Entanglement entropy of aperiodic quantum spin chains

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Abstract – We study the entanglement entropy of blocks of contiguous spins in non-periodic (quasi-periodic or more generally aperiodic) critical Heisenberg, XX and quantum Ising spin chains, e.g. in Fibonacci chains. For marginal and relevant aperiodic modulations, the entanglement entropy is found to be a logarithmic function of the block size with log-periodic oscillations. The effective central charge, $c_{\text{eff}}$, defined through the constant in front of the logarithm may depend on the ratio of couplings and can even exceed the corresponding value in the homogeneous system. In the strong modulation limit, the ground state is constructed by a renormalization group method and the limiting value of $c_{\text{eff}}$ is exactly calculated. Keeping the ratio of the block size and the system size constant, the entanglement entropy exhibits a scaling property, however, the corresponding scaling function may be nonanalytic.

Introduction. – Recently, the entanglement properties of strongly correlated systems have attracted great attention both in condensed-matter physics \cite{1} and in quantum information theory \cite{2}, for a review see \cite{3}. Much work is devoted to homogeneous one-dimensional systems in which the entanglement entropy of $L$ contiguous spins, defined as the von Neumann entropy of the density matrix

$$S_L = -\text{Tr} \rho_L \log_2 \rho_L,$$

of the block, scales at the critical point as

$$S_L = \frac{c}{3} \log_2 L + k,$$

where $c$ is the central charge of the associated conformal field theory and $k$ is a non-universal constant. In the vicinity of the quantum critical point, $L$ in eq. (1) is replaced by the correlation length \cite{1}.

Inhomogeneities of different kinds (localized or extended defects, quenched disorder, etc.) are able to modify the local critical behavior of the system \cite{4} and as a consequence, the scaling properties of $S_L$ in eq. (1) can also be changed. We expect that in case of weak perturbations caused by inhomogeneities the entropy scaling remains invariant or is modified depending on the stability of the local critical behavior at the boundary of the block. For irrelevant perturbations the critical properties of the system at the boundary of the block remain unchanged and it is natural to assume that the same scaling law holds for the entanglement entropy as in the homogeneous system. On the contrary, for relevant perturbations the local critical behavior at the block boundary is governed by a new fixed point and consequently the scaling of the entanglement entropy is expected to be modified. Finally, for marginal perturbations the local critical behavior is characterized by continuously varying local exponents, thus, also the prefactor of the logarithmic entropy scaling is presumably a continuously varying function of the strength of the inhomogeneity.

This scenario has been checked \cite{5} for a single defect coupling located at the boundary of the block in the spin-$\frac{1}{2}$ XXZ chain defined by the Hamiltonian

$$H_{XXZ} = \sum_{i=1}^{N} J_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z),$$

where the $S_i^\alpha$'s ($\alpha = x, y, z$) are spin-$\frac{1}{2}$ operators and $J_i = J$ for $i \neq L$ and $J_L \neq J$. Concerning the behavior of the entanglement entropy, this type of perturbation is found to be irrelevant in the ferromagnetic domain ($\Delta < 0$) and relevant in the antiferromagnetic (AF) domain ($\Delta > 0$) in complete agreement with the local critical behavior of the system. More interestingly, the boundary defect is a (truly) marginal perturbation in the XX chain (i.e. with $\Delta = 0$), where the logarithmic
scaling form in eq. (1) is still valid, although $c$ is replaced by a so-called effective central charge, $c_{\text{eff}}$, which is found to depend continuously on the strength of the defect [6]. We have observed a similar marginal behavior with a continuously varying effective central charge in case of a single defect in the critical quantum Ising chain (QIC) defined by the Hamiltonian

$$H_L = -2 \sum_{i=1}^{N} J_i S_i^x S_{i+1}^x - h \sum_{i=1}^{N} S_i^z$$

with $J_i = J$ for $i \neq L$ and $J_L \neq J$. Quenched random disorder is a relevant perturbation both for the QIC and for the AF $XXZ$ model [9]. An arbitrarily small random perturbation drives the system to an infinite randomness fixed point (IRFP), which can be studied in the framework of an asymptotically exact renormalization group (RG) method [10–12]. In accordance with this, it was found that the effective central charge jumps to the value characteristic for the IRFP for an arbitrarily weak random modulation [13–15].

