Infomechanics of Independent and Identically Distributed Particles

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Abstract—The paper moves a step towards the full integration of statistical mechanics and information theory. Starting from the assumption that the thermodynamical system is composed by particles whose quantized energies can be modelled as independent and identically distributed random variables, the paper proposes an approach whose cornerstone is the information-theoretic typical set and the conditional equiprobability of microstates given certain macrostates of the system. When taken together, these two concepts explain why the standard assumption of equally probable microstates is non-necessary, if not misleading. Several new specific results of physical relevance are derived from this approach, among which are the probability distribution of the occupancy numbers of the quantum states and an exact formula for the ideal gas in a container that gives the entropy of the gas also at low temperature. These specific results are pieces of a self-consistent and unified framework that encompasses the cases of low and high temperature, of distinguishable and indistinguishable particles, of small and large number of particles.

I. INTRODUCTION

The following passage of an interview with Shannon can be found in [1]: "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, no one really knows what entropy really is, so in a debate you will always have the advantage."

Starting from the concept of entropy that Information Theory (IT) and Statistical Mechanics (SM) share, many authors built in the past bridges between them. Among the works that more contributed to the strengthen link between the two disciplines we cite the paper of Landauer [2], that showed the equivalence between heat and logical information. This major result is today proved experimentally [3] and it is widely accepted that (quantum) thermodynamics can be treated by (quantum) information-theoretic tools, see for instance the tutorial paper [4]. With reference to the connections between classical thermodynamics and classical information theory, we limit ourselves to mention the recent survey [5], the pioneering work of Jaynes [6] and the large attention that has been attracted in the past by the connections between information theoretic inequalities and the irreversibility of certain thermodynamical processes, see [7] and Chapter 4 of [8]. Recently, the development of quantum information theory has brought the community of information theory researchers closer to quantum thermodynamics than ever before, see for instance the recent tutorial [9]. Making a comprehensive review of the bibliography that links information theory and thermodynamics and, more generally, of the extremely vast bibliography that, in various manners, touches the topics that are treated in this paper, is out of our scope. We will limit ourselves to cite and to comment along the paper the bibliography that we find relevant to the specific point at hand.

Despite the evidence that heat and logical information are equivalent, still today the standard textbook approach to statistical mechanics and thermal physics is strongly physically oriented, leaving to classical and quantum information theory only a minor role. Although many textbooks have a chapter or a section devoted to information theory, quantities as random entropy, conditional entropy, mutual information, Holevo accessible information, are often overlooked. This happens because these quantities and the associated concepts, that are of fundamental importance in information theory, actually seem not to have yet found their role in classical and quantum statistical mechanics. The identification of these information-theoretic quantities with the corresponding physical quantities is the vision that guides the research reported in this paper. In our understanding, more than proposing a theory, this paper proposes a vision, the infomechanical vision, where the hybridization between the two disciplines is deep as never it has been before.

Assuming that particles can be modelled as independent subsystems and that the probability distribution of particle’s quantum state is the same for all the particles, and starting from the guiding idea that macrostates are random global attributes of the system that play the role of random conditions in the conditional probability of microstates, we demonstrate the following specific results of physical relevance that, to our best knowledge, are new:

- the probability distribution of the occupancy numbers in a system of a fixed number of particles that can take many energy values is the multinomial distribution,
- microstates of the above system are conditionally equiprobable given the occupancy numbers,
- an exact formula for the entropy of the ideal gas in a container, that holds with equality also at low temperature.

These specific results are pieces of a puzzle where low and high temperature, indexed (distinguishable) and non-indexed (indistinguishable) particles, small and large number of par-
articles, coexist and find their own place in harmony between them.

The outline of the paper is as follows. In section II we present the notation and the main definitions. Although this material is standard in information theory, we present it because, since it could be not part of the background of researchers of statistical mechanics, it contributes to make the paper self-contained. Section III presents the assumptions that we make and the system model. Here we pass from the representation of the system in the phase space to the representation of the system in the space of its quantum states. This leads to a naively quantum definition of entropy, that does not requires quantization of the phase space and the subsequent need for a natively quantum definition of entropy, that does not requires presentation of the system in the phase space to the representation we make and the system model. Here we pass from the representation of the system in the phase space to the representation of the system in the space of its quantum states. This leads to a naively quantum definition of entropy, that does not requires quantization of the phase space and the subsequent need for approximations at low temperature, see e.g. [10]. In section IV, systems made by non-indexed particles are considered. The main conceptual point of this section is the identification of the entropy of indistinguishable particles with the entropy of the occupancy macrostate. The crucial point from the technical point of view is the observation that the probability distribution of the occupancy numbers is the multinomial distribution, a result that, as claimed before, seems to be new. Section V is devoted to the application of the findings of section IV to systems at the thermal equilibrium. One specific instance of non-indexed particles is the ideal dilute gas in a container, that is studied in section VI, where it is given an exact entropy formula that describes the thermodynamics of the gas both at low and at high temperature. In section VII the main points of the paper are summarized and comments about open points that could be addressed in the future are presented. The appendixes address specific points and propose historical remarks that can be skipped at the first reading.

II. NOTATION AND DEFINITIONS

Let the uppercase calligraphic character, e.g. \( \mathcal{L} \), denote a random variable and let \( \{ \mathcal{L} \} \) be the support set of the random variable. Unless explicitly stated, in the following we will refer to discrete random variables. We denote \( |\mathcal{L}| \) the number of elements of the support set of the discrete random variable and we indicate the probability \( Pr(\mathcal{L} = l) \) with the shorthand \( p_\mathcal{L}(l) \), that is

\[
p_\mathcal{L}(l) \overset{\text{def}}{=} Pr(\mathcal{L} = l), \quad \forall \ l \in \{ \mathcal{L} \}.
\]

The probability distribution, or, simply, distribution, of the random \( \mathcal{L} \), is the set \( \{ p_\mathcal{L}(l) \}, \ \forall \ l \in \{ \mathcal{L} \} \), that will be often hereafter indicated with the shorthand \( p_\mathcal{L} \). In the following we will use the angular brackets to denote the expectation (when it exists) of a function of random variable with respect to the probability distribution of the random variable (the calligraphic character) that is inside the brackets:

\[
\langle \epsilon(\mathcal{L}) \rangle \overset{\text{def}}{=} \sum_{l \in \{ \mathcal{L} \}} p_\mathcal{L}(l) \epsilon(l),
\]

where \( \epsilon(\cdot) \) is a deterministic function of its argument. The above notation can be extended in a straightforward way to the case of functions of many random variables, by taking the expectation over the joint probability distribution of the many random variables that are inside the angular brackets. Let us consider the random variable

\[
\mathcal{E} = \epsilon(\mathcal{L}).
\]

When the context leaves no room to ambiguity about the deterministic function \( \epsilon(\cdot) \) that maps \( \mathcal{L} \) onto \( \mathcal{E} \), we will use the familiar notation \( \mu_\mathcal{E} \) and \( \sigma_\mathcal{E}^2 \) for mean value and variance of \( \mathcal{E} \):

\[
\mu_\mathcal{E} \overset{\text{def}}{=} \langle \epsilon(\mathcal{L}) \rangle,
\]
\[
\sigma_\mathcal{E}^2 \overset{\text{def}}{=} \langle \epsilon^2(\mathcal{L}) \rangle - \langle \epsilon(\mathcal{L}) \rangle^2.
\]

In general, when we want to shorten the notation of expectation we put the random variable in the subscript, while when we want to indicate a deterministic function of a random variable we put the random variable inside the round bracket. The special case \( \epsilon(\cdot) = \delta(\cdot) \), where \( \delta(\cdot) \) is the indicator function,

\[
\delta(x) = \begin{cases} 
1, & x = 0, \\
0, & x \neq 0,
\end{cases}
\]

shows two interpretations of the function \( p_\mathcal{L}(\cdot) \). If the argument of \( p_\mathcal{L}(\cdot) \) is deterministic, then the deterministic \( p_\mathcal{L}(\cdot) \) expresses probability as expectation:

\[
p_\mathcal{L}(l) = \sum_{k \in \{ \mathcal{L} \}} p_\mathcal{L}(k) \delta(k - l) = \delta(\mathcal{L} - l).
\]

Instead, if the argument of \( p_\mathcal{L}(\cdot) \) is random, then \( p_\mathcal{L}(\cdot) \) is the random variable that is obtained by mapping the outcome of the random argument into its probability:

\[
p_\mathcal{L}(\mathcal{L}) = \sum_{l \in \{ \mathcal{L} \}} p_\mathcal{L}(l) \delta(l - \mathcal{L}).
\]

The reader could find the above discussion about the meaning of \( p_\mathcal{L}(l) \) and \( p_\mathcal{L}(\mathcal{L}) \) redundant, if not trivial, but we want to stress the difference between \( p_\mathcal{L}(l) \) and \( p_\mathcal{L}(\mathcal{L}) \) because, in this paper, this difference is crucial; in the rest of the paper, \( p_\mathcal{L}(l) \) means the deterministic quantity [1] while \( p_\mathcal{L}(\mathcal{L}) \) means the random quantity [2].

**Surprise, uncertainty, information**

In classical information and communication theory, the random entropy \( H(\mathcal{L}) \) is the following deterministic function of the discrete random variable \( \mathcal{L} \):

\[
\infty > H(\mathcal{L}) \overset{\text{def}}{=} -k \log(p_\mathcal{L}(\mathcal{L})) \geq 0,
\]

where \( k > 0 \) is a constant that depends on the context and the inequalities are obvious because \( 0 < p_\mathcal{L}(\mathcal{L}) \leq 1 \) (we exclude from the support set of \( \mathcal{L} \) events with zero probability to guarantee that the random entropy is limited). In physics \( k = k_B \), while, in information and communication theory,

\[
k = \frac{1}{\log(2)},
\]

or, equivalently, one takes the base-2 logarithm and \( k = 1 \).

In what follows, we drop the multiplicative constant when it
is unnecessary, being understood that it must be recovered from the context when it becomes necessary. Information and communication theory researchers often call $H(L)$ *surprise*, because it quantitatively expresses the surprise that one experiences when he observes the result $L$ of the random experiment. Being a deterministic function of a random variable, see (2) and the relevant discussion about its meaning, the above $H(L)$ is a random variable itself. The expectation of $H(L)$ with respect to the probability distribution $p_L$ is the Shannon entropy of $L$:

$$H_L \overset{\text{def}}{=} - \sum_{l \in \{L\}} p_L(l) \log(p_L(l)) \geq 0,$$

where we use the shorthand notation

$$H_L = \langle H(L) \rangle$$

and the inequality becomes equality only when $L$ is non-random.

The extension to random vectors is straightforward. The random entropy of the random vector $\bar{L}$ is

$$H(\bar{L}) \overset{\text{def}}{=} - \log(p_{\bar{L}}(\bar{l})).$$

Its expectation, that is the Shannon entropy of the random vector, is

$$H_{\bar{L}} \overset{\text{def}}{=} - \sum_{l \in \{\bar{L}\}} p_{\bar{L}}(\bar{l}) \log(p_{\bar{L}}(\bar{l})).$$

The above entropy is called in thermodynamics *Gibbs entropy*.

