Extensive nonadditive entropy in quantum spin chains

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Abstract. We present details on a physical realization, in a many-body Hamiltonian system, of the abstract probabilistic structure recently exhibited by Gell-Mann, Sato and one of us (C.T.), that the nonadditive entropy \( S_q = k [1 - \text{Tr} \, \rho^q] / [q - 1] \) (\( \rho \equiv \) density matrix; \( S_1 = -k \text{Tr} \ln \rho \)) can conform, for an anomalous value of \( q \) (i.e., \( q \neq 1 \)), to the classical thermodynamical requirement for the entropy to be extensive. Moreover, we find that the entropic index \( q \) provides a tool to characterize both universal and nonuniversal aspects in quantum phase transitions (e.g., for a \( L \)-sized block of the Ising ferromagnetic chain at its \( T = 0 \) critical transverse field, we obtain \( \text{lim}_{L \to \infty} S_1(\hat{\rho}_{[L]}(L)) = 3.56 \pm 0.03 \)). The present results suggest a new and powerful approach to measure entanglement in quantum many-body systems. At the light of these results, and similar ones for a \( d = 2 \) Bosonic system discussed by us elsewhere, we conjecture that, for blocks of linear size \( L \) of a large class of Fermionic and Bosonic \( d \)-dimensional many-body Hamiltonians with short-range interaction at \( T = 0 \), we have that the additive entropy \( S_1(L) \propto (L^{d-1} - 1)/(d - 1) \) (i.e., \( \ln L \) for \( d = 1 \), and \( L^{d-1} \) for \( d > 1 \)), hence it is not extensive, whereas, for anomalous values of the index \( q \), we have that the nonadditive entropy \( S_q(L) \propto L^d \) (\( \forall q \)), i.e., it is extensive. The present discussion neatly illustrates that entropic additivity and entropic extensivity are quite different properties, even if they essentially coincide in the presence of short-range correlations.

Keywords: quantum spin chains, entanglement, quantum phase transitions, nonextensive statistical mechanics, nonadditive entropy

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INTRODUCTION

The appearance of long-range correlations in the ground state of a quantum many-body system, undergoing a quantum phase transition at zero temperature, is due to the entanglement [1]. Quantum spin chains, composed by a set of localized spins coupled through short-range exchange interaction in an external transverse magnetic field, capture the essence of these intriguing phenomena and have been extensively studied [3, 2, 4, 5, 6]. The degree of entanglement between a block of \( L \) contiguous spins and the rest of the chain in its ground state, as measured by the von Neumann block entropy \( S_1(L) \equiv -k \text{Tr} \hat{\rho}_L \ln \hat{\rho}_L \) (\( \hat{\rho}_L \equiv \text{Tr}_{N \to \infty} \hat{\rho}_N \)) is the reduced density matrix of a \( L \)-sized block within a \( N \to \infty \) chain with density matrix \( \hat{\rho}_N \), typically saturates (i.e., \( \lim_{L \to \infty} S_1(L) < \infty \)) or is logarithmically unbounded (i.e., \( S_1(L) \propto \ln L \)) for large block size, off or at the critical point, respectively. Here we show that the nonadditive entropy [7, 8] \( S_q(L) \equiv k [1 - \text{Tr} \, \rho^q] / [q - 1] \) of the block of \( L \) spins of the ground state of quantum spin chains in the neighborhood of a quantum phase transition is extensive (i.e., for \( L \gg 1 \), \( S_q(L) \propto L \)) for special values of \( q < 1 \). The additive von Neumann entropy \( S_1(L) = -k \text{Tr} \ln \hat{\rho}_L \)
is (like the additive Renyi entropy) nonextensive; indeed, \( \lim_{L \to \infty} S_1(L)/L = 0 \) in all considered cases. We present here details of the first physical realization (this as well as another, Bosonic, physical realization have been discussed in [9]), in a many-body Hamiltonian system, of the abstract mathematical examples shown in Ref. [10], that, for anomalous values of \( q \), the nonadditive entropy \( S_q \), can be extensive, as expected from the Clausius thermodynamical requirement for the entropy. We find that the index \( q \) provides a new and efficient tool to characterize different universality classes in quantum phase transitions, and to quantify entanglement [11, 12, 13] in quantum many-body systems, by using a nonadditive measure [14, 15, 16, 17, 18, 19, 20, 21].

