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Entropy, von Neumann and the von Neumann entropy *

Dedicated to the memory of Alfred Wehrl

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The highway of the development of entropy is marked by many great names, for example, Clausius, Gibbs, Boltzmann, Szilárd, von Neumann, Shannon, Jaynes, and several others. In this article the emphasis is put on von Neumann and on quantum mechanics. The selection of the subjects reflects the taste (and the knowledge) of the author and it must be rather restrictive. In the past 50 years entropy has broken out of thermodynamics and statistical mechanics and invaded communication theory, ergodic theory and shown up in mathematical statistics, social and life sciences. It is practically impossible to present all of its features. The favourite subjects of entropy is about macroscopic phenomena, irreversibility and incomplete knowledge. In the strictly mathematical sense entropy is related to the asymptotics of probabilities or it is a kind of asymptotic behaviour of probabilities.

This paper is organized as follows. After a short introduction to entropy, von Neumann's gedanken experiment is repeated, which led him to the formula of thermodynamic entropy of a statistical operator. In the analysis of his ideas we stress the role of (the lack of) superselection sectors and summarize von Neumann's knowledge about quantum mechanical entropy. The final part of this article is devoted to some important developments of the von Neumann entropy which were discovered long after von Neumann's work. Subadditivity and interpretation of the von Neumann entropy as the capacity of a communication channel are among those.

1 General introduction to entropy

The word "entropy" was created by Rudolf Clausius and it appeared in his work "Abhandlungen über die mechanische Wärmetheorie" published in 1864. The word has a Greek origin, its first part reminds us of "energy" and the second part is from "tropos" which means turning point. Clausius' work is the foundationstone of classical thermodynamics. According to Clausius, the change of entropy of a system is obtained by adding the small portions of heat quantity received by the system divided by the absolute temperature during the heat absorption. This definition is satisfactory from a mathematical point of view and gives nothing other than an integral in precise mathematical terms. Clausius postulated that the entropy of a closed system cannot decrease, which is generally referred to as the second law of thermodynamics. On the other hand, he did not provide any heuristic argument to support the law. This fact might partly be responsible for the mystery surrounding entropy for a long time. As an extreme, we can cite Alfred Wehrl who had the opinion in 1978 that "the second law of thermodynamics does not appear to be fully understood yet" [13].

The concept of entropy was really clarified by Ludwig Boltzmann. His scientific program was to deal with the mechanical theory of heat in connection with probabilities. Assume that a macroscopic system consists of a large number of microscopic ones, we simply call them particles. Since we have ideas of quantum mechanics in mind, we assume that each of the particles is in one of the energy levels $E_1 < E_2 < \ldots < E_m$. The number of particles in the level E_i is N_i, so $\sum_i N_i = N$ is the total number of

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particles. A macrostate of our system is given by the occupation numbers $N_1, N_2, \ldots, N_m$. The energy of a macrostate is $E = \sum_i N_i E_i$. A given macrostate can be realized by many configurations of the N particles, each of them at a certain energy level E_i. Those configurations are called microstates. Many microstates realize the same macrostate. We count the number of ways of arranging N particles in m boxes (i.e., energy levels) such that each box has $N_1, N_2, \ldots, N_m$ particles. There are

$$\left(\begin{array}{c} N \\ N_1, N_2, \cdots, N_m \end{array} \right) := \frac{N!}{N_1!\, N_2! \ldots N_m!} \tag{1}$$

such ways. This multinomial coefficient is the number of microstates realizing the macrostate $(N_1, N_2, \ldots, N_m)$ and it is proportional to the probability of the macrostate if all configurations are assumed to be equally likely. Boltzmann called (1) the thermodynamical probability of the macrostate, in German "thermodynamische Wahrscheinlichkeit", hence the letter W was used. Of course, Boltzmann argued in the framework of classical mechanics and the discrete values of energy came from an approximation procedure with "energy cells".