The effect of non-periodic (quasi-periodic or more generally aperiodic) disorder has many similarities to the effect of quenched random perturbations. After the discovery of quasicrystals [16], aperiodic systems have become the subject of intensive studies, both experimentally and theoretically [17,18]. Contrary to random disorder, these types of perturbations may also be irrelevant or marginal. The relevance of an aperiodic perturbation on the critical behavior of a quantum chain is related to the sign of the cross-over exponent [19], $\phi = 1 + \nu(\omega - 1)$, where $\nu$ is the correlation length critical exponent of the pure chain and $\omega$ is the wandering exponent of the aperiodic model. According to a heuristic criterion [19] the perturbation is relevant if $\phi > 0$, marginal if $\phi = 0$ and irrelevant if $\phi < 0$. Later aperiodic QICs [20–22] and XX chains [23] were studied by an RG method and the low-energy properties were exactly calculated. For aperiodic $XXZ$ chains, field-theoretical methods [24] and a variant of the strong disorder RG approach have been applied [25–28]. For all models with marginal or relevant perturbations anisotropic scaling behavior is observed which manifests itself in the scaling of the energy gap $\epsilon \sim N^{-z}$, where the dynamical exponent $z$ is greater than one.

In this paper, we study the entanglement properties of critical aperiodic quantum spin chains as a function of the strength of aperiodicity, measured by the ratio of the different couplings, $r$. We investigate systematically the effect of different type of non-periodic perturbations, such as irrelevant, relevant or marginal ones and examine the scaling form of the entropy in these critical, but not conformally invariant systems. It is known that the spectrum of aperiodic systems have many unusual features [17] and we are interested in how these singularities are reflected in the entanglement properties. Spin chains both with continuous symmetry ($XX$ and $XXX$ models) and with discrete symmetry ($QIC$) are considered.

**Methods.** In the case of QIC and $XX$ models, which can be mapped to a system of free-fermions by means of standard techniques [29], we have performed large-scale numerical calculations. Here, one determines first the restricted correlation matrix, $G_{ij}$, $i,j = 1,2,\ldots,L$, which is the corresponding $L \times L$ minor of the matrix defined in eq. (2.32c) in ref. [29]. Then one determines the eigenvalues $\nu_j^2$ ($j = 1,2,\ldots,L$) of the positive definite symmetric matrix $[7] G^T L G^T$, where $G^T$ denotes the transpose of $G$. In this representation, the entanglement entropy is given as a sum of binary entropies of the non-collimated fermionic modes [2,30]:

$$S_L(N) = \sum_{l=1}^{N} -\lambda_l \log_2(\lambda_l) - (1 - \lambda_l) \log_2(1 - \lambda_l),$$

where $\lambda_l = (1 + \nu_l)/2$.

In the actual calculations, we considered blocks of size $L$ which are given by finite approximants of the aperiodic sequence in order to get rid of log-periodic oscillations. The complete system then consists of $N = 2L$ spins with periodic boundary conditions and the entropy is generally averaged over the $L$ different starting positions of the block.

For the aperiodic sequences we used in this paper, we also consider the strong aperiodic modulation limit, $r \rightarrow 0$ or $1/r \rightarrow 0$, when the average entanglement entropy is studied by a variant of the strong disorder RG method. For the aperiodic AF $XX$ and Heisenberg chains, the ground state in this limit is of an aperiodic singlet form, which is analogous to the random singlet phase of disordered chains. The entanglement entropy is then given by the number of singlet bonds connecting the block with the rest of the system. For the strongly aperiodic QIC, the ground state is of an aperiodic embedded cluster form and the entropy is obtained by counting the clusters connecting the block with the rest of the system. The implementation of the RG method is described in details where the specific problems are treated. The aperiodic sequences we study in this paper are selected in such a way to illustrate the general properties of the entropy in aperiodic quantum chains. The considered sequences are summarized in table 1, in which we have also given the stability of the two fixed points: the pure system’s fixed point ($r = 1$) and the strongly aperiodic system’s fixed point ($r = 0$). The applied methods used for the different models in the given range of the ratio $r$ are also indicated.
Table 1: Summary of sequences (Fib.: Fibonacci, Tripl.: tripling, P.D.: period doubling, Hier.: hierarchical) studied for different models (QIC, XX and XXX) in this paper. The relevance of the aperiodic perturbation at the fixed points ($r=1$ pure system, $r=0$ extreme aperiodic system) are indicated as I: irrelevant, M: marginal, R: relevant, whereas letter D refers to a noncritical dimerized ground state. The applied methods of investigations in the given range of $r$ are also shown as: FF: free-fermion numerical calculation, RG: analytical renormalization group study.