**NONEXTENSIVE STATISTICAL MECHANICS**

The aim of statistical mechanics is to establish a direct link between the mechanical microscopic laws and classical thermodynamics. The most famous classical theory in this field has been developed by Boltzmann and Gibbs (BG) and it is considered one of the cornerstones of contemporary physics. The connection between micro- and macro-world is described by the so called BG entropy:

\[
S_{BG} = -k \sum_{i=1}^{W} p_i \ln p_i
\]

where \( k \) is a positive constant, \( W \) is the number of microscopic states and \( \{p_i\}_{i=1,...,W} \) is a normalized probability distribution. One of the crucial properties of the entropy in the context of classical thermodynamics is extensivity, namely proportionality with the number of elements of the system. The BG entropy satisfies this prescription if the subsystems are statistically (quasi-) independent, or typically if the correlations within the system are generically local. In such cases the system is called extensive.

In general, however, the situation is not of this type and correlations may be far from negligible at all scales. In such cases the BG entropy may be nonextensive. Nonetheless, for an important class of such systems, an entropy exists which is extensive in terms of the microscopic probabilities [10]. The additive BG entropy can be generalized into the nonadditive \( q \)-entropy [7]

\[
S_q = k \frac{1 - \sum_{i=1}^{W} p_i^q}{q - 1}, \quad q \in \mathbb{R} \quad (S_1 = S_{BG}).
\]

This is the basis of the so called nonextensive statistical mechanics [8], which generalizes the BG theory.

Additivity (for two probabilistically independent subsystems \( A \) and \( B \)) is generalized by the following pseudo-additivity: \( S_q(A,B)/k = S_q(A)/k + S_q(B)/k + (1 - q)S_q(A)S_q(B)/k^2 \); the cases \( q < 1 \) and \( q > 1 \) correspond to super-additivity and sub-additivity, respectively. For subsystems that have special probability correlations, extensivity is not valid for \( S_{BG} \), but may occur for \( S_q \) with a particular value of the index \( q \neq 1 \). Such systems are sometimes referred to as nonextensive [10, 8].

A physical system may exhibit genuine quantum aspects. In particular, quantum correlations, quantified by the entanglement, can be present. The classical probability
concepts are replaced by the density matrix operator $\hat{\rho}$, in terms of a more general probability amplitude context. Therefore the quantum counterpart of the BG entropy in Eq. (1), which is called von Neumann entropy, is given by $S_1(\hat{\rho}) = -k \text{Tr} \hat{\rho} \ln \hat{\rho}$, while the classical $q$-entropy, Eq. (2), is replaced by:

$$S_q(\hat{\rho}) = k \frac{1 - \text{Tr} \hat{\rho}^q}{q - 1}. \quad (3)$$

The pseudo-additivity property is now given by

$$\frac{S_q(\hat{\rho}_1 \otimes \hat{\rho}_2)}{k} = \frac{S_q(\hat{\rho}_1)}{k} + \frac{S_q(\hat{\rho}_2)}{k} + (1 - q) \frac{S_q(\hat{\rho}_1)}{k} \frac{S_q(\hat{\rho}_2)}{k};$$

from now on $k = 1$.

**XY MODEL**

In this paper we analyze a quantum system in which strong non-classical correlations occur between its components. We focus our investigations on a one-dimensional spin-$1/2$ ferromagnetic chain with an exchange (local) coupling and in the presence of an external transverse magnetic field, i.e., the quantum XY model. The Hamiltonian of the XY model with open boundary conditions is:

$$\hat{H} = -N-1 \sum_{j=1}^{N-1} \left[ (1 + \gamma) \hat{\sigma}_j^x \hat{\sigma}_{j+1}^x + (1 - \gamma) \hat{\sigma}_j^y \hat{\sigma}_{j+1}^y + 2\lambda \hat{\sigma}_j^z \right]. \quad (4)$$

