Nonadditive entropy for random quantum spin-S chains

A. Saguia, M. S. Sarandy

Instituto de Física, Universidade Federal Fluminense, Av. Gal. Milton Tavares de Souza s/n, Gragoatá, 24210-346, Niterói, RJ, Brazil.

Abstract

We investigate the scaling of Tsallis entropy in disordered quantum spin-S chains. We show that an extensive scaling occurs for specific values of the entropic index. Those values depend only on the magnitude S of the spins, being directly related with the effective central charge associated with the model.

Keywords: Quantum Spin Chain; Disordered System; Nonextensive Statistical Mechanics.

1. Introduction

Correlations among parts of a quantum system are behind remarkable phenomena, such as a quantum phase transition (QPT) \[1, 2\]. In particular, the relationship between correlations and QPTs is revealed by the behavior of entanglement at criticality as measured, e.g., by the von Neumann entropy \(S\) (see, for instance, Ref. \[3\]). Given a quantum system in a pure state \(|\psi\rangle\) and a bipartition of the system into two subsystems \(A\) and \(B\), the von Neumann entropy between \(A\) and \(B\) reads

\[
S = -\text{Tr} (\rho_A \ln \rho_A) = -\text{Tr} (\rho_B \ln \rho_B),
\]

where \(\rho_A = \text{Tr}_B \rho\) and \(\rho_B = \text{Tr}_A \rho\) denote the reduced density matrices of \(A\) and \(B\), respectively, with \(\rho = |\psi\rangle \langle \psi|\). If \(A\) and \(B\) are probabilistic independent (such that \(\rho = \rho_A \otimes \rho_B\)), the von Neumann entropy is additive, i.e., \(S_{AB} = S_A + S_B\). As a consequence, \(S\) is extensive for uncorrelated subsystems, namely, \(S(L) \propto L\), where \(L\) denotes the size of a block of the system. On the other hand, \(S\) becomes nonextensive in presence of correlations. Indeed, for critical systems in one dimension, which are known to be highly entangled, conformal invariance implies a diverging logarithmic scaling given by \(S(L) \propto (c/3) \ln L\) (or, more specifically, \(S(L) = (c/3) \ln L + \text{constant}\)), where \(c\) is the central charge associated with the Virasoro algebra of the underlying conformal field theory \[4, 5, 6\].

For noncritical (gapful) systems in one dimension, entanglement saturates at a constant value \(k\), i.e., \(S(L) \rightarrow k\) as \(L \rightarrow \infty\). More generally, for higher dimensions, noncritical systems are expected to obey the area law, which implies that the von Neumann entropy of a region scales as the surface area of the region instead of the volume of the region itself. In other words, the area law establishes that \(S(L) \propto L^{D-1}\) \((L \rightarrow \infty)\), where \(D\) is the dimension of the system.

Remarkably, it has recently been shown in Refs. \[7, 8\] that a quantum system may exhibit specific probability correlations among its parts such that an extensive entropy can be achieved even for highly correlated subsystems. This has been obtained by generalizing the von Neumann entropy into the nonadditive Tsallis \(q\)-entropy \[9, 10\]

\[
S_q[\rho] = \frac{1}{1-q} (\text{Tr} \rho^q - 1),
\]

with \(q \in \mathbb{R}\). One can show that the von Neumann entropy is a particular case of Eq. \(2\) by taking \(q = 1\). Tsallis entropy has been successfully applied to handle a variety of physical systems, in particular those exhibiting long-range interactions. Recent experimental results for its predictions can be found, e.g., in Refs. \[11, 12\]. In Tsallis statistics, the additivity of the von Neumann entropy for independent subsystems is replaced by the pseudo-additivity relation of the \(S_q\) entropy

\[
S_q[\rho_A \otimes \rho_B] = S_q[\rho_A] + S_q[\rho_B] + (1-q) S_q[\rho_A] S_q[\rho_B].
\]
The investigation of $S_q$ in conformal invariant quantum systems has revealed that the extensivity of the entropy can be achieved for a particular choice $q_{\text{ext}}$ of the entropic index $q$ in Eq. (2). In particular, $q_{\text{ext}}$ is directly associated with the central charge $c$. More specifically, the extensivity of $S_q$ occurs for

$$q_{\text{ext}} = \frac{\sqrt{9 + c^2} - 3}{c}.$$  

(4)

