Operational thermodynamics from purity

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This is an extended abstract based on the preprint [15]. We propose four information-theoretic axioms for the foundations of statistical mechanics in general physical theories. The axioms—Causality, Purity Preservation, Pure Sharpness, and Purification—identify purity as a fundamental ingredient for every sensible theory of thermodynamics. Indeed, in physical theories satisfying these axioms, called *sharp theories with purification*, every mixed state can be modelled as the marginal of a pure entangled state, and every unsharp measurement can be modelled as a sharp measurement on a composite system. We show that these theories support a well-behaved notion of entropy and of Gibbs states, by which one can derive Landauer's principle. We show that in sharp theories with purification some bipartite states can have negative conditional entropy, and we construct an operational protocol exploiting this feature to overcome Landauer's principle.

Thermodynamics is one of the most successful paradigms of physics, as the scope of its fundamental principles ranges across different fields of science, from theoretical physics to nanotechnology, chemistry, and computation [34, 7, 21, 44]. Since thermodynamic laws do not make any explicit reference to the underlying physical theory, a natural question is whether they have an inherently fundamental character, or they can be derived from more primitive notions. The development of statistical mechanics [36, 37, 9, 19] led to a reduction of the laws of thermodynamics to the laws of an underlying dynamic of particles. However, new questions arose from the resulting tension between the statistical description, associated with the incomplete knowledge of an agent, or to fictitious ensembles, and the picture provided by classical mechanics, where there is no place for ignorance at the fundamental level. Many proposals have been put forward [8, 38, 29, 33, 27, 28], yet this tension has not been eased completely.

In this scenario, quantum theory offers a totally new opportunity, as a system and its environment can be jointly in a pure state, whilst the system is individually in a mixed state. Here the mixed state is not associated with an ensemble of identical systems, but rather represents the state of a *single* quantum system. Based on this idea, some authors [39, 20] have proposed that entanglement could be the starting point for a new foundation of statistical mechanics. The idea is that, when the environment is large enough, the system is approximately in the equilibrium state, for the typical joint *pure* states of the system and the environment.

In this work we want to push this approach even further, and turn entanglement into an axiomatic ingredient for the foundations of statistical mechanics in general physical theories. Specifically, we explore the hypothesis that the physical systems admitting a well-behaved statistical mechanics are exactly those where, at least in principle, mixed states can be modelled as the local states of larger systems, globally in a pure state. We adopt the framework of general probabilistic theories (GPTs) [23, 6, 2, 18, 11, 12, 5, 24, 25, 10, 17], which allows one to treat quantum theory, classical theory, and

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a variety of hypothetical post-quantum theories on common grounds. In this framework we demand the validity of four information-theoretic axioms [14, 15], informally stated as follows:

Causality No signal can be sent from the future to the past.

Purity Preservation The composition of two pure transformations is a pure transformation.

Pure Sharpness Every system has at least one pure sharp observable.

Purification Every state can be modelled as the marginal of a pure state. Such a modelling is unique up to local reversible transformations.

These principles enforce purity as a fundamental property of all physical systems, and pure-state entanglement as a feature of the composition of systems. We call the theories satisfying the above axioms *sharp theories with purification*. They include quantum theory both with complex and real amplitudes, as well as a suitable extension of classical probability theory where classical systems can be entangled with other, non-classical, systems [15]. In general, it can be shown that the systems of these theories correspond to Euclidean Jordan algebras [4].

These theories support sensible definitions of the resource theories of purity [26, 22, 13, 16], which is the simplest thermodynamic resource theory in the presence of a trivial Hamiltonian. Moreover, every state can be diagonalised, i.e. decomposed into a random mixture of perfectly distinguishable pure states [14], with unique coefficients [15], called the *eigenvalues* of the state. The eigenvalues encode the information about the purity of a state; indeed, if a state ρ is purer than σ, the spectrum of ρ majorises the spectrum of σ [16]. The converse implication is instead slightly subtler [16].

Given the characterisation of the purity preorder in terms of majorisation, one can define a special class of mixedness monotones on the state space from Schur-concave functions of the eigenvalues of states [35, 15] (see also Refs. [31, 1, 32] for a related approach based on different axioms). Among them a special place is occupied by Rényi entropies

$$S_\alpha\left(\rho\right) := H_\alpha\left(\mathbf{p}\right), \tag{1}$$

where $\mathbf{p}$ is the spectrum of ρ, and H_α is the α-Rényi entropy ($\alpha \in [0,+\infty]$). We show [15] that in sharp theories with purification, Rényi entropies defined in Eq. (1) coincide, for every α, with their definition in terms of *measurement entropies* [3, 43, 30]

$$S_\alpha^{\mathrm{meas}}\left(\rho\right) := \inf H_\alpha\left(\mathbf{q}\right),$$

where the infimum is over all pure measurements, and $\mathbf{q}$ is the vector of the probabilities arising from such measurements; and *preparation entropies* [3, 43, 30]

$$S_\alpha^{\mathrm{prep}}\left(\rho\right) := \inf H_\alpha\left(\lambda\right),$$

where the infimum is over all convex decompositions of ρ into pure states, with coefficients λ. In short, $S_\alpha\left(\rho\right) = S_\alpha^{\mathrm{meas}}\left(\rho\right) = S_\alpha^{\mathrm{prep}}\left(\rho\right)$. This result has been linked to the absence of higher-order interference in certain theories [32].

