Power law violation of the area law in quantum spin chains

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Entanglement between two quantum systems is a non-classical correlation between them. Entanglement is a feature of quantum mechanics which does not appear classically, and it serves as a resource for quantum technologies. In condensed matter theory, the area law says that the amount of entanglement between a subsystem and the rest of the system is proportional to the area of the boundary of the subsystem [1]. A system that obeys an area law can be simulated more efficiently than an arbitrary quantum system, and an area law provides useful information about the low-energy physics of the system [1–3]. The area law has only been proved for one-dimensional systems with a constant-energy spectral gap [4]. However, it is widely believed that for physically reasonable quantum systems, the area law could not be violated by more than a logarithmic factor in the system's size [5]. Here, we introduce a class of exactly solvable one dimensional models that have exponentially more entanglement than previously expected, and violate the area law by a square root factor. In addition to using recent advances in quantum information theory, we have drawn upon various branches of mathematics in our work. We hope that the tools we have developed may be useful for other problems in physics as well.

The study of quantum many-body systems (QMBS) is the study of matter. One of the properties of the QMBS is the amount of entanglement contained in them. Entanglement can be used as a resource for quantum technologies and information processing [6]; however, at a fundamental level it provides information about the quantum state of matter such as near criticality [3, 7]. Moreover, systems that posses a large amount of entanglement are usually hard to simulate on a classical computer [1, 2]. The area law says that entanglement entropy between two subsystems of a system is proportional to the area of the boundary between them. The ground state and low energy excited states of a QMBS are expected to obey the area law up to a logarithmic factor [1]. A generic state does not obey an area law [8]; therefore obeying an area law implies that a QMBS possesses a lot less amount of quantum correlations than generically expected.

How hard is it to simulate QMBS? How much entanglement can simple physical quantum systems posses? One can imagine that any given problem has inherent constraints such as underlying symmetries, locality of interaction [9], etc. that restrict the states to reside on special sub-manifolds and render their efficient simulation.

The interactions in QMBS are usually, to a good approximation, local [9] a consequence of which is the sub-volume scaling of the entanglement entropy [1]. The rigorous proof of an general area law does not exist; however, Hastings proved that it holds for one dimensional gapped systems [4]. That is 1D gapped systems have a constant, independent of the number of particles, amount of entanglement. Later Wolf et al proved that the information contained in part of a system in thermal equilibrium obeys an area law [10]. Brandão and Horodecki showed that in 1D, exponential decay of correlations implies an area law as expected [11].

Since the AKLT model [12] we have come to believe that one dimensional systems are typically easy to simulate. Later density matrix renormalization group (DMRG) [13] and its natural representation by matrix product states (MPS) [14, 15] gave systematic recipes for truncating the

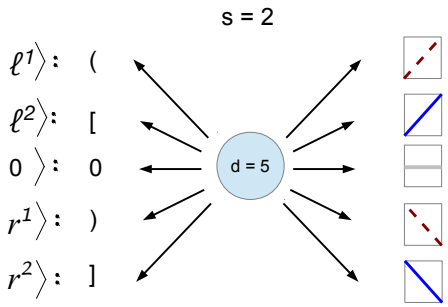

Figure 1: Labeling the states for $s = 2$.

Hilbert space based on ignoring zero and small singular values in specifying the states of 1D systems. DMRG and MPS have been tremendously successful in practice for capturing the properties of QMBS in physics and chemistry [16–19]. One wonders about the limitations of DMRG.

Swingle and Senthil [5] defined what constitutes a "physically reasonable" model and based on scaling arguments argued that local Hamiltonians with unique ground states can violate the area law by at most a $\log(n)$ factor, where n is the number of particles. This implies that $\log(n)$ is the maximum expected entanglement entropy in physical spin chains. There are various interesting examples of Hamiltonians [20, 21] that have larger, even linear, scaling of entanglement entropy with the system's size but these do not satisfy the "physically reasonable" criteria.