If we are interested in the thermodynamic limit N increasing to infinity, we use the relative numbers $p_i := N_i/N$ to label a macrostate and, instead of the total energy $E = \sum_i N_i E_i$, we consider the average energy pro particle $E/N = \sum_i p_i E_i$. To find the most probable macrostate, we wish to maximize (1) under a certain constraint. The Stirling approximation of the factorials gives

$$\frac{1}{N} \log \left(\begin{array}{c} N \\ N_1, N_2, \cdots, N_m \end{array} \right) = H(p_1, p_2, \ldots, p_m) + O(N^{-1} \log N), \tag{2}$$

where

$$H(p_1, p_2, \ldots, p_m) := \sum_i -p_i \log p_i. \tag{3}$$

If N is large then the approximation (2) yields that instead of maximizing the quantity (1) we can maximize (3). For example, maximizing (3) under the constraint $\sum_i p_i E_i = e$, we get

$$p_i = \frac{e^{-\lambda E_i}}{\sum_j e^{-\lambda E_j}}, \tag{4}$$

where the constant λ is the solution of the equation

$$\sum_i E_i \frac{e^{-\lambda E_i}}{\sum_j e^{-\lambda E_j}} = e.$$

Note that the last equation has a unique solution if $E_1 < e < E_m$, and the distribution (4) is known as the discrete Maxwell-Boltzmann law today.

Let $p_1, p_2, \ldots, p_n$ be the probabilities of different outcomes of a random experiment. According to Shannon, the expression (1) is a measure of our ignorance prior to the experiment. Hence it is also the amount of information gained by performing the experiment. (1) is maximum when all the p_i's are equal. In information theory logarithms with base 2 are used and the unit of information is called bit (from binary digit). As will be seen below, an extra factor equal to Boltzmann's constant is included in the physical definition of entropy.

2 Von Neumann's contribution to entropy

The comprehensive mathematical formalism of quantum mechanics was first presented in the famous book "Mathematische Grundlagen der Quantenmechanik" published in 1932 by Johann von Neumann. In the traditional approach to quantum mechanics, a physical system is described in a Hilbert space: Observables correspond to selfadjoint operators and statistical operators are asssociated with the states. In fact, a statistical operator describes a mixture of pure states. Pure states are the really physical states and they are given by rank one statistical operators, or equivalently by rays of the Hilbert space.

Von Neumann associated an entropy quantity to a statistical operator in 1927 [5] and the discussion was extended in his book [6]. His argument was a gedanken experiment on the ground of phenomenological thermodynamics. Let us consider a gas of $N(\gg 1)$ molecules in a rectangular box K. Suppose that the gas behaves like a quantum system and is described by a statistical operator D which is a mixture $\lambda|\varphi_1\rangle\langle\varphi_1| + (1-\lambda)|\varphi_1\rangle\langle\varphi_2|$, $|\varphi_i\rangle \equiv \varphi$ is a state vector $(i = 1, 2)$. We may take λN molecules in the pure state φ_1 and $(1-\lambda)N$ molecules in the pure state φ_2. On the basis of phenomenological thermodymanics we assume that if φ_1 and φ_2 are orthogonal, then there is a wall which is completely permeable for the φ_1-molecules and isolating for the φ_2-molecules. (In fact, von Neumann supplied an argument that such a wall exists if and only if the state vectors are orthogonal.) We add an equally large empty rectangular box K' to the left of the box K and we replace the common wall with two new walls. Wall (a), the one to the left is impenetrable, whereas the one to the right, wall (b), lets through the φ_1-molecules but keeps back the φ_2-molecules. We add a third wall (c) opposite to (b) which is semipermeable, transparent for the φ_2-molecules and impenetrable for the φ_1-ones. Then we push slowly (a) and (c) to the left, maintaining their distance. During this process the φ_1-molecules are pressed through (b) into K' and the φ_2-molecules diffuse through wall (c) and remain in K. No work is done against the gas pressure, no heat is developed. Replacing the walls (b) and (c) with a rigid absolutely impenetrable wall and removing (a) we restore the boxes K and K' and succeed in the separation of the φ_1-molecules from the φ_2-ones without any work being done, without any temperature change and without evolution of heat. The entropy of the original D-gas (with density N/V) must be the sum of the entropies of the φ_1- and φ_2-gases (with densities $\lambda N/V$ and $(1-\lambda)N/V$, respectively.) If we compress the gases in K and K' to the volumes λV and $(1-\lambda)V$, respectively, keeping the temperature T constant by means of a heat reservoir, the entropy change amounts to $\kappa\lambda N \log\lambda$ and $\kappa(1-\lambda)N\log(1-\lambda)$, respectively. Indeed, we have to add heat in the amount of $\lambda_i N\kappa T \log\lambda_i$ (< 0) when the φ_i-gas is compressed, and dividing by the temperature T we get the change of entropy. Finally, mixing the φ_1- and φ_2-gases of identical density we obtain a D-gas of N molecules in a volume V at the original temperature. If $S_0(\psi, N)$ denotes the entropy of a ψ-gas of N molecules (in a volume V and at the given temperature), we conclude that