Shannon-von Neumann entropy is probably the best known among Rényi entropies. In sharp theories with purification it satisfies some of the properties of its quantum version [15], following from an operational version of the Klein's inequality for relative entropy [42, 15, 32]. For instance, for a bipartite state one has [15]

$$\left|S\left(\rho_{\mathrm{A}}\right) - S\left(\rho_{\mathrm{B}}\right)\right| \leq S\left(\rho_{\mathrm{AB}}\right) \leq S\left(\rho_{\mathrm{A}}\right) + S\left(\rho_{\mathrm{B}}\right).$$

On a more physical level, we prove that the joint reversible evolution of a system S and its environment E leads to the inequality [15, 40]

$$S\left(\rho_{\mathrm{S}}'\right)+S\left(\rho_{\mathrm{E}}'\right)\geq S\left(\rho_{\mathrm{S}}\right)+S\left(\rho_{\mathrm{E}}\right), \tag{2}$$

where the primes denote the state after the reversible evolution.

This inequality is the starting point for an operational reconstruction of Landauer's principle [34] along the lines of Ref. [40]. Clearly, first we must define the thermal state operationally. To do that, we resort to the maximum entropy principle [27, 28]: once we fix the expectation value of some "energy observable" [15], we show that the state that maximises the Shannon-von Neumann entropy is precisely of the Gibbs form [15]. Then to derive Landauer's principle, we consider again a system S, with the environment initially in a thermal state at temperature T. Some manipulations of Eq. (2) lead finally to Landauer's bound [15, 40]

$$\left\langle H_{\mathrm{E}}'\right\rangle-\left\langle H_{\mathrm{E}}\right\rangle\geq k_{\mathrm{B}}T\left[S\left(\rho_{\mathrm{S}}\right)-S\left(\rho_{\mathrm{S}}'\right)\right], \tag{3}$$

where $\left\langle H_{\mathrm{E}}\right\rangle$ denotes the expectation value of the energy observable H on the (initial) state of the environment. A decrease in the entropy of the system must be accompanied by an increase in the expected energy of the environment, which manifests itself as heat.

One may wonder if sharp theories with purification, allowing pure-state entanglement [11], allow also for the thermodynamic advantages of non-classical correlations, usually captured by the negativity of the conditional entropy [41]. Indeed, sharp theories with purifications admit bipartite states with negative conditional entropy. Given the bipartite state ρ_{AB}, define the conditional entropy as $S\left(\mathrm{A}|\mathrm{B}\right)_{\rho_{\mathrm{AB}}}:=S\left(\rho_{\mathrm{AB}}\right)-S\left(\rho_{\mathrm{B}}\right)$ [15]. If ρ_{AB} is a pure entangled state, it is easy to show that the conditional entropy is negative [13, 15]. We provide an operational protocol for overcoming Landauer's bound (3), based on the negativity of conditional entropy [41]. This shows that the power of entanglement in thermodynamics goes even beyond the realm of quantum theory, and has a nice operational characterisation in terms of information-theoretic principles. However, this part has yet to appear in the preprint [15][1], so further mathematical details are provided in appendix A for the interested reader.

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A Overcoming Landauer's bound

Combining the settings of Ref. [41] and Ref. [40], we can explore the thermodynamic meaning of negative conditional entropy in sharp theories with purification. We will show that it allows us to overcome Landauer's bound (3): exploiting non-classical correlations, we can reduce the entropy of the system without heating up the environment.

Consider again a system S initially uncorrelated with its environment E, which is again initially in a thermal state. However, now there is an additional system M, the *memory*, which contains some information about the system S encoded in correlations between S and M. Now consider the case where the joint system $\mathrm{S}\otimes\mathrm{E}\otimes\mathrm{M}$ is in the state $\rho_{\mathrm{SM}}\otimes\gamma_{\mathrm{E},\beta}$, with γ_β a Gibbs state. We also assume that the joint reversible evolution does not increase the entropy of the memory, viz. $S(\rho'_{\mathrm{M}})\leq S(\rho_{\mathrm{M}})$ [41]. It is easy to show that

$$S\left(\rho'_{\mathrm{SM}}\right)-S(\rho_{\mathrm{SM}})+S\left(\rho'_{\mathrm{E}}\right)-S(\rho_{\mathrm{E}})=I(\mathrm{SM}:\mathrm{E})_{\rho'_{\mathrm{SME}}}, \tag{4}$$