Bravyi et al [22] proposed the first example of a frustration free (FF) translationally invariant spin-1 chain with a local Hamiltonian that has a unique ground state and non-trivial entanglement. It was found that the Schmidt rank is $\chi = n+1$ and that the entanglement entropy $S = \frac{1}{2}\log n + c$ where c is a constant. Moreover, the gap was proved to be poly$(1/n)$.

We generalize the spin-1 model of Bravyi et al [22] to all integer spin-s chains, whereby we introduce a class of exactly solvable models that are physical and exhibit signatures of criticality, yet violate the area law by a power law. The proposed Hamiltonian is local and translationally invariant in the bulk. We prove that it is FF and has a unique ground state. Moreover, we prove that the energy gap scales as n^{-c}, where using the theory of Brownian excursions we prove that the constant $c \geq 2$. This rules out the possibility of these models being describable by a conformal field theory and it improves the previous bounds in [22]. We analytically show that the Schmidt rank grows exponentially with n and that the half-chain entanglement entropy to the leading order scales as $\sqrt{n}$. Lastly, we introduce an external field which allows us to remove the boundary terms yet retain the desired properties of the model. We now describe the details of the model.

Let us consider an integer spin$-s$ chain of length $2n$. It is convenient to label the $d = 2s+1$ spin states by $\{0, \ell^1, \ell^2, \cdots, \ell^s, r^1, r^2, \cdots, r^s\}$ where ℓ means a left parenthesis (or a step up) and r a right parenthesis (or a step down) as shown in Fig. 1. We distinguish each *type* of steps (or parenthesis) by associating a color from the s colors shown as superscripts on ℓ and r.

A Motzkin walk on $2n$ steps is any walk from $(x, y) = (0, 0)$ to $(x, y) = (2n, 0)$ with steps $(1, 0)$, $(1, 1)$ and $(1, -1)$ that never passes below the x-axis, i.e., $y \geq 0$. An example of such a walk is shown in Fig. 2. The height in the middle is $0 \leq m \leq n$ which results from m steps up with the balancing steps down on the second half of the chain. In our model the unique ground state is the $s-$colored Motzkin state which is defined to be the uniform superposition of all s colorings of Motzkin walks on $2n$ steps. The nonzero heights in the middle is the source of the mutual information between the two halves and the large entanglement entropy of the half-chain (Fig. 2).

The Schmidt rank is $\frac{s^{n+1}-1}{s-1} \approx \frac{s^{n+1}}{s-1}$, and using a two dimensional saddle point method, the

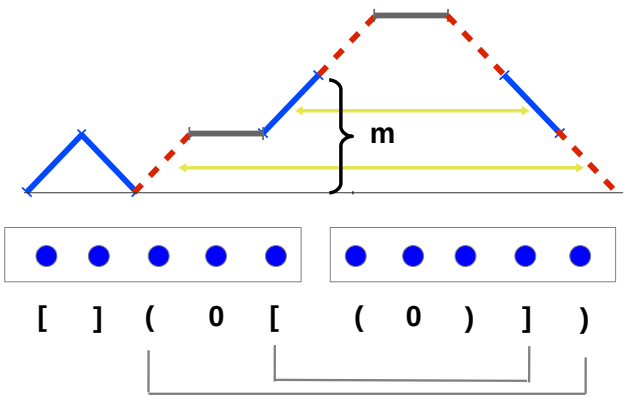

Figure 2: A Motzkin walk with $s = 2$ colors of length $2n = 10$. The height m quantifies the degree of correlation between the two halves.

half-chain entanglement entropy asymptotically is

$$S \;=\; 2\log_2(s)\,\sqrt{\frac{2\sigma}{\pi}}\,\sqrt{n} + \frac{1}{2}\log_2(2\pi\sigma n) + \left(\gamma - \frac{1}{2}\right)\log_2 e \quad \text{bits}$$

where $\sigma = \frac{\sqrt{s}}{2\sqrt{s}+1}$ and γ is the Euler constant. The ground state is a pure state (which we call the Motzkin state), whose entanglement entropy is zero. However, the entanglement entropy quantifies the amount of disorder produced (i.e., information lost) by ignoring half of the chain. The leading order $\sqrt{n}$ scaling of the entropy establishes that there is a large amount of quantum correlations between the two halves.

