Entanglement entropy from coarse-graining in pure and mixed multipartite systems

Joseph Schindler,* Dominik Šafraňek,† and Anthony Aguirre
SCIPP and Department of Physics, University of California, Santa Cruz, California 95064, USA
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We study quantum coarse-grained entropy and demonstrate that the gap in entropy between local and global coarse-graining is a natural generalization of entanglement entropy to mixed states in multipartite systems. This quantity is additive over independent systems, is invariant under local unitary operations, vanishes on states with strictly classical correlations, and reduces to the standard value for bipartite pure states. It quantifies how well a quantum system can be understood via local measurements, and ties directly to non-equilibrium thermodynamics, including representing a lower bound on the quantum part of thermodynamic entropy production. We discuss two other measures of nonclassicality to which this entropy is equivalent, and argue that together they provide a unique thermodynamically distinguished measure.

Keywords: quantum information, quantum coarse-graining, entanglement entropy, thermodynamics

I. INTRODUCTION

Entanglement entropy is an important measure of non-local correlations in quantum systems, with uses ranging from information theory [1–4], to many-body theory [5–9], quantum thermodynamics [10, 11], quantum phase transitions [12–14], and the description of the holographic principle and black hole entropy [15–18]. It is defined for pure states of a bipartite quantum system as $S_{\text{ent}}(|\psi\rangle\langle\psi|) = S_{\text{VN}}(\rho_A) = S_{\text{VN}}(\rho_B)$, with $|\psi\rangle$ a global pure state and $\rho_A, \rho_B$ the reduced density operators in each subsystem, and with $S_{\text{VN}}(\rho) = -\text{tr}(\rho \log \rho)$ the von Neumann entropy.

There are several generalizations of entanglement entropy to mixed and/or multipartite states, including both entanglement measures [3, 4] and measures of nonclassicality [19, 20]. These are usually motivated by characterizing the usefulness of states in performing information tasks, such as quantum communication [21–24], metrology [25–28], or computation [29–31], where entanglement is a key resource. It is now known that both entanglement and nonclassicality can be used as resources for such tasks [32–34].

Among such measures, most are either measures of some type of utility (e.g. distillable entanglement [35, 36], entanglement of formation [37], entanglement cost [38]), or of distance from some distinguished set of states (e.g. relative entropy of entanglement [39]). But they do not retain a clear interpretation as entropy, in the sense of statistical mechanics.

Meanwhile, there are also many related but distinct notions of entropy. These range from the classical Gibbs and quantum von Neumann entropies, which are informational measures of the inherent uncertainty in a state, to “microstate-counting entropies” such as the classical Boltzmann entropy, and ultimately to the thermodynamic entropy and its application to heat and work.

In this context it is well known that the relationship between informational entropies and thermodynamic entropy is related to the concept of coarse-graining, as is the case with classical Boltzmann entropy. Recently, a precise formulation of coarse-graining in quantum systems, which was originally discussed by von Neumann [40], has been revived [42, 43] and shown to provide a comprehensive framework for connecting quantum entropies to thermodynamics [41–45]. A key aspect of this connection is that while coarse-graining a system in energy provides a relation to equilibrium thermodynamic entropy, non-equilibrium thermodynamic entropy relates to local energy coarse-grainings.

In this article we study local coarse-grainings more generally, and find that there is a gap in entropy between local and global coarse-grainings that is naturally identified as entanglement entropy. This “multipartite entanglement entropy”—defined as the difference between the infimum local and global coarse-grained entropies—is the natural extension of entanglement entropy to general systems, in both the informational and thermodynamic sense. It quantifies the uncertainty associated with local measurements, and, we will see, forms a direct contribution to non-equilibrium thermodynamic entropy.

In addition to its interpretation as thermodynamic entropy, the quantity we study is also important as a measure of nonclassicality—in fact it is equal to two other measures, the relative entropy of quantum discord [46–50] (a measure of distance from the set of classically correlated states), and the zero-way quantum deficit [50–52] (a measure of work extractable by certain local operations). The equivalence of these three measures, each with quite different meanings, suggest that together they provide a unique, thermodynamically distinguished, measure of non-classicality. With this in mind, this paper aims to provide a self-contained treatment in terms of the statistical mechanics of coarse-graining.

