

The Role of Thermodynamics in Understanding

Quantum Mechanics

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Abstract

Thermodynamics is a highly successful macroscopic theory widely used across the natural sciences and for the construction of everyday devices, from car engines to solar cells. With thermodynamics predating quantum theory, research now aims to uncover the thermodynamic laws that govern finite size systems which may in addition host quantum effects. Recent theoretical breakthroughs include the characterization of the efficiency of quantum thermal engines, the extension of classical non-equilibrium fluctuation theorems to the quantum regime and a new thermodynamic resource theory has led to the discovery of a set of second laws for finite size systems. These results have substantially advanced our understanding of nanoscale thermodynamics, however putting a finger on what is genuinely *quantum* in quantum thermodynamics has remained a challenge. Here we identify information processing tasks, the so-called *projections* that can only be formulated within the framework of quantum mechanics. We show that the physical realisation of such projections can come with a non-trivial thermodynamic work only for quantum states with coherences. This contrasts with information erasure, first investigated by Landauer, for which a thermodynamic work cost applies for classical and quantum erasure alike. Repercussions on quantum work fluctuation relations and thermodynamic single-shot approaches are also discussed.

Introduction

When Landauer argued in 1961 that any physical realisation of erasure of information has a fundamental thermodynamic work cost he irrevocably linked thermodynamics and information theory 1:2:3:4:5:6:7:8:9. A practical consequence of this insight is that all computers must dissipate a minimal amount of heat in each irreversible computing step, a threshold that is becoming a concern with future computer chips entering atomic scales. The treatment of general quantum information processing tasks within the wider framework of quantum thermodynamics has only recently begun13. Quantum mechanics differs from classical mechanics in at least three central aspects: the special nature of measurement, the possibility of a quantum system to be in a superposition and the existence of quantum correlations. The thermodynamic energy needed to perform a (selective) measurement has been investigated10 and the total work for a closed thermodynamic measurement cycle explored11. The catalytic role of quantum superposition states when used in thermal operations has been uncovered12 and it has been shown that work can be drawn from quantum correlations 13,14 in a thermodynamic setting, see Fig. 1. In particular, del Rio et al. 14 showed that contrary to Landauer's principle, it is possible to extract work while performing erasure of a system's state when the system is correlated to a memory. This can occur if and only if the initial correlations imply a negative conditional entropy, a uniquely quantum feature. The thermodynamic process does however now require operation on degrees of freedom external to the system, i.e. the memory's.



Results

Projections and the optimal work value of removing coherences

Our motivation is here to shed light on the implications of performing a measurement on a quantum state that has coherences. We will consider this task in the thermodynamic setting of Landauer's erasure, involving a heat bath at fixed temperature T and operation on $N \rightarrow \infty$ uncorrelated and identically prepared copies of the system (i.i.d. limit). This is of interest in the context of the quantum Jarzynski equality, for example and will also be central for experiments testing quantum thermodynamic predictions in the future. To tackle this question we define the information-theoretic "projection" $\rho \rightarrow \eta^{\mathcal{P}} = \sum_k \prod_k^{\mathcal{P}} \rho \prod_k^{\mathcal{P}} \int_{\Gamma_k} \rho \prod_k^{\mathcal{P}} \rho \prod_k^{\mathcal{$ given initial quantum state ρ and a complete set of mutually orthogonal projectors $\{\Pi_k^P\}_k$. Such state transformation can be seen as analogous to the state transfer of erasure, $\rho \rightarrow |0\rangle$, to a blank state $|0\rangle$. Physically, this projection can be interpreted as the result of an unread, or unselective15, measurement of an observable \mathcal{P} that has eigenvector projectors $\{\Pi_k^{\mathcal{P}}\}_k$. In an unselective measurement the individual measurement outcomes are not recorded and only the statistics of outcomes is known. In the literature the implementation of unselective measurements is often not specified, although it is typically thought of as measuring individual outcomes, e.g. with a Stern-Gerlach experiment, see Fig. 2a, followed by mixing. The crux is that the information-theoretic projection $\rho \rightarrow \eta^{\mathcal{P}}$ can be implemented in many physical ways. The associated thermodynamic heat and work will differ depending on how the projection was done and we will refer to the various realisations as "thermodynamic projection processes". One possibility is $\{\Pi_k^{\text{pointer}}\}_{k, a}$ thermodynamic process where an decohering16 the state in the so-called pointer basis, environment removes coherences in an uncontrolled manner resulting in no associated work. In general it is possible to implement the state transfer in a finely controlled fashion achieving optimal thermodynamic heat and work values.

