Highly entangled quantum spin chains^{*}

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Abstract

We mainly discuss a highly entangled quantum spin chain with local interactions, called as (colored) Motzkin spin chain, in which entanglement entropy for its ground state grows as a square root of the volume. Since this is beyond logarithmic behavior in the ordinary critical systems, it is important to study such a model to reveal novel features of quantum entanglement. We explain how the model yields the extraordinary growth of the entanglement entropy, and then compute the Rényi entropy for the same model. As a result, we find a new phase transition with respect to the Rényi parameter, which has been never seen in any other spin chain studied so far.

PACS: 02.30.Ik, 03.65.Ud, 03.67.Bg, 05.30.-d, 12.40.Ee

1. Introduction

Quantum entanglement is one of the most surprising features of quantum theory, and gives correlations that cannot be explained in classical mechanics. This comes from the fact that superpositions of states are possible in quantum mechanics. As a measure of the entanglement, entanglement entropy (EE) is defined as follows. First, we divide a total system S into a subsystem A and the rest B. Starting with the density matrix of the total system ρ , we obtain the reduced density matrix of A by tracing out ρ by the Hilbert space belonging to B: $\rho_A = \text{Tr}_B \rho$. Then, the EE is defined as the von Neumann entropy of ρ_A :

$$S_A = -\operatorname{Tr}_A \rho_A \ln \rho_A. \tag{1}$$

In case that the system S has a unique ground state, its density matrix is a pure state ($\rho = |\text{GS}\rangle\langle\text{GS}|$) and its von Neumann entropy is zero. However, the reduced density matrix ρ_A can become a mixed state and the EE can

^{*} The author is grateful to all the organizers and participants of the 10th Mathematical Physics Meeting (MPHYS10) for their warm hospitality and discussions. He also thanks Vladimir Korepin and Pramod Padmanabhan for collaborations and discussions.

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be nonzero. The mixed state reflects information of interactions between A and B, some of which is measured by the EE. Thus, different behavior of the EE implies difference of the structure of the ground state, i.e., different phase structure, and the EE can be regarded as a new order parameter of the system.

Let us consider ground states of quantum many-body systems with local interactions. Typically, the EE of such systems grows proportionally to the area of the boundary of A and B ("Area law") [1]. For systems with gap, it is naturally understood since correlation length is finite and interactions contributing to the EE localize around the boundary. A mathematical proof of the area law has been given in gapped systems in one spatial dimension [2]. Actually, in conformal field theory (CFT) in (1 + 1)dimensions, which is gapless, logarithmic violation of the area law has been observed [3, 4, 5], where the EE grows as $\ln L$ with L length scale of the subsystem A^{-1} .

For gapless systems in general spatial dimensions (D), it had been believed that the EE violates the area law $(S_A = O(L^{D-1}))$ by at most logarithmic corrections $(S_A = O(L^{D-1} \ln L))$. Recently, Movassagh and Shor has constructed a spin chain model that gives a counterexample for the belief. In their model, called as colored Motzkin spin chain, the EE violates the area law by a square-root correction $(S_A = O(\sqrt{L}))$ that is much larger than the logarithmic behavior [6]. Since this behavior is beyond the behavior for the ordinary critical systems, they called it as supercritical entanglement.

In this article, we explain the spin chain given by Movassagh and Shor, and discuss how such a large correction arises in the EE. Then, we compute the Rényi entropy of the spin chain and find a new phase transition that has not been observed in any other spin chain.

This paper is organized as follows. We introduce the Motzkin spin chain in section 2. and its colored version in section 3. with computing the EE for each case. After introducing the Rényi entropy in section 4., we compute the Rényi entropy for colorless and colored Motzkin spin chains in sections 5. and 6.. Section 7. is devoted to a summary and possible future directions.

2. Motzkin spin chain

Let us consider a quantum spin chain defined on sites of the one-dimensional lattice with length 2n: $\{1, 2, \dots, 2n\}$. The local Hilbert space at each site consists of spin-1 degrees of freedom, up $|u\rangle$, zero $|0\rangle$ and down $|d\rangle$, which we can correspond to up, flat and down steps, respectively. Then, each spin configuration corresponds to a length 2n walk on the two-dimensional (x, y)-plane. Fig. 1 shows an example for length 2n = 6.