* jeschind@ucsc.edu
† dsafrane@ucsc.edu

1 And see [41] for a detailed account of the history of this idea.
The analysis in terms of coarse-graining leads to a distinction between three types of entropy:

- **von Neumann entropy** is inherent to the state $\rho$, and quantifies fundamental uncertainty in a system due to being in a mixed state;
- **entanglement entropy** depends on a partition into subsystems, and quantifies the additional uncertainty in a multipartite system if one can only make subsystem-local measurements;
- **coarse-grained entropy** depends on a division of the state space into macrostates, and quantifies uncertainty associated with describing a system in terms of these macrostates.

The first two each contribute to the third: the entropy of any possible coarse-graining is bounded below by von Neumann entropy, while the entropy of any local coarse-graining is bounded below by the sum of von Neumann and entanglement entropies.

In this way multipartite entanglement entropy provides a key piece to a unified treatment of quantum statistical/thermodynamic entropy, along with a direct link to important measures in quantum information theory.

### II. ENTANGLEMENT ENTROPY FROM QUANTUM COARSE-GRAINED ENTROPY

In the theory of quantum coarse-grained entropy [40–44], a coarse-graining $\mathcal{C} = \{\hat{P}_i\}$ is a collection of Hermitian $(\hat{P}_i^\dagger = \hat{P}_i)$ orthogonal projectors $(\hat{P}_i \hat{P}_j = \delta_{ij} \hat{1})$ forming a partition of unity $(\sum_i \hat{P}_i = \hat{1})$. A coarse-graining is the set of outcomes of some projective measurement. Each subspace generated by $\hat{P}_i$ is called a "macrostate."

Given a coarse-graining $\mathcal{C}$ the "coarse-grained entropy" (or "observational entropy") of a density operator $\rho$ is

$$S_\mathcal{C}(\rho) = -\sum_i p_i \log \left( \frac{p_i}{V_i} \right),$$

where $p_i = \text{tr}(\hat{P}_i \rho)$ is the probability to find $\rho$ in each macrostate, and $V_i = \text{tr}(\hat{P}_i)$ is the volume of each macrostate. The coarse-grained entropy is defined both in and out of equilibrium, obeys a second law, and (with a properly chosen coarse-graining) is equal to thermodynamic entropy in appropriate cases [41–45, 53–55].

One way to specify a coarse-graining is via the spectral decomposition of an observable operator $\hat{Q} = \sum_q q \hat{P}_q$, with associated coarse-graining $\mathcal{C}_\mathcal{Q} = \{\hat{P}_q\}$. If $\hat{Q}$ has a full spectrum of distinct eigenvalues, then $S_{\mathcal{C}_\mathcal{Q}}(\rho)$ is merely the Shannon entropy of measuring $\hat{Q}$. On the other hand $\hat{Q}$ may have larger eigenspaces. If $\rho$ has a definite value $q$ then $S_{\mathcal{C}_\mathcal{Q}}(\rho)$ is the log of the dimension of the $q$ eigenspace of $\hat{Q}$ (i.e. the volume of the $q$ macrostate), a quantum analog of the Boltzmann entropy. Evidently the coarse-grained entropy provides a quantum generalization of both the Shannon and Boltzmann entropies of a measurement, and represents the uncertainty an observer making measurements assigns to the system.

Given a density operator $\rho$, the minimum value of coarse-grained entropy, minimized over all coarse-grainings $\mathcal{C}$, is

$$\inf_{\mathcal{C}} \left( S_\mathcal{C}(\rho) \right) = S_{\mathcal{C}_\rho}(\rho) = S_{VN}(\rho),$$

the von Neumann entropy [40, 42, 43]. The second equality states that the von Neumann entropy $S_{VN}(\rho) = -\text{tr}(\rho \log \rho)$ is equal to the coarse-graining entropy $S_{\mathcal{C}_\rho}(\rho)$ in the coarse-graining $\mathcal{C}_\rho$ consisting of eigenspaces of $\rho$.

Thus (2) expresses that no measurement can be more informative than measuring the density matrix itself.

Now consider an arbitrary multipartite system $AB\ldots C$, whose Hilbert space is the tensor product $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \otimes \ldots \otimes \mathcal{H}_C$.