Another approach to entropy in thermodynamics is the following. Let the $l$-th random occupancy number $N_L(l)$ be the number of elements of $L^N$ whose value is $l$:

$$N_L(l) \overset{\text{def}}{=} \sum_{i=1}^N \delta(l - L_i), \quad \forall l \in \{L\},$$

with

$$\sum_{l \in \{L\}} N_L(l) = N.$$  \hspace{1cm} (5)

Assuming that the entries of the random vector $L^N$ are independent and identically distributed (i.i.d) discrete random variables, one can write

$$H_{\bar{L}} = -N \sum_{l} p_{\bar{L}}(l) \log(p_{\bar{L}}(l))$$

$$= - \sum_{l} \langle N_L(l) \rangle \log \left( \frac{\langle N_L(l) \rangle}{N} \right) \overset{\text{Stirling}}{\approx} \log \left( \frac{N!}{\prod_l (\langle N_L(l) \rangle)!} \right) = \log \left( W_M(\langle N_L \rangle) \right),$$

where $W_M(\cdot)$ is the multinomial coefficient,

$$\langle N_L(l) \rangle = N p_L(l)$$

is the expectation of the $l$-th random occupancy number and

$$\log(n) \overset{\text{Stirling}}{\approx} n(\log(n) - 1)$$

is Stirling’s approximation. The gamma function can be used in place of the factorial when $\langle N_L(l) \rangle$ is non-integer. The multinomial coefficient is interpreted in standard combinatorics as the number of distinct permutations of the elements of the vector, where distinct means that if the positions of two elements with the same value are permuted, then the vector before and after the permutation is the same and the permutation must not be counted as a distinct permutation. For instance, the number of distinct permutations of a vector of four elements with two zeros and two ones is six. When all the elements have distinct values, as it happens with unit probability when the $N$ elements are the outcomes of continuous random variables, all the permutations are distinct and the multinomial coefficient is equal to $N!$. Although the identification of the above multinomial coefficient with the $W$ appearing in (70) leads to the identification of the Boltzmann-Planck entropy with the Gibbs entropy, see e.g. eqn. (18.14) of [11], still today researchers are actively trying to put in a coherent relation the two, see e.g. [12]. The better succeeded of these attempts is, to our opinion, paper [13]. We will return on [13] in Appendix B to discuss the relation between this paper and [13].

Given two random variables $L$ and $X$, the conditional random entropy of $L$ given $X$ is

$$H(L|X) \overset{\text{def}}{=} - \log(p_{L|X}(L,X)),$$

where the familiar notation is used for the conditional probability distribution. The expectation of the conditional random entropy over the joint probability distribution of $L$ and $X$ is the conditional entropy of $L$ given $X$, that is

$$H_L \overset{\text{def}}{=} H_{L|X} \overset{\text{def}}{=} \sum_{y \in \{Y\}} p_X(y) H_{L|X} \geq 0,$$  \hspace{1cm} (7)

where

$$H_{L|X} \overset{\text{def}}{=} - \sum_{l \in \{L\}} p_{L|X}(l,x) \log(p_{L|X}(l,x))$$

is the conditional entropy of $L$ with deterministic condition $X = x$, see chapter 2 of [8] for the definition of conditional entropy and for the inequalities in (7). The conditional entropy of $L$ given $X$ is a measure of the uncertainty that we have about the unknown $L$ given the outcome of $X$. One of the most fundamental quantities in classical information theory is the information $I_{L:X}$ between $L$ and $X$:

$$I_{L:X} \overset{\text{def}}{=} H_L - H_{L|X} \geq 0,$$

where the inequality becomes equality only when $L$ and $X$ are independent random variables, in which case the uncertainty that we have about the unknown $L$ is unchanged by the given $X$. The above quantity, introduced by Shannon in [14], is interpreted as the reduction of uncertainty about $L$ achieved thanks to the given $X$, that is, the information that $X$ brings about the unknown $L$. By straightforward use of Bayes rule one has

$$I_{L:X} = H_L - H_{L|X} = H_X - H_X|L = I_{X:L}.$$  \hspace{1cm} (8)
For this reason, often the information is called mutual information. The extension to random vectors is straightforward and is not pursued for brevity.

III. SYSTEM MODEL

One quantum particle is modelled as the probabilistic mixture of pure states and is represented by the density operator

$$\hat{\rho} = \sum_{l \in \{\mathcal{L}\}} p_{\mathcal{L}}(l) |\phi(l)\rangle \langle \phi(l)|,$$

(9)

where the bra-ket notation is used for quantum states and

$$\{|\phi(l)\rangle\}, \quad l \in \{\mathcal{L}\}$$

are the eigenstates resulting from the solution of the one-particle time-independent Schrödinger equation. Since the eigenstates $\{|\phi(l)\rangle\}$ forms an orthonormal basis of the Hilbert space of the one-particle system, equation (9) gives the density operator in the form of its spectral decomposition. In this case, the Von Neumann entropy $S(\hat{\rho})$ coincides with the Shannon entropy of the classical random variable $\mathcal{L}$:

$$S(\hat{\rho}) \overset{\text{def}}{=} -\text{Tr}(\hat{\rho} \log(\hat{\rho})) = H_{\mathcal{L}}.$$

(10)

In this model, the particle takes discrete energy values that belong to the set $\{\epsilon(l)\}$ of the eigenvalues associated to the eigenstates. One popular example is the set of energy eigenvalues of the quantum harmonic oscillator, where

$$\epsilon(l) = l\omega \hbar + \frac{1}{2} \omega \hbar, \quad l \in \{0, 1, \cdots\},$$

(11)

where $l$ is the quantum number,

$$\hbar = 1.05 \cdot 10^{-34} \quad \text{J} \cdot \text{s}$$

is the reduced Planck constant, $\omega$ is the angular frequency of the oscillation and

$$\epsilon(0) = \frac{1}{2} \omega \hbar$$

is the energy of the ground state. Another example is that of a particle of mass $m$ in an one-dimensional box of length $L$, for which the solutions of the time-independent Schrödinger equation with aperiodic boundary conditions have eigenvalues

$$\epsilon(l) = l^2 \frac{\pi^2 \hbar^2}{2mL^2}, \quad l \in \{1, 2, \cdots\}.$$  

(12)

A system made by $N$ quantum particles of the same species is modelled by the density operator

$$\hat{\rho} = \sum_{l \in \{\mathcal{L}\}} p_{\mathcal{L}}(l) |\phi(l)\rangle \langle \phi(l)|,$$

(13)

where $\{|\phi(l)\rangle\}$ form an orthonormal basis of the Hilbert space of the system, therefore

$$S(\hat{\rho}) = H_{\mathcal{L}^N}.$$  

(14)

Vector $\vec{l}$ completely describes the system at the microscopic level. For this reason, in statistical mechanics and thermal physics, $\vec{l}$ is called the microstate of the system, see for instance 1.1. of [15]. Distinct microstates of the system are obtained by permuting any two elements of the vector, unless the values of the two permuted elements are the same, in which case the permutation does not lead to a distinct microstate.

Our main assumption is that the $N$ classical random variables of the random vector $\mathcal{L}$ are independent and identically distributed (i.i.d.):

$$p_{\mathcal{L}}(\vec{l}) = \prod_{i=1}^{N} p_{\mathcal{L}_i}(l_i),$$

(15)

$$p_{\mathcal{L}_i}(l) = p_{\mathcal{L}_2}(l) = \cdots = p_{\mathcal{L}_N}(l) = p_{\mathcal{L}}(l).$$

Writing the basis states of system’s Hilbert space as the tensor product of the basis states of the Hilbert subspaces of the individual particles, we see that the density operator $\hat{\rho}$ can be factored into the density operators of the $N$ particles:

$$\hat{\rho} = \hat{\rho}_1 \otimes \hat{\rho}_2 \otimes \cdots \otimes \hat{\rho}_N,$$

(16)

where $\otimes$ denotes the tensor product,

$$\hat{\rho}_i = \sum_{l \in \{\mathcal{L}\}} p_{\mathcal{L}}(l) |\phi(l)\rangle_i \langle \phi(l)|_i, \quad i = 1, 2, \cdots, N,$$

are independent and identically distributed (i.i.d.) and form an orthonormal basis for the Hilbert subspace of the $i$-th particle. Equation (16), which means that particles of the ensemble represented by $\hat{\rho}$ are non entangled between them, imports inside $\hat{\rho}$ the standard assumption of non-interacting particles. Identical distribution seems to be a physically sound assumption for systems at the thermal equilibrium even if, in principle, this assumption is an abstract one that could not limit the system model to systems at the thermal equilibrium.

From (14) and from the i.i.d. assumption it follows that

$$S(\hat{\rho}) = N H_{\mathcal{L}}.$$  

(17)

Other very well known consequences of the i.i.d. assumption are that the total energy of the system is the sum of the energies of the particles, the partition function of the system is the product of the partition functions of the individual particles, the distribution of system’s energy that maximizes the entropy of the system is the Boltzmann distribution.

IV. MACROSTATES

In this section we consider a system made by a deterministic number $N$ of particles, the case of a random number of particles being treated in Appendix A. We assume that the size $|\mathcal{L}|$ of the set of quantum state numbers is finite and

1When the number of quantum state numbers is infinite, to obtain a vector of occupancy numbers with a finite number of elements we truncate the set $\{\mathcal{L}\}$ to a subset $\{\mathcal{L}’\}$ with finite number of elements. The truncation is such that

$$\text{Pr}(\mathcal{L} \notin \{\mathcal{L}’\})$$

is small enough for our purposes. When the event $\mathcal{L} \notin \{\mathcal{L}’\}$ happens, we force $\mathcal{L}$ to the closest energy level in $\{\mathcal{L}’\}$. This transformation of $\mathcal{L}$ produces a new random vector $\mathcal{L}’$ that we consider in place of $\mathcal{L}$. The probability distribution of $\mathcal{L}’$ and the occupancy numbers follow in a straightforward way.
call $\bar{n}_\Sigma$ the generic vector of the $|\mathcal{L}|$ occupancy numbers, see \cite{15} for the definition of the occupancy number. For any given vector $\bar{n}_\Sigma$ of occupancy numbers, the occupancy macrostate is the set of microstates

$$\{\bar{l}(\bar{n}_\Sigma)\} = \{\bar{l}_1(\bar{n}_\Sigma), \bar{l}_2(\bar{n}_\Sigma), \ldots, \bar{l}_{W_M(\bar{n}_\Sigma)}(\bar{n}_\Sigma)\},$$

where $\bar{l}_i(\bar{n}_\Sigma)$ is a vector whose occupancy numbers are the elements of $\bar{n}_\Sigma$, the subscript $i$ indicates the $i$-th distinct permutation of the $N$ elements of $\bar{l}_1(\bar{n}_\Sigma)\}$ and the number of elements $W_M(\bar{n}_\Sigma)$ of the set of distinct permutations is the multinomial coefficient, which has been already introduced in \cite{6}.

In the case of non-indexed particles, often referred to as indistinguishable particles, the permutation of any two particles doesn’t change the state of the system. In this case, the system is modelled by the random vector $\bar{N}_\Sigma$ of the occupancy numbers and system’s physical entropy is $H_{\bar{N}_\Sigma}$ multiplied by Boltzmann’s constant.

