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A Fundamental Property of Quantum-Mechanical Entropy

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We have proved the strong subadditivity of quantum-mechanical entropy and the Wigner-Yanase-Dyson conjecture.

There are some properties of entropy, such as concavity and subadditivity, that are known to hold (in classical and in quantum mechanics) irrespective of any assumptions on the detailed dynamics of a system. These properties are consequences of the definition of entropy as

$$S(\rho) = -\mathrm{Tr}\rho\ln\rho \text{ (quantum)}, \tag{1a}$$

$$S(\rho) = -\int\rho\ln\rho \text{ (classical continuous)}, \tag{1b}$$

$$S(\rho) = -\sum\rho_i\ln\rho_i \text{ (classical discrete)}, \tag{1c}$$

where Tr means trace, ρ is a density matrix in (1a), and ρ is a distribution function (usually on R^{6N}) in (1b). In (1c) the ρ_i are discrete energy level probabilities.

One such property, strong subadditivity (SSA), was known to hold for classical systems and was only conjectured for quantum systems. The observation that classical entropy has SSA (this, in fact, is a theorem in information theory) and that SSA implies strong results about the thermodynamic limit of entropy per unit volume is due to Robinson and Ruelle.[1] Later, Lanford and Robinson[2] conjectured that SSA holds for quantum systems as well, and Baumann and Jost[3,4] were able to prove this when ρ has a special form. Araki and Lieb[5] proved a weakened form of SSA, but one which held for general ρ and which was sufficient for many of the purposes to which SSA had been put in Ref. 1. The physical significance of SSA is explained below [item (f) of Table I].

Prior to these developments, Wigner and Yanase[6] proposed a different definition of entropy (or negative information) which was generalized by Dyson.[6] The conjecture that this generalized entropy was concave in ρ was also proved by Baumann and Jost[3,7] in special cases, but it was not realized that this concavity problem and the SSA problem were related; in fact they are equivalent.

Here, we wish to announce that both of these problems have been solved affirmatively. The proofs, which are too long for this note, will be given in two papers.[8,9]

A density matrix is a positive semidefinite operator with $\mathrm{Tr}\rho = 1$. The Wigner-Yanase-Dyson p-entropy of ρ with respect to a self-adjoint operator (observable) K is

$$S_p(\rho, K) = \tfrac{1}{2}\mathrm{Tr}[\rho^p, K][\rho^{1-p}, K], \tag{2}$$

where $[A, B] = AB - BA$ and $0 \le p \le 1$ is fixed. We can think of (2) as defined for all $\rho \ge 0$ and ask whether $S_p(\rho, K)$ is concave as a function of ρ. The term $-\frac{1}{2}\mathrm{Tr}\rho K^2$ is obviously concave since it is linear, so the problem reduces to that of the concavity of $\mathrm{Tr}\rho^p K\rho^{1-p}K$. This was proved[6] when $p = \frac{1}{2}$. We have proved the following:

Theorem: For each fixed K (not necessarily self-adjoint), $\mathrm{Tr}\rho^p K^\dagger \rho^r K$ is a concave function of ρ for $\rho \ge 0$ whenever $p \ge 0$, $r \ge 0$, and $p + r \le 1$. This theorem is obviously stronger than necessary.

Returning to the conventional entropy (1a), we suppose that the Hilbert space of the system is a tensor product of three spaces, $H = H^1 \otimes H^2 \otimes H^3$. Thus, the system has three sets of degrees of freedom; for example, these may be thought of as the degrees of freedom of a gas in three disjoint regions in space (R^3). Given a density matrix ρ^{123} on H, we can define a density matrix ρ^{12} on $H^1 \otimes H^2$ by partial trace, i.e., $\rho^{12} = \mathrm{Tr}_3\rho^{123}$. In like manner we can form ρ^{23}, ρ^2, etc., and for each of these we have an entropy given by (1a). Denoting $S(\rho^{123})$ by S^{123}, etc., subadditivity states that

$$S^{12} \le S^1 + S^2, \tag{3}$$

while SSA states that

$$S^{123} + S^2 \le S^{12} + S^{23}. \tag{4}$$

We first show that $S^1 - S^{12}$ is convex in ρ^{12}. This implies SSA because, as was pointed out previously,[5] in the quantum or classical discrete case SSA is equivalent to

$$F \equiv (S^1 - S^{12}) + (S^3 - S^{23}) \le 0, \tag{5}$$

but as F is convex in ρ^{123}, it is less than its maximum value on extremal points, which latter are those ρ^{123} that are pure states. For pure states, $F = 0$.

We also prove some other related theorems,

TABLE I. Fundamental properties of entropy and their truth (T) or falsity (F) in three kinds of mechanics.

	Classical discrete	Classical continuous	Quantum
(a) $S(\rho)$ is concave in ρ	T	T	T
(b) $S^{12} \le S^1 + S^2$	T	T	T
(c) $S(\rho) \ge 0$	T	F	T
(d) $S^{12} \ge S^1$	T	F	F
(e) $S^{12} \ge \lvert S^1 - S^2 \rvert$	T	F	T
(f) $S^{123} + S^2 \le S^{12} + S^{23}$	T	T	T
(g) $S^{12} - S^1$ is concave in ρ^{12}	T	T	T

among which is the following:

Theorem: Let K be self-adjoint on a Hilbert space H and fixed. Then $\mathrm{Tr}[\exp(K + \ln\rho)]$ is a concave function of ρ for $\rho > 0$. Closer inspection shows that this theorem is a generalization of the Golden-Thompson inequality[10,11] to three operators.

To conclude, in Table I we append a list of the known fundamental entropy [Eq. (1)] inequalities and their physical significance. The following remarks clarify the physical significance of Table I. The letters (a)–(g) refer to entries in Table I.

(a) states that if two different ensembles are united, the entropy of the resulting ensemble is greater than the average entropy of the component ensembles.[6]

(b) is a statement of subadditivity and is the basic tool for proving that the entropy per unit volume has a thermodynamic limit (which may, however, depend on the particular sequence of domains).

(c) expresses a well-known defect of classical continuous statistical mechanics with respect to the third law of thermodynamics.

(d) expresses an intuitive defect of quantum and classical continuous statistical mechanics. An example occurs when ρ^{12} is a pure state, so that $S^{12} = 0$. Thus, the entropy of the universe can remain zero while the entropy of Earth increases without limit.

(e) is a consequence of SSA in the alternative form of inequality (5) (cf. Ref. 5) and is included as partial compensation for (d).

(f) is the statement of SSA. As a technical tool it allows one to prove that the entropy per unit volume for quantum continuous systems is independent of shape, at least for rectangular parallelepipeds of fixed orientation (cf. Ref. 5). If one is willing to assume that the entropy of every bounded region is finite [which cannot be proved, as (d) is false quantum mechanically], then the limit exists for arbitrary regions in the sense of Van Hove. However, (f) has a more heuristic interpretation. Although the connection between entropy and information is hedged with controversy, we may suppose, along with the Copenhagen school, that when we measure a system its density matrix is reduced to that of a pure state and the entropy is reduced to zero. Thus, entropy measures the information gain in an experiment. $S^{23} - S^{2}$ can be thought of as the information gained upon measuring a total system (23) when a subsystem (2) is known. In quantum mechanics it may be negative because of (d). $S^{123} - S^{12} \leq S^{23} - S^{2}$ states that this incremental information is smaller when the initial information [(12) as against (2)] is larger. This, at least, is the interpretation given in information theory.

(g) states that the incremental information, like the entropy itself, increases when two ensembles are united.

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