In this background one can consider a subclass of coarse-grainings, the "local" coarse-grainings, defined by

$$\mathcal{C}_A \otimes \mathcal{C}_B \otimes \ldots \otimes \mathcal{C}_C = \{\hat{P}_i^A \otimes \hat{P}_m^B \otimes \ldots \otimes \hat{P}_n^C\},$$

where $\mathcal{C}_A = \{\hat{P}_i^A\}$ is a coarse-graining of $A$, and so on for the other subsystems. These are precisely the coarse-grainings describing local measurements (i.e. consisting of only local operators). Applying the definition (1) in such a coarse-graining yields the entropy

$$S_{\mathcal{C}_A \otimes \ldots \otimes \mathcal{C}_C}(\rho) = -\sum_{lm\ldots n} p_{lm\ldots n} \log \left( \frac{p_{lm\ldots n}}{V_{lm\ldots n}} \right),$$

where $p_{lm\ldots n} = \text{tr}(\hat{P}_i^A \otimes \hat{P}_m^B \otimes \ldots \otimes \hat{P}_n^C \rho)$ are the probabilities to find the system in each macrostate, and $V_{lm\ldots n} = \text{tr}(\hat{P}_i^A \otimes \hat{P}_m^B \otimes \ldots \otimes \hat{P}_n^C \rho)$ are the volumes of each macrostate.

One can now ask: what is the minimum entropy of any set of local measurements? That is, what is the infimum value

$$\inf_{\mathcal{C} = \mathcal{C}_A \otimes \ldots \otimes \mathcal{C}_C} \left( S_\mathcal{C}(\rho) \right)$$

of the coarse-grained entropy, if the minimum is taken only over local coarse-grainings?
There are two possibilities. Either the minimum value $S_{VN}(\rho)$ can be saturated by local coarse-grainings, or it cannot. Which of these is the case depends on the density matrix. If the minimum fails to be saturated, then there is an entropy gap $\Delta S$ above the minimum which is inherent to any local measurements.

A natural question is then: how is this entropy gap, associated with restricting to local coarse-grainings, related to entanglement entropy? Two observations provide a foundation for answering this question. The first, quite nontrivial, observation is that the entropy gap is equal to the usual entanglement for bipartite pure states. The second is that the entropy gap is zero for any product state. These facts suggest that entanglement entropy should in general be identified with this entropy gap. The aim of this article is to make precisely that identification and show that it leads to an intuitive and useful framework.

The observations above motivate the definition

$$S_{AB...C}^{ent}(\rho) \equiv \inf_{C=CA\otimes \ldots \otimes CC} (S_C(\rho) - S_{VN}(\rho))$$

(6)

of the multipartite entanglement entropy $S_{AB...C}^{ent}(\rho)$. The subscript denotes the partition into subsystems, allowing various partitions of the same system.

In other words, the entanglement entropy is the difference in coarse-grained entropy between the best possible local coarse-graining and the best possible global coarse-graining. This definition can be evaluated exactly for a variety of states using the properties introduced below, and can also be implemented numerically.

### III. PROPERTIES

The multipartite entanglement entropy $S^{ent}$, defined by Eq. (6), has the following properties. Proofs are given in the appendix.\(^4\)

(Ia) A bipartite system $AB$ in a pure state $\rho = |\psi\rangle\langle\psi|$, with reduced densities $\rho_A$ and $\rho_B$ in the $A$ and $B$ subsystems, has entanglement entropy

$$S_{AB}^{ent}(\rho) = S_{VN}(\rho_A) = S_{VN}(\rho_B).$$

(7)

This is equal to the usual value.

(Ib) More generally, for any multipartite state of the special (“maximally correlated” $[51, 57]$) form

$$\rho = \sum_{ij} \sigma_{ij} |a_i b_i \ldots c_i \rangle \langle a_j b_j \ldots c_j|,$$

(8)

where $\sigma_{ij}$ are complex coefficients and $|a_1 \rangle, |b_1 \rangle, \ldots, |c_n \rangle$ are orthonormal bases for the $A, B, \ldots, C$ subsystems, the entanglement entropy is

$$S_{AB...C}^{ent}(\rho) = \left( - \sum_i \sigma_{ii} \log \sigma_{ii} \right) - S_{VN}(\rho).$$

(9)

Note that for $\rho$ to be a state requires $\sigma_{ij} = \sigma_{ji}^*$ and $\sum_i \sigma_{ii} = 1$. These states include all pure states of the form $|\psi\rangle = \sum_k \alpha_k |a_k b_k \ldots c_k \rangle$, and thus all bipartite pure states by virtue of the Schmidt decomposition. The infimum defining entanglement entropy is achieved by coarse-graining in the $|a_i b_i \ldots c_i \rangle$ basis.