¹In one spatial dimension, the boundary of A and B is point(s), and the area law means that the EE asymptotically approaches to some finite constant.



Figure 1: An example of spin configurations for length 6, and its corresponding walk. Indices of the state vectors indicate sites.

The Motzkin spin chain (or colorless Motzkin spin chain) is defined by the Hamiltonian [7]

$$H_{\rm M} = \sum_{j=1}^{2n-1} \left\{ |D\rangle_{j,j+1} \langle D| + |U\rangle_{j,j+1} \langle U| + |F\rangle_{j,j+1} \langle F| \right\} + |d\rangle_1 \langle d| + |u\rangle_{2n} \langle u|$$
(2)

with

$$|D\rangle = \frac{1}{\sqrt{2}} (|0\rangle|d\rangle - |d\rangle|0\rangle), \qquad |U\rangle = \frac{1}{\sqrt{2}} (|0\rangle|u\rangle - |u\rangle|0\rangle),$$

$$|F\rangle = \frac{1}{\sqrt{2}} (|0\rangle|0\rangle - |u\rangle|d\rangle). \tag{3}$$

In (2), three terms inside of the sum are projection operators acting to adjacent sites j and j + 1 as indices indicate, whereas the last two terms are boundary terms acting to sites 1 and 2n. The Hamiltonian consists of a sum of local projection operators. Since projection operators are positive-semi definite operators, the Hamiltonian is also. Therefore, if we find a zero-energy eigenstate for (2), it must be a ground state of the system. Such a ground state is a zero-energy ground state in terms of walks. First, the boundary terms forbid a down (up) step at the left (right) edge. Second, the projection operators with respect to the three states (3) mean that a sum of walks corresponding to the ground state should be invariant under the three moves at any adjacent two steps:

From these, it turns out that the zero-energy ground state is unique and corresponds to random walks from (0,0) to (2n,0) without entering the

region y < 0. Such a kind of random walks is called as Motzkin walk, which is the origin of the name of the spin chain. For example, the ground state for length 2n = 4 is

$$|P_4\rangle = \frac{1}{\sqrt{9}} [|0000\rangle + |ud00\rangle + |0ud0\rangle + |00ud\rangle + |u0d0\rangle + |0u0d\rangle + |u00d\rangle + |udud\rangle + |uudd\rangle]$$
(5)

and the corresponding Motzkin walk is given as



We pick a left-half of the system $\{1, 2, \dots, n\}$ as a subsystem A and compute the EE. The ground state is decomposed as a linear combination of the tensor product of a state belonging to A and a state belonging to the rest $B = \{n + 1, \dots, 2n\}$ (Schmidt decomposition):

$$|P_{2n}\rangle = \sum_{h=1}^{n} \sqrt{p_{n,n}^{(h)}} \left| P_n^{(0\to h)} \right\rangle \otimes \left| P_n^{(h\to 0)} \right\rangle,\tag{7}$$

where $|P_n^{(0\to h)}\rangle$ is a sum of states, corresponding to length-*n* walks from (0,0) to (n,h) and belonging to *A*, while $|P_n^{(h\to 0)}\rangle$ belongs to *B*. By using the number of the walks of $|P_{2n}\rangle$ denoted by M_{2n} and that of $|P_n^{(0\to h)}\rangle$ by $M_n^{(h)}$, $p_{n,n}^{(h)}$ in the coefficient is expressed as $p_{n,n}^{(h)} = (M_n^{(h)})^2 / M_{2n}$. From combinatorics, the numbers are given by

$$M_{2n} = \sum_{k=0}^{n} \frac{1}{k+1} {\binom{2k}{k}} {\binom{2n}{2k}},$$

$$M_{n}^{(h)} = \sum_{r=0}^{n-h} \frac{1+(-1)^{n-r+h}}{2} {\binom{n}{r}} \frac{h+1}{\frac{n-r+h}{2}+1} {\binom{n-r}{\frac{n-r+h}{2}}}, \quad (8)$$

and $p_{n,n}^{(h)}$ asymptotically behaves as

$$p_{n,n}^{(h)} \sim \frac{3\sqrt{6}}{\sqrt{\pi}} \frac{(h+1)^2}{n^{3/2}} e^{-\frac{3}{2}\frac{(h+1)^2}{n}} \times \left[1 + O(n^{-1})\right] \qquad (n \to \infty).$$
(9)