$$\begin{aligned} &S_0(\varphi_1, \lambda N) + S_0(\varphi_2, (1-\lambda)N) \\ &\quad = S_0(D, N) + \kappa\lambda N\log\lambda + \kappa(1-\lambda)N\log(1-\lambda) \end{aligned}$$

must hold, where κ is Boltzmann's constant. Assuming that $S_0(\psi, N)$ is proportional to N and dividing by N we have

$$\begin{aligned} &\lambda S(\varphi_1) + (1-\lambda)S(\varphi_2) \\ &\quad = S(D) + \kappa\lambda\log\lambda + \kappa(1-\lambda)\log(1-\lambda)\,, \end{aligned} \tag{5}$$

where S is certain thermodynamical entropy quantity (relative to the fixed temperature and molecule density). We arrived at the mixing property of entropy, but we should not forget about the initial assumption: φ_1 and φ_2 are supposed to be orthogonal. Instead of a two-component mixture, von Neumann operated by an infinite mixture, which does not make a big difference, and he concluded that

$$S\Big(\sum_i \lambda_i|\varphi_i\rangle\langle\varphi_i|\Big) = \sum_i \lambda_i S(|\varphi_i\rangle\langle\varphi_i|) - \kappa\sum_i \lambda_i\log\lambda_i. \tag{6}$$

Before we continue to follow his considerations, let us note that von Neumann's argument does not require that the statistical operator D is a mixture of pure states. What we really needed is the property $D = \lambda D_1 + (1-\lambda)D_2$ in such a way that the possible mixed states D_1 and D_2 are disjoint. D_1 and D_2 are disjoint in the thermodynamical sense, when there is a wall which is completely permeable for the molecules of a D_1-gas and isolating for the molecules of a D_2-gas. In other words, if the mixed states D_1 and D_2 are disjoint, then this should be demonstrated by a certain filter. Mathematically, the disjointness of D_1 and D_2 is expressed in the orthogonality of the eigenvectors corresponding to nonzero eigenvalues of the two density matrices. The essential point is in the remark that equation (5) must hold also in a more general situation when possibly the states do not correspond to density matrices

but orthogonality of the states makes sense:

$$\begin{aligned}&\lambda S(D_1) + (1-\lambda)S(D_2)\\ &\quad = S(D) + \kappa\lambda\log\lambda + \kappa(1-\lambda)\log(1-\lambda)\end{aligned} \tag{7}$$

Equation (6) reduces the determination of the (thermodynamical) entropy of a mixed state to that of pure states. The so-called Schatten decomposition $\sum_i \lambda_i |\varphi_i\rangle\langle\varphi_i|$ of a statistical operator is not unique even if $\langle\varphi_i, \varphi_j\rangle = 0$ is assumed for $i \neq j$. When λ_i is an eigenvalue with multiplicity, then the corresponding eigenvectors can be chosen in many ways. If we expect the entropy $S(D)$ to be independent of the Schatten decomposition, then we are led to the conclusion that $S(|\varphi\rangle\langle\varphi|)$ must be independent of the state vector $|\varphi\rangle$. This argument assumes that there are no superselection sectors, that is, any vector of the Hilbert space can be a state vector. On the other hand, von Neumann wanted to avoid degeneracy of the spectrum of a statistical operator (as well as the possible degeneracy of the spectrum of observables as we shall see below).