The aim of this work is to consider the scaling of the nonadditive entropy $S_q$ and, consequently, its extensivity in quantum critical spin chains under the effect of disorder into the exchange couplings among the spins. Indeed, disorder appears as an essential feature in a number of condensed matter systems, motivating a great deal of theoretical and experimental research (see, e.g., Refs. [13, 14]). In particular, it is well known that, in the case of a spin-$S$ random exchange Heisenberg antiferromagnetic chain (REHAC), disorder can drive the system to the so-called random singlet phase (RSP), which is a gapless phase described by spin singlets distributed over arbitrary distances [15]. In recent years, it has been observed that the entanglement entropy in critical random spin chains displays a logarithmic scaling that closely resembles the behavior of pure (non-disordered) systems. Indeed, for a block of spins of length $L$, we have that the von Neumann entropy reads $S(L) \propto (c_{\text{eff}}/3) \ln L$, where $c_{\text{eff}}$ is an effective central charge that governs the scale of the entropy [16]. Moreover, it has been shown that in the case of the RSP, $c_{\text{eff}}$ is determined solely in terms of the magnitude $S$ of the spin in the chain [17, 18, 19] (see Ref. [21] for a review of entanglement in random systems and Ref. [22] for other connected results). Here, we will show that the extensivity of $S_q$ can also be obtained for random critical spin chains, with $q_{\text{ext}}$ governed by $c_{\text{eff}}$. Hence, $q_{\text{ext}}$ will be given as a unique function of the spin $S$. Moreover, as we will see, around the extensivity point $q_{\text{ext}}$, $S_q(L) \propto L^\gamma$, with the exponent $\gamma$ of the power law given by a quadratic function of $q$.

2. Nonadditive entropy for a set of random singlets

We begin by considering the typical arrange of a quantum spin-$S$ chain in the RSP, which is provided by a set of spin singlets distributed over arbitrary distances, as sketched by Fig. 1.

In order to evaluate $S_q$ in the RSP, we begin by considering a number $n$ of singlets connecting a contiguous block composed by $L$ spins with the rest of the chain. In this situation, the pseudo-additivity of $S_q$ implies that Tsallis entropy is given by the Proposition below.

**Proposition 1.** For a bipartite system composed of a number $n$ of spin-$S$ singlets connecting two blocks, with $n \in \mathbb{N}$, Tsallis entropy $S_q^{(n)}$ for each block is given by

$$S_q^{(n)} = \frac{1}{1-q} \left[ (2S+1)^{n(1-q)} - 1 \right].$$

(5)

**Proof.** The proof can be obtained by finite induction. Indeed, the single-site reduced density operator $\rho_A$ for a spin-$S$ singlet can be represented by a $D$-dimensional diagonal matrix given by $\rho_A = \text{diag}(D^{-1}, \cdots, D^{-1})$, with $D = 2S + 1$. Therefore, from Eq. (2), we obtain that $S_q^{(1)} = (1-q)^{-1}(D^{1-q} - 1)$. For two singlets, the pseudo-additivity of $S_q$ given by Eq. (4) implies that $S_q^{(2)} = (1-q)^{-1}(D^{2(1-q)} - 1)$. By taking the general expression for the entropy for $n$ singlets as $S_q^{(n)} = (1-q)^{-1}(D^{n(1-q)} - 1)$, we obtain for $(n+1)$ singlets that $S_q^{(n+1)} = (1-q)^{-1}(D^{(n+1)(1-q)} - 1)$. Hence, Eq. (5) holds for any $n \in \mathbb{N}$. □

Tsallis entropy for the RSP can then be obtained by numerically averaging $S_q^{(n)}$ over a sample of random couplings along the chain. These random configurations are generated by following a gapless probability distribution, which drives the system to the RSP, with the entropy of each configuration computed by counting the spin singlets via a renormalization group approach described in the next section.