(IIa) In finite dimensions, $S_{AB...C}^{ent}(\rho) = 0$ if and only if $\rho$ is a classical state—that is, if there exists a locally orthonormal product basis diagonalizing $\rho$. Explicitly, classical states are those that can be put in the form

$$\rho = \sum_{lm\ldots n} p_{lm\ldots n} |a_l b_m \ldots c_n \rangle \langle a_l b_m \ldots c_n|$$

(10)

where $|a_l \rangle, \ldots, |c_n \rangle$ form orthonormal bases in $A, \ldots, C$, and $p_{lm\ldots n}$ form a set of real probabilities. These are the states with strictly classical correlations, as has been studied extensively $[34, 46, 48, 50, 51, 58-60]$. Classical states include all product states, and form a strict subset of the separable states.

(IIb) In general (finite or infinite dimensions), $\rho$ is a classical state if and only if both $\inf C=CA\otimes \ldots \otimes CC S_C(\rho)$ is realized as a minimum and $S_{AB...C}^{ent}(\rho) = 0$. In finite dimensions the infimum is always realized.

(III) For any product coarse graining $C_A \otimes \ldots \otimes C_C$,

$$S_{C_A\otimes \ldots \otimes C_C}(\rho) \geq S_{VN}(\rho) + S_{AB...C}^{ent}(\rho).$$

(11)

That is, any observer who can make only local measurements observes at least as much uncertainty as the inherent uncertainty in the joint state (the von Neumann entropy) plus an additional contribution (the entanglement entropy) due to their inability to make a nonlocal joint measurement.

(IV) In general $0 \leq S_{AB...C}^{ent}(\rho) \leq \log \dim \mathcal{H} - S_{VN}(\rho)$.

Additional bounds can be computed directly from local von Neumann entropies. A family of lower bounds is given by

$$S_{AB...C}^{ent}(\rho) \geq S_{VN}(\rho_{loc}) - S_{VN}(\rho),$$

(12)

where $\rho_{loc}$ is any local reduced density matrix obtained by tracing out some of the subsystems. An upper bound is given by

$$S_{AB...C}^{ent}(\rho) \leq \left( \sum_X S_{VN}(\rho_X) \right) - S_{VN}(\rho),$$

(13)

where $X \in \{A, B, \ldots, C \}$ is an index summing over all the subsystems, with $\rho_X$ the reduced density in each one.

(V) If $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ and $\mathcal{H}_B = \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2}$ then for a fixed $\rho$ on $\mathcal{H}$,

$$S_{AB_1B_2}^{ent}(\rho) \geq S_{AB}^{ent}(\rho).$$

(14)

\(^4\) Note that properties (I), (IIa), (VII), and equations (12), (16), have appeared before in the literature in the context of equivalent measures (see section VI for further discussion). Also Bravyi [56] has evaluated an equivalent measure on the so-called determinant and hexacode pure states.
That is, further splitting up the system into smaller subsystems can only increase entanglement entropy.

(VI) If $H = H_A \otimes H_B$ and $H_B = H_{B_1} \otimes H_{B_2}$ then
\[ S_{ent}^{AB_1B_2}(\rho_A \otimes \rho_B) = S_{ent}^{B_1B_2}(\rho_B). \] (15)

If also $H_A = H_{A_1} \otimes H_{A_2}$ then
\[ S_{ent}^{A_1A_2B_1B_2}(\rho_A \otimes \rho_B) = S_{ent}^{A_1A_2}(\rho_A) + S_{ent}^{B_1B_2}(\rho_B). \] (16)

That is, $S_{ent}$ is additive on independent systems.

(VII) $S_{ent}^{AB...C}(\rho)$ is invariant under local unitary operations. That is, if $\tilde{\rho} = (U_A \otimes \ldots \otimes U_C) \rho (U_A^\dagger \otimes \ldots \otimes U_C^\dagger)$, then $S_{ent}^{AB...C}(\tilde{\rho}) = S_{ent}^{AB...C}(\rho)$, where $U$ are local unitaries.