From the density matrix of the ground state $\rho = |P_{2n}\rangle\langle P_{2n}|$, the EE is obtained as

$$S_A = -\sum_{h=0}^n p_{n,n}^{(h)} \ln p_{n,n}^{(h)}, \qquad (10)$$

whose asymptotic form becomes

$$S_A \sim \frac{1}{2} \ln n + \frac{1}{2} \ln \frac{2\pi}{3} + \gamma - \frac{1}{2}$$
 (11)

with γ being the Euler constant. We suppressed terms vanishing as $n \to \infty$.

Although (11) violates the area law logarithmically, the system cannot be described by relativistic CFT. Another investigation shows that the gap of the system behaves like $O(n^{-z})$ with $z \ge 2$, whereas the gap of the relativistic CFT scales as $O(n^{-1})$ [6]. We will present another evidence for this issue in computing Rényi entropy.

3. Colored Motzkin spin chain

In this section, we discuss a spin chain obtained by adding color degrees of freedom to the up and down spins in the model in the previous section. Let us add s kinds of color degrees of freedom in the up and down spins, namely $|u^k\rangle$ and $|d^k\rangle$ $(k = 1, \dots, s)$. As we will see, this contributes to the square-root violation of the area law.

The Hamiltonian is defined as a sum of projection operators:

$$H_{cM,s} = \sum_{j=1}^{2n-1} \sum_{k=1}^{s} \left\{ \left| D^{k} \right\rangle_{j,j+1} \left\langle D^{k} \right| + \left| U^{k} \right\rangle_{j,j+1} \left\langle U^{k} \right| + \left| F^{k} \right\rangle_{j,j+1} \left\langle F \right| \right\} + \sum_{j=1}^{2n-1} \prod_{j,j+1}^{cross} + \sum_{k=1}^{s} \left\{ \left| d^{k} \right\rangle_{1} \left\langle d^{k} \right| + \left| u^{k} \right\rangle_{2n} \left\langle u^{k} \right| \right\},$$
(12)

where $|D^k\rangle$, $|U^k\rangle$ and $|F^k\rangle$ are given in (3) with d and u replaced by d^k and u^k , respectively. The term

$$\Pi_{j,j+1}^{\text{cross}} \equiv \sum_{k \neq k'} \left| u^k \right\rangle_j \left| d^{k'} \right\rangle_{j+1} \left\langle u^k \right|_j \left\langle d^{k'} \right|_{j+1}$$
(13)

is a peculiar to the colored model, which realizes color-matched up-down pairs in zero-energy states.

From similar argument to the previous section, we can see that (12) has a unique zero-energy eigenstate corresponding to colored Motzkin walk. For length 2n = 4 case, the ground state and the corresponding colored Motzkin walk are

$$|P_{4,s}\rangle = \frac{1}{\sqrt{1+6s+2s^2}} \Biggl[|0000\rangle + \sum_{k=1}^{s} \left\{ \left| u^k d^k 00 \right\rangle + \left| 0u^k d^k 0 \right\rangle + \left| 00u^k d^k \right\rangle + \left| u^k 00d^k \right\rangle + \left| u^k 00d^k \right\rangle \right\} + \sum_{k,k'=1}^{s} \left\{ \left| u^k d^k u^{k'} d^{k'} \right\rangle + \left| u^k u^{k'} d^{k'} d^k \right\rangle \right\} \Biggr]$$
(14)

and

The number in the normalization $1 + 6s + 2s^2$ gives the number of the colored Motzkin walks of length 4.