| Seq. | $r$ | QIC | XX | XXX |
|------|-----|-----|----|-----|
| Fib. | 1   | I   | M  | R   |
|      | 0   | I FF| M  | R   |
| Tripl.| 1  | M   | FF | R   |
|      | 0  | M FF| M  | R   |
| P.D. | 1  | M   | D  | D   |
|      | 0  | M RG| D  | D   |
| Hier.| 1  | M   | D  | D   |
|      | 0  | M RG| D  | D   |

**Fibonacci modulation.** – Many basic features of entropy scaling can be seen for the Fibonacci modulation, which is irrelevant for the QIC ($\nu = 1, \omega = -1$), marginal for the XX chain ($\nu = 1, \omega = 0$) and relevant for the XXX chain ($\nu = 2/3, \omega = 0$). The Fibonacci sequence, which consists of two different letters $a$ and $b$, is defined by the inflation rule: $a \rightarrow ab$ and $b \rightarrow a$, so that we have by iteration: $a, ab, aba, ababa, \ldots$, and the length of the sequence in the $l$-th iteration is the Fibonacci number, $F_l$. In the quantum chains, the couplings take two values, $J_a = r$ and $J_b = 1$, depending on the underlying letter. To check the effect of an irrelevant perturbation for the QIC, we have calculated the size-dependence of the entropy for a strong modulation, $r = 0.01$, and plotted the results in the inset of the upper panel of fig. 1. We can see that the entropy has the same scaling form as in the homogeneous system with a central charge, $c = 0.500(1)$. Hence this value is found indeed to be independent of the value of $r$.

Repeating the same type of calculation for the Fibonacci XX model, the effective central charge is found to be $r$-dependent, see the extrapolated values in the upper panel of fig. 1, which is in agreement with the marginal nature of the perturbation for this system. $c_{\text{eff}}(r)$ is monotonously decreasing with decreasing $r < 1$ and approaches a finite limiting value at $r = 0$ with a correction of $O(r^2)$.

We have calculated $\lim_{r \to 0} c_{\text{eff}}(r) \equiv c_{\text{eff}}(0)$ for the XX Fibonacci chain exactly by a variant of the strong disorder RG approach [12]. For details of the application of the method, we refer to refs. [25–28].

Fig. 1: Upper panel: average effective central charge of the Fibonacci XX chain as a function of the coupling ratio, $r$. In the inset $S_L$ vs. $\log_2 L$ is shown for the QIC at $r = 0.01$. Lower panel: the same for the tripling sequence.

A maximally entangled singlet and the words $aba$ and $ababa$ are renormalized into the letters $b'$ and $a'$, representing the new effective couplings $J_a' \approx \kappa r^2$ and $J_b' \approx \kappa^2 r^3$, respectively. For the XX model, the prefactor is $\kappa = 1$. We note that this renormalization step corresponds to the reversed triple application of the inflation transformation described earlier. The renormalized infinite chain is again a Fibonacci chain with $J_a'/J_b' = r$, so that one can repeat the transformation and finally the ground state of the system consists of a set of singlet pairs. The entanglement entropy in this case is given by the number of singlet bonds connecting the block with the rest of the system [13]. The effective central charge can be determined by calculating the difference $\Delta S = S_L - S_{L'}$ of the entanglement entropies belonging to blocks of length $L = F_{l+3}$ and $L' = F_l$. In order to do this, we notice that $L/L' = \rho = r^3$ for large $l$, where $\tau = (1 + \sqrt{5})/2$ is the golden-mean ratio. The ratio of the length of the renormalized letters is $\lambda(a')/\lambda(b') = \tau$ and the ratio of the density of the letters is given by $\mu(a')/\mu(b') = \tau$, thus the singlet bonds represented by letter $b'$, cover a fraction $n_{\text{cov}} = 1/(\tau^2 + 1)$ of the chain. In this case, we obtain

$$\Delta S = \frac{c_{\text{eff}}(0)}{3} \log_2 \rho = 2n_{\text{cov}},$$

and $c_{\text{eff}}(0) = 2/[(\tau^2 + 1) \log_2 \tau] = 0.7962$ which is in excellent agreement with the numerical findings (see the arrow in the upper panel of fig. 1). A more detailed derivation of $c_{\text{eff}}$ based on the distribution of singlet lengths in the infinite system can be found in ref. [31].