3. Renormalization group method for random spin systems

The RSP can be conveniently handled via a perturbative real-space renormalization group method introduced by Ma, Dasgupta and Hu (MDH) [22, 23], which was successfully applied to the spin-1/2
REHAC. This approach was proven to be asymptotically exact, which allowed for a fully characterization of the properties of the RSP \cite{16}. Considering a set of random Heisenberg antiferromagnetic interactions $J_i$ between neighbouring spins $S_i$ and $S_{i+1}$, the original MDH method consists in finding the strongest interaction $\Omega$ between a pair of spins $(S_2$ and $S_1$ in Fig. 2a) and treating the couplings of this pair with its neighbors ($J_1$ and $J_2$ in Fig. 2a) as a perturbation. Diagonalization of the strongest bond leads at zeroth order in perturbation theory to a singlet state between the spins coupled by $\Omega$. Then, the singlet is decimated away and an effective interaction is always smaller than those eliminated. Now suppose $J_1 > J_2$ and $J_1 > 3\Omega/[2S(S+1)]$. In this case, we consider the trio of spins-$S$ coupled by the two strongest interactions of the trio, $J_1$ and $\Omega$ and solve it exactly (see Fig. 2b). This trio of spins is then substituted by one effective spin interacting with its neighbors through new renormalized interactions obtained by degenerate perturbation theory for the ground state of the trio. This method has been used to successfully investigate the quantum phase diagram of the spin-1/2 \cite{25} and spin-3/2 \cite{26} Heisenberg spin chains and will be here applied to the computation of the nonadditive entropy.

4. Scaling of nonadditive entropy in the RSP

Let us apply now the generalized MDH approach to analyze the behavior of $S_q$ in the RSP of antiferromagnetic spin chains. We start with a REHAC, whose Hamiltonian is given by

$$H_{Heis} = \sum_{i=1}^{N} J_i \vec{S}_i \cdot \vec{S}_{i+1} \tag{7}$$

where $\{J_i\}$ are random exchange couplings obeying a probability distribution $P(J)$ and $\{\vec{S}_i\}$ are spin-S operators, with periodic boundary conditions adopted. The numerical investigation of $S_q$ is performed as follows. We begin by considering spin chains with 200,000 sites, whose couplings $\{J_i\}$ are randomly generated by using a gapless power law distribution $P(J) \propto J^{-0.8}$, for which trio renormalizations are negligible. Results are then obtained by averaging over a sample of $M = 40,000$ configurations for $\{J_i\}$ \cite{25}. For each random configuration $j$, we decimate the spins out via the generalized MDH technique and compute the number $n_j$ of singlets that cross a block of length $L$. The number $n_j$ is counted by following Ref. \cite{17}. In turn, if a singlet is decimated and the spins composing the singlet are in different blocks, this singlet adds one to the total number $n_j$. On the other hand, in the case of a trio elimination, nothing is added to $n_j$, since one effective spin is returned to the chain (see also Ref. \cite{16}).

\footnote{It is worth observing that a considerably larger amount of configurations is demanded for the evaluation of Tsallis entropy in comparison with the von Neumann entropy (see, e.g., Ref. \cite{15}).}
for a similar approach). The decimation procedure is iterated until the elimination of all spins in the chain. After all configurations computed, Tsallis entropy is then obtained by averaging over all of them, i.e.,

$$S_q = \frac{\sum_{j=1}^{M} S_q^{(n_j)}}{M}, \quad (8)$$

with $S_q^{(n_j)}$ given by Eq. (8). The results for spin-1/2, spin-1, and spin-3/2 REHACs are shown in Figs. 3-5. Note that an extensive $S_q$ can be found for specific negative values $q_{ext}$ in the examples above. These values are clearly distinct for different spin magnitudes $S$. In turn, a remarkable fact is that $q_{ext}$ depends only on $S$ for a system in the RSP and not on the specific model considered.