**Multinomial distribution of the occupancy numbers**

A consequence of the i.i.d. assumption that we make for the random energy levels is that the probability distribution of the random vector $\bar{N}_\Sigma$ is the multinomial distribution:

$$p_{\bar{N}_\Sigma}(\bar{n}_\Sigma) = W_M(\bar{n}_\Sigma) \prod_{l \in \{\mathcal{L}\}} (p_{\mathcal{L}}(l))^{n_{\mathcal{L}}(l)},$$

Randomness of macrostates is discussed in Appendix B. To our best knowledge, it is observed here for the first time that the distribution of the occupancy numbers is the multinomial distribution \cite{19}. Although the multinomial coefficient is a recurring figure in statistical mechanics since the times of Boltzmann, the term $\prod_{l \in \{\mathcal{L}\}} (p_{\mathcal{L}}(l))^{n_{\mathcal{L}}(l)}$ that appears in \cite{19} is not present in Boltzmann neither, to our best knowledge, in the subsequent literature, at least with the meaning that it has in \cite{19}. It could seem obvious, but it is worth remarking that, while the multinomial coefficient is a number, the product between the multinomial coefficient and the probability distribution $\prod_{l \in \{\mathcal{L}\}} (p_{\mathcal{L}}(l))^{n_{\mathcal{L}}(l)}$ is a probability distribution! In the open literature, the multinomial distribution is considered only when the probability distribution $p_{\mathcal{L}}$ is uniform. In this case, see e.g. \cite{16}, \cite{17} and II.5 of \cite{18}, the uniform distribution of course is not the distribution of energy levels. The multinomial distribution appears in eqn. (8) of 6.2 of \cite{15} with the same meaning as here, but in the cited reference it appears only in a passage of a mere algebraic manipulation of a partition function that allows to calculate the partition function itself by the help of the multinomial theorem. Actually, the authors of \cite{15} seem not to give to the multinomial distribution any other meaning than that of a term involved in an algebraic manipulation. In \cite{15}, eqn. 6.3.12, the authors claim that the distribution of the occupancy numbers in the canonical ensemble is the Poisson distribution. However, the occupancy numbers cannot follow the Poisson distribution if the total number of particles is deterministic, as it actually is in the canonical ensemble, hence this claim is not compatible with the constraint on the total number of particle of eqn. 6.2.3 of the same book. An interesting use of the multinomial distribution is made in \cite{19}, but, in that paper, entropy is defined in the phase space and the multinomial distribution is used to describe the occupancy of space, not of the energy levels.

**Conditional equiprobability of microstates given the occupancy numbers**

Since

$$\prod_{l \in \{\mathcal{L}\}} (p_{\mathcal{L}}(l))^{n_{\mathcal{L}}(l)} = p_{\mathcal{L}}(\bar{l}), \quad \forall \bar{l} \in \{\bar{l}(\bar{n}_\Sigma)\},$$

equation \cite{19} can be written as

$$p_{\mathcal{L}}(\bar{l}) = (W_M(\bar{n}_\Sigma))^{-1} p_{\bar{N}_\Sigma}(\bar{n}_\Sigma), \quad \forall \bar{l} \in \{\bar{l}(\bar{n}_\Sigma)\},$$

which shows that microstates’ probability depends only on the occupancy numbers, or, in other words, that microstates are equiprobable given the occupancy numbers. We express this concept by saying that microstates are conditionally equiprobable given the occupancy numbers.

To obtain a formal expression of conditional equiprobability we must use conditional probability distributions. Since $\bar{N}_\Sigma$ is known given $\mathcal{L}$, the conditional probability distribution of $\bar{N}_\Sigma$ given $\mathcal{L}$ is

$$p_{\bar{N}_\Sigma|\mathcal{L}}(\bar{n}_\Sigma, \bar{l}) = \left\{ \begin{array}{ll} 1, & \bar{l} \in \{\bar{l}(\bar{n}_\Sigma)\}, \\ 0, & \bar{l} \notin \{\bar{l}(\bar{n}_\Sigma)\}, \end{array} \right.$$

hence, by Bayes formula,

$$p_{\mathcal{L}|\bar{N}_\Sigma}(\bar{l}, \bar{n}_\Sigma) = \left\{ \begin{array}{ll} \frac{p_{\mathcal{L}}(\bar{l})}{p_{\bar{N}_\Sigma|\mathcal{L}}(\bar{n}_\Sigma)}, & \bar{l} \in \{\bar{l}(\bar{n}_\Sigma)\}, \\ 0, & \bar{l} \notin \{\bar{l}(\bar{n}_\Sigma)\}. \end{array} \right.$$ 

Substituting \cite{20} in \cite{22} we get

$$p_{\mathcal{L}|\bar{N}_\Sigma}(\bar{l}, \bar{n}_\Sigma) = \left\{ \begin{array}{ll} \frac{1}{W_M(\bar{n}_\Sigma)}, & \bar{l} \in \{\bar{l}(\bar{n}_\Sigma)\}, \\ 0, & \bar{l} \notin \{\bar{l}(\bar{n}_\Sigma)\}, \end{array} \right.$$ 

which shows that microstates are conditionally equiprobable given the occupancy numbers. Note that conditional equiprobability is here demonstrated starting from the i.i.d. assumption of the elements of $\mathcal{L}$.

**Entropy, conditional entropy and mutual information**

For the conditional random entropies associated to the conditional probabilities \cite{21} and \cite{23} we have

$$H(\bar{N}_\Sigma|\mathcal{L}) = 0,$$

leading to

$$H_{\bar{N}_\Sigma|\mathcal{L}} = 0,$$

$$H_{\mathcal{L}|\bar{N}_\Sigma} = \log(W_M(\bar{n}_\Sigma)),$$
\begin{align}
H_{\bar{E}|\bar{N}_S} &= \sum_{\bar{n}_S \in \{\bar{N}_S\}} p_{\bar{N}_S}(\bar{n}_S) \log(W_{M}(\bar{n}_S)) \\
&= \langle \log(W_{M}(\bar{N})) \rangle. \quad (24)
\end{align}

By (8) we have
\begin{equation}
I_{\bar{E}|\bar{N}_S} = H_{\bar{E}} - H_{\bar{E}|\bar{N}_S} = H_{\bar{N}_S} \geq 0, \quad (25)
\end{equation}
where the inequality becomes equality only when \( \bar{N}_S \) is non-random. The above inequality says that, while \( H(\bar{E}) \) is an unbiased estimator of the Gibbs entropy, \( H(\bar{E}|\bar{N}_S) \) is not. Substituting (24) in (25) we have
\begin{equation}
\begin{split}
H_{\bar{N}_S} &= H_{\bar{E}N} - \log(N!) + \sum_{l \in \{\mathcal{L}\}} \langle \log(\bar{N}_S(l)) \rangle \\
&= NH_{\bar{E}} - \log(N!) + \sum_{l \in \{\mathcal{L}\}} \langle \log(\bar{N}_S(l)) \rangle \\
&= NH_{\bar{E}} - \log(N!) + \sum_{l \in \{\mathcal{L}\}} \langle \log(B(l)) \rangle,
\end{split}
\end{equation}
where \( B(l) \) is a binomial random variable with parameter \( p = p_{\bar{E}}(l) \) and \( N \) trials, see (20).
\begin{equation}
\langle \log(B(l)) \rangle = \sum_{n=0}^{N} \binom{N}{n} p_{\bar{E}}^n(l)(1-p_{\bar{E}}(l))^{N-n} \log(n!), \quad (28)
\end{equation}
which has been recently calculated in integral form in (21). Substituting (8) in (26) we get
\begin{equation}
\begin{split}
H_{\bar{N}_S} &\approx \log(W_M(\langle \bar{N} \rangle)) - \langle \log(W_M(\bar{N})) \rangle \\
&= \sum_{l \in \{\mathcal{L}\}} \langle \log(\bar{N}_l) \rangle - \langle \log(\bar{N}_l) \rangle \geq 0, \quad (29)
\end{split}
\end{equation}
where the inequality is obtained by applying to all the terms of the sum the Jensen inequality for the convex (upward) function \( f(x) = \log(x!) \):
\begin{equation}
\langle f(\bar{N}) \rangle \geq f(\langle \bar{N} \rangle).
\end{equation}
Note that if we put
\begin{equation}
\langle \log(W(\bar{N})) \rangle \approx \log(W(\langle \bar{N} \rangle))
\end{equation}
we get zero entropy of the random occupancy macrostate! Instead, \( H_{\bar{N}_S} \) is approximated with the quality of the Stirling approximation by the sum of the Jensen gaps in the sum (29).

By (25), \( H_{\bar{N}_S} \) is equal to the classical mutual information \( I_{\bar{E}N|\bar{N}_S} \) between \( \bar{E}^{N} \) and \( \bar{N}_S \), which can be related to the quantum entropy as follows. Writing the density operator \([13]\) as
\begin{equation}
\hat{\rho} = \sum_{\bar{n}_S \in \{\bar{N}_S\}} p_{\bar{N}_S}(\bar{n}_S)\hat{\rho}(\bar{n}_S), \quad (30)
\end{equation}
with
\begin{equation}
\hat{\rho}(\bar{n}_S) = \sum_{i \in \{\mathcal{N}\}} p_{\bar{E}N|\bar{N}_S}(i|\bar{n}_S) \ket{\phi(iN)} \bra{\phi(iN)}, \quad (31)
\end{equation}
we recognize that \( H_{\bar{N}_S} \) is equal to the Holevo upper bound \( \chi \) above the accessible information:
\begin{equation}
\chi \defeq S(\hat{\rho}) - \sum_{\bar{n}_S \in \{\bar{N}_S\}} p_{\bar{N}_S}(\bar{n}_S)S(\hat{\rho}(\bar{n}_S)) \quad (32)
\end{equation}
\begin{equation}
= H_{\bar{E}N} - H_{\bar{E}N|\bar{N}_S} \quad (33)
\end{equation}
\begin{equation}
= H_{\bar{N}_S}, \quad (34)
\end{equation}
where, by the diagonal nature of the density operator \( \hat{\rho}(\bar{n}_S) \),
\begin{equation}
S(\hat{\rho}(\bar{n}_S)) = H_{\bar{E}N|\bar{n}_S},
\end{equation}
\begin{equation}
\sum_{\bar{n}_S \in \{\bar{N}_S\}} p_{\bar{N}_S}(\bar{n}_S)S(\hat{\rho}(\bar{n}_S)) = H_{\bar{E}N|\bar{N}_S}.
\end{equation}
Note that factorization of \( \hat{\rho} \) in (16) does not imply factorization of \( \hat{\rho}(\bar{n}_S) \), basically because factorization of \( p_{\bar{E}N} \) does not imply factorization of \( p_{\bar{E}N|\bar{N}_S} \). Therefore, while the particles of the system represented by \( \hat{\rho} \) are not entangled between them, the particles of the preparation \( \hat{\rho}(\bar{n}_S) \) may be entangled between them. The deep connection between information and thermodynamics has been enlightened by the paper of Landauer [22], that showed the equivalence between heat and logical information. Landauer’s result is today proved experimentally [3] and it is widely accepted that (quantum) thermodynamics can be treated by (quantum) information-theoretic tools, see for instance the tutorial paper [4].