For the XXX-chain the Fibonacci modulation is a relevant perturbation and the fixed point at $r = 0$ is strongly attractive. Indeed, the RG-procedure described for the XX-model leads to the same form of renormalized couplings but with a prefactor $\kappa = 1/2$, thus the ratio
Tripling modulation. – The next sequence we consider is a tripling sequence, which is (for small perturbations) marginal both for the QIC and for the XX model \((\nu = 1, \omega = 0)\) and relevant for the XXX model \((\nu = 2/3, \omega = 0)\). This sequence consists of three different letters, \(a, b, \) and \(c\) and is defined by the inflation rule: \(a \rightarrow aba, b \rightarrow cbc\) and \(c \rightarrow abc\). In the following, we consider \(J_b > J_c > J_a\) and use the parameterization: \(J_c/J_a = J_b/J_a = r\). For the QIC, the size-dependence of the entropy for \(r = 0.01\) is shown in the inset of the lower panel of fig. 1, which is characterized by a central charge \(c_{\text{eff}} = 0.560(5)\). For the XX model, the shift in the effective central charge is even greater, see the extrapolated values in the lower panel of fig. 1. Surprisingly, this type of inhomogeneity enhances the entanglement as opposed to random and single defect perturbations in these models. We mention that in some special chains of spins with many components also random disorder can enhance entanglement [32]. In the XX case, we have also calculated the small \(r\) limiting behavior by the RG method, in which singlets form over the spins with many components also random disorder can enhance entanglement [32]. In the XX case, we have also calculated the small \(r\) limiting behavior by the RG method, in which singlets form over the spin states, in which there is a strong bond at \(L = N/2\). By eliminating this bond, an effective cluster is formed, which connects the block with the rest of the system, such that in the limit \(1/r \rightarrow 0\), the entropy \(S_L(N) = 1\) and \(c_{\text{eff}}(0) = 0\) in accordance with the numerical results presented in fig. 2. In the free-fermion representation, this result follows from eq. (4) in which there is only one mixed non-correlated fermionic mode in the subsystem with a non-zero eigenvalue \(\lambda_1 = 1/2\) \((i.e., \lambda_i = 0, \text{for } i = 2, 3, \ldots, L)\). The perturbative correction to this term for \(1/r \ll 1\) can be estimated as follows. For \(n = 2\), \(i.e., \text{for } N = 16\), we obtain the sequence \(\overline{abbab}\) after the first RG step, while by eliminating the two strong \(b\) bonds in the second RG step, a super-cluster is formed over the boundary of the block. The entanglement contribution due to this super cluster is calculated perturbatively leading to a new mixed fermionic mode
with non-zero eigenvalue: $\lambda_2 = r^{-2/3}/16$. For $n = 3$, i.e. for $N = 64$, three RG steps can be performed, which results in a new super-cluster and a new mixed mode, so that there are then two non-zero sub-leading eigenvalues: $\lambda_2 = \lambda_3 = r^{-2/3}/16$. For a general $n$, we then have $n$ embedded clusters and there are $n-1$ non-zero sub-leading eigenvalues: $\lambda_2 = \lambda_3 = \ldots = \lambda_n = r^{-2/3}/16$. The entanglement entropy for small $1/r$ indeed scales with $n-1 \sim 1/\log_2 N/N - 1$ and the effective central charge is given by: $c_{\text{eff}}(r) = r^{-2/3}(\log_2 r/8 + \text{const})$. The symmetry of the effective central charge $c_{\text{eff}}(r) = c_{\text{eff}}(1/r)$ observed numerically can also be seen in the perturbative treatment for small $r$. Hence, the function $c_{\text{eff}}(r)$ is indeed singular at $r = 0$ in accordance with the numerical results in the inset of fig. 2.

Hierarchical modulation. -- The last sequence we consider in this paper is the hierarchical one in which the couplings are given by [34]

$$J_i = J r^n, \quad i = 2^n(2m + 1), \quad n, m = 0, 1, \ldots$$  \hfill (6)

The hierarchical sequence is limit periodic [35] and can be generated through substitution with an infinite alphabet. For the QIC, the critical point is located at [8] $h_c = J r$ and by setting $J = 1/r$, we have $h_c = 1$. The excitation energy scales as $\epsilon \sim N^{-2}$, with a dynamical exponent $z = \ln(r + 1/r)/\ln 2$ [20,21]. (For the XX and XXX models this type of modulation drives the system to a dimerized phase.)

In the numerical study we considered open Ising chains of length $N = 2^n$ and calculated the entanglement entropy of the half of the system, i.e. with $L = N/2$. As can be seen in fig. 2, the entropy approaches a finite limiting value for any $r \neq 1$. Saturation of the entropy is found also at $L = N/4$ and $L = N/8$ and expected to hold for any $L = N/2^p$, $p = 1, 2, \ldots$, since at these special positions there are very small couplings, which act in the infinite system as an effective cut. Repeating the calculation with a block of size $L = [N/3]_{\text{int}}$, where $[y]_{\text{int}}$ denotes the integer part of $y$, we obtain the usual logarithmic dependence as can be seen in fig. 2. In this case $c_{\text{eff}}(r)$ is found to be a continuous function of $r$ (see the extrapolated values in the inset of fig. 2). We have thus the surprising conclusion that the scaling function $S(x = L/N) = \lim_{N \to \infty} S_L(N)/\log_2 N$ is non-analytic at $x = 2^{-p}$, $p = 1, 2, \ldots$, in contrast to the behavior in homogeneous systems [1].