IV. RELATIONSHIP TO SUBSYSTEM ENTROPIES AND MUTUAL INFORMATION

In order to understand the entanglement entropy it is instructive to see how the entropy of a local coarse-graining is minimized, by considering the identity
\[ S_{C_A \otimes \ldots \otimes C_C}(\rho) = \left( \sum_X S_{C_X}(\rho_X) \right) - I_{C_A \otimes \ldots \otimes C_C}(\rho), \] (17)

where $X \in \{A, B, \ldots, C\}$ labels the subsystems, with $\rho_X$ the reduced density in each one, and
\[ I_{C_A \otimes \ldots \otimes C_C}(\rho) = \sum_{lm\ldots n} p_{lm\ldots n} \log \left( \frac{p_{lm\ldots n}}{p_{l}^{A} p_{m}^{B} \ldots p_{n}^{C}} \right) \] (18)

is the mutual information of the joint measurement. The $p_{l}^{X} = \sum_{m\ldots n} p_{lm\ldots n} = \text{tr}(P_{l}^{X} \rho_A)$ and so on are marginal probabilities, and subadditivity of Shannon entropy implies $I \geq 0$.

In computing the entanglement entropy one might hope to maximize the subsystem entropies $S_{C_X}$ while maximizing $I_{C_A \otimes \ldots \otimes C_C}$ in (17). These extrema cannot, in general, be achieved simultaneously, so an optimal coarse-graining must obtain some balance of these contributions.

Pure states of the form $|\psi\rangle = \sum_k a_k |a_k b_k \ldots c_k\rangle$ (cf. property (Ib)) provide a special case where the subsystem entropies and mutual information can be simultaneously extremized. In the optimal coarse-graining, assuming $N$ subsystems, one then finds $\sum_X S_{C_X}(\rho_X) = NS_0$ and $I = (N - 1)S_0$, where $S_0 = -\sum_k |a_k|^2 \log (|a_k|^2)$. Subtracting these two contributions leads in this special case to
\[ S_{ent}^{AB...C}(\rho) = S^{VN}(\rho_A) = \ldots = S^{VN}(\rho_C) = S_0, \] (19)

an equality which could be somewhat misleading, since in general the entanglement entropy and subsystem von Neumann entropies will not be equal.

V. EXAMPLES

To demonstrate calculability we exhibit two simple examples of some relevance to the literature. Example (A) compares “two Bell pair” versus GHZ entanglement in different partitions, relevant to genuine multipartite non-locality [61–63]. Example (B) considers a prototypical “separable but not classical” state, relevant to local indistinguishability [64].

(A) In a 4-partite system labelled $A_1 \otimes A_2 \otimes B_1 \otimes B_2$, define $|\phi_{GHZ}\rangle = ((000) + (1111))/\sqrt{2}$ and $|\phi_{Bell}\rangle = |\phi^+\rangle_A B_1 \otimes |\phi^+\rangle_A B_2$, where $|\phi^+\rangle = ((00) + (11))/\sqrt{2}$, each with density $\rho = |\phi\rangle \langle \phi|$. By properties (I,VI) above, we find for the 4-partite case $S_{ent}^{A_1A_2B_1B_2}(\rho_{Bell}) = 2$ bits, while in two bipartite cases $S_{ent}^{A_1B_1A_2B_2}(\rho_{Bell}) = 0$ and $S_{ent}^{AB}(\rho_{Bell}) = 2$ bits. Meanwhile $S_{ent}(\rho_{GHZ}) = 1$ bit in all these partitions.

(B) In a bipartite system $A \otimes B$ define $\rho = 1/2(|00\rangle + |11\rangle)/\sqrt{2}$. Properties (IV,II) provide an analytical bound $\alpha \geq S_{ent}(\rho) > 0$ (where $\alpha \approx 0.6$ bits is a number derived from (13)). Numerical minimization estimates $S_{ent}(\rho_{GHZ}) = 0.50$ bits.

VI. EQUIVALENCE TO OTHER MEASURES

Equivalent measures to the entropy considered here have arisen with various motivations and in various guises throughout the literature. The first seems to have been considered (in the special case of pure states) by Bravyi [56] as a minimal Shannon entropy of measurement outcomes. The motivation was essentially similar to here, only lacking the connection to coarse-graining and statistical mechanics. This was generalized to mixed states by SaiToh et. al. [47], though without reference to Bravyi. In between those studies the concept of quantum deficit was introduced by Oppenheim et. al. [51] and in subsequent studies [50, 52] the zero-deficit was shown (implicitly) to be equal to the measure of Bravyi and SaiToh et. al. and also (explicitly) to the relative entropy distance to classically correlated states. That distance was then proposed as an important measure of nonclassicality in its own right by Groisman et. al. [48], and systematically related to other relative entropy based measures by Modi et. al. [46], who called it the relative entropy of quantum discord.