Of particular importance in thermodynamics is the projection $\rho \rightarrow \eta^H$ of the system's initial state ρ onto the set of energy eigenstates $\{\Pi_k^H\}_k$ of the system's Hamiltonian $H = \sum_k E_k \Pi_k^H$ with E_k the energy eigenvalues. Here the state's off-diagonals with respect to the energy eigenbasis are removed - a state transformation that is frequently employed in quantum thermodynamic derivations and referred to as "dephasing" or "measuring the energy". Our key observation is that there exists a thermodynamic projection process realising this transformation and allowing to draw from the quantum system a non-trivial *optimal average work* of

$$\langle W_{\text{opt}} \rangle = k_B T (S(\eta^H) - S(\rho)).$$
 (1)

Here *T* is the temperature of the heat bath with which the system is allowed to interact, see illustration <u>Fig.</u> <u>1</u>, k_B is the Boltzmann constant and *S* is the von Neumann entropy. Crucially, this work is strictly positive

for quantum states with coherences. Extending the key observation to general projections $\rho \rightarrow \eta^{\mathcal{P}}$ one finds that optimal thermodynamic projection processes can be implemented that allow to draw an average work of

$$\langle W_{\text{opt}} \rangle = k_B T (S(\eta^{\mathcal{P}}) - S(\rho)) - \text{Tr}[H(\eta^{\mathcal{P}} - \rho)], \quad (2)$$

where an additional internal energy change term appears.

Physical interpretation and assumptions made to derive the optimal work

The optimal work values stated in Eqs. (1) and (2) are valid for processes applied to classical and quantum states alike. While for a classical ensemble the entropy change, $\Delta S^{\mathcal{P}} = S(\eta^{\mathcal{P}}) - S(\rho)$, will be zero this is not so in the general quantum situation, where initial non-diagonal quantum states result in a strictly positive entropy change<u>17</u>. We note that while the optimal work values are in principle attainable, practical implementations may be suboptimal resulting in a reduced work gain or a higher work cost.

The physical meaning of $\Delta S^{\mathcal{P}}$ can be grasped by considering a lower bound <u>18</u> on $\Delta S^{\mathcal{P}} \ge 1/2 \left\| \rho - \frac{1}{d} \right\|_2^2 \Delta A^{\mathcal{P}}$, see Supplement. Here *d* is the dimension of the system and $\| \cdot \|_2$ denotes the Hilbert-Schmidt norm. The first factor quantifies the distance of the initial state from the fully mixed state, while the second factor, $\Delta A^{\mathcal{P}}$, quantifies the angle between the diagonal basis of ρ and the projection basis $\{\Pi_k^{\mathcal{P}}\}_k$. These terms correspond to incoherent and coherent mixing contributions. The entropy change is non-trivially bounded only if the initial state is not an incoherent mixture with respect to that basis. The entropy bound is the largest for pure initial states whose basis is mutually unbiased with respect to $\{\Pi_k^{\mathcal{P}}\}_k$. In this case the optimal entropy change is $\Delta S^{\mathcal{P}} = k_B T \ln d$.

One may wonder where the work has gone to. There are two equivalent approaches to the accounting of work. In the present analysis the focus is on the work that the system exchanges, as done in statistical physics $5 \cdot 19 \cdot 20 \cdot 21 \cdot 22$. In this approach it is often not explicitly mentioned where the work goes to, but the only place work can go to are the externally controlled energy sources. Similarly, the heat, i.e. the energy change minus the work, is established implicitly. For example, in the experimental realisation of classical Landauer erasure with a colloidal silica bead trapped in an optical tweezer 21, the dissipated heat of erasure was calculated by knowing the applied tilting forces and integrating over the bead's dynamics. The second approach is to collect work in a separate work storage system 23, as illustrated by the weight in Fig. 1 and detailed in the Supplement. Both the implicit and the explicit treatment of work are equivalent in the sense that the results obtained in one approach can be translated into the other.