A comment is in order about the interpretation of the word accessible between Holevo and information in this specific context. It is indistinguishability that makes part of the entropy \( H_{\bar{E}N} \) of distinguishable particles non accessible. Actually, from equations (32) and (33) is clear that lack of indexing (hence indistinguishability) makes impossible to know which among the \( W(\bar{N}_S) \) microstates is visited by the system whose macrostate is \( \bar{N}_S \), hence lack of indexing prevents the access to the corresponding \( \log(W(\bar{N}_S)) \) nats of information, that, in the average, are just \( H_{\bar{E}N|\bar{N}_S} \) nats.

Finally, note that, using Stirling’s formula and
\begin{equation}
\lim_{N \to \infty} \frac{\bar{N}_S(l)}{N} = p_{\bar{E}}(l),
\end{equation}
it is straightforward to manipulate the random \( W_M(\bar{N}_S) \) to show that
\begin{equation}
\lim_{N \to \infty} \frac{\log(W_M(\bar{N}_S))}{N} = H_{\bar{E}}, \quad (35)
\end{equation}
\begin{equation}
\lim_{N \to \infty} \frac{H_{\bar{E}N} - H_{\bar{E}N|\bar{N}_S}}{N} = \lim_{N \to \infty} \frac{H_{\bar{N}_S}}{N} = 0. \quad (36)
\end{equation}
Hence, for \( N \to \infty \), the randomness of \( \bar{N}_S \) impacts only the conditional entropy, not the conditional entropy per particle, which is actually equal to the entropy per particle. Equation (35) expresses what in information theory is called Asymptotic Equipartition Property (AEP), which stands at the basis of the information-theoretic typicality. Appendix C reports a discussion of the celebrated \( \log(W) \) formula at the light of the AEP and of the information-theoretic typicality.
Other random macrostates than the occupancy macrostate can be obtained by the union of all the microstates associated to the same value of the random sum

\[ \mathcal{M}_\Sigma = \sum_{i=1}^{N} m(L_i), \]

where \( m(\cdot) \) is a deterministic function of the quantum number. For instance, the random energy macrostate, which is characterized by the total energy \( \mathcal{E}_\Sigma \), is the union of all the microstates whose total energy is

\[ \mathcal{E}_\Sigma = \sum_{i=1}^{N} \epsilon(L_i). \]

The random occupancy macrostate is the most detailed random macrostate because from it any other random macrostate can be derived by writing

\[ \mathcal{M}_\Sigma = \sum_{i=1}^{N} m(L_i) = \sum_{\ell \in \{\mathcal{L}\}} N_{\mathcal{L}}(l)m(l), \quad (37) \]

where the second equality can be seen as the random version of the expectation of \( m(L) \), with \( N_{\mathcal{L}} \) in the role of "random" probability distribution multiplied by the number of particles. The probability of a macrostate is the probability that comes out a microstate that belongs to the macrostate, hence the probability of the macrostate can be identified with the probability of the sum:

\[ Pr(L \in \{ l(m\Sigma) \}) = p_{\mathcal{M}_\Sigma}(m\Sigma). \]

The set of vectors belonging to \( \{ l(m\Sigma) \} \) can be partitioned into non-overlapping subsets of the type \( \mathcal{L} \), hence the probability distribution of the macrostate is

\[ p_{\mathcal{M}_\Sigma}(m\Sigma) = \sum_{\bar{N}_{\Sigma}: \sum_{\ell \in \{\mathcal{L}\}} n_{\mathcal{L}}(l)m(l)=m\Sigma} p_{\bar{N}_{\Sigma}}(\bar{n}_{\Sigma}), \quad (38) \]

and the number of microstates belonging to the macrostate is

\[ W(m\Sigma) = \sum_{\bar{n}_{\Sigma}: \sum_{\ell \in \{\mathcal{L}\}} n_{\mathcal{L}}(l)m(l)=m\Sigma} W_{\mathcal{L}}(\bar{n}_{\Sigma}). \quad (39) \]

Any generic random macrostate \( \bar{M}_{\Sigma} \) is known given \( \bar{N}_{\Sigma} \), therefore \( H_{\bar{M}_{\Sigma}|\bar{N}_{\Sigma}} = 0 \), leading to

\[ I_{\bar{N}_{\Sigma}:\bar{M}_{\Sigma}} = H_{\bar{N}_{\Sigma}} - H_{\bar{N}_{\Sigma}|\bar{M}_{\Sigma}} = H_{\bar{M}_{\Sigma}} - H_{\bar{M}_{\Sigma}|\bar{N}_{\Sigma}} = H_{\bar{M}_{\Sigma}}, \]

\[ I_{\bar{L}:\bar{M}_{\Sigma}} = H_{\bar{M}_{\Sigma}} = I_{\bar{N}_{\Sigma}:\bar{M}_{\Sigma}}. \]

Since

\[ H_{\bar{N}_{\Sigma}} \geq H_{\bar{M}_{\Sigma}}, \]

also the entropy per particle of any macrostate becomes vanishingly small as \( N \to \infty \).

V. THERMAL EQUILIBRIUM

Suppose that the system is at the thermal equilibrium with a heat bath at known temperature \( T \) Kelvin degrees. Even if, besides the temperature and the number of particles, other constraints are imposed, e.g., in the case of a gas, the volume occupied by the particles, the constraints can be not enough to uniquely define the probability distribution \( p_{\mathcal{L}} \). To find this distribution, Jaynes proposed in [6] to maximize the entropy of the microstate \( H_{\mathcal{L}} \) under the temperature constraint. This is the famous maxent principle, which become an universally accepted standard after Jaynes. In our approach, the entropy to be maximized should be the entropy of the occupancy macrostate \( H_{\bar{N}_{\Sigma}} \). However, the sum appearing in (26) makes maximization difficult. If the sum in (26) is neglected, the result of the maximization of \( H_{\bar{N}_{\Sigma}} \) is the same as that of the maximization of \( H_{\mathcal{L}} \), because the term \( \log(N!) \) of (26) is independent of the probability distribution. Since the \( N \) entries of the random vector \( \mathcal{L}^N \) are assumed to be i.i.d., the entropy \( H_{\mathcal{L}^N} \) is \( N \) times the entropy of one particle, therefore in the maximization we can consider the one-particle entropy. Maximization of \( H_{\mathcal{L}} \) can be worked out by the Lagrange multipliers method, the Lagrangian being

\[ \Lambda = - \sum_{l \in \{ \mathcal{L} \}} p_{\mathcal{L}}(l) \left( \log(p_{\mathcal{L}}(l)) + \beta \epsilon(l) + \alpha \right), \]

where \( \beta \) and \( \alpha \) are the Lagrange multipliers. The Lagrange multiplier \( \alpha \) is found by imposing the constraint

\[ \sum_{l} p_{\mathcal{L}}(l) = 1. \]

The Lagrange multiplier \( \beta \) is found by imposing that \( k_B H_{\mathcal{L}} \) is the thermodynamical (Clausius) entropy per particle, the quantity usually denoted \( S/N \), that is by imposing

\[ \frac{\partial H_{\mathcal{L}}}{\partial p_{\mathcal{L}}(l)} = \frac{1}{k_B T}. \quad (40) \]

The partial derivatives of the Lagrangian are

\[ \frac{\partial \Lambda}{\partial p_{\mathcal{L}}(l)} = - \log(p_{\mathcal{L}}(l)) - 1 - \beta \epsilon(l) - \alpha, \quad \forall l \in \{ \mathcal{L} \}, \]

the solution is therefore

\[ p_{\mathcal{L}}(l) = e^{-\beta \epsilon(l) - \alpha - 1}, \quad (41) \]

where \( \alpha \) is such that

\[ \sum_{l \in \{ \mathcal{L} \}} e^{-\beta \epsilon(l) - \alpha - 1} = 1, \]

hence

\[ e^{\alpha + 1} = \sum_{l \in \{ \mathcal{L} \}} e^{-\beta \epsilon(l)}. \]

The above sum takes the name of (one-particle) canonical partition function and is usually indicated with the symbol \( Z \):

\[ Z = e^{\alpha + 1} = \sum_{l \in \{ \mathcal{L} \}} e^{-\beta \epsilon(l)}. \quad (42) \]
Substituting (42) in (41) one gets the Boltzmann distribution in the familiar form

\[ p_{\mathcal{E}}(l) = \frac{1}{Z} e^{-\beta \epsilon(l)}. \]  

(43)

The probability distribution of the discrete energy is

\[ p_{\mathcal{E}}(\epsilon) = \frac{g_{\epsilon}}{Z} e^{-\beta \epsilon}, \]

where \( g_{\epsilon} \) is the degeneracy of the energy eigenvalue \( \epsilon \), that is the number of distinct eigenstates with the same energy eigenvalue \( \epsilon \). The Boltzmann distribution (43) can now be used to find the one-particle random entropy and its expectation:

\[ H(\mathcal{L}) = \log(Z e^{\beta \epsilon(\mathcal{L})}), \]

\[ H_{\mathcal{L}} = \sum_{l \in \mathcal{L}} (Z e^{\beta \epsilon(l)})^{-1} \log(Z e^{\beta \epsilon(l)}). \]  

(44)

We can manipulate the above two formulas as follows:

\[ H(\mathcal{L}) = \log(Z) + \beta \epsilon(\mathcal{L}), \]

\[ H_{\mathcal{L}} = \log(Z) + \beta \mu_{\mathcal{L}}, \]  

(45)

where

\[ \mu_{\mathcal{L}} = \frac{1}{Z} \sum_{l \in \mathcal{L}} \epsilon(l)e^{-\beta \epsilon(l)} \]  

(46)

is the expected energy per particle, a quantity often called \( U/N \) in standard textbooks, where \( U \) is system’s internal energy. If desired, \( \beta \) can be found as a function of \( \mu_{\mathcal{L}} \) by solving for \( \beta \) the transcendental equation (46). However, when the entropy-\( \beta \) relation is the concern, there is no need of expressing \( \beta \) as a function of the expected energy per particle, it is enough to use directly (44), or, equivalently, to substitute (46) in (45).

