

Study
Edition

M. Ohya
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Quantum Entropy and Its Use



Springer

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Preface to the Corrected Second Printing

Since our monograph was published first in 1993, quantum information theory has developped a lot in connection with the revolutionary achievements in the fields of quantum computing and quantum algorithms. Von Neumann entropy and quantum relative entropy have got several new applications and interpretations and many examples of quantum communication channels have been discovered and discussed.

The second edition keeps the original structure of the first one. At the end of the chapters a short summary is given about some of the new results obtained after the first addition was published. The results covered by the summary sections are selected in a rather arbitrary way and they cannot give an abstract of the huge number of papers published in quantum information theory in the recent years. The bibliography of the book is slightly extended as well. The new items are indicated by a star.

The second edition has benefitted from comments from a number of people and the authors are grateful to many colleagues who helped to correct misprints. The index of the book has been made more comprehensive to help those readers who wants to find some specific subjects.

Masanori Ohya
Dénes Petz

Preface to the First Edition

Entropy is a concept which appears in several fields and it is in the center of interest both in mathematical and physical subjects, sometimes even at other places, for example in communication engineering. The birthplace of quantum entropy was in quantum statistical mechanics. Quantum entropy is not a single concept but rather a family of notions which started with the von Neumann entropy of a density matrix and has developed in a number of directions. The heritage of quantum entropies from quantum mechanics is their strong relation to Hilbert space.

This book begins with the entropy of a state and through the entropy of coarse graining it proceeds to the quantum dynamical entropy. A bunch of topics shows the direct physical relevance of the entropy methods. The mathematical formalism is based on operator theory and mostly the language of operator algebras is used. The use of the concepts and methods of functional analysis not only makes the theory of quantum entropy more uniform and lucid, but it essentially simplifies and extends it. A comprehensive presentation without these elements would not be possible.

Chapters 1–3 are elementary and require of the reader only a basic knowledge of linear algebra and function theory. (Some series expansions may be beyond this level but they are standard in mathematical physics and an exact source indication provides assistance in the few cases they show up.) Most of the results of Chapters 1 and 3 are repeated in Part 2 in a more general setting. Part 1 of the book intends to demonstrate that although the quantum entropy is a more technical subject than the classical one, the basic concepts and properties are accessible without heavy mathematics.

The theory of operator algebras becomes more necessary in Parts 2–4. The very essentials are contained in any standard book on operator algebras but we suggest “Operator Algebras and Quantum Statistical Mechanics 1” by Olla Bratteli and Derek W. Robinson if a reader really would like to see a systematic treatment of this subject. What is badly needed for quantum entropy theory is concisely summarized in Chapter 4. It might be informative to emphasize that the bulk of entropy results are fully understandable without a deep knowledge of functional analysis but the proofs at a general level require sometimes sophisticated tools.

Part 5 is a collection of independent subjects which provide wide space for application of the abstract theory. In our opinion one can get a real insight into these topics without a thorough reading of all the previous chapters but with the understanding of Part 1. Precise references help those readers who have not gone through the preceding chapters.

Almost all the results in this book are accompanied with detailed rigorous proofs. Our attitude is contained in the following motto.

“Even things that are true can be proved.”
(O. Wilde)

The end of a proof is indicated by the symbol \square . Each chapter is closed by a section “Notes and Remarks”. Here one can find the main sources used by the authors in the presentation and references to related results if the authors were aware of those. The literature on quantum entropy is huge and on entropy it is even more tremendous. Our selection must be very subjective and it mostly indicates our sources rather than evaluation of the literature. To find the balance between classical entropy and quantum entropy theory was a delicate point for the authors. Typically the classical theory is neither assumed nor explained in detail in the book. Of course, any slight knowledge of probabilistic entropy concepts is very helpful for the reader and yields a deeper understanding.

We want to thank many colleagues for their kind help in the preparation of the manuscript. We cannot name all of them but we ought to mention Luigi Accardi, Imre Csiszár, András Dévényi, Matthew J. Donald, Mark Fannes, Fumio Hiai, Heide Narnhofer, Walter Thirring and André Verbeure.