In order to compute the EE of the half chain, let us consider the Schmidt decomposition of the ground state $|P_{2n,s}\rangle$. We divide any path of the colored Motzkin walks from (0,0) to (2n,0) into two length-*n* paths, corresponding to the subsystems *A* and *B*. For the midpoint (n,h) in the division, the left-half path from (0,0) to (n,h) has colors of *h* up-steps unmatched inside *A*, which should be matched to colors of *h* down steps in the right-half path from (n,h) to (2n,0). We show an example of length 2n = 8 and h = 2 in Fig. 2.

 κ_m denotes a color of the unmatched up-step from height m-1 to m in the left-half. By expressing the left-half (right-half) path with unmatched colors $\kappa_1, \dots, \kappa_h$ as $P_{n,s}^{(0\to h)}(\{\kappa\})$ ($P_{n,s}^{(h\to 0)}(\{\kappa\})$), the Schmidt decomposition has the form

$$|P_{2n,s}\rangle = \sum_{h=0}^{n} \sum_{\kappa_1=1}^{s} \cdots \sum_{\kappa_h=1}^{s} \sqrt{p_{n,n,s}^{(h)}} \Big| P_{n,s}^{(0\to h)}(\{\kappa\}) \Big\rangle \otimes \Big| P_{n,s}^{(h\to 0)}(\{\kappa\}) \Big\rangle.$$
(16)

The number of paths in the colored Motzkin walks of length 2n is denoted by $M_{2n,s}$, and the number of $P_{n,s}^{(0\to h)}(\{\kappa\})$ by $\tilde{M}_{n,s}^{(h)}$. Then, $p_{n,n,s}^{(h)} =$



Figure 2: Division of a path with length 2n = 8 and h = 2. The colors k and k' are matched inside A and B respectively, whereas the colors κ_1 and κ_2 are matched across the boundary.

$$\left(\tilde{M}_{n,s}^{(h)}\right)^{2}/M_{2n,s}.$$
 The numbers are obtained by combinatorics as

$$M_{2n,s} = \sum_{k=0}^{n} \frac{1}{k+1} \binom{2k}{k} \binom{2n}{2k} s^{k},$$

$$M_{n,s}^{(h)} = \sum_{r=0}^{n-h} \frac{1+(-1)^{n-r+h}}{2} \binom{n}{r} \frac{h+1}{\frac{n-r+h}{2}+1} \binom{n-r}{\frac{n-r+h}{2}} s^{\frac{n-r+h}{2}}.$$
(17)

Assuming $n,r,n-r\pm h\gg 1,$ we evaluate the sums by the saddle point method, and obtain

$$p_{n,n,s}^{(h)} \sim \frac{s^{-h}}{\sqrt{\pi} s^{1/4}} \frac{(2n)^{3/2}}{(2\sqrt{s}+1)^{2n+\frac{3}{2}}} \frac{n^{2n+1}}{r_0^{2n+3}} \frac{(h+1)^2}{[4sn^2 - (4s-1)h^2]^{1/2}} \times \left(\frac{n-r_0-h}{n-r_0+h}\right)^{h+1} \times \left[1+O(n^{-1})\right],$$
(18)

where the saddle point value of r is $r_0 + O(n^0)$ with

$$r_0 \equiv \frac{n}{4s-1} \left[-1 + \sqrt{4s - (4s-1)\frac{h^2}{n^2}} \right].$$
 (19)

When, $h \leq O(n^{1/2})$, (18) reduces to

$$p_{n,n,s}^{(h)} \sim \frac{\sqrt{2} \, s^{-h}}{\sqrt{\pi} \, (\sigma n)^{3/2}} \, (h+1)^2 e^{-\frac{(h+1)^2}{2\sigma n}} \times \left[1 + O(n^{-1})\right] \tag{20}$$