The temperature constraint can be imposed by observing that

\[ \frac{\partial \log(Z)}{\partial \beta} = \frac{\partial \log(Z) \partial Z}{\partial Z \partial \beta} \]

\[ = \frac{1}{Z} \left( - \sum_{l \in \mathcal{L}} \epsilon e^{-\beta \epsilon(l)} \right) \]

\[ = - \mu_{\mathcal{L}}, \]

henceforth

\[ \frac{\partial H_{\mathcal{L}}}{\partial \mu_{\mathcal{L}}} = \frac{\partial \log(Z)}{\partial \mu_{\mathcal{L}}} + \beta + \mu_{\mathcal{L}} \frac{\partial \beta}{\partial \mu_{\mathcal{L}}} \]

\[ = \frac{\partial \log(Z) \partial \beta}{\partial \beta \partial \mu_{\mathcal{L}}} + \beta + \mu_{\mathcal{L}} \frac{\partial \beta}{\partial \mu_{\mathcal{L}}} \]

\[ = \beta = \frac{1}{k_B T}. \]

where the last equality is the constraint (40). All the classical thermodynamics of systems at the equilibrium can be obtained from the identification of \( \beta \) with the inverse temperature and of \( k_B H_{\mathcal{L}} \) with the Clausius entropy per particle. For instance, since

\[ \frac{\partial T \log(Z)}{\partial T} = H_{\mathcal{L}}, \]

from (45) we have that the Helmholtz free energy per particle \( F/N \) is

\[ \frac{F}{N} \overset{\text{def}}{=} -k_B T \log(Z) = \mu_{\mathcal{L}} - k_B T H_{\mathcal{L}}, \]

an equation that in the standard textbook notation reads

\[ F = U - T S. \]

The probability distribution of microstates is

\[ p_{\mathcal{L}}(\mathcal{L}) = \prod_{i=1}^{N} p_{\mathcal{E}}(l_i) \]

\[ = \prod_{i=1}^{N} e^{-\beta \epsilon(l_i)} \]

\[ = \frac{e^{-\beta \sum_{i=1}^{N} \epsilon(l_i)}}{Z^N}. \]  

(47)

For the random system entropy, from (47) we have

\[ H(\mathcal{L}) = N \log(Z) + \beta \sum_{i=1}^{N} \epsilon(l_i), \]

whose expectation is

\[ \overline{H_{\mathcal{L}}} = N(\log(Z) + \beta \mu_{\mathcal{L}}). \]

The Boltzmann distribution (47) for systems at the thermal equilibrium is one of the central results of thermal physics and statistical mechanics. A derivation very similar to ours but based on the constrained maximization of the multinomial coefficient can be found, for instance, in 18.1 of [11] and in 3.2 of [15]. Another derivation of (47) can be obtained by separating the system from the heat bath and by assuming equiprobability of microstates of the heat bath after separation, see for instance 19.1 of [11], 3.1 of [15].

**Quantum harmonic oscillator at the thermal equilibrium**

For the quantum harmonic oscillator (11) at the thermal equilibrium, the probability distribution of the energy levels, the entropy, the partition function and the energy-temperature ratio can be found in closed form by calculating the two sums in (42) and (46). To our knowledge, calculus of (42) and (46) dates back to Einstein [23], [24] and was applied to the entropy in Section II of [25]. The partition function (42) turns out to be a geometric series, whose calculation gives

\[ Z = e^{-\frac{\beta \omega}{k_B}} \sum_{l=0}^{\infty} e^{-\beta l \omega} = \frac{e^{\frac{\beta \omega}{k_B}}}{e^{\frac{\beta \omega}{k_B}} - 1}. \]  

(48)

As in 3.8 of [15], for completeness we consider the energy of the ground state in the calculations. However, as observed in 16.3 of [11] and in [25], adding the energy of the ground state produces only a shift that does not impact neither the probability distribution nor the entropy.
Using (48) in (43), we see that the probability distribution of the random quantum number $L$ of (11) is the geometric distribution:

$$p_L(l) = (1 - p)^l p, \quad l = 0, 1, \ldots, \quad (49)$$

with

$$p = e^{-\beta \omega h} = 1 - \frac{e^{-\beta \omega h}}{Z}, \quad (50)$$

see 7.5.6 of [26] for the derivation of (49) in a full quantum-mechanical approach. The mean value and the variance of the geometric distribution are known to be

$$\mu_L = \frac{p}{1 - p} = \frac{e^{-\beta \omega h}}{1 - e^{-\beta \omega h}} = \frac{1}{e^{\beta \omega h} - 1}, \quad (52)$$

$$\sigma_L^2 = \frac{p}{(1 - p)^2} = \mu_L (1 + \mu_L) = \frac{e^{-\beta \omega h}}{(1 - e^{-\beta \omega h})^2}. \quad (53)$$

At high temperature, where

$$e^{\pm \beta \omega h} \approx 1 \pm \beta \omega h,$$

we have

$$\sigma_L \approx \mu_L \approx \frac{1}{\beta \omega h}. \quad (54)$$

Taking the mean value as a parameter, the geometric distribution can be expressed in the form

$$p_L(l) = \frac{1}{1 + \mu_L} \left( \frac{\mu_L}{1 + \mu_L} \right)^l, \quad l = 0, 1, \ldots,$$

leading, for the random entropy and for the entropy, to

$$H(L) = \log(1 + \mu_L) + L \log(1 + \mu_L^{-1}),$$

$$H_L = \log(1 + \mu_L) + \mu_L \log(1 + \mu_L^{-1}) = (1 + \mu_L) \log(1 + \mu_L) - \mu_L \log(\mu_L),$$

where the last line is the form used by Planck in the analysis of the blackbody radiation spectrum, but for Planck the energy of the ground state is zero, so after formula (10) of his 1901 paper [27] he puts $\mu_L / \omega h$ in place of $\mu_L$. Substituting the last term of (52) in place of $\mu_L$ in the above equation, the entropy-temperature relation results

$$H_L = \log \left( \frac{1}{1 - e^{-\beta \omega h}} \right) + \frac{\beta \omega h}{e^{\beta \omega h} - 1}. \quad (55)$$

Substituting (53) in the above equation, at high temperature we have

$$H_L \approx \log \left( \frac{1}{1 - e^{-\beta \omega h}} \right) + 1, \quad (56)$$

which, compared to (55), shows that

$$\beta \mu_L = \frac{\omega h}{2} + \frac{\beta \omega h}{e^{\beta \omega h} - 1} \approx \frac{\beta \omega h}{e^{\beta \omega h} - 1} \approx 1.$$ Equivalently, since at high temperature $\mu_L$ is large, we can put

$$\log(1 + \mu_L^{-1}) \approx \mu_L^{-1}$$

in (54), leading to

$$H_L \approx \log(1 + \mu_L) + 1,$$

which, on substitution of (52), is (56). See appendix D for a system of $N$ monochromatic quantum harmonic oscillators.

**Particle in a box at the thermal equilibrium**

The Boltzmann distribution for the particle in a box with aperiodic boundary conditions (12) is

$$p_L(l) = Z^{-1} e^{-\beta l^2 \omega^2 l^2 / 2mL^2}, \quad l = 1, 2, \ldots. \quad (57)$$

Here the partition function cannot be calculated in closed form, even if numerical evaluation is possible.

At high temperature, where quantization effects become negligible, sums are approximated to integrals, discrete random variables are approximated to dense random variables, and the gas behaves approximately as a classical gas made by hard balls. Specifically, the sums (42) and (46) can be approximated to the discretization with unit step of the following two integrals

$$Z \approx \int_{l=0}^{\infty} e^{-\beta l^2 \omega^2 l^2 / 2mL^2} dl = \sqrt{\frac{mL^2}{2\beta \pi \hbar^2}}, \quad (58)$$

and

$$A = \frac{\pi^2 \hbar^2}{2mL^2} \int_{l=0}^{\infty} l e^{-\beta l^2 \omega^2 l^2 / 2mL^2} dl = \sqrt{\frac{mL^2}{8\beta^3 \pi \hbar^2}},$$

respectively, leading to

$$\mu_L \approx \frac{A}{Z} \approx \frac{1}{2\beta},$$

$$H_L = \log(Z) + \beta \mu_L \approx \frac{1}{2} \left( \log \left( \frac{mL^2}{2\beta \pi \hbar^2} \right) + 1 \right). \quad (59)$$

The probability density function of dense (continuous) random $L$ is obtained by looking at the quantization rule appearing in the exponent of the Boltzmann distribution as at a continuous function of continuous variable. The normalization of the dense distribution is just the division by the integral of equation (58), leading to

$$f_L(l) = \sqrt{\frac{2\beta \pi \hbar^2}{mL^2}} e^{-\frac{\omega^2 l^2}{2mL^2}}, \quad l > 0,$$
where \( f_X(\cdot) \) indicates the probability density function of the continuous random variable \( X \). The probability density function of the continuous random energy, that again we call \( \mathcal{E} \), is found by making the following change of random variable from the continuous energy level \( \mathcal{L} \) to the continuous energy \( \mathcal{E} \):

\[
\mathcal{E} = \frac{\pi^2 \hbar^2}{2mL^2} \mathcal{L}^2,
\]

hence

\[
\mathcal{L} = \sqrt[\frac{2mL^2}{\pi^2 \hbar^2}] \mathcal{E}.
\]

Calling \( \epsilon \) the continuous variable that spans the support of \( \mathcal{E} \), the change of random variable provides us with

\[
f_\mathcal{E}(\epsilon) = f_\mathcal{L} \left( \frac{2mL^2 \epsilon}{\pi^2 \hbar^2} \right) \frac{d}{d\epsilon} \frac{2mL^2 \epsilon}{\pi^2 \hbar^2} = \sqrt{\frac{2\beta\pi\hbar^2}{mL^2}} e^{-\beta\epsilon} \sqrt{\frac{mL^2}{2\pi^2 \hbar^2} \epsilon} = \sqrt{\frac{\beta}{\pi}} e^{-\beta\epsilon} = \frac{1}{\Gamma(0.5)} \sqrt{\frac{\beta}{\pi}} e^{-\beta\epsilon}, \epsilon > 0,
\]

that is a Gamma distribution \( \Gamma(k, \theta) \) with shape parameter \( k = 0.5 \) and scale parameter \( \theta = \beta^{-1} \), or, equivalently, a \( \chi^2 \) distribution with one degree of freedom and mean value \((2\beta)^{-1}\). The probability density function of momentum of the classical one-dimensional gas particle at the thermal equilibrium is in fact known to be normal with zero mean value and variance \( m\beta^{-1} \), therefore, since the energy is wholly kinetic, the probability density function of the continuous energy must be \( \chi^2 \) with one degree of freedom and mean value \((2\beta)^{-1}\), as it actually is.

VI. IDEAL GAS IN A CONTAINER

The pseudo-quantum model for a particle of an ideal gas in a container is that of the particle in a box, whose energy levels are given in \(\mathcal{L} \). As we will see, through the quantization rule \(\mathcal{L} \) the volume of the container will be imported in the probability distribution of energy levels and, as a consequence, in the entropy formula. In the following, we take as a deterministic constraint the Boltzmann distribution for the energy of gas' particles, even if this could be not the entropy-maximizing distribution, because entropy maximization should take into account also the third term of \(\mathcal{E} \), which is important at low temperature. However, this maximization is out of the scope of the present paper.

When the \( N \) particles have \( D \) degrees of freedom, the energy level becomes a \( D \)-dimensional vector \( l = (l_1, l_2, \ldots, l_D) \), the energy level of the \( i \)-th particle is the \( D \)-dimensional vector \( l_i = (l_{i,1}, l_{i,2}, \ldots, l_{i,D}) \) and the occupancy number is the number of particles that are found in a vector of energy levels, hence the occupancy number is

\[
\mathcal{N}_{\mathcal{L}_i}(l^D) = \sum_{i=1}^{N} \prod_{d=1}^{D} \delta((l_i - l_d),
\]

where \( \mathcal{L}_{i,d} \) is the random energy level of the \( i \)-th particle in the \( d \)-th dimension and

\[
\sum_{i=1}^{N} \mathcal{N}_{\mathcal{L}_i}(l^D) = N.
\]

With a \( D \)-dimensional box with sides all of length \( L \) and, as a consequence, in the entropy formula. In the following, we take as a deterministic distribution of energy levels and, as a consequence, in the third term of \(\mathcal{E} \), which is important at low temperature. However, this maximization is out of the scope of the present paper.