The thermodynamic assumptions made to prove Eq. (2) are congruent with current literature 9:23:24:25; specifically they are: (T0) an isolated system is a system that only exchanges work and not heat; (T1) the validity of the *first law* relating the internal energy change, ΔU , of the system during a process to its average heat absorbed and work drawn, $\Delta U = \langle Q^{abs} \rangle - \langle W \rangle$; (T2) the validity of the *second law* relating the

system's entropy change to its average absorbed heat, $k_B T\Delta S \ge \langle Q^{abs} \rangle$, when interacting with a bath at temperature *T*, with equality attainable by an optimal process; (T3) the thermodynamic entropy to be equal to the von Neumann entropy in equilibrium as well as out-of-equilibrium, $S_{th} = S_{vN}$. In addition we make the following standard quantum mechanics assumptions: (Q0) an isolated system evolves unitarily; (Q1) control of a quantum system includes its coherences. Details of the proof are in the Methods Summary. We note that in the single-shot setting whole families of second laws apply<u>7.8</u> that differ from (T2) stated above. However, in the limit of infinitely many independent and identically prepared copies of the system these collapse to the standard second law, (T2), on the basis of which Eq. (2) is derived.

From the information-theory point of view the projections considered here constitute just one example of the larger class of trace-preserving completely positive (TPCP) maps characterising quantum dynamics. Of course, all TPCP maps can be interpreted thermodynamically with the assumptions stated above, resulting in an optimal average work given by a free energy difference. Erasure is another such map whose study forged the link between information theory and thermodynamics. The benefit of discussing "projections" here lies in the insight that this focus provides: it uncovers that coherences offer the potential to draw work making it a genuine and testable quantum thermodynamic feature. This work is non-trivial even when the thermodynamic process is operated on the system alone, not involving any side-information<u>14</u> stored in other degrees of freedom.

Discussion of implications

To conclude, erasure is not the only irreversible information processing task – in the quantum regime a second fundamental process exists that mirrors Landauer's erasure. In contrast to the minimum heat limit of erasure, thermodynamic projection processes have a maximum work limit. While the former is non-zero for the erasure of classical *and* quantum bits, optimal thermodynamic projection processes have a non-zero work *only* when applied to quantum states with coherences. The optimal average work stated in Eqs. (1) and (2) constitutes an experimentally accessible quantum thermodynamic prediction. Future experiments testing this optimal work may be pursued with current setups, for instance with NMR/ESR techniques26·27 or single atoms33 and promise to be accessible with other platforms entering the quantum regime, such as single electron boxes22. Experiments will be limited by practical constraints, such as achieving a quasistatic process and obtaining the maximum work for pure states which may require, for instance, very large B-fields.

The derivation of the optimal work value is mathematically straightforward, just like that of Landauer's principle. The result's significance is that it opens new avenues of thought and provides key input for the construction of a future quantum thermodynamic framework. For example, the developed approach opens the door to investigate the connection between microscopic statistical physics and macroscopic thermodynamics in the quantum regime. While it is straightforward to identify the thermodynamic work of quantum processes involving macroscopic ensembles, what is needed is a microscopic concept of work that when averaged, gives the correct macroscopic work. The microscopic work concept should be valid for general (open) quantum processes and quantum states (including coherences) and only require access to properties of the system. While single-shot approaches have discarded coherences<u>29:30</u>, fluctuating work approaches cannot be applied directly to a system undergoing open quantum evolution<u>20</u>.

The observation is also important from the experimental perspective as testing quantum thermodynamic predictions will involve measurement – a projection process. We have argued that measurements, such as those required in establishing the Jarzynski equality, are not necessarily thermodynamically neutral. Indeed, they can be implemented in different physical ways and in general play an active role in thermodynamics, contributing a non-zero average heat and work. This new perspective gives physical meaning to the change of entropy in the debated quantum measurement process - it provides a capacity to draw work. Specifically, work can be drawn when *coherences* of a state are removed during an unselective measurement.