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with $\sigma = \sqrt{s}/(2\sqrt{s}+1)$. For the density matrix of the ground state $\rho = |P_{2n,s}\rangle\langle P_{2n,s}|$, the EE is obtained as

$$S_A = -\sum_{h=0}^n s^h p_{n,n,s}^{(h)} \ln p_{n,n,s}^{(h)}, \qquad (21)$$

where the factor s^h arises from the sums of κ 's in (16). Here, since $h \leq O(n^{1/2})$ dominantly contributes to the sum, we may use (20) in evaluating the EE. The result is

$$S_A \sim (2\ln s)\sqrt{\frac{2\sigma n}{\pi}} + \frac{1}{2}\ln n + \frac{1}{2}\ln(2\pi\sigma) + \gamma - \frac{1}{2} - \ln s$$
 (22)

up to terms vanishing as $n \to \infty$. The first term grows as $O(\sqrt{n})$ and provides a new violation of the area law much greater than the logarithm that have ever seen. This reproduces the result in the colorless case (11) in the limit $s \to 1$. We can see that the leading term of S_A comes from the expectation value of $h \ln s$ under the weight $s^h p_{n,n,s}^{(h)} \sim e^{-\frac{(h+1)^2}{2\pi n}}$. Due to the Gaussian distribution, the expectation value scales as $\sqrt{n} \ln s$.

For spin-1/2 case, a model exhibiting the same square-root violation has been constructed [8, 9]. By introducing a parameter that controls the randomness of the walks, models realizing the extensive EE that scales as O(n) have also been discovered [10, 11, 12].

4. Rényi entropy

Rényi entropy is a genralization of the EE and defined by [13]

$$S_{A,\alpha} = \frac{1}{1-\alpha} \ln \operatorname{Tr}_A \rho_A^{\alpha}, \qquad (23)$$

where α is a positive number not equal to 1. It is easy to see that (23) reduces to (1) in the limit $\alpha \to 1$. The Rényi entropy has further importance than the EE, because the whole spectrum (entanglement spectrum) of ρ_A or equivalently of the entanglement Hamiltonian

$$H_{\text{ent},A} = -\ln \rho_A \tag{24}$$

can be obtained once the Rényi entropy is known as a function of α .

 $S_{A,\alpha}$ (0 < α < 1) for gapped systems in one space-dimension is proven to exhibit the area law [14]. For CFT in (1 + 1) dimensions, the Rényi entropy behaves as [3, 15]

$$S_{A,\alpha} \sim \frac{c}{6} \left(1 + \frac{1}{\alpha} \right) \ln L,$$
 (25)

where c is the central charge of the CFT, and L is a length scale of the subsystem A.

In terms of (24), the Rényi entropy takes a form analogous to the "thermal free energy" with the "temperature" $1/\alpha$:

$$S_{A,\alpha} = \frac{1}{1-\alpha} \ln \operatorname{Tr}_{A} e^{-\alpha H_{\operatorname{ent},A}}.$$
 (26)

In the next section, we compute the Rényi entropy in the colorless and colored Motzkin spin chains, and observe a new phase transition with respect to the parameter α [16].

5. Rényi entropy of colorless Motzkin spin chain

First, let us compute asymptotic behavor of the Rényi entropy (23) as $n \to \infty$ for colorless case s = 1. Since ρ_A is diagonal, (23) becomes

$$S_{A,\alpha} = \frac{1}{1-\alpha} \ln \sum_{h=0}^{n} \left(p_{n,n}^{(h)} \right)^{\alpha}$$
(27)

with $p_{n,n}^{(h)}$ given in (9). The sum $\sum_{h=0}^{n} \left(p_{n,n}^{(h)} \right)^{\alpha}$ can be evaluated by converting to an integral. Elementary calculations lead to

$$S_{A,\alpha} = \frac{1}{2} \ln n + \frac{1}{1-\alpha} \ln \Gamma \left(\alpha + \frac{1}{2} \right) \\ - \frac{1}{2(1-\alpha)} \left\{ (1+2\alpha) \ln \alpha + \alpha \ln \frac{\pi}{24} + \ln 6 \right\}$$
(28)

up to terms vanishing as $n \to \infty$. This logarithmically grows as the CFT case (25), but the dependence of α is different, which shows that the colorless Motzkin spin chain cannot be described by CFT. The result is consistent with the computation in [17].

6. Rényi entropy of colored Motzkin spin chain

Next, we consider the colored case (s > 1). What we compute is the asymptotic behavior of

$$S_{A,\alpha} = \frac{1}{1-\alpha} \ln \sum_{h=0}^{n} \left(s^{h} p_{n,n,s}^{(h)} \right)^{\alpha}$$
(29)

with (20). Note that the summand has a factor $s^{(1-\alpha)h}$. Due to this, the summand exponentially grows as h increases for $0 < \alpha < 1$, whereas it exponentially decays for $\alpha > 1$.