where $\hat{\sigma}_j^\alpha (\alpha = x, y, z)$ are the Pauli matrices of the $j$-th spin, $N$ is the number of spins of the chain, $\gamma$ and $\lambda$ characterize, respectively, the strength of the anisotropy parameter and of a transverse magnetic field along the $z$ direction. This model for $0 < |\gamma| \leq 1$ belongs to the Ising universality class and it actually reduces to the quantum Ising chain for $|\gamma| = 1$. This system undergoes a quantum phase transition at the critical point $|\lambda_c| = 1$ in the thermodynamic limit $N \to \infty$. For $\gamma = 0$ it is the isotropic XX model, which is critical for $|\lambda| \leq 1$ [1]. Let us stress that in the following we will solve analytically the ground state in the limiting case of an infinite chain, i.e. $N \to \infty$. Therefore, the coupling being ferromagnetic, the results will not depend on our particular choice of the boundary conditions.

The entanglement in the neighborhood of the quantum phase transition has been recently widely investigated, thus establishing a direct connection between quantum information theory and condensed matter physics [2, 3, 4, 5, 6]. In particular it has been shown that one-site and two-site entanglement between nearest or next-to-nearest spins display a peak near or at the critical point [2, 3]. On the other side, the entanglement between a block of $L$ contiguous spins and the rest of the chain in the ground state, quantified by the von Neumann entropy, presents a logarithmic divergence with $L$ at criticality, while it saturates in a non-critical regime [4, 5, 6].

The inadequacy of the additive von Neumann entropy as a measure of the information content in a quantum state has been pointed out in Ref. [15]. A theoretical observation
that the measure of quantum entanglement may not be additive has been discussed in Refs. [16, 14, 15, 17, 18, 19, 20, 21]. Recently, Ref. [22] suggested to abandon the \textit{a priori} probability postulate going beyond the usual BG situation.

Here we propose to extend the definition of the von Neumann entropy to a wider class of entropy measures which naturally include it, thus generalizing the notion of the block entanglement entropy. The block $q$-entropy of a block of size $L$ is simply defined as the $q$-entropy, Eq. (3), of the reduced density matrix $\hat{\rho}_L$ of the block, when the total chain is in the ground state. In the following we show that, contrary to the von Neumann entropy, there exists a $q$ value for which $S_q(\hat{\rho}_L)$ is extensive. This value does depend on the critical properties of the chain and it is consistent with the universality hypothesis.

The XY model in Eq. (4) can be diagonalized exactly with a Jordan-Wigner transformation, followed by a Bogoliubov rotation [23, 24, 25, 26]; this allows one to analytically consider the thermodynamic limit $N \to \infty$. The normal modes of the system are linear combinations of the following non–local Majorana fermions:

$$\hat{c}_{2l} \equiv \left( \prod_{k=0}^{l-1} \hat{\sigma}_z^k \right) \hat{\sigma}_x^l; \quad \hat{c}_{2l+1} \equiv \left( \prod_{k=0}^{l-1} \hat{\sigma}_z^k \right) \hat{\sigma}_y^l. \quad (5)$$

These operators are Hermitian and obey the anti-commutation rules $\{\hat{c}_m, \hat{c}_n\} = 2 \delta_{mn}$.

The ground state $|\Psi_g\rangle$ is completely characterized by the scalar product $\langle c_m c_n \rangle = \delta_{mn} + i \Gamma_{mn}$, where

$$\Gamma^{(N)} = \begin{bmatrix} \Pi_0 & \Pi_1 & \cdots & \Pi_{N-1} \\
\Pi_1 & \Pi_0 & \cdots & \vdots \\
\vdots & \ddots & \ddots & \vdots \\
\Pi_{1-N} & \cdots & \Pi_0 & \Pi_0 \end{bmatrix}, \quad \Pi_l = \begin{bmatrix} 0 & g_l \\
-g_l & 0 \end{bmatrix}$$

with real coefficients $g_l$ given, for an infinite chain, by $g_l = \frac{1}{2\pi} \int_0^{2\pi} d\phi e^{-i\lambda \phi - i\gamma \sin \phi} \cos \phi \begin{bmatrix} \cos \phi - i \gamma \sin \phi \\
\cos \phi + i \gamma \sin \phi \end{bmatrix}$.