In fact, let us consider the spin-1 random exchange biquadratic antiferromagnetic chain, whose Hamiltonian is given by

$$H_{Biq} = \sum_{i=1}^{N} J_i \left( \vec{S}_i \cdot \vec{S}_{i+1} \right)^2. \quad (9)$$

Application of the generalized MDH procedure here results only in the formation of singlets, with the renormalized exchange coupling reading [24]

$$J' = \frac{2 J_1 J_2}{9 \Omega}. \quad (10)$$

where $J_1$ and $J_2$ are the nearest neighbors of the strongest bond $\Omega$. As in the Heisenberg case, we consider spin chains with 200,000 sites, whose couplings $\{J_i\}$ are randomly generated by using a gapless power law distribution $P(J) \propto J^{-0.8}$ and averaged over a sample of $M = 40,000$ configurations for $\{J_i\}$. This model produces the same result for $q_{ext}$ as the spin-1 REHAC in the RSP. In order to illustrate this equivalence and obtain a numerical value for $q_{ext}$, let us consider the relationship between $S_q$ and $L$ close to the extensivity index $q_{ext}$. As indicated in Figs. 3-5, we obtain that $S_q \propto L^\gamma$ around the extensive point $\gamma = 1$. Indeed, the aim of Figs. 3-5 is precisely show this dependence as $q$ is varied across extensivity. Moreover, as shown in Fig. 6 for the REHACs (with different spin magnitudes $S$) as well as for the spin-1 biquadratic chain, the exponent $\gamma$ shows a quadratic dependence on $q$, namely,

$$\gamma = uq^2 + vq + w, \quad (11)$$
dure. Indeed, from ∆ obtained from a standard error propagation procedure, the error bar ∆ for different magnitudes S of spin in the chain. In particular, note the collapse of the spin-1 REHAC and biquadratic curves, indicating that qext is uniquely determined by S.

Moreover, qext can be directly obtained by imposing γ = 1 in Eq. (11). The values for qext as well as their relationship with the effective central charge are summarized in Table 1. Concerning the estimation of the error bar ∆qext, it can be directly obtained from a standard error propagation procedure. Indeed, from ∆γ = |∂γ/∂q| ∆q, we obtain ∆qext = ∆γ/|2 u qext + v|. Although the analytical

\[ c_{eff} = \ln (2S + 1). \] (12)

is obtained. This behavior is indeed displayed in Fig. 6 in terms of 1/cff for REHACs in the RSP. In particular, note that a linear behavior can be inferred between qext and 1/cff, which reads

\[ q_{ext} = 1 - \frac{1.67}{c_{eff}} \] (13)

Therefore, as given by Eq. (11) for the pure case, we can also determine an expression for qext in terms of cff for disordered systems, which reinforces the universal properties of the entropic index q in critical systems.

5. Conclusions

In summary, we have investigated the scaling of Tsallis entropy Sq in spin-S random critical quantum spin chains. By focusing on the RSP, we have shown that, for specific values qext of the entropic index, Sq becomes an extensive quantity, which reconciles the quantum scaling with the Clausius-like prescription for classical thermodynamics. It is important to emphasize that the extensivity of the nonadditive entropy does not imply absence of correlations between the parts of the quantum system. In this context, there is no contradiction with the behavior of block entanglement as measured by the von Neumann entropy. Remarkably, qext is directly associated with the effective central charge cff that governs bipartite entanglement in random spin chains, which means that qext is solely determined by the magnitude S of the spin in the chain. Moreover, we have inferred a linear algebraic relationship between qext and 1/cff. An analytical investigation of this relationship as well as the

Table 1: Entropic indices qext that yield the extensivity of Sq for different magnitudes S and their corresponding effective central charges.
behavior of $q_{ext}$ in other critical phases of random spin chains (e.g., Griffiths phase) are challenges under research. Moreover, the scaling of $S_q$ far from the extensivity point is also relevant in connection with the scaling of $\text{Tr} \rho^q$ (see, e.g., Refs. [29, 30]).

We intend to address such topics in a future work.

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