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Some Properties of Quantum Entropy.

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Summary

We consider finite degree of freedom systems, the states of which are described by density matrices ϱ : $\varrho \geq 0$, $\mathrm{Tr}\, \varrho = 1$ The entropy associated with ϱ reads $S(\varrho) = - k \mathrm{Tr}\, \varrho \ln \varrho$, k beeing Boltzmann's constant. To become technically not too involved let us further assume ϱ to be a finite-dimensional matrix. Then $0 \leq S'(\varrho) < \infty$ always and $S'(\varrho) = 0$ iff ϱ is a pure state. We describe three general properties of the entropy.

1. Entropy and general canonical ensembles. The following is well known. Let us consider some observables $A_1, A_2, \ldots, A_m$ There observed averages may be $a_1, a_2, \ldots, a_m$. Let us consider the set Φ of all density matrices satisfying $\mathrm{Tr}\, A_j \varrho = a_j$ If Φ is not emty, there is just one state $\omega \in \Phi$ with $S(\omega) \geq S'(\varrho)$ for all $\varrho \in \Phi$. If there are real numbers $\alpha_1, \alpha_2, \ldots, \alpha_m$ such that $\omega' = Z^{-1} \exp\{\alpha_1 A_1 + \ldots + \alpha_m A_m\} \in \Phi$ then $\omega = \omega'$. The most important examples are provided by Gibbsian canonical and grand canonical ensembles. More general ones have been used in non-equilibrium thermodynamics.

2. Subadditivity and related questions. If the basic Hilbert space $\mathcal{H}$ of a system is decompoes into a Kronecker product

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \ldots \otimes \mathcal{H}_q$$

of some other Hilbert spaces we say, the system is decomposed into subsystems characterised by the spaces $\mathcal{H}_j$. In such a decomposition the subspaces are "in a special position" relative one-to-another. If ϱ is a density matrix of $\mathcal{H}$, there is a unique density matrix ϱ_1 of $\mathcal{H}_1$ describing the same state

ϱ as viewed by an observer only observing properties connected with $\mathcal{H}_1$, i.e. operators of the form $A_1 \otimes 1 \otimes 1 \ldots$. ϱ_1 is called the reduction of ϱ to $\mathcal{H}_1$ ("reduced density matrix = partial trace over all other subsystems). Though in classical physics the entropy of a subsystem is always smaller than that of the total system, this is not so in quantum statistics (loss of monotonicity)! One easely constructs examples with $S(\varrho) < S(\varrho_1)$. (Given ϱ_1 one even finds a pure state ϱ which reduces to ϱ_1 if $\mathcal{H}_2$ is sufficient large.) On the other hand, if $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, one knows the triangle inequality

$$| S(\varrho_1) - S(\varrho_2) | \le S(\varrho)$$

Subadditivity, on the contrary, reads

$$S(\varrho) \le S(\varrho_1) + S(\varrho_2)$$

and equality holds iff $\varrho = \varrho_1 \otimes \varrho_2$, i.e. iff there are no correlations between the subsystems. Correlations, interactions, between the subsystems restrict somehow the possible states of the total system as seen from the subsystems.

The famous strong subadditivity property can be explained with three subsystems, $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$. If ϱ is a density matrix of $\mathcal{H}$, its reduction to $\mathcal{H}_1 \otimes \mathcal{H}_2$, $\mathcal{H}_2 \otimes \mathcal{H}_3$, $\mathcal{H}_2$, respectively may be denoted by ϱ_{12}, ϱ_{23}, ϱ_2. Then one has

$$S(\varrho) + S(\varrho_2) \le S(\varrho_{12}) + S(\varrho_{23})$$

3. Concavity properties. Properties 1) and 2) are due to the special behaviour of the function $-x \ln x$. With no other ansatz one can get either property 1) nor 2). In contrast to this there is a property of entropy shared by several other state functions, namely, concavity. Concavity is essential (though not sufficient) in understanding the connection between entropy

and irreversibility. Given density matrices $\varrho_1, \varrho_2, \ldots, \varrho_m$ and probabilities $p_1 \ge 0, \ldots, p_m \ge 0$; $\sum p_j = 1$, we construct

$$\varrho = p_1 \varrho_1 + p_2 \varrho_2 + \ldots + p_m \varrho_m$$

ϱ is called Gibbsian mixture of $\varrho_1, \ldots, \varrho_m$ with weights $p_1, \ldots, p_m$. Under this operation one always destroys some relative phases, correlations, informations,... and some state functions "measure" this: Let $F = F(\varrho)$ be a state function. It is concave if always

$$F(\varrho) \ge p_1 F(\varrho_1) + \ldots + p_m F(\varrho_m)$$

The entropy is concave. The more, define $F(\varrho) = \mathrm{Tr}\, f(\varrho)$ with $f(x)$ fullfilling $f''(x) \le 0$. Then F is concave. This is the reason why, historically, also different notations for entropy had appeared - and disappeared! But how to use these "entropy-like quantities"? One defines $\varrho \succ \omega$ for two density matrices and calls ϱ more mixed (more chaotic, less pure) than ω iff $F(\varrho) \ge F(\omega)$ for all concave and unitarilly invariant state functions F hold. Obviously, this relation, if it is true, is much stronger than a single inequality. Hence, it only defines a (pre-) semiordering of the density matrices, the "order structure of states". $\varrho \succ \omega$ iff ϱ is a Gibbsian mixture of states which are unitarilly equivalent to ω. $\succ$ points in the direction of a certain diffusion of the eigenvalues: Let $\lambda_1 \ge \lambda_2 \ge \ldots$; $\mu_1 \ge \mu_2 \ge \ldots$ denote the eigenvalues of ϱ and ω then $\varrho \succ \omega$ if and only if for all naturals k

$$\sum_{j=1}^{k} \lambda_j \le \sum_{j=1}^{k} \mu_j$$

i.e. the larger eigenvalues decrease, the lower increase and all together flatten out by going to more and more mixed states.

There will appear a review article by A. Wehrl in Rev. Mod. Phys. where the reader can find proofs, examples and references.