The spectrum of $\hat{\rho}_L$ in an infinite chain in its ground state can then be exactly evaluated [6]. Indeed, the matrix $\hat{\rho}_L$ can be written as a tensor product in terms of $L$ uncorrelated non–local Fermionic modes, which are linear combinations of the operators $\hat{c}_n$ in Eq. (5): $\hat{\rho}_L = \hat{\tau}_1 \otimes \cdots \otimes \hat{\tau}_L$, where $\hat{\tau}_l$ denotes the mixed state of mode $l$. The eigenvalues of $\hat{\tau}_l$ are $(1 \pm v_l)/2$, where $v_l$ is the imaginary part of the eigenvalues of the matrix $\Gamma^{(L)}$. The entropy in Eq. (3) is then easily computed by using the pseudo-additivity, Eq. (4), and by noticing that the trace of $\hat{\tau}_l^q$ is simply $\text{Tr} \hat{\tau}_l^q = [(1 + v_l)/2]^q + [(1 - v_l)/2]^q$. Notice that the required computational time scales polynomially with the block size $L$, thus allowing one to reliably analyze blocks with up to a few hundreds of spins.

**RESULTS**

We first analyze the anisotropic quantum XY model, Eq. (4) with $\gamma \neq 0$, that has a critical point in $\lambda_c = 1$. The block $q$-entropy as a function of the block size can show completely different asymptotic behaviors, by varying the entropic index $q$. In particular, here we are interested in a thermodynamically relevant quantity, namely the slope,
noted \( s_q \), of \( S_q \) versus \( L \). It is generically not possible to have a finite value of \( s_1 \); the entanglement entropy, evaluated by the von Neumann entropy, either saturates or diverges logarithmically in the thermodynamic limit, for respectively non–critical or critical spin chains [4, 5, 6]. The situation dramatically changes by using the entropy in Eq. (3): qualitatively it happens that, regardless the presence or absence of criticality, a \( \lambda \)-dependent value of \( q \), noted \( q_{\text{ent}} \), exists such that, in the range \( 1 \ll L \ll \xi \) (\( \xi \) being the correlation length), \( s_{q_{\text{ent}}} \) is finite, whereas it vanishes (diverges) for \( q > q_{\text{ent}} \) \((q < q_{\text{ent}})\). We note that here the nonextensivity \((\text{i.e., } q \neq 1)\) features are not due to the presence of say long-range interactions [27] but they are triggered only by the fully quantum nonlocal correlations. In Fig. 1 we show, for the critical Ising model \((\lambda = 1, \gamma = 1)\), the behavior of the block \( q \)-entropy with respect to the block size: \( S_q(\hat{\rho}_L) \) becomes extensive \((\text{i.e., } 0 < \lim_{L \to \infty} S_q(\hat{\rho}_L)/L < \infty)\) for \( q_{\text{ent}} \simeq 0.0828 \pm 10^{-4} \) (with a corresponding entropic density \( s_{q_{\text{ent}}} \simeq 3.56 \pm 0.03 \)), thus satisfying the classical thermodynamical prescription.

A very similar behavior is shown for non–critical Ising model, as well as for critical and non–critical XY models with \( 0 < \gamma < 1 \). The value of \( q_{\text{ent}} \), for which \( S_q(\hat{\rho}_L) \) is extensive, is obtained maximizing numerically the linear correlation coefficient \( r \) of \( S_q(\hat{\rho}_L) \), in the range \( 1 \ll L \ll \xi \), with respect to \( q \), as shown in the bottom inset in Fig. 2. Let us stress that, at precisely the critical point, \( \xi \) diverges, hence \( L \) is unrestricted and can run up to infinity. The index \( q_{\text{ent}} \) depends on the distance from criticality and it increases as \( \lambda \) approaches \( \lambda_c \) (Fig. 2). It is worth stressing that our numerical results satisfy the duality symmetry \( \lambda \to 1/\lambda \), investigated in Ref. [29].