Finally, it is apparent that optimal thermodynamic projection processes require use of knowledge of the initial state ρ , i.e. its basis and eigenvalues. One may be inclined to exclude use of such knowledge, particularly when considering projections in the context of measurement which is often associated with the acquisition of knowledge. Such restriction would necessarily affect the set of assumptions (T0-T3, Q0-Q1) in the quantum regime. These could be changed, for example, by dropping the possibility of saturating the second law inequality (cf. T2) or choosing a new quantum non-equilibrium entropy that only considers the state's diagonal entries (cf. T3). The latter would mean a departure from standard quantum information theory where entropies are basis-independent. Thus whichever approach one takes - not making or making a restriction - quantum coherences will contribute a new dimension to thermodynamics. They either lead to non-classical work extraction or they alter the link between information theory and thermodynamics in the quantum regime. The line drawn here between the assumptions (T0-T3, Q0-Q1) and results (Eqs. (1) and (2)) establishes a frame for this possibility to be investigated.

Methods Summary

Further underlying research materials can be accessed in the <u>supplementary information</u> that accompanies this article.

Proof of Eq. (2)

Using the first law (T1) the average work drawn in a thermodynamic projection process $\rho \rightarrow \eta^{\mathcal{P}}$ is simply $\langle W \rangle = \langle Q^{abs} \rangle - \Delta U^{\mathcal{P}}$, where $\Delta U^{\mathcal{P}}$ is the average energy change for that process. Relating the average heat absorbed by the system during the process to its entropy change one then obtains $\langle W \rangle \leq k_B T \Delta S^{\mathcal{P}}$ (T2). Here $\Delta S^{\mathcal{P}}$ is the difference of von Neumann entropies of the system's state before and after the projection (T3). The average work drawn is thus $\langle W \rangle \leq k_B T \Delta S^{\mathcal{P}} - \Delta U^{\mathcal{P}}$, where the entropy change is non-negative and the energy change can be either positive or negative. The stated *optimal* work, $\langle W_{opt} \rangle$, is achieved when the inequality is saturated by an optimal process (T2) the implementation of which may require knowledge of the initial state and control of coherences (Q1). In the special case of a projection onto the energy eigenbasis $\{\Pi_k^H\}_k$ the internal energy change is zero, $\Delta U^H = 0$ and one obtains Eq. (1).

Optimality of three-step process for finite-dimensional systems

It is straightforward to generalise the proof of optimality from the two-dimensional spin-1/2 example to thermodynamic projection processes in dimension d. Again the projectors $\{\Pi_k^H\}_k$ map onto the energy eigenspaces of the Hamiltonian, $H = \sum_{k} E_{k}^{(0)} \Pi_{k}^{H}$, where $E_{k}^{(0)}$, k = 1, ..., d, are the energy eigenvalues. A general initial state can be written as $\rho = \sum_{j=1}^{d} a_{j} |j\rangle\langle j|$ where $a_{j} \ge 0$ are probabilities, $\sum_{j=1}^{d} a_{j} = 1, |j\rangle\langle j|$ are rank-1 projectors on the corresponding eigenvectors $|j\rangle$ and j = 1, ..., d. A unitary operation, V, is now chosen such that it brings the initial configuration (ρ, H) into the new diagonal and thermal configuration $(\rho_1 = V \rho V^{\dagger}, H^{(1)})$ where $\rho_1 = \sum_k a_k \Pi_k^H$ and $H^{(1)} = \sum_k E_k^{(1)} \Pi_k^H$. The new energy eigenvalues, $E_k^{(1)}$, are adjusted such that the probabilities a_k are thermally distributed with respect to $H^{(1)}$ for the bath temperature T. Adjusting the Hamiltonian eigenvalues while letting the state thermalise isothermal at all times now results quasi-static operation in a from $(\rho_1, H^{(1)})_{to} (\eta^H = \sum_k p_k \Pi_k^H, H^{(2)} = \sum_k E_k^{(2)} \Pi_k^H)$. Here the new energy eigenvalues, $E_k^{(2)}$, are chosen