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Introduction

The task of statistical mechanics is to derive macroscopic or bulk properties of matter from the laws governing a huge number of individual particles. (The word particle is used here for the sake of simplicity, one can think of molecules in a gas, electrons in a plasma, etc.) Entropy relates macroscopic and microscopic aspects and the concept is as old as modern thermodynamics. The name “entropy” is due to Clausius and the main steps towards the concept were taken by Boltzmann and Gibbs. Any study leading to the understanding of entropy must go through probability theory. The Boltzmann-Gibbs-Shannon entropy of a finite probability distribution (p_1, p_2, \dots, p_k) is the quantity

$$H(p_1, p_2, \dots, p_k) = - \sum_{i=1}^k p_i \log p_i, \quad (1)$$

which is strongly related to the asymptotics of certain probabilities. This is the very reason why the same quantity appears in different subjects, statistical mechanics, information theory, ergodic theory, for example.

$$W_N(p_1, p_2, \dots, p_k) = \frac{N!}{(p_1 N)! (p_2 N)! \dots (p_k N)!} \quad (2)$$

is the number of ways one can put N objects (say, particles) into k boxes (say, cells of the phase space) so that the different boxes contain objects with proportions p_1, p_2, \dots, p_k . Suppose we are interested in the behavior of W_N for large N . Using Stirling bounds for the factorials one can see that

$$\left| \frac{1}{N} \log W_N(p_1, p_2, \dots, p_k) - H(p_1, p_2, \dots, p_k) \right| = O(n^{-1} \log n). \quad (3)$$

Boltzmann interpreted the number $\log W_N(p_1, p_2, \dots, p_k)$ as the “thermodynamical probability” of the macro-state (p_1, p_2, \dots, p_k) . He had to divide the phase space into cells in order to speak of the number of “micro-states”. In quantum mechanics such discretization is not necessary because contained in the theory.

Before we turn to entropy in quantum systems we summarize the abstract logical foundations of quantum theory. The primary mathematical structure associated with the set \mathcal{P} of all propositions on a physical system is an ordered structure. (In place of proposition “question”, “event” and “yes-no experiment” are used in the literature.) On the set \mathcal{P} a reflexive antisymmetric

transitive relation (that is, an order relation) is given, which is customarily denoted by \leq . The relation $p \leq q$ is interpreted as stating that q is true whenever p is proven to be true. Any (finite) collection $(p_i)_i$ of elements of \mathcal{P} admits a greatest lower bound $\bigwedge_i p_i$ and a least upper bound $\bigvee_i p_i$. We write $p \wedge q$ and $p \vee q$ if we have to do with two elements. \mathcal{P} is called a lattice in the language of algebra and it has a least element and a greatest element, which are denoted by O and I respectively. Another algebraic operation on \mathcal{P} is the orthocomplementation. This is a mapping $p \mapsto p^\perp$ of \mathcal{P} onto itself such that

- (i) $p^{\perp\perp} = p$,
- (ii) $p \leq q$ implies $p^\perp \geq q^\perp$,
- (iii) $p \wedge p^\perp = O$ and $p \vee p^\perp = I$.

Two elements p and q of \mathcal{P} are said to be disjoint or orthogonal if $p \leq q^\perp$ (or equivalently $q \leq p^\perp$). Without deeply entering quantum logics we recall that the logical differences between quantum and classical behavior concerns the distributivity of the lattice \mathcal{P} .

In this book we always suppose that \mathcal{P} is the set of all orthoprojections (i.e., idempotent self-adjoint elements: $p = p^2 = p^*$) of a $*$ -algebra \mathcal{A} . In usual quantum mechanics \mathcal{A} is the set of all bounded operators on a Hilbert space. On the set of projections of \mathcal{A} the ordering is defined by

$$p \leq q \iff pq = p$$

and orthocomplementation is defined by

$$p^\perp = I - p$$

where I is the unit element of \mathcal{A} . (I is the largest projection.) The lattice operations are not directly expressed by product and sum. In the Hilbert space formulation of quantum mechanics \mathcal{P} is the set of all orthogonal projections of a Hilbert space \mathcal{H} . Let $p, q \in \mathcal{P}$ be projections onto the closed subspaces \mathcal{H}_1 and \mathcal{H}_2 , respectively. Then the join $p \vee q$ is the orthogonal projection onto the closed subspace generated by \mathcal{H}_1 and \mathcal{H}_2 and the meet $p \wedge q$ projects onto the intersection of \mathcal{H}_1 and \mathcal{H}_2 .