where the mutual information of a bipartite system $\mathrm{A}\otimes\mathrm{B}$ is defined as $I(\mathrm{A}:\mathrm{B})_{\rho_{\mathrm{AB}}}:=S(\rho_{\mathrm{A}})+S(\rho_{\mathrm{B}})-S(\rho_{\mathrm{AB}})$ [15]. Repeating the calculations for the derivation of Landauer's principle [15, 40], and recalling Eq. (4), one founds that, under the hypotheses explained above

$$\left\langle H'_{\mathrm{E}}\right\rangle-\langle H_{\mathrm{E}}\rangle=k_{\mathrm{B}}T\left[S(\mathrm{S}|\mathrm{M})_{\rho_{SM}}-S(\mathrm{S}|\mathrm{M})_{\rho'_{SM}}+\right.$$

$$\left.+\,S(\rho_{\mathrm{M}})-S\left(\rho'_{\mathrm{M}}\right)+I(\mathrm{SM}:\mathrm{E})_{\rho'_{\mathrm{SME}}}+D\left(\rho'_{\mathrm{E}}\parallel\gamma_{\mathrm{E},\beta}\right)\right].$$

where $D\left(\rho'_{\mathrm{E}}\parallel\gamma_{\mathrm{E},\beta}\right)$ is the relative entropy, defined in [15], and such that $D(\rho\parallel\sigma)\geq 0$. Since we also have $I(\mathrm{SM}:\mathrm{E})_{\rho'_{\mathrm{SME}}}\geq 0$ [15], and $S(\rho'_{\mathrm{M}})\leq S(\rho_{\mathrm{M}})$ by hypothesis, Landauer's bound (3) becomes

$$\left\langle H'_{\mathrm{E}}\right\rangle-\langle H_{\mathrm{E}}\rangle\geq k_{\mathrm{B}}T\left(S(\mathrm{S}|\mathrm{M})_{\rho_{SM}}-S(\mathrm{S}|\mathrm{M})_{\rho'_{SM}}\right) \tag{5}$$

Comparing this with Eq. (3), we notice the presence of conditional entropies which may be *negative*. In the particular case of $\mathrm{S}\otimes\mathrm{M}$ in a *pure* state, $S(\mathrm{S}|\mathrm{M})_{\rho_{\mathrm{SM}}}=-S(\rho_{\mathrm{S}})$. Then Eq. (5) reads

$$\left\langle H'_{\mathrm{E}}\right\rangle-\langle H_{\mathrm{E}}\rangle\geq k_{\mathrm{B}}T\left(S\left(\rho'_{\mathrm{S}}\right)-S(\rho_{\mathrm{S}})\right), \tag{6}$$

where the roles of the initial and final states are swapped with respect to Eq. (3). Now we will show that this feature allows us to perform the erasure of a mixed state of S to a fixed pure state of S, at *no* thermodynamic cost, thus overcoming Landauer's bound.

Suppose $\mathrm{S}\otimes\mathrm{M}$ is initially in a *pure entangled* state Ψ; in this case ρ_{S} is mixed [13], and we have $S(\rho_{\mathrm{M}})=S(\rho_{\mathrm{S}})>0$ [15]. Suppose we want to erase ρ_{S} to a fixed pure state ψ_0 of S. Now, let us consider the joint reversible evolution of $\mathrm{S}\otimes\mathrm{M}\otimes\mathrm{E}$ to be $\mathscr{U}_{\mathrm{SM}}\otimes\mathscr{I}_{\mathrm{E}}$, where $\mathscr{U}_{\mathrm{SM}}$ is the reversible channel mapping Ψ to $\psi_0\otimes\varphi_0$, where φ_0 is some pure state of the memory M. Clearly this reversible evolution respects the hypotheses explained above because $0=S(\rho'_{\mathrm{M}})<S(\rho_{\mathrm{M}})$, so it performs the erasure of ρ_{S} to ψ_0. Let us evaluate its thermodynamic cost $\langle H'_{\mathrm{E}}\rangle-\langle H_{\mathrm{E}}\rangle$. Since initially the environment is uncorrelated in the state $\gamma_{\mathrm{E},\beta}$, and the evolution is $\mathscr{U}_{\mathrm{SM}}\otimes\mathscr{I}_{\mathrm{E}}$, we have $\rho'_{\mathrm{E}}=\gamma_{\mathrm{E},\beta}$, whence the erasure occurs at *zero* thermodynamic cost. Note that Eq. (6) is satisfied, indeed its LSH vanishes, while its RSH is negative and equal to $-k_{\mathrm{B}}TS(\rho_{\mathrm{S}})$.

Again, non-classical correlations, captured by the negativity of the conditional entropy, allow us to overcome Landauer's principle and perform erasure at no thermodynamic cost, similarly to what happens in quantum theory [41].