Von Neumann's proof of the property that $S(|\varphi\rangle\langle\varphi|)$ is independent of the state vector $|\varphi\rangle$ was different. He did not want to refer to a unitary time development sending one state vector to another, because that argument requires great freedom in choosing the energy operator H. Namely, for any $|\varphi_1\rangle$ and $|\varphi_2\rangle$ we would need an energy operator H such that

$$e^{\mathrm{i}tH}|\varphi_1\rangle = |\varphi_2\rangle.$$

This process would be reversible. (It is worthwhile to note that the problem of superselection sectors appears also here.)

Von Neumann proved that $S(|\varphi_1\rangle\langle\varphi_1|) \leq S(|\varphi_2\rangle\langle\varphi_2|)$ by constructing a great number of measurement processes sending the state $|\varphi_1\rangle$ into an ensemble, which differs from $|\varphi_2\rangle\langle\varphi_2|$ by an arbitrarily small amount. The measurement of an observable $A = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$ in a state $|\varphi\rangle$ yields an ensemble of the pure states $|\psi_i\rangle\langle\psi_i|$ with weights $|\langle\varphi|\psi_i\rangle|^2$. This was a basic postulate in von Neumann's measurement theory when the eigenvalues of A are non-degenerate, that is, λ_i's are all different. In a modern language, von Neumann's measurement is a conditional expectation onto a maximal Abelian subalgebra of the algebra of all bounded operators acting on the given Hilbert space. Let $(|\psi_i\rangle)_i$ be an orthonormal basis consisting of eigenvectors of the observable under measurement. For any bounded operator T we set

$$E(T) = \sum_i \langle\psi_i|T|\psi_i\rangle|\psi_i\rangle\langle\psi_i|. \tag{8}$$

The linear transformation E possesses the following properties:

(i) $E = E^2$.

(ii) If $T \geq 0$ then $E(T) \geq 0$.

(iii) $E(I) = I$.

(iv) $\mathrm{Tr}\,\big(E(T)\big) = \mathrm{Tr}\,T$.

In particular, for a statistical operator D its transform $E(D)$ is a statistical operator as well. It follows immediately from definition (8) that

$$E(|\varphi\rangle\langle\varphi|) = \sum_i |\langle\varphi|\psi_i\rangle|^2 |\psi_i\rangle\langle\psi_i|$$

and the conditional expectation E acts on the pure states exactly in the same way as it is described in the measurement procedure. It was natural for von Neumann to assume that

$$S(D) \leq S\big(E(D)\big), \tag{9}$$

at least if the statistical operator D corresponds to a pure state. Inequality (9) is nothing other than the manifestation of the second law for the measurement process.

In the proof of the inequality $S(|\varphi_1\rangle\langle\varphi_1|) \le S(|\varphi_2\rangle\langle\varphi_2|)$ one can assume that the vectors $|\varphi_1\rangle$ and $|\varphi_2\rangle$ are orthogonal. The idea is to construct measurements $E_1, E_2, \dots, E_k$ such that

$$E_k\Big(\dots\big(E_1(|\varphi_1\rangle\langle\varphi_1|)\big)\dots\Big) \tag{10}$$

is in a given small neighbourhood of $|\varphi_2\rangle\langle\varphi_2|$. The details are well-presented in von Neumann's original work, but we confine ourselves here to his definition for E_n. He set a unit vector

$$\psi^{(n)} = \cos\frac{\pi n}{2k}|\varphi_1\rangle + \sin\frac{\pi n}{2k}|\varphi_2\rangle$$

and extended it to a complete orthonormal system. The measurement conditional expectation E_n corresponds to this basis ($1 \le n \le k$). It is elementary to show that (10) tends to $|\varphi_2\rangle\langle\varphi_2|$ as $k \to \infty$. We stress again that the argument needs that $|\varphi_1\rangle$ and $|\varphi_2\rangle$ are in the same superselection sector, so that their linear combinations may be state vectors.