The two approximations \(\mathcal{E} \) and \(\mathcal{L} \) rule out two different quantum effects that become negligible at high temperature. The quantum effect neglected in \(\mathcal{E} \), which impacts the conditional entropy \( H_{\mathcal{L}|\mathcal{N}_{\mathcal{L}}} \), is represented by the multiple sum appearing in \(\mathcal{L} \). This multiple sum accounts for the probability that two or more particles are found in the same vector of energy levels, hence its nature is clearly quantistic. The approximation \(\mathcal{L} \), which impacts the entropy \( H_{\mathcal{L}} \), is the approximation of the discrete energy to a dense variable that has been discussed before, see \(\mathcal{E} \). Stirling’s approximation finally leads to the \( D \)-dimensional version of the Sackur-Tetrode entropy formula \(\mathcal{L} \). At low temperature, the entropy \( H_{\mathcal{L}} \) cannot be calculated in closed form, but numerical evaluation is possible, as well as it is possible numerical evaluation of the sum in the first line of \(\mathcal{L} \).

The results of Figs. \(\mathcal{L} \) report the entropy (or terms that contribute to the entropy) in \( k_B \) units versus temperature in Kelvin degrees. All the results are obtained for volume of the cubic box \( V = 10^{-27} \) cubic meters and mass of one

\[\text{Note that the sum in the first line of \(\mathcal{L} \), whose generic term is}
\]

\[
\langle \log(\mathcal{N}_{\mathcal{L}_i}(l^D)) \rangle = \sum_{n=0}^{N} \binom{N}{n} (p_{\mathcal{L}_D}(l^D))^{n} (1 - p_{\mathcal{L}_D}(l^D))^{N-n} \log(n!),
\]

is a multiple sum over \( D \) indexes, hence its numerical evaluation can become demanding for large \( D \). The complexity of the evaluation can be mitigated by suitably truncating the set \(\mathcal{L}^D \) to those whose probability is non-negligible. At low temperature, vectors with non-negligible probability have entries that their values with high probability in the first few one-dimensional energy levels, while at high temperature this quantum effect can be neglected. In practice, this means that we can take \(\mathcal{L}^D = |L|^D \) with \(|L| \) that becomes smaller and smaller as \( D \) increase.
particle \( m = 1.67 \cdot 10^{-27} \) kilograms. With these parameters, the energy of the one-dimensional ground state is
\[
\epsilon(1) = \frac{\pi^2 \hbar^2}{2mL^2} = 3.25 \cdot 10^{-23}.
\]

In Figs. 1, 2, 3 the size of the set of energy level has been truncated to \( |L| = 1000 \), having verified that the probability of \( L > 1000 \) is so small that it does not impact the graphs in the entire range of temperature. We hasten to point out that the graphs reported in the following are intended to be only a numerical exercise based on the formulas presented in this paper, therefore they will describe the behavior of a real physical system only inside the range of validity of the assumptions that we made.

Fig. 1 shows the approximation (59) and the numerical evaluation of the entropy \( 3H_L \) of one particle in three dimensions. The energy/temperature term \( \beta \mu_L \) is reported in Fig. 2. At \( T = 1 \) Kelvin this term is approximately equal to 2.37, which corresponds to the following expected energy per dimension
\[
\mu_L |_{T=1} = 1.005 \cdot \epsilon(1).
\]

Since the mean value of the energy per degree of freedom is lower bounded by \( \epsilon(1) \) and since the lower bound is virtually reached at 1 Kelvin, at temperature below 1 Kelvin the energy/temperature term \( \beta \mu_L \) is forced to grow hyperbolically. In passing, we observe that the energy/temperature term \( \beta \mu_L \) strongly resembles a hyperbola in the entire range of temperature. The heuristic hyperbolic fit
\[
\beta \mu_L \approx \frac{1}{2} + \frac{\epsilon(1)}{k_B T}
\]
(64)
is the dash-dotted line in Fig. 2. At high-temperature, the energy/temperature term reaches the horizontal asymptote of the hyperbola, that, as predicted by the high temperature approximation, is equal to 0.5. However, in the transition region, say \( 0.3 < T < 3 \), the approximation error is appreciable. For instance, for \( T = 1 \) the numerical calculation gives \( \beta \mu_L = 2.37 \), while the heuristic hyperbolic fit (64) gives \( \beta \mu_L = 2.86 \).

Figs. 3 and 4 report the results obtained numerically for \( N = 30 \) three-dimensional particles. The number of energy levels considered in the triple sum of equation (60) is 15, which generates \( 15^3 \) terms of the triple sum, but we have verified that also only 5 terms do virtually not impact graphs. The graph shows that the entropy of indexed particles and, consequently, the entropy of non indexed particles, which must be between zero and the entropy of indexed particles, drops virtually to zero at the “cutoff” temperature of about 1.3 Kelvin, where the entropy of the 30 three-dimensional indexed particles is 1.44 (1.44/90 per degree of freedom), while the entropy of the non-indexed particles is 1.18. A so low value of entropy is compatible with the fact, already pointed out, that the expected energy per particle is close to that of the ground state, meaning that particles are with high probability in the ground state. Fig. 4 reports the relative quantum correction, that is
\[
\frac{\sum_{P \in \{\mathbb{Z}^N\}} \log(N_L(P))}{\log(N!)}
\]
virtually equal to the denominator, hence that the third term of (60) completely compensates the term \( \log(N!) \), preventing negative values of the entropy. As expected, the quantum correction tends quickly to zero at high temperature. At 10 Kelvin it is still appreciably above zero, but at 100 Kelvin it becomes negligible.

VII. CONCLUSIONS

A step towards a full information-theoretic paradigm for the statistical mechanics of systems made by independent particles has been proposed in the paper. This approach, we would say, this vision, is based on the identification of information theoretic concepts as typicality, conditional entropy, mutual information, Holevo accessible information, with the corresponding physically equivalent quantities. Our paradigm rules out the postulate of equally probable microstate, which has been object of debate since when it was originally proposed by Einstein. The renounce to the postulate not only is compatible with all the results that we know about many-particle systems, but also leaves space to an harmonic and unified treatment of low and high temperature, small and large number of particles, systems of indexed and of non-indexed particles.

Much work is to be done along the direction taken by this paper. We hereafter mention few points that are not covered in this paper and that could be considered in the future. One point that needs investigation is the role of the assumption of identical distribution. For systems at the thermal
equilibrium, it seems that this assumption is reasonable, but, even if in principle this assumption could be made also for a system that is not at the thermal equilibrium, it could become questionable and could lead to misleading conclusions when the system evolves towards equilibrium through non-reversible transformations. For instance, when two gases at different temperatures are mixed, can the mixture be described by one probability distribution obtained by the weighted sum of the two and, if so, till what extent? Finally, we mention that another open point is how and if the Bose-Einstein condensed state can be inserted inside the framework sketched in this paper.

VIII. APPENDIX A: RANDOM NUMBER OF PARTICLES

Let us consider the case where the system can randomly exchange particles with the environment. This happens, for instance, when the system occupies a region of space that is not bounded by impenetrable walls, so that particles can freely come in and out of the region of interest. Let us start the analysis by observing that, in the case of a fixed number of particles, the probability distribution of the random state can be written by multiplying the multinomial probability distribution by a delta-type distribution that imposes the total number of particles:

\[ p(\bar{n}_\Sigma) = \frac{\delta \left( N - \sum_{l \in \ell} n_\Sigma(l) \right)}{N!} \prod_{l \in \ell} \left( \frac{p_\ell(l)}{n_\Sigma(l)!} \right)^{n_\Sigma(l)} \]

If, in place of being deterministic, the total number of particles is random, then probability distribution \( p_{N_\Sigma} \) of the total random number of particles takes the place of the delta-type distribution and the factorial of the fixed number of particles becomes the factorial of the random number of particles, leading to

\[ p_{N_\Sigma}(\bar{n}_\Sigma) = p_{N_\Sigma}(n_\Sigma) \prod_{l \in \ell} \left( \frac{p_\ell(l)}{n_\Sigma(l)!} \right)^{n_\Sigma(l)}. \]

We assume that the position where a particle can be detected is a continuous random variable with uniform distribution over a virtually unbounded region of space that includes the region of interest and the surroundings. This assumption is reasonable for systems at the thermal equilibrium, in which case the system is one element of the grand canonical ensemble. If, besides the uniform distribution, we also assume that two
particles cannot be detected in the same position and that the positions where particles are detected are independent random variables, then the random number \( N_{\Sigma}(l) \) of particles that occupy the \( l \)-th energy level inside the region of interest follows the Poisson distribution, therefore

\[
p_{N_{\Sigma}(l)}(n_{\Sigma}(l)) = \frac{(\lambda(l))^{n_{\Sigma}(l)}e^{-\lambda(l)}}{n_{\Sigma}(l)!},
\]

where \( \lambda(l) \) is the expected number of particles inside the region of interest that occupy the \( l \)-th energy level. Since the sum of Poisson random variables is a Poisson random variable,

\[
p_{N_{\Sigma}}(n_{\Sigma}) = \frac{\lambda^{n_{\Sigma}}e^{-\lambda}}{n_{\Sigma}!},
\]

where

\[
\lambda = \sum_{l \in \{L\}} \lambda(l).
\]

The Poisson distribution has been used in the past in very many cases. A case that is worth mentioning because it looks very close to ours is that of London’s bombing in the second war, where the random number of bombs (in the distributions of V-1 bombs and of V-2 rockets, the “flying bombs,” are analyzed) falling in a sub-area of an area subject to almost uniform bombing is modelled by the Poisson distribution. Here, in place of the random number of particles with different energies. It is easy to see that the entries of the random vector \( N_{\Sigma} \) are independent between them. Independency between the occupancy numbers is not that obvious. For instance, the occupancy numbers of the multinomial distribution are not independent between them, because their sum is forced to be equal to a deterministic number. Substituting the Poisson distribution for \( p_{N_{\Sigma}}(n_{\Sigma}) \) in \( (65) \) one gets

\[
p_{N_{\Sigma}}(\tilde{n}_{\Sigma}) = \lambda^{\tilde{n}_{\Sigma}}e^{-\lambda} \prod_{l \in \{L\}} \frac{(p_{L}(l))^{n_{\Sigma}(l)}e^{-\lambda(l)}}{n_{\Sigma}(l)!}.
\]

Substituting

\[
\lambda(\tilde{n}_{\Sigma}) = \prod_{l \in \{L\}} \lambda^{n_{\Sigma}(l)}(l),
\]

\[
e^{-\lambda} = \prod_{l \in \{L\}} e^{-\lambda(l)}
\]

and

\[
\lambda(l) = p_{L}(l) \lambda
\]

in equation \( (66) \), one finds

\[
p_{N_{\Sigma}}(\tilde{n}_{\Sigma}) = \prod_{l \in \{L\}} \frac{(\lambda(l))^{n_{\Sigma}(l)}e^{-\lambda(l)}}{n_{\Sigma}(l)!}.
\]