6.1. $0 < \alpha < 1$ case

For $0 < \alpha < 1$, we find a saddle point value of the sum with (18) as

$$h_* = n \frac{s^{1/(2\alpha)} - s^{1-1/(2\alpha)}}{s^{1/(2\alpha)} + s^{1-1/(2\alpha)} + 1} + O(n^0).$$
(30)

Since $h_* = O(n)$, here we cannot reduce (18) to (20). Saddle point analysis around (30) provides the result

$$S_{A,\alpha} = n \frac{2\alpha}{1-\alpha} \ln \left[\sigma \left(s^{\frac{1-\alpha}{2\alpha}} + s^{-\frac{1-\alpha}{2\alpha}} + s^{-1/2} \right) \right] + \frac{1+\alpha}{2(1-\alpha)} \ln n \qquad (31)$$

up to $O(n^0)$ terms. The leading term linearly grows with respect to the volume n. We should note that the limit $\alpha \to 1$ or $s \to 1$ does not commute with the large-n limit. When $\alpha \to 1$ or $s \to 1$, the leading term of O(n) in (30) vanishes, and thus the saddle point analysis cannot be trusted.

6.2. $\alpha > 1$ case

For $\alpha > 1$, it can be seen that $h \leq 1/((\alpha - 1) \ln s) = O(n^0)$ dominantly contributes to the sum (29). Using (20), we end up with

$$S_{A,\alpha} = \frac{3\alpha}{2(\alpha - 1)} \ln n + O(n^0).$$
(32)

This grows logarithmically. Again, the limit $\alpha \to 1$ or $s \to 1$ does not commute with the $n \to \infty$ limit.

6.3. Phase transition

We saw that $S_{A,\alpha}$ grow as as O(n) for $0 < \alpha < 1$, while as $O(\ln n)$ for $\alpha > 1$. There is nonanalyticity at $\alpha = 1$. As discussed in section 4., α can be regarded as the inverse temperature. From this point of view, our result means a phase transition takes place at the inverse temperature $\alpha = 1$. The transition point itself form a phase, where the EE behaves as a square-root of the volume. We summarize the result in Fig. 3.

7. Conclusions

We have mainly discussed quantum entanglement of the ground state for the Motzkin spin chain and its colored version, the latter of which significantly violates the area law by the square-root correction in spite of local interactions of the model. Then, we proceed with the computation of the Rényi entropy of the same model, and find a phase transition at the parameter $\alpha = 1$. This is a new phase transition never seen in any other spin chain studied so far.

Following future directions seem to be worth pursuing:



Figure 3: Phase diagram along the "temperature" $1/\alpha$. In high temperature, the Rényi entropy linearly grow with respect to n, to which h = O(n)dominantly contributes. On the other hand, in low temperature, the Rényi entropy logarithmically grows, to which $h = O(n^0)$ mainly contributes. Finally, the third phase appears at the transition point $\alpha = 1$, where main contribution comes from $h = O(\sqrt{n})$ to give the EE growing as \sqrt{n} .

- The behavior of the EE is beyond the logarithmic growth at the ordinary critical point. So, it is interesting to investigate if the colored Motzkin spin chain is described as any quantum field theory. If so, it would have exotic properties that are not seen in the conventional quantum field theory.
- We also constructed models exhibiting the same square-root violation of the EE by using symmetric inverse semigroups [18, 19]. It would be interesting to compute the Rényi entropy for the systems.
- If we construct a higher-dimensional analog of the model, its ground state would be expressed as a sum of higher-dimensional objects, namely a sum of surfaces for a two-dimensional model. It could have some connection to string theory.
- From the viewpoint of gauge/gravity duality or holography, it would be interesting to interpret the square-root violation of the EE as a geodesic of some bulk space geometry. Since the same square-root scaling has been discovered for a geodesic in a two-dimensional fluctuating surface, i.e., two-dimensional quantum gravity [20, 21], This direction might provide a new formulation of quantum gravity.

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