Here we are interested in the equivalence of three quantities. The zero-deficit quantum discord, which measures a difference in work extractable by local versus global operations, is defined by [50]
\[ \Delta^0(\rho) = \inf_{\Lambda \in \text{CLOCC}} [S(\rho'_A) + \ldots + S(\rho'_C)] - S(\rho), \] (20)

where $\Delta^0(\rho)$ is a zero-deficit CLOCC operation (see [50]), $\rho' = \Lambda(\rho)$, and $\rho'_A = \text{tr}_{B...C}(\rho')$ and so on are the reduced densities. The relative entropy of quantum discord measures distance to the nearest classical state, and
is defined by [46]
\[
S^{\text{REQ}}(\rho) = \inf_{\chi \in S_C} S(\rho \| \chi),
\]
where \( S_C \) is the set of all classical states as defined by (10) and \( S(\rho \| \chi) = \text{tr}(\rho \log \rho - \rho \log \chi) \) is the quantum relative entropy. And \( S^{\text{ent}}(\rho) \) is defined by (6).

It is well known that \( \Delta^0 = S^{\text{REQ}} \) [19, 50]. It is easy to also show \( S^{\text{ent}} = S^{\text{REQ}} \). By Thm. 3 of [43], every coarse-graining can be refined to rank-1 without increasing coarse-grained entropy, so that (6) can be rewritten as an infimum over rank-1 local projectors. Then an application of Lemma 1 from [50] leaves the composition of two infima which combine to the one in (21) above. Thus \( \Delta^0 = S^{\text{REQ}} = S^{\text{ent}} \).

This measure therefore has three significant and complementary interpretations: (1) in terms of work extracted by local operations, (2) as a measure of nonclassicality as the distance from the set of classical states, and (3) as a statistical mechanical entropy related to non-equilibrium thermodynamics. Given this breadth of meaning, these three quantities seem to provide a thermodynamically distinguished measure of nonclassicality.

VII. DISCUSSION AND CONCLUSIONS

Consider a state \( \rho \) in a multipartite system. The coarse-grained entropy of \( \rho \), when minimized over all possible coarse-grainings, has a minimum given by the von Neumann entropy. But if one minimizes over only local coarse-grainings, the minimum may be higher. This entropy gap is what we call the multipartite entanglement entropy.

This definition treats pure and mixed states, and multipartite systems with any number of subsystems, all on equal footing. It is also a measure of nonclassicality: it is equal to the zero-way quantum deficit and to the relative entropy of quantum discord. Together these provide a clear interpretation: this entropy arises because no set of local measurements can reveal all information about a nonclassical state.

The given definition can also be extended immediately to classical systems (described by phase space density distributions) in the context of classical coarse-grained entropy [44], but in the classical case \( S^{\text{ent}} \) is always zero. This reflects that, like classically correlated quantum states (cf. (10)), the state of a classical system is exactly determined by local measurements.

In addition to measuring nonclassicality, this entropy has a role in thermodynamics. So far quantum coarse-grained entropy has been formally applied to non-equilibrium thermodynamics in two main scenarios.

In one scenario, Strasberg and Winter [41] considered a system-bath interaction where total thermodynamic entropy was identified as \( S_{C_S \otimes C_E} \) in the present notation, where \( C_E \) is an energy coarse-graining of the bath, and \( C_S \) is any coarse-graining of the system. This entropy was shown to be produced by non-equilibrium processes in accordance with standard thermodynamic laws. The present work indicates that one driving factor behind entropy production is the development of nonclassical correlations between the system and bath, and in particular \( S_{C_S \otimes C_E} \geq S^{\text{ent}}_{\text{SB}}(\rho) + S^{\text{VN}}(\rho) \). Interestingly, they have also split the entropy production up into classical and quantum parts. Comparing to their (42), \( S^{\text{ent}} \) is in fact a lower bound on the quantum part alone. Inserting local projectors into their (21) and comparing with (21) above also shows this identity holds more broadly.