The probability distribution \( (68) \) is the product of Poisson distributions with parameters \( \lambda(l) \), hence the individual random variables are independent between them. The random entropy and the entropy of the Poisson random variable \( N \) with parameter \( \lambda \) are

\[
H(N) = -N \log(\lambda) + \lambda + \log(N!),
\]

\[
H_N = -\lambda(\log(\lambda) - 1) + \langle \log(N_{\Sigma}(l)!)) \rangle,
\]

where

\[
\langle \log(N_{\Sigma}(l)!) \rangle = e^{-\lambda} \sum_{n=0}^{\infty} \frac{\lambda^n \log(n!)}{n!}.
\]

An integral form for the above expectation has been recently worked out in \([21]\). The Shannon entropy of the vector of independent random variables is the sum of the individual entropies, therefore

\[
H_{N_{\Sigma}} = \sum_{l \in \{L\}} H_{N_{\Sigma}(l)}
\]

\[
= \lambda H_{\Sigma} - \lambda(\log(\lambda) - 1) + \sum_{l \in \{L\}} \langle \log(N_{\Sigma}(l)!)) \rangle
\]

\[
\approx \lambda H_{\Sigma} - \lambda(\log(\lambda) + 1) + \sum_{l \in \{L\}} \langle \log(N_{\Sigma}(l)!)) \rangle,
\]

where in the second equality we use \([67]\) and, in the last line, which is obtained by Stirling’s formula, for non-integer \( \lambda \) one uses the gamma function in place of the factorial. Putting \( \lambda = N \) we immediately appreciate the strong similarity between the above entropy and that of the multinomial random variable \( (27) \). The conclusion that, when the system exchanges particles with the environment, the probability distribution of \( N_{\Sigma}(l) \) is Poisson, is achieved, by different arguments, also in the standard treatment of the classical ideal gas at high temperature, see for instance 21.2.4-21.2.6 of \([11]\) where, however, independency between the random occupancy numbers is not discussed. Here the Poisson distribution for the random number of particles descends directly from the uniformity of the spatial distribution of particles in the unbounded region of space that includes the region of interest, an assumption that seems reasonable also at low temperature.

**IX. Appendix B: Randomness of Macrostates**

Deterministic constraints imposed on the system must be distinguished from macrostates. A deterministic constraint is the expectation of the corresponding macrostate divided by the number of particles. The most detailed deterministic constraint is the entire probability distribution,

\[
p_{L}(l) = \frac{1}{N} \langle N_{\Sigma}(l) \rangle, \quad \forall l \in \{L\}.
\]

The probability distribution allows for the computation of any other deterministic constraint, exactly as the occupancy numbers do with any other random macrostate through \([21]\). Our distinction between deterministic constraint and macrostate is compatible with the Gibbsian view of a canonical ensemble of systems, where the systems of the ensemble are assumed to be at the thermal equilibrium at a given temperature and the number of particles is the same for all the systems of the ensemble, therefore the deterministic constraint is the
Boltzmann distribution with a prescribed number of particles and a prescribed expected energy per particle that depends on the temperature, while the random macrostate is system's total energy which, in the random experiment of picking the system of interest from the ensemble, comes together with the picked system. It should be added that, with the assumption of i.i.d. particles, we don't need an ensemble of systems: an ensemble of particles is all we need if we build the system of interest by randomly picking \( N \) particles from the ensemble of particles. This ensemble of particles is equivalent to the Gibbsonian canonical ensemble of systems and the two are compatible with the time evolution of an ergodic system resulting from the random interaction of the system with the surrounding environment.

Randomness of macrostates in the canonical ensemble is universally recognized since the times of Maxwell. The randomness that is present in the total system energy makes it possible that system's energy fluctuates around its expectation. One can figure out the extreme situation where a system made by only one particle is in contact with the heat bath. Even if, occasionally, the energy of the one-particle system is below (above) what expected, it can get even lower (higher) if, in the "contact" with the heat bath, the particle of the system kicks a slower (faster) particle of the heat bath. Quoting from [29]: 

\[ \text{As Maxwell points out, measurable thermodynamic quantities are averages over many molecular quantities; if the molecular quantities exhibit fluctuations that are probabilistically independent of each other, these fluctuations will tend to be washed out as the number of molecules considered is increased.} \]

However, the consequences of this randomness seem not to be fully exploited in the standard treatment of statistical mechanics, at least in the sense pursued in this paper. Specifically, we cannot find equation [25], that for systems of the canonical ensemble reads

\[ H_{\bar{E}} = H_{\bar{E}|\bar{E}_S} + H_{\bar{E}_L}, \]

in anyone of the many textbooks that we consulted, where, in fact, also the conditional probability distribution \( p_{\bar{E}|\bar{E}_S} \) is overlooked. All these textbooks deeply consider the canonical entropy \( H_{\bar{E}} \) and the microcanonical entropy \( H_{\bar{E}|\bar{E}_S} \). The canonical system imports macrostate's randomness through the Boltzmann distribution, an approach that does not need to explicitly show macrostate's probability distribution and macrostate's entropy. In the microcanonical system, the "given" macrostate \( \bar{E}_S \) is treated as a deterministic condition that is often taken equal to the expectation of system's energy. In the end, neither the canonical approach nor the microcanonical approach explicitly analyze macrostate's probability distribution and, with it, macrostate's entropy. This has made impossible in the past, with the exception of [13] that we are going to discuss, to explain with a simple formula like [29] the relation between the canonical entropy and the microcanonical entropy and, more generally, between the Gibbs entropy and the Boltzmann-Planck entropy.

We argue that the incomplete consideration of macrostates' randomness originates from a fallacy in the argument that supports the last part of the passage of [29] quoted above. In thermodynamics, where \( N \) is large, the random sum that characterizes the random macrostate becomes virtually equal to its expectation within a small relative random error, which, in the case of the random total entropy, can be seen as the random version of the deterministic entropy that appears in [24]-[28]. At the same time, for \( N \to \infty \), equation [36] shows that macrostate's entropy per particle becomes vanishingly small. At a first glance, this argument could seem convincing because, physically speaking, one could think that the relative error and the entropy per particle are what really matters to all practical purposes. However, it remains that, for \( N \to \infty \), the random sum does not converge to any deterministic value. On the contrary, if we represent the randomness of the random sum with its standard deviation, we see that it increases with the square root of the number of particles. Therefore the fallacy of this argument is that it is not true that this randomness is washed out when \( N \to \infty \), what is washed out is the relative randomness. The distinction between absolute and relative randomness is not a mere sophism or a subtle technicality that has no impact on reality. First, the contribution of the term \( H_{\bar{E}_S} \) to system's entropy \( H_{\bar{E}} \) can significantly impact the entropy of systems of few particles, till to become the only contribution to the entropy of a system made by one particle, for which macrostate and microstate coincide. Second, in a forthcoming section of this paper we will show that randomness of macrostates is the only randomness that contributes to the macroscopic entropy of systems of a large number of non-indexed particles.

Paper [13] is the only one, among the very many papers that we studied during this research, that fully catches randomness of macrostates in the sense discussed above. Specifically, what the authors of [13] call the probability distribution of the macroscopic state of the system and denote \( P(a) \) can be identified with our \( p_{\bar{E}_S}(\bar{n}_S) \) and what they call \( W(a) \) can be identified with our \( W_M(\bar{n}_S) \). With this identification, our \( H(\bar{E}|\bar{n}_S) \) is what they call Boltzmann entropy in their eqn. (6) and our \( H_{\bar{E}|\bar{E}_S} \) is what they call the mean value of the Boltzmann entropy in their eqn. (7). Then they use this mean value of Boltzmann entropy in the entropic relation [25]. In our opinion, paper [13] is particularly important because, to our best knowledge, it is the first paper that makes use in a physical context of the concepts of random entropy and of conditional entropy and that recognizes that Gibbs entropy \( H_{\bar{E}} \) is the sum of the term \( H_{\bar{E}|\bar{n}_S} \), which is due to the randomness of the macrostate, and of the term \( H_{\bar{E}|\bar{E}_S} \), which is due to the randomness of the microstates whose union form the macrostate. However, it should be added that the authors of [13] seem not to be aware that their Boltzmann entropy is a conditional entropy. As a matter of fact, they do not make any explicit use of conditional probability distributions. They hide the conditional probability distribution \( p_{\bar{E}|\bar{E}_S} \) behind the corresponding multinomial coefficient \( W_M(\bar{n}_S) \) and implicitly consider understood the equality [21]. Also, they claim but don't prove that the probability distribution of the occupancy numbers is multinomial, neither they use the multinomial
distribution, in fact they consider the Gaussian approximation in place of the exact multinomial distribution. Finally, the big difference with our paper is that the authors of [13] still assume that microstates are conditionally equiprobable.

X. APPENDIX C: INFORMATION-THEORETIC TYPICALITY

The commonly accepted definition of entropy in statistical mechanics and thermal physics is

\[ S = k_B \log(W), \]

(70)

where \( S \) is the entropy, \( \log(x) \) is the natural logarithm of \( x \),

\[ k_B = 1.38 \cdot 10^{-23} \text{ J} \cdot \text{K}^{-1} \]

is Boltzmann’s constant and \( W \) is the number of microstates that are compatible with the constraints imposed on the system. The phrase of Von Neumann that opens the introduction of this paper reflects the fact that the above entropy, called by many authors Boltzmann-Planck entropy, has been for a long time and is still today object of discussion. Actually, the right side of the equality is an entropy only if the \( W \) microstates are equally probable but, still today, there is not any mathematical proof of microstates’ equiprobability. Nonetheless, equation (70) is universally recognized to be the very foundation of thermal physics and statistical mechanics, that, in the absence of a mathematical proof but, at the same time, in the presence of strong physical evidences, take it as a postulate. Einstein was the first who, in [24], suggested to postulate or, using the original German verb, verlangt, equiprobability of microstates: Neither Mr. Boltzmann nor Mr. Planck gave a definition of \( W \). They put purely formally \( W = \) number of complexions of the state under consideration. If one now demands that these complexions be equally probable...

There is wide skepticism in the research community about the possibility of producing a mathematical proof of microstates equiprobability. This skepticism dates back to the following quotation from Khinchin [30], that is widely reported in the open bibliography, e.g. [31], [32]: All existing attempts to give a general proof of this postulate must be considered as an aggregate of logical and mathematical errors superimposed on a general confusion in the definition of the basic quantities. About fifteen years ago, by arguments based on typicality, the two papers [33] and [34] proved that microstates cannot be equiprobable, but, at the same time, they showed that microstates converge to equiprobability as the number of particles grows. Paper [33] claims in the abstract that ...the main postulate of statistical mechanics, the equal a priori probability postulate, should be abandoned as misleading and unnecessary. This claim is substantiated by a theorem based on the law of large numbers. The two papers [33] and [34] have attracted noticeable interest, see for instance [35], and can be considered a cornerstone of modern quantum thermodynamics, see [36], [37]. A result similar to that of [33] and [34] has been recently published by this author in [38]. The approach of [38], although relying on typicality as [33] and [34], is much more information-theoretically oriented than [33] and [34]. Hereafter we report the main points of [38].