to be thermal (at *T*) for the state's probabilities which are given by $p_k = \operatorname{Tr}[\rho \Pi_k^H]$. Finally, a quench brings the thermal configuration $(\eta^H, H^{(2)})$ quickly into the non-equilibrium state (η^H, H) . The average work for this overall process $\langle W \rangle = \sum_{j=1}^3 \langle W^{(j)} \rangle$ where $\langle W^{(1)} \rangle = -\operatorname{Tr}[H^{(1)}\rho_1 - H\rho]$ and $\langle W^{(3)} \rangle = -\operatorname{Tr}[H\eta^H - H^{(2)}\eta^H]$ because the first and third steps are unitary (Q0+T0). The quasistatic step's work

 $is_{25\cdot29} \langle W^{(2)} \rangle = -F_T^{(2)} + F_T^{(1)}$ where $F_T^{(1)} = Tr[H^{(1)}\rho_1] - k_B TS(\rho_1)$ is the thermal equilibrium free energy for Hamiltonian $H^{(1)}$ and similarly, $F_T^{(2)} = Tr[H^{(2)}\eta^H] - k_B TS(\eta^H)$. Summing up and using $Tr[H(\rho - \eta^H)] = 0$, one obtains $\langle W \rangle = k_B T(S(\eta^H) - S(\rho)) \equiv \langle W_{opt} \rangle$ concluding the optimality proof of the process sequence.

Additional Information

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References

- Scully, M. O., Zubairy, M. S., Agarwal, G. S. & Walther, H. Extracting Work from a Single Heat Bath via Vanishing Quantum Coherence. Science 299, 862 (2003).
- Kosloff, R. & Levy, A. Quantum Heat Engines and Refrigerators: Continuous Devices. Annu. Rev. Phys. Chem. 65, 365 (2014).
- Roßnagel, J., Abah, O., Schmidt-Kaler, F., Singer, K. & Lutz, E. Nanoscale Heat Engine Beyond the Carnot Limit. Phys. Rev. Lett. 112, 030602 (2014).
- Mukamel, S. Quantum extension of the Jarzynski relation: Analogy with stochastic dephasing. Phys. Rev. Lett. 90, 170604 (2003).
- Talkner, P., Lutz, E. & Hänggi, P. Fluctuation theorems: Work is not an observable. Phys. Rev. E 75, 050102 (R) (2007).
- Janzing, D., Wocjan, P., Zeier, R., Geiss, R. & Beth, T. Thermodynamic cost of reliability and low temperatures: tightening Landauer's principle and the second law. Int. J. Theor. Phys. 39, 2717 (2000).
- Brandão, F. G. S. L., Horodecki, M., Ng, N. H. Y., Oppenheim, J. & Wehner, S. The second laws of quantum thermodynamics. PNAS 112, 3275 (2015).
- Lostaglio, M., Jennings, D. & Rudolph, T. Description of quantum coherence in thermodynamic processes requires constraints beyond free energy. Nat. Commun. 6, 6383 (2015).
- Landauer, R. Dissipation and heat generation in the computing process. IBM J. Res. Develop. 5, 148–156 (1961).
- Jacobs, K. Quantum measurement and the first law of thermodynamics: The energy cost of measurement is the work value of the acquired information. Phys. Rev. E 86 040106(R) (2012).
- Erez, N. Thermodynamics of projective quantum measurements. Phys. Scr. 151, 014028 (2012).
- Åberg, J. Catalytic Coherence. Phys. Rev. Lett. 113, 1504022 (2014).
- Zurek, W. H. Quantum discord and Maxwell's demons. Phys. Rev. A 67, 012320 (2003).

- del Rio, L., Åberg, J., Renner, R., Dahlsten, O. &Vedral, V. The thermodynamic meaning of negative entropy. Nature 474, 61 (2011).
- Erez, N., Gordon, G., Nest, M. &Kurizki, G. Thermodynamic control by frequent quantum measurements. Nature 452, 724 (2008).