Let us summarize von Neumann's discussion of the thermodynamical entropy of a statistical operator D. First of all, he assumed that $S(D)$ is a continuous function of D. He carried out a reversible process to obtain the mixing property (5) for orthogonal pure states, and he concluded (6). He referred to the second law again when assuming (9) for pure states. Then he showed that $S(|\varphi\rangle\langle\varphi|)$ is independent of the state vector $|\varphi\rangle$ so that

$$S\Big(\sum_i \lambda_i|\varphi_i\rangle\langle\varphi_i|\Big) = -\kappa\sum_i \lambda_i \log\lambda_i \tag{11}$$

up to an additive constant which could be chosen to be 0 as a matter of normalization. (11) is von Neumann's celebrated entropy formula; it has a more elegant form

$$S(D) = \kappa \mathrm{Tr}\,\eta(D), \tag{12}$$

where $\eta : \mathbb{R}^+ \to \mathbb{R}$ is the continuous function $\eta(t) = -t\log t$. (The modern notation for $-t\log t$ comes from information theory which did not exist at that time.)

When von Neumann deduced (12), his natural intention was to make mild assumptions. For example, the monotonicity (9) was assumed only for pure states. If we already have (12) as a definition, then (9) can be proved for an arbitrary statistical operator D. The argument is based on the Jensen inequality, and von Neumann remarked that for

$$S_f(D) = \mathrm{Tr}\, f(D)$$

with a differentiable concave function $f : [0,1] \to \mathbb{R}$,

$$S_f(D) \le S_f\big(E(D)\big) \tag{13}$$

holds for every statistical operator D. His analysis also indicated that the measurement process is typically irreversible, the finite entropy of a statistical operator definitely increases if a state change occurs.

Von Neumann solved the maximization problem for $S(D)$ under the constraint $\mathrm{Tr}\, DH = e$. This means the determination of the ensemble of maximal entropy when the expectation of the energy operator H is a prescribed value e. It is convenient to rephrase his argument in terms of conditional expectations. $H = H^*$ is assumed to have a discrete spectrum and we have a conditional expectation E determined by the eigenbasis of H. If we pass from an arbitrary statistical operator D with $\mathrm{Tr}\, DH = e$ to $E(D)$, then the entropy is increasing on the one hand and the expectation of the energy does not change on the other hand, so the maximizer should be searched among the operators commuting with H. In this way we are (and von Neumann was) back to the classical problem of statistical mechanics treated at the beginning of this article. In terms of operators the solution is in the form

$$\frac{\exp(-\beta H)}{\mathrm{Tr}\,\exp(-\beta H)},$$

which is called the Gibbs state today.

3 Some topics about entropy from von Neumann to the present

After Boltzmann and von Neumann, it was Shannon who initiated the interpretation of the quantity $-\sum_i p_i \log p_i$ as "uncertainty measure" or "information measure". The American electrical engineer/scientist Claude Shannon created communication theory in 1948. He posed a problem in the following way:

> "Suppose we have a set of possible events whose probabilities of occurence are $p_1, p_2, \ldots, p_n$. These probabilities are known but that is all we know concerning which event will occur. Can we find a measure of how much "choice" is involved in the selection of the event or how uncertain we are of the outcome?"

Denoting such a measure by $H(p_1, p_2, \ldots, p_n)$ he listed three very reasonable requirements which should be satisfied. He concluded that the only H satisfying the three assumptions is of the form

$$H = -K \sum_{i=1}^{n} p_i \log p_i \,,$$

where K is a positive constant. For H he used different names such as information, uncertainty and entropy. Many years later Shannon said [12]:

> "My greatest concern was what to call it. I thought of calling it 'information', but the word was overly used, so I decided to call it 'uncertainty'. When I discussed it with John von Neumann, he had a better idea. Von Neumann told me, 'You should call it entropy, for two reasons. In the first place your uncertainty function has been used in statistical mechanics under that name, so it already has a name. In the second place, and more important, nobody knows what entropy really is, so in a debate you will always have the advantage."

Shannon's postulates were transformed later into the following axioms:

(a) Continuity: $H(p, 1-p)$ is continuous function of p.

(b) Symmetry: $H(p_1, p_2, \ldots, p_n)$ is a symmetric function of its variables.

(c) Recursion: For every $0 \le \lambda < 1$ the recursion $H(p_1, \ldots, p_{n-1}, \lambda p_n, (1-\lambda)p_n) = H(p_1, \ldots, p_n) + p_n H(\lambda, 1-\lambda)$ holds.