Next, we turn to a perturbative RG treatment for small $r$ and focus on the block composed of the first $L$ spins at the left boundary but now we consider the thermodynamic limit $N \to \infty$. As for the period-doubling modulation, we eliminate the strongest bonds, which are at odd positions (i.e. with $n = 0$), and create renormalized two-spin clusters subjected to an effective transverse field of $h \approx h^2/J = r$. The renormalized chain has now $N/2$ sites with the same hierarchical structure of couplings. In the repeated use of the transformation, bonds with $n = 1$ (then with $n = 2$, etc) are decimated out and super-clusters with a hierarchical structure are created. Then for any value of $L$, the block is connected to the environment through one super-cluster, thus the entanglement entropy is $S_L = 1$ and $c_{\text{eff}}(0) = 0$ in accordance with the results presented in the inset of fig. 2. This result can also be derived using the free-fermionic representation of the system, when in the limit $r \to 0$, the density matrices of the non-correlated fermionic modes have eigenvalues ($\lambda_i = 1 - \lambda_i$) given by $\lambda_1 = 1/2$ and $\lambda_2 = 0$, for $L = 2, 3, \ldots$. Thus $S_L = 1$.

For a small but finite $r$, there are perturbative corrections, which depend on the value of $L$. In the simplest case $L = 3$, these corrections are due to correlations between the spin-clusters (1, 2) and (3, 4). In the non-correlated free-fermionic description, the eigenvalues are up to $O(r^2)$: $\lambda_1 = 1/2 + O(r^2)$, $\lambda_2 = r^2/4$ and $\lambda_3 = 0$, for $L = 3 \ldots L$. For $L = 5$ there are two perturbative cluster-cluster contributions which will result in $\lambda_2 = r^2/4$, whereas the other eigenvalues remain unchanged, at least up to $O(r^2)$. Generally, for $L_\kappa = 2^\kappa + 1$, $\kappa = 0, 1, \ldots$ there are $\kappa$ perturbative contributions and in the limit $\kappa r^2 \ll 1$ we have $\lambda_2 = \kappa r^2/4$. (cf. the form of perturbative cluster correction in the case of the period-doubling sequence.) Thus we obtain for the entanglement entropy

$$S_L = 1 + \kappa r^2 \left[ -\frac{1}{4} \log_2(\kappa r^2) + \frac{1}{2} \frac{1}{4 \ln 2} + O(\kappa^2 r^4) \right].$$  \hfill (7)

For a general value of $L = 2^n(2m + 1)$, the number of independent perturbative (cluster) contributions, $\kappa$, does not depend on $n$ and given by $\kappa = [\log_2 m]_{\text{int}} + 1$. In this case the entanglement entropy in the leading order is given in eq. (7). We thus conclude, that $S_L(r)$ has log-periodic oscillations in $L$ and the leading $L$ dependence is faster than logarithmic in the range ($\log_2 L)r^2 \ll 1$, although for ($\log_2 L)r^2 \gg 1$, a logarithmic $L$ dependence is expected.

Summary. -- Summing up, we have studied the entanglement properties of critical quantum spin chains, such as the antiferromagnetic Heisenberg and XX models, as well as the quantum Ising chain in the presence of aperiodic modulations of the couplings. As far as the critical properties of the systems are concerned, an aperiodic inhomonogeneity can be irrelevant, marginal or relevant, depending on the model and on the fluctuation properties of the aperiodic sequence. An irrelevant aperiodicity alters neither the logarithmic scaling of the entropy nor the constant in front of the logarithm, i.e. the growth of the entropy is determined by the central charge $c$ of the pure system. For marginal and relevant modulations, the average entropy is still scaling logarithmically with the size of the block, however, the prefactor is modified compared to that of the homogeneous system i.e. $c_{\text{eff}} \neq c$ and in addition to this, log-periodic oscillations appear. Interestingly, $c_{\text{eff}}$ can exceed the corresponding value in the homogeneous system and for marginal perturbations, it is a continuously varying function of the coupling.
ratio \( r \). In the \( r \to 0 \) limit, where the ground state of several aperiodic sequences can be exactly constructed, the average effective central charge was analytically calculated.

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