Given an orthocomplemented partially ordered set \mathcal{P} we say that a real-valued function μ on \mathcal{P} is a probability measure on \mathcal{P} if

- (i) $0 \leq \mu(p) \leq 1$ for all $p \in \mathcal{P}$, $\mu(O) = 0$ and $\mu(I) = 1$,
- (ii) for every sequence (p_i) of pairwise orthogonal elements in \mathcal{P} the additivity $\sum_i \mu(p_i) = \mu(\bigvee_i p_i)$ holds.

The additivity property (ii) may be called finite or countable additivity depending on the sequence required. When \mathcal{P} is the set of projections of a $*$ -algebra and φ is a linear functional on \mathcal{A} such that $0 \leq \varphi(p) \leq 1$ for every projection and $\varphi(I) = 1$, then φ restricted to \mathcal{P} gives rise to a finitely additive measure on \mathcal{P} . This is a consequence of the simple fact that for disjoint projections p and q the equality $p \vee q = p + q$ holds. In order to obtain a measure

on \mathcal{P} by the restriction of a linear functional φ we need to pose some further conditions on φ . A linear functional φ will be called a state if $\varphi(I) = 1$ and $\varphi(x^*x) \geq 0$ for every $x \in \mathcal{A}$. The states of a *-algebra supply an important class of measures on the set of projections of the algebra but certainly not all the measures may be obtained in this way. A pair (\mathcal{A}, φ) consisting of a *-algebra \mathcal{A} and of a state φ will be called a probability algebra. Given a probability space (X, \mathcal{F}, μ) the set of all complex-valued bounded measurable functions form a *-algebra with pointwise conjugation as involution, on which integration with respect to μ provides a state. On the basis of this example, we are tempted to borrow terminology from classical probability theory when dealing with probability algebras.

In Hilbert space quantum mechanics states are given by statistical operators. A positive operator $D \in B(\mathcal{H})$ is called a statistical operator or density if its spectrum consists only of eigenvalues and the sum of eigenvalues is 1. When the physical system is in a state described by the density D , the expected value of the bounded (self-adjoint) observable $A \in B(\mathcal{H})$ is

$$\text{Trace } DA = \sum_i \lambda_i \langle f_i | A | f_i \rangle \quad (4)$$

if $D = \sum_i \lambda_i |f_i\rangle\langle f_i|$ in an orthonormal basis $|f_i\rangle$. In physics the underlying Hilbert space is often infinite dimensional and so is the *-algebra $B(\mathcal{H})$. However, because of their technical simplicity it is useful to consider finite dimensional *-algebras which readily admit an abstract trace functional. An abstract trace functional is a linear functional Tr taking the value 1 on each minimal projection (that is, on the atoms of the corresponding logic). So $\text{Tr } I$ measures the size of the algebra; it is the number of pairwise orthogonal minimal projections the sum of which is the unity I . By means of Tr the states are described by density matrices in the form

$$\varphi(a) = \text{Tr } D_\varphi a \quad (a \in \mathcal{A}).$$

Here the density matrix D_φ is positive (semidefinite) and $\text{Tr } D_\varphi = 1$ comes from the normalization $\varphi(I) = 1$. In this formalism for the case of the commutative algebra $\mathcal{A} = \mathbb{C}^n$ we have

$$\text{Tr } (c_1, c_2, \dots, c_n) = \sum_{i=1}^n c_i.$$

In this case the density “matrix” or “statistical operator” becomes a probability distribution on the n -point-space. It is certainly an advantage of the *-algebraic approach to the foundations of quantum theory that it includes traditional probability theory and on the other hand the “matrix mechanics” of quantum systems is covered by the same formalism.