These axioms determine a function H up to a positive constant factor. Excepting the above story about a conversation between Shannon and von Neumann, we do not know about any mutual influence. Shannon was interested in communication theory and von Neumann's thermodynamical entropy was in the formalism of quantum mechanics. Von Neumann himself never made any connection between his quantum mechanical entropy and information. Although von Neumann's entropy formula appeared in 1927, there was not much activity concerning it for several decades. At the end of the 1960's, the situation changed. Rigorous statistical mechanics came into being [10] and soon after that the needs of rigorous quantum statistical mechanics forced new developments concerning von Neumann's entropy formula.

Von Neumann was aware of the fact that statistical operators form a convex set whose extreme points are exactly the pure states. He also knew that entropy is a concave functional, so

$$S\Big(\sum_i \lambda_i D_i\Big) \ge \sum_i \lambda S(D_i) \tag{14}$$

for any convex combination. To determine the entropy of a statistical operator, he used the Schatten decomposition, which is an orthogonal extremal decomposition in our present language. For a statistical operator D there are many ways to write it in the form

$$D = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$$

if we do not require the state vectors to be orthogonal. The geometry of the statistical operators, that is the state space, allows many extremal decompositions and among them there is a unique orthogonal one if the spectrum of D is not degenerate. Non-orthogonal pure states are essentially nonclassical. They are between identical and completely different. Jaynes recognized in 1956 that from the point of view of information the Schatten decomposition is optimal. He proved that

$$\begin{aligned} S(D) \quad = \quad & \sup\Big\{ -\sum_i \lambda_i \log \lambda_i : D = \sum_i \lambda_i D_i \\ & \qquad \text{for some convex combination and statistical operators} \Big\}. \end{aligned}$$

This is Jaynes contribution to the von Neumann entropy [2]. (However, he became known for the very strong advocacy of the maximum entropy principle.)

Certainly the highlight of quantum entropy theory in the 70's was the discovery of subadditivity. Before we state it in precise mathematical form, we describe the setting where this property is crucial. A one-dimensional quantum lattice system is a composite system of $2N+1$ subsystems, indexed by the integers $-N \le n \le N$. Each of the subsystems is described by a Hilbert space $\mathcal{H}_n$; those Hilbert spaces are isomorphic if we assume that the subsystems are physically identical, and even the very finite dimensional case $\dim \mathcal{H}_n = 2$ can be interesting if the subsystem is a "spin 1/2" attached to the lattice site n. The finite chain of $2N+1$ spins is described in the tensor product Hilbert space $\otimes_{n=-N}^{N} \mathcal{H}_n$, whose dimension is $(\dim \mathcal{H}_n)^{2N+1}$. For a given Hamiltonian H_N and inverse temperature β the equilibrium state maximizes the free energy functional

$$F_N(D_N) = \mathrm{Tr}_N H_N D_N - \frac{1}{\beta} S(D_N), \tag{15}$$

and the actual maximizer is the Gibbs state

$$\frac{\exp(-\beta H_N)}{\mathrm{Tr}\, \exp(-\beta H_N)}. \tag{16}$$

It seems that this was already known in von Neumann's time but not the thermodynamical limit, $N \to \infty$. Rigorous statistical mechanics of spin chains was created in the 70's. Since entropy, energy, and free energy are extensive quantities, the infinite system should be handled by their normalized versions, called entropy density, energy density, etc. One possibility to describe the equilibrium of the infinite system is to carry out a limiting procedure from the finite volume equilibrium states, and another is to solve the variational principle for the free energy density on the state space of the infinite system. In a translation invariant theory the two approaches lead to the same conclusion, but many technicalities are involved. The infinite system is modeled by a C^*-algebra and their states are normalized linear functionals instead of statistical operators. The rigorous statistical mechanics of quantum spin systems was one of the successes of the operator algebraic approach. [11] and Sec. 15 of [7] are suggested further readings about details of quantum spin systems. One of the key points in this approach is the definition of entropy density of a state of the infinite system which goes back to the subadditivity of the von Neumann entropy. Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be possibly finite dimensional Hilbert spaces corresponding to two quantum systems. A mixed state of the composite system is determined by a statistical operator D_{12} acting on the tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$. Assume that we are to measure observables on the first subsystem. What is the statistical operator we need? The statistical operator D_1 has to fulfill the condition