We have also checked other values of \( \gamma \) for the XY model and the results are very similar to those presented here. This fact is consistent with the universality hypothesis. On one hand, XY and Ising model (Ising universality class) have the same behavior as regards the extensivity of \( S_q(\hat{\rho}_L) \); in Fig. 3 we report the variation of \( s_{q_{\text{ent}}} \) with respect to \( \lambda \). On the other hand, for the isotropic XX model \((\gamma = 0)\) in the critical region \(|\lambda| \leq 1\) we find \( q_{\text{ent}} \simeq 0.15 \pm 0.01 \) \((\simeq 2q_{\text{XY}}^{\text{ent}} \text{ with } q_{\text{XY}}^{\text{ent}} \simeq 0.08)\) for which \( S_q(\hat{\rho}_L) \) becomes extensive.
FIGURE 2. The $\lambda$-dependence of the index $q_{\text{ent}}$ in the Ising ($\gamma = 1$, circle) and XY ($\gamma = 0.75$, square) chains. At bottom: Determination of $q_{\text{ent}}$ through numerical maximization of the linear correlation coefficient $r$ of $S_q(\hat{\rho}_L)$. The error bars for the Ising chain are obtained considering the variation of $q_{\text{ent}}$ when using the range $100 \leq L \leq 400$ in the search of $S_q(\hat{\rho}_L)$ linear behavior. Actually, at the present numerical level, we cannot exclude finite-size effects off criticality.

FIGURE 3. The $\lambda$-dependence of the $q$-entropic density $s_{q_{\text{ent}}}$ in the Ising ($\gamma = 1$, circle) and XY ($\gamma = 0.75$, square) models. For $\lambda = 1$, the slopes are $3.56$ and $2.63$, for $\gamma = 1$ and $\gamma = 0.75$, respectively.

Ref. [28] enables us to analytically confirm, at the critical point, our numerical results. The continuum limit of a (1+1)-dimensional critical system is a conformal field theory with central charge $c$. In this quite different context, the authors re-derive the result $S_1(\hat{\rho}_L) \sim (c/3) \ln L$ for a finite block of length $L$ in an infinite critical system. To obtain the von Neumann entropy, they find an analytical expression for $\text{Tr} \hat{\rho}_L^q$, namely $\text{Tr} \hat{\rho}_L^q \sim L^{-c/6(q-1/q)}$. Here, we use this expression quite differently. We impose the
extensivity of $S_q(\hat{\rho}_L)$ finding the value of $q$ for which $-c/6(q_{\text{ent}} - 1/q_{\text{ent}}) = 1$, i.e.,

$$q_{\text{ent}} = \frac{\sqrt{9 + c^2} - 3}{c}.$$  \hspace{1cm} (6)

Consequently, $\lim_{L \to \infty} S_{q(\hat{\rho}_L)}(L)/L < \infty$. When $c$ increases from 0 to infinity (see Fig. 4), $q_{\text{ent}}$ increases from 0 to unity (von Neumann entropy); for $c = 4$ (dimension of physical space-time), $q = 1/2$; $c = 26$ corresponds to a 26-dimensional Bosonic string theory, see [30]. It is well known that for critical quantum Ising and XY models the central charge is equal to $c = 1/2$ (indeed they are in the same universality class and can be mapped to a free Fermionic field theory). For these models, at $\lambda = 1$, the value of $q$ for which $S_q(\hat{\rho}_L)$ is extensive is given by $q_{\text{ent}} = \sqrt{37} - 6 \approx 0.0828$, in perfect agreement with our numerical results in Fig. 2. The critical isotropic XX model ($\gamma = 0$ and $|\lambda| \leq 1$) is, instead, in another universality class, the central charge is $c = 1$ (free Bosonic field theory) and $S_q(\hat{\rho}_L)$ is extensive for $q_{\text{ent}} = \sqrt{10} - 3 \approx 0.16$, as found also numerically. We finally notice that, in the $c \to \infty$ limit, $q_{\text{ent}} \to 1$. We do not clearly understand the physical interpretation of this fact. However, since $c$ in some sense plays the role of a dimension (see [30]), this limit could correspond to some sort of mean field approximation. If so, it is along a line such as this one that a mathematical justification could emerge for the widely spread use of BG concepts in the discussion of mean-field theories of spin-glasses (within the replica-trick and related approaches). Indeed, BG statistical mechanics is essentially based on the ergodic hypothesis. It is firmly known that glassy systems (e.g., spin-glasses) precisely violate ergodicity, thus leading to an intriguing and fundamental question. Consequently, a mathematical justification for the use of BG entropy and energy distribution for such complex mean-field systems would be more than welcome.