The other scenario [42, 43] is that of an isolated system with local interactions. In this case the system is split into small but macroscopic local systems, with the relevant thermodynamic entropy ("factorized observational entropy") \( S_{C_E \otimes ... \otimes C_E} \) arising from local energy coarse-graining. This represents a thermodynamic entropy both in and out of equilibrium. Starting out of equilibrium, over time it approaches the canonical equilibrium value (up to some corrections dependent upon finite-size effects and on the initial state), even though the system is isolated, and perhaps pure. At some intermediate time \( t \) (when the system has only partially equilibrated) its value can be interpreted as the equilibrium thermodynamic entropy the system would attain in the long-time limit if (hypothetically) starting from time \( t \) the subsystems were not allowed to exchange either energy or particles [44]. Comparison with an equivalent classical scenario shows that this entropy increases in both situations [44]. The present work shows that, in the quantum system, creation of nonclassical correlations is an extra factor that drives the entropy upwards.

In both cases, non-equilibrium thermodynamic entropy can be seen as arising from some appropriate local coarse-graining, and thus has three additive (non-negative) contributions: (1) \( S^{\text{VN}}(\rho) \), the mixedness of the global state; (2) \( S^{\text{ent}}(\rho) \), the entropy of nonclassical correlation between the relevant subsystems; and (3) an additional contribution depending on the specific coarse-graining relevant to the problem. This provides useful insight into the generic relations between thermalization, entropy production, and nonclassical correlation.

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Appendix

This Appendix provides proofs of the properties (I–VII) of \( S^{\text{ent}} \) listed in the main text.

(Ia) Every bipartite pure state can be put in the
form (8) by Schmidt decomposition. The result then follows from (Ib).

(Ib) Let $S_0 = -\sum_i \sigma_{ii} \log \sigma_{ii} - S_{VN}(\rho)$. $C = \{\{a_i|a_i\}\} \cdots \{\{c_n|c_n\}\}$ is a local coarse-graining such that $S_C(\rho) = S_0 + S_{VN}(\rho)$. So $S_{\text{ent}}^{AB\cdots C}(\rho) \leq S_0$. But (IV) with $\rho_{\text{loc}} = \rho_A$ gives also $S_{\text{ent}}^{AB\cdots C}(\rho) \geq S_0$. Thus $S_{\text{ent}}^{AB\cdots C}(\rho) = S_0$.

(IIa) Follows from (Iib).

(Iib) ($\Rightarrow$) Suppose $\{a_1 \ldots c_n\}$ is a product basis diagonalizing $\rho$. Then $C = \{\{a_i|a_i\}\} \cdots \{\{c_n|c_n\}\}$ is a local coarse-graining finer than $C_0$, which implies $S_C(\rho) = S_{VN}(\rho)$ (Thm. 3 of [43]), which is the infimum by (2). ($\Leftarrow$) Assume $\min_{C = C_A \otimes \cdots \otimes C_C} S_C(\rho)$ exists and is equal to $S_{VN}(\rho)$. The coarse-graining $C_0 = \{P_i \otimes \cdots \otimes P_n\}$ attaining the minimum is finer than $C_0$ (Thm. 3 of [43]), thus it diagonalizes $\rho$. Thus $\rho = \sum_{i_1 \ldots i_n} P_{i_1} \otimes \cdots \otimes P_n$ where $P_{i_1 \ldots i_n}$ are real numbers. Writing each projector into rank-1 orthogonal projectors $P_i = \sum_k |a_{ik}\rangle \langle a_{ik}|$ yields the classical separable form (10). Then $\{a_{i_1} \ldots a_{i_k}\}$ is a product basis diagonalizing $\rho$. (Finite Dimensions) Only coarse-grainings involving rank-1 projectors need be considered in the infimum since others can be refined (Thm. 2 of [43]). These can be written in terms of unitary operators $U_A, \ldots, U_C$ such that $\inf_{C = C_A \otimes \cdots \otimes C_C} S_C(\rho) = \inf_{U_A, \ldots, U_C} S(U_A, \ldots, U_C)$ where $\tilde{S} = -\sum_{i_1 \ldots i_n} \log p_{i_1 \ldots i_n}$ with $p_{i_1 \ldots i_n} = tr(\rho (U_A \otimes \cdots \otimes U_C) P_{i_1 \ldots i_n})(U_A \otimes \cdots \otimes U_C)$ and $P_{i_1 \ldots i_n}$ are projectors of any rank-one local coarse-graining. Then $\tilde{S} : \mathcal{U}_A \times \cdots \times \mathcal{U}_C \to \mathbb{R}$ with $\mathcal{U}_A$ the set of unitary operators on $\mathcal{H}_A$, etc. If each subsystem has finite dimension then, in an appropriate topology, $\tilde{S}(U_A, \ldots, U_C)$ is the real continuous image of a compact set, so it attains its infimum.