$$\mathrm{Tr}_1 A D_1 = \mathrm{Tr}_{12}(A \otimes I) D_{12} \tag{17}$$

for any observable A. Indeed, the left hand side is the expectation of A in the subsystem and the right hand side is that in the total system. It is easy to see that condition

$$\langle \psi | D_1 | \psi \rangle = \sum_i \langle |\psi\rangle \otimes |\varphi_i\rangle, D_{12} |\psi\rangle \otimes |\varphi_i\rangle \,\rangle \tag{18}$$

gives the statistical operator D_1, where $|\psi\rangle \in \mathcal{H}_1$ and $|\varphi_i\rangle$ is an arbitrary orthonormal basis in $\mathcal{H}_2$. (In fact equation (18) is obtained from (17) by putting $|\psi\rangle\langle\psi|$ in place of A.) It is not difficult to state the subadditivity property now:

$$S(D_{12}) \leq S(D_1) + S(D_2). \tag{19}$$

This is a particular case of the strong subadditivity

$$S(D_{123}) \leq S(D_{12}) + S(D_{23}) - S(D_2) \tag{20}$$

for a system consisting of three subsystems. (We hope that the notation is selfexplanatory, otherwise see [4], [13] or p. 23 in [7].) If the second subsystem is lacking, (20) reduces to (19). (19) was proven first by Lieb and Ruskai in 1973 [4].

The measurement conditional expectation was introduced by von Neumann as the basic irreversible state change, and it is of the form

$$D \mapsto \sum_i P_i D P_i, \tag{21}$$

where P_i are pairwise orthogonal projections and $\sum_i P_i = I$. (We are in the Schrödinger picture.) The measurement conditional expectation has the following generalization. Assume that our quantum system is described by an operator algebra $\mathcal{M}$ whose positive linear functionals correspond to the states. A functional $\tau : \mathcal{M} \to \mathbb{C}$ is a state if $\tau(A) \geq 0$ for any positive observable A and $\tau(I) = 1$. An operational partition of unity is a finite subset $\mathcal{W} = (V_1, V_2, \ldots, V_n)$ of $\mathcal{M}$ such that $\sum_i V_i^* V_i = I$. In the Heisenberg picture $\mathcal{W}$ acts on the observables as

$$A \mapsto \sum_i V_i^* A V_i$$

and the corresponding state change in the Schrödinger picture is

$$\tau(\,\cdot\,) \mapsto \tau\Big(\sum_i V_i^* \,\cdot\, V_i\Big).$$

Let us compare this with the traditional formalism of quantum mechanics. If $\tau(A) = \operatorname{Tr} DA$, then

$$\tau\Big(\sum_i V_i^* A V_i\Big) = \operatorname{Tr}\Big(D \sum_i V_i^* A V_i\Big) = \operatorname{Tr}\Big(\sum_i V_i D V_i^*\Big) A,$$

hence the transformation of the statistical operator is

$$D \mapsto \sum_i V_i D V_i^*$$

which is an extension of von Neumann's measurement conditional expectation (21). Given a state τ of the quantum system, the observed entropy of the operational process is defined to be the von Neumann entropy of the finite statistical operator

$$\big[\tau(V_i^* V_j)\big]_{i=j=1}^n,$$

which is an $n \times n$ positive semidefinite matrix of trace 1. If we are interested in the entropy of a state, we perform all operational processes and compute their entropy. If the operational process changes the state of our system, then the observed operational entropy includes the entropy of the state change. Hence we have to restrict ourself to state invariant operational processes when focusing on the entropy of the state. The formal definition

$$S^L(\tau) = \sup\Big\{S\big(\big[\tau(V_i^* V_j)\big]_{i=j=1}^n\big)\Big\}$$

is the operational (or Lindblad) entropy of the state τ if the least upper bound is taken over all operational partitions of unity $\mathcal{W} = (V_1, V_2, \ldots, V_n)$ such that