The set of all states, the state space, is a convex set. In the example $\mathcal{A} = \mathbb{C}^n$ the state space is nothing else but the standard n -simplex

$$\mathbf{S}_n = \{(c_1, c_2, \dots, c_n) \in \mathbb{R}^n : c_i \geq 0, \sum_{i=1}^n c_i = 1\}.$$

The extreme points of the state space are called pure states. (Pure states can not be mixtures of other states.) The simplex \mathbf{S}_n has n extreme points and every element is uniquely represented by their convex combination. (A convex set is called “Choquet simplex” if all points are unique mixtures of the extremal boundary.) The state space of a typical quantum system is far from being a simplex. Consider the algebra \mathcal{A} of a single particle of spin $1/2$ which is simply $\mathcal{A} = M_2(\mathbb{C})$, the algebra of 2×2 complex matrices. The state space with an appropriate parameterization may be identified with the three dimensional unit ball. The pure states correspond to surface points and all the inner points are mixtures of pure states in many ways.

Turning to thermodynamical entropy we repeat a gedanken experiment of John von Neumann. Let us have a gas of $N (\gg 1)$ molecules in a rectangular box K . Suppose that the gas behaves as a quantum system and it is described by a probability algebra (\mathcal{A}, φ) in a certain physical state. If φ is a mixture $\lambda\varphi_1 + (1 - \lambda)\varphi_2$, then we may think that λN molecules are in state φ_1 and $(1 - \lambda)N$ ones are in the state φ_2 . On the ground of phenomenological thermodynamics we assume that if φ_1 and φ_2 are disjoint, then there is a wall which is completely permeable for the φ_1 -molecules and isolating for the φ_2 -molecules. (If the states φ_1 and φ_2 are disjoint, then this should be demonstrated by a certain filter. Mathematically the disjointness of φ_1 and φ_2 is expressed in the orthogonality of the eigenvectors corresponding to nonzero eigenvalues of the density matrices of the states φ_1 and φ_2 .) 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 semi-permeable, transparent for the φ_2 -molecules and impenetrable for the φ_1 -ones. Then we push slowly (a) and (c) to the left, keeping 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 φ -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 constant by means of a heat reservoir, the entropy change amounts to $\kappa_B \lambda N \log \lambda$ and $\kappa_B (1 - \lambda) N \log(1 - \lambda)$, respectively. Finally, mixing the φ_1 - and φ_2 -gases of identical density we obtain a φ -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

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

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

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

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 starting assumption: φ_1 and φ_2 are supposed to be disjoint. In order to get the entropy of a φ -gas with statistical operator D_φ we need one more postulate: We shall assume that the entropy of pure states vanishes. If $D_\varphi = \sum_i \lambda_i p_i$ is the spectral decomposition of the statistical operator (p_i 's are pairwise orthogonal minimal projections), then

$$S(\varphi) = -\kappa_B \sum \lambda_i \log \lambda_i \quad (6)$$

is easily inferred by repeated application of the mixing equation (5). In this book Boltzmann's constant κ_B will be taken 1. This choice makes the entropy dimensionless (and correspondingly, the temperature should be measured in erg instead of Kelvin). The above gedanken experiment is a heuristical motivation for von Neumann's entropy formula (6). During the deduction we overlooked a problem arising from the ambiguity of the decomposition $\varphi = \lambda \varphi_1 + (1 - \lambda) \varphi_2$. Nevertheless, a closer inspection shows that a different decomposition $\varphi = \mu \psi_1 + (1 - \mu) \psi_2$ would not yield a contradicting conclusion.

The statistical operator is fundamental in quantum theory, but one should be aware of the fact that not all states of any quantum system can be described by a statistical operator. For example, type III von Neumann algebras appearing typically in quantum field theory do not have pure normal states. Notwithstanding this, the von Neumann entropy of a density matrix is right way to understand quantum entropy. Entropy is not an observable like position or angular momentum. There does not exist self-adjoint operator such that its expectation value in a state would yield the entropy of this state. The von Neumann entropy is a functional on the states of the quantum system which can not be represented by an operator.

The von Neumann entropy of a state expresses the degree of "mixing". Pure states have vanishing entropy. Since the state space of a quantum system is never a Choquet simplex, a state φ may have several extremal decompositions like

$$\varphi = \sum_i \lambda_i \varphi_i \quad \left(\sum_i \lambda_i = 1, \quad \lambda_i \geq 0 \right), \quad (7)$$

where every φ_i is a pure state by definition. Then

$$S(\varphi) = \inf \{ H(\lambda_1, \lambda_2, \dots) : \varphi = \sum_i \lambda_i \varphi_i \}$$