(III) True by definition (6).

(IV) The loose bounds follow immediately from (6) with (2). (Upper Bound) By (17), since $I \geq 0$, $S_{C_{\rho_A \otimes \cdots \otimes C_{\rho_C}}}(\rho) \leq \sum S_{\rho_{\gamma X}}(\rho_X) = \sum S_{VN}(\rho_X)$. But $S_{AB\cdots C}^{\text{ent}}(\rho) \leq S_{C_{\rho_A \otimes \cdots \otimes C_{\rho_C}}}(\rho) - S_{VN}(\rho)$ since it is the infimum. (Lemma) Let $p_{i_1 \ldots i_n}$ and $V_{i_1 \ldots i_n}$ be the probabilities and volumes defining $S_{C_{\rho_A \otimes \cdots \otimes C_{\rho_C}}}(\rho)$. Likewise let $q_{i_1 \ldots i_n}$ and $W_{i_1 \ldots i_n}$ be those defining $S_{C_{\rho_A \otimes \cdots \otimes C_{\rho_C}}}(\rho_{B\cdots C})$, where $\rho_{B\cdots C} = tr_A(\rho)$. It follows that $q_{i_1 \ldots i_n} = \sum_{i_1 \ldots i_n} p_{i_1 \ldots i_n} V_{i_1 \ldots i_n} = tr(P_iW_{i_1 \ldots i_n})$. Thus $q_{i_1 \ldots i_n} \geq \frac{v_{i_1 \ldots i_n}}{v_{i_1 \ldots i_n}}$ for all $i_1, \ldots, i_n$, and since $-\log(x)$ is monotonic decreasing, $-\sum_{i_1 \ldots i_n} p_{i_1 \ldots i_n} \log \frac{v_{i_1 \ldots i_n}}{v_{i_1 \ldots i_n}} = -\sum_{i_1 \ldots i_n} q_{i_1 \ldots i_n} \log \frac{v_{i_1 \ldots i_n}}{v_{i_1 \ldots i_n}}$. Thus $S_{C_{\rho_A \otimes \cdots \otimes C_{\rho_C}}}(\rho) \geq S_{C_{\rho_A \otimes \cdots \otimes C_{\rho_C}}}(\rho_{B\cdots C})$. (Lower Bound) By repeated application of the lemma above, $S_{C_{\rho_A \otimes \cdots \otimes C_{\rho_C}}}(\rho) \geq S_{C_{\rho_A \otimes \cdots \otimes C_{\rho_{B\cdots F}}}}(\rho)$. (2) implies $S_{C_{\rho_A \otimes \cdots \otimes C_{\rho_{B\cdots F}}}}(\rho) \geq S_{VN}(\rho_{B\cdots F})$. Ordering of subsystems is irrelevant, so this is general.

(V) Any coarse-graining of the form $C_A \otimes C_{B_1} \otimes C_{B_2}$ is also a coarse-graining of the form $C_A \otimes C_B$. So one minimization strictly includes the other.

(VI) $S_{C_{\rho_A \otimes \rho_B}}(\rho_A + \rho_B) = S_{C_A}(\rho_A) + S_{C_B}(\rho)$ since $V_{i_1} = V_i V_j$ and for $\rho = \rho_A \otimes \rho_B$ also $p_{i_1 j_1} = p_{i_1} p_{j_1}$. Also $S_{VN}(\rho_A \otimes \rho_B) = S_{VN}(\rho_A) + S_{VN}(\rho_B)$. Thus $S_{\text{ent}}$ is additive since after splitting each term is infinum independent. Then (15) follows from $S_{\text{ent}}^{\text{inf}}(\rho_A) = 0$.

(VII) Write the infimum of (6) in terms of local unitaries as in the proof of (Iib). The local unitaries defining $\tilde{\rho}$ are absorbed into the infimum, so the infimum is invariant. Since also $S_{VN}(U\rho U^\dagger) = S_{VN}(\rho)$, $S_{\text{ent}}^{AB\cdots C}$ is invariant.

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