![Graph](image-url)

**FIGURE 4.** $q_{\text{ent}}$ versus $c$ with the $q$-entropy, $S_q(\hat{\rho}_L)$, being extensive, i.e., $\lim_{L \to \infty} S_{q(\hat{\rho}_L)}(L)/L < \infty$. When $c$ increases from 0 to infinity, $q_{\text{ent}}$ increases from 0 to unity (von Neumann entropy); for $c = 4$, $q = 1/2$ and for $c \gg 1$, see Ref. [30]. Inset: for the critical quantum Ising and XY models $c = 1/2$ and $q_{\text{ent}} = \sqrt{37} - 6 \approx 0.0828$, while for the critical isotropic XX model $c = 1$ and $q_{\text{ent}} = \sqrt{10} - 3 \approx 0.16$. 
It is worth to mention that the Renyi entropy of a block of critical XX spin chains has been derived analytically in Ref. [31]. Since the Renyi entropy is simply connected to the entropy $S_q$, it is possible to re-derive $q_{ent}$ for the critical XX model also from that analytical expression.

CONCLUDING REMARKS

Summarizing, we have presented: (i) Details on the first physical realization (in a 1/2-spin $d = 1$ quantum system), in a many-body Hamiltonian system, of the abstract probabilistic structure shown in Ref. [10], that $S_q$ conforms, for a special value of $q$, to the classical thermodynamical requirement for the entropy to be extensive (the second physical realization, in a $d = 2$ Bosonic system, can be seen in [9]); (ii) A new connection, Eq. (6), between nonextensive statistical mechanical concepts and BG statistical mechanics at criticality (see [32] for another such analytical connection); (iii) A novel and simple manner to characterize entanglement through the pair $(q_{ent}, s_{q_{ent}})$.

Let us point out also that the reduction of the pure ground state of the full chain (at $T = 0$) to a finite block of $L$ spins results in a mixed state with quantum fluctuations. A mapping of this subsystem within a zero temperature XX infinite chain to a finite system which is thermalized at some finite temperature has been recently exhibited [33], thus defining an $L$-dependent effective temperature of the block. The use of a non-Boltzmannian distribution (e.g., the one emerging within nonextensive statistical mechanics) might enable defining an effective temperature which would not depend on $L$, as physically desirable. Indeed, this approach has been successfully implemented for $e^-e^+$ collision experiments [34].

Finally, let us emphasize the difference between additivity and extensivity for the entropy. Additivity only depends on the mathematical definition of the entropy; therefore, $S_1$ is additive, whereas $S_q$ ($q \neq 1$) is nonadditive. Extensivity is more subtle, since it also depends on the specific system. The $T = 0$ block entropies of the present 1/2-spin $d = 1$ quantum system at criticality are given by $S_1(L) \propto \ln L$ (i.e., nonextensive), and $S_{\sqrt[4]{\gamma + \gamma e^{-\Delta}}} (L) \propto L$ (i.e., extensive). It is known (see [35] and references therein) that, for $d$-dimensional Bosonic systems (e.g., a black hole [36]), $S_1$ follows the area law, i.e., $S_1(L) \propto L^{d-1}$ (i.e., nonextensive). A logarithmic behavior for $d = 1$, and the area law for $d > 1$ can be unified through $S_1(L) \propto [L^{d-1} - 1] / (d - 1) \equiv \ln_{2-d} L$ [37] (i.e., nonextensive), which would correspond to a large class (yet not completely identified) of fully entangled quantum systems. For all these systems, one could expect that a value of $q$ exists such that $S_q(L) \propto L^d$ (i.e., extensive). In addition to the present example, a $d = 2$ Bosonic system has been shown [9] to satisfy this conjecture.

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