$$\tau(A) \mapsto \tau\Big(\sum_i V_i^* A V_i\Big),$$

for every observable A. For a statistical operator D we have

$$S^L(D) = 2S(D),$$

and we may imagine that the factor 2 is removable by appropriate normalization, so that we are back to the von Neumann entropy. The operational entropy satisfies von Neumann's mixing condition and is a concave functional on the states even in the presence of superselection rules. However, it has some new features. To see a concrete example, assume that there are two superselection sectors and the operator algebra is $M_2(\mathbb{C}) \oplus M_3(\mathbb{C})$, that is, the direct sum of two full matrix algebras. Let a state τ_0 be the mixture of the orthogonal pure states $|\psi_i\rangle$ with weights λ_i, where $|\psi_1\rangle, |\psi_2\rangle$ are in the first sector and $|\psi_3\rangle$ is in the second. This assumption implies that there is no dynamical change sending $|\psi_1\rangle$ into $|\psi_3\rangle$, and superpositions of those states are also prohibited. One computes

$$\begin{aligned} S^L(\tau_0) &= -2\sum_i \lambda_i \log \lambda_i \\ &\quad -(\lambda_1+\lambda_2)\log(\lambda_1+\lambda_2) - (\lambda_1+\lambda_2+\lambda_3)\log(\lambda_1+\lambda_2+\lambda_3), \end{aligned}$$

which shows that this entropy is really sensitive to the superselection sectors. (For further properties on S^L we refer to pp. 121–124 of [7].)

Nowdays some devices are based on quantum mechanical phenomena, and this holds also for information transmission. For example, in optical communication a polarized photon can carry information. Although von Neumann apparently did not see an intimate connection between his entropy formula and the formally rather similar Shannon information measure, many years later an information theoretical reinterpretation of von Neumann's entropy is becoming common. Communication theory deals with coding, transmission, and decoding of messages. Given a set $\{a_1, a_2, \dots, a_n\}$ of messages, a coding procedure assigns to each a_i a physical state, say a quantum mechanical state $|\psi_i\rangle$. The states are transmitted and received. During the transmission some noise can enter. The receiver uses some observables to recover the transmitted message. Shannon's classical model is stochastic, so it is assumed that each message a_i should be teleported with some probability λ_i, $\sum_i \lambda_i = 1$. Hence in the quantum model the input state of the channeling transformation is a mixture; its statistical operator is $D_{\rm in} = \sum_i p_i |\psi_i\rangle\langle\psi_i|$. This is the state we need to transmit, and after transmission it changes into $T(D_{\rm in}) = D_{\rm out}$ which is formally a statistical operator but may correspond to a state of a very different system. Input and output could be far away in space as well as in time. The observer measures the observable A_j and $p_i = \mathrm{Tr}\, D_{\rm out} A_i$ is the probability with which he concludes the message a_j was transmitted. Here we need $\sum_j A_j = I$ and $0 \le A_i$. More generally, we assume that

$$p_{ji} = \mathrm{Tr}\, T(|\psi_i\rangle\langle\psi_i|)A_j$$

is the probability that the receiver deduces the transmission of the message a_j when actually the message a_i was transmitted. If we forget about the quantum mechanical coding, transmission and decoding (measurement), we see a classical information channel in Shannon's sense. According to Shannon, the amount of information going through the channel is

$$I = \sum_{ij} p_{ji} \log \frac{p_{ji}}{p_i}.$$

One of the basic problems of communication theory is to maximize this quantity subject to certain constraints. For the sake of simplicity, assume that there is no noise. This may happen when the channel is actually the memory of a computer; storage of information might be a noiseless channel in Shannon's sense. We have then $T =$identity, $D_{\rm in} = D_{\rm out} = D$ and the inequality

$$I \le S(D)$$

holds. If we fix the channel state D and optimize with respect to the probabilities λ_i, the states $|\psi_i\rangle$ and the observables A_j, then the maximum information transmittable through the channel is

exactly the von Neumann entropy. What we are considering is a simple example, probably the simplest possible. However, it is well demonstrated that the von Neumann entropy is actually the capacity of a communication channel. Recently, there has been a lot of discussion about capacities of quantum communication channels, which is outside of the scope of the present article. However, the fact that von Neumann's entropy formula has much to do with Shannon theory and possesses an interpretation as measure of information must be conceptually clear without entering more sophisticated models and discussions. More details are in [8] and a mathematically full account is [1].

Further sources about quantum entropy and quantum information are [3], [9] and [7].

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