Rev. A* **61** 062314
- [9] Turgut S 2009 *Phys. Rev. E* **79** 041102
- [10] Dahlstein O C O 2013 *Entropy* **15** 5346–61
- [11] Reeb D and Wolf M M 2014 *New J. Phys.* **16** 103011
- [12] Bérut A, Arakelyan A, Petrosyan A, Ciliberto S, Dillenschneider R and Lutz E 2012 *Nature* **483** 187
- [13] Jun Y, Gavrilov M and Bechhoefer J 2014 *Phys. Rev. Lett.* **113** 190601
- [14] Martini L *et al* 2016 *Nano Energy* **19** 108–16
- [15] Anderson N G 2008 *Phys. Lett. A* **372** 5552
- [16] Sagawa T and Ueda M 2009 *Phys. Rev. Lett.* **102** 250602
- [17] Aksak Ç and Turgut S 2011 *J. Phys. A: Math. Theor.* **44** 275304
- [18] del Rio L, Åberg J, Renner R, Dahlsten O and Vedral V 2011 *Nature* **474** 61
- [19] Kim S W, Sagawa T, De Liberato S and Ueda M 2011 *Phys. Rev. Lett.* **106** 070401
- [20] Sagawa T 2012 *Lectures on Quantum Computing, Thermodynamics and Statistical Physics* (Kinki University Series on Quantum Computing) ed M Nakahara and S Tanaka (Singapore: World Scientific)
- [21] Goold J and Modi K 2014 *Phys. Rev. E* **90** 020101(R)
- [22] Goold J, Paternostro M and Modi K 2015 *Phys. Rev. Lett.* **114** 060602
- [23] Binder F, Vinjanampathy S, Modi K and Goold J 2015 *Phys. Rev. E* **91** 032119
- [24] Peterson J P S, Sarthour R S, Souza A M, Oliveira I S, Goold J, Modi K, Soares-Pinto D O and Céleri L C 2016 *Proc. R. Soc. A* **472** 20150813
- [25] Solinas P and Gasparinetti S 2015 *Phys. Rev. E* **92** 042150
- [26] Kammerlander P and Anders J 2016 *Sci. Rep.* **6** 22174
- [27] Elouard C, Auffèves A and Clusel M 2015 arXiv:1507.00312
- [28] Schumacher B W 1995 *Phys. Rev. A* **51** 2738–47
- [29] Partovi M H 1989 *Phys. Lett. A* **137** 440
- [30] Maroney O J E *The Physical Basis of the Gibbs-von Neumann Entropy* arXiv:quant-ph/0701127
- [31] Nielsen M A and Chuang I L 2010 *Quantum Computation and Quantum Information* (Cambridge: Cambridge University Press)
- [32] Maroney O J E 2005 *Stud. Hist. Phil. Mod. Phys.* **36** 355–74
- [33] Veldhorst M *et al* 2015 *Nature* **526** 410
- [34] Bennett C H 1973 *IBM J. Res. Dev.* **17** 525
- [35] Maroney O J E *Are All Reversible Computations Tidy?* arXiv:quant-ph/0403079
- [36] Esposito M, Lindenberg K and Van den Broeck C 2010 *New J. Phys.* **12** 013013
- [37] Audenaert K M R and Eisert J 2011 *J. Math. Phys.* **52** 112201
- [38] Hiai F, Ohya M and Tsukada M 1981 *Pac. J. Math.* **96** 99
- [39] Skrzypczyk P, Short A J and Popescu S 2014 *Nat. Commun.* **5** 4185
- [40] Anders J and Giovannetti V 2013 *New J. Phys.* **15** 033022