When the \( N \) random variables of the random vector \( \mathcal{L}^N \) are i.i.d. we have

\[
\lim_{N \to \infty} \frac{1}{N} H(\mathcal{L}^N) = \lim_{N \to \infty} -\frac{1}{N} \log(p_{\mathcal{L}^N}(\mathcal{L}^N)) = \lim_{N \to \infty} -\frac{1}{N} \sum_{i=1}^{N} \log(p_{\mathcal{L}_i}(\mathcal{L}_i)) = \lim_{N \to \infty} -\frac{1}{N} \sum_{i=1}^{N} \log(p_{\mathcal{L}_i}(\mathcal{L}_i)) = H_{\mathcal{L}},
\]

(71)

where (71) is the assumption of independency, (72) is the assumption of identical distribution, and (73) is the law of large numbers. The convergence of the limit (71) to (73) is in various senses. Our main concern is the case of large but finite \( N \), hence we consider convergence in probability, that is

\[
\lim_{N \to \infty} \text{Pr} \left( \left| \frac{1}{N} \log(p_{\mathcal{L}^N}(\mathcal{L}^N)) + H_{\mathcal{L}} \right| > \eta \right) = 0,
\]

(74)

for every \( \eta > 0 \). The above limit is a pillar of classical information theory. In chapter 3 of their book [8], Cover and Thomas call it the Asymptotic Equipartition Property (AEP).

In the context of ergodic theory, many authors refer to (74) as to the Shannon-McMillan theorem. Almost everywhere convergence, that strengthens convergence in probability, is known as the Shannon-McMillan-Breiman theorem.

Starting from (74) we arrive at the concept of typical set \( \{ \mathcal{T}_\eta^N \} \), which is a subset of the set \( \{ \mathcal{L}^N \} \),

\[
\{ \mathcal{T}_\eta^N \} \subseteq \{ \mathcal{L}^N \},
\]

(75)

whose definition is based on the random probability (2). Specifically, the typical set is made by those random vectors whose random probability, for every \( \eta \) and for sufficiently large \( N \), is a random number that lies in the narrow range

\[
e^{-N(H_{\mathcal{L}}+\eta)} \leq p_{\mathcal{L}^N}(\mathcal{T}_\eta^N) \leq e^{-N(H_{\mathcal{L}}-\eta)}.
\]

(76)

The properties of the typical set are that the number of its elements is in the narrow range

\[
e^{N(H_{\mathcal{L}}+\eta)} \geq |\mathcal{T}_\eta^N| \geq (1-\eta)e^{N(H_{\mathcal{L}}-\eta)}
\]

(77)

and that the probability that the outcome of the random vector \( \mathcal{L}^N \) belongs to the typical set is

\[
\text{Pr}(\mathcal{L}^N \in \{ \mathcal{T}_\eta^N \}) > 1 - \eta,
\]

(78)

see again [8]. Using the language of statistical mechanics, we can look at the elements of the typical set as at the accessible microstates. For \( N \) large enough, inequalities (76), (78) show that their number is nearly \( e^{N(H_{\mathcal{L}})} \) and that their overwhelming majority is nearly equiprobable. Compared to the standard approach, where microstates are either accessible (with uniform probability) or non-accessible (zero probability of access), here all the microstates that have non-zero probability are in principle accessible, but with different probabilities.

\footnote{Here it is the probability that is equally partitioned, not the energy, hence this AEP has nothing to do with the classical energy equipartition property.}
XI. Appendix D: Historical Positioning of the Paper

Ideal gas in a container

Looking at (27), we see that the term $-\log(N!)$ is the one introduced by Gibbs to make the phase-space entropy of non-indexed particles compatible with his famous paradox. The genesis of the term $-\log(N!)$ has been in the past object of debate. Many authors report that this term was introduced by Gibbs as an *ad hoc* correction of the entropy of indexed particles to ensure extensivity of entropy, but Jaynes argues in [39] that an early work of Gibbs contains an analysis that correctly explains the presence of the term $-\log(N!)$ in the entropy formula.

After Gibbs, Tetrode followed a reasoning that brought him very close to (27). He considered quantization of the phase space into cells of area $2\pi\hbar$ and argued that gas states obtained by permutation of particles should not be counted as different, see [40]. At high temperature all the particles occupy different cells of the phase space, hence the number of permutations expressed by the multinomial coefficient becomes equal to $N!$, whose logarithm is just the correction term considered by Tetrode. Basically, equation (27) can be seen as a consequence of Tetrode’s approach, it is enough to consider the random multinomial coefficient as it is and then to take the expectation of its logarithm. The denominator of the multinomial coefficient, overlooked by Tetrode, generates the sum that appears in (26). This sum becomes important at low temperature, where many particles occupy the same quantum state, reducing significantly below $N!$ the number of distinct permutations. If this term is overlooked, at temperature low enough the correction represented by $-\log(N!)$ becomes too large and the entropy falls below zero, as it actually happens in the Sackur-Tetrode entropy formula. The difference with our approach is that in the Sackur-Tetrode approach what is quantized is the phase space, while here we consider a truly quantum approach that in the Sackur-Tetrode approach what is quantized is the phase-space entropy formula. The difference with our approach is that in the Sackur-Tetrode approach what is quantized is the phase space, while here we consider a truly quantum approach that in the Sackur-Tetrode approach what is quantized is the phase-space entropy formula. The difference with our approach is that in the Sackur-Tetrode approach what is quantized is the phase space, while here we consider a truly quantum approach that in the Sackur-Tetrode approach what is quantized is the phase-space entropy formula. The difference with our approach is that in the Sackur-Tetrode approach what is quantized is the phase space, while here we consider a truly quantum approach that in the Sackur-Tetrode approach what is quantized is the phase-space entropy formula.

The random total quantum number $\mathcal{L}_\Sigma$ is defined by

$$\mathcal{L}_\Sigma = \sum_{i=1}^{N} \mathcal{L}_i,$$

is the sum of $N$ i.i.d. geometric random variables, therefore its distribution is the negative binomial distribution:

$$p_{\mathcal{L}_\Sigma}(l_\Sigma) = W_NB(l_\Sigma)p^N(1 - p)^{l_\Sigma},$$

where $l_\Sigma$ spans the support set of $\mathcal{L}_\Sigma$ and

$$W_{NB}(l_\Sigma) = \frac{(l_\Sigma + N - 1)!}{l_\Sigma!(N - 1)!}$$

is the negative binomial coefficient, which Planck calls $R$ after equation (4) of [27]. The interested reader is referred to chapter 5 of [33] for the relation between the geometric distribution and the negative binomial distribution and to [21] for the entropy of the negative binomial distribution. To our best knowledge, it is recognized in [42] for the first time that the probability distribution of the random total quantum number $\mathcal{L}_\Sigma$ of a system of $N$ i.i.d. quantum harmonic oscillators all oscillating with the same angular frequency is negative binomial. Equation (39) becomes

$$W_{NB}(l_\Sigma) = \sum_{\tilde{\eta}_\Sigma: \sum_{\ell \in \eta}_\Sigma = l_\Sigma} W_M(\tilde{\eta}_\Sigma).$$

Boltzmann already pointed out that the negative binomial coefficient, that he calls $J$ in [44], is *the sum of all possible complexion*.

As the multinomial coefficient, also the negative binomial coefficient is a recurring figure in statistical mechanics and quantum mechanics. It can be calculated by the *stars and bars* method, which, as reported in [45], was introduced in 1914 in a paper by Ehrenfest and Kamerlingh-Onnes and was later brought by Feller [18] in a context different to physics. The stars and bars method counts the number of distinct arrangements of $l_\Sigma$ stars (energy quanta) into $N$ cells (oscillators) separated by $N - 1$ bars plus two additional bars at the beginning and at the end of the pattern. This number is the number of distinct vectors $^N\text{V}$ whose sum is $l_\Sigma$.

Thanks to the negative binomial distribution, Mandel demonstrates in [42] that all the $W_{NB}(\mathcal{L}_\Sigma)$ arrangements of energy quanta are *conditionally equiprobable* given the total...
number $L_{\Sigma}$ of energy quanta. Here the random condition is $L_{\Sigma}$ and, with arguments analogous to those that led to (23), for the conditional probability of microstates we get

$$p_{\tilde{L}l} = \begin{cases} \frac{1}{W_{NB}(l_{\Sigma})}, & \tilde{L} \in \{l(l_{\Sigma})\}, \text{elsewhere,} \end{cases}$$

(81)

This conditional equiprobability has the same interpretation as (23). What changes between the two is only the random condition and its probability distribution. Since

$$H(L_{\Sigma}) = \text{constant},$$

$$H_{L_{\Sigma}|l} = 0,$$

the entropic relation analogous to (25) is

$$H_{L_{\Sigma}} - H_{L_{\Sigma}|l} = H_{L_{\Sigma}} \geq 0,$$

where the inequality is satisfied with equality only when $L_{\Sigma}$ is actually deterministic, that is, at the ground state, where $L_{\Sigma} = 0$.

**Boltzmann’s total number of complexes and Planck’s entropy**

Planck takes Boltzmann’s total number of complexes (79), forcing inside it the mean value of the total quantum number

$$\langle L_{\Sigma} \rangle = N \mu_{L},$$

(82)

see [27], see also 16.3 of [11] and 3.8 of [15]. The gamma function can be used in the factorials in case of non-integer $\langle L_{\Sigma} \rangle$. Then Planck, citing Boltzmann, claims that the logarithm of the above $W_{NB}(L_{\Sigma})$ is entropy, even if Boltzmann never assigned to the logarithm of the above $W_{NB}(L_{\Sigma})$ the role of entropy. In fact, nobody understands why the logarithm of the negative binomial coefficient should be entropy. But, undoubtedly, it works.

A question naturally arises. Bose’s entropy

$$\log(W_M(\langle N_{\Sigma} \rangle))$$

and Planck’s entropy

$$\log(W_{NB}(L_{\Sigma}))$$

are the logarithms of two different numbers, how can they be the same entity? Luckily, as Von Neumann said to Shannon, no one really knows what entropy really is, therefore everyone can feel free to put inside that logarithm whatever he likes. Provided that it works, we add. In fact, for large $N$, the two logarithms are both a good approximation to the Gibbs entropy, because in (80) the term $W_M(\langle N_{\Sigma} \rangle)$ dominates the sum, see problem 3.4 of [15]. What changes is the accuracy of the approximation, that, for finite $N$, can be different in the two cases. Specifically, Planck’s entropy can be manipulated as follows

$$\log(W_{NB}(L_{\Sigma})) \approx \log((\langle L_{\Sigma} \rangle + N)!)/\langle L_{\Sigma} \rangle!)$$

Stirling

$$\approx \langle L_{\Sigma} \rangle \log(1 + N/\langle L_{\Sigma} \rangle) + N \log(1 + L_{\Sigma}/N)$$

$$= N(\mu_{L} \log(1 + \mu_{L}^{-1}) + \log(1 + \mu_{L}))$$

$$= H_{L}. \quad \text{[15]}$$

Compared to (6), the above equation shows why Planck can use the negative binomial coefficient in place of the multinomial coefficient.

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