Consider the following local operations to any Motzkin walk: interchanging zero with a non-flat step (i.e., $0r^k \leftrightarrow r^k 0$ or $0\ell^k \leftrightarrow \ell^k 0$) or interchanging a consecutive pair of zeros with a peak of a given color (i.e., $00 \leftrightarrow \ell^k r^k$). Any $s-$colored Motzkin walk can be obtained from another one by a sequence of these local changes. To construct a local Hamiltonian with projectors as interactions that has the uniform superposition of the Motzkin walks as its zero energy ground state, each of the local terms of the Hamiltonian has to annihilate states that are symmetric under these interchanges. Local projectors as interactions have the advantage of being robust against certain perturbations [23]. This is important from a practical point of view and experimental realizations.

Therefore, the local Hamiltonian, with projectors as interactions, that has the Motzkin state as its unique zero energy ground state is

$$H = \Pi_{boundary} + \sum_{j=1}^{2n-1} \Pi_{j,j+1} + \sum_{j=1}^{2n-1} \Pi^{cross}_{j,j+1}, \tag{1}$$

where $\Pi_{j,j+1}$ implements the local changes discussed above and is defined by

$$\Pi_{j,j+1} \equiv \sum_{k=1}^{s} \Big[R^k\rangle_{j,j+1}\langle R^k + L^k\rangle_{j,j+1}\langle L^k + \varphi^k\rangle_{j,j+1}\langle\varphi^k\Big]$$

with $R^k\rangle \sim \big[0r^k\rangle - r^k 0\rangle\big]$, $L^k\rangle \sim \big[0\ell^k\rangle - \ell^k 0\rangle\big]$ and $\varphi^k\rangle \sim \big[00\rangle - \ell^k r^k\rangle\big]$. The projectors $\Pi_{boundary} \equiv \sum_{k=1}^{s}\big[r^k\rangle_1\langle r^k + \ell^k\rangle_{2n}\langle\ell^k\big]$ select out the Motzkin state by excluding all walks that start and end at non-zero heights. Lastly, $\Pi^{cross}_{j,j+1} = \sum_{k\neq i}\ell^k r^i\rangle_{j,j+1}\langle\ell^k r^i$ ensures that balancing is

well ordered (i.e., prohibits $00 \leftrightarrow \ell^k r^i$); these projectors are required only when $s > 1$ and do not appear in [22].

The difference between the ground state energy and the energy of the first excited state is called the gap. One says a system is gapped when the difference between the two smallest energies is at least a fixed constant in the thermodynamical limit ($n \to \infty$). Otherwise the system is gapless.

Whether a system is gapped and, when gapless, the scaling by which the gap vanishes as a function of the the system's size, have important consequences for its physics. For example, gapped systems have exponentially decaying correlation functions [21], and quantum critical systems are necessarily gapless [24]. Moreover, systems that obey a conformal field theory are gapless but the gap must vanish as $1/n$ [25]. Therefore, to quantify the physics, it is desirable to find new techniques for analyzing the gap that can be applied in other scenarios.

The model proposed here is gapless and the gap scales as n^{-c} where $c \geq 2$ is a constant. We prove this by finding two function both of which are inverse powers of n such that the gap is always smaller than one of them (called an upper bound) and greater than the other (called a lower bound). We utilize techniques from various branches of mathematics and computer science.

To prove an upper bound on the gap one needs a state $\phi\rangle$ that has a small constant overlap with the ground state and such that $\langle\phi|H|\phi\rangle \geq \mathcal{O}\left(n^{-2}\right)$. Take

$$\phi\rangle = \frac{1}{\sqrt{M_{2n}}} \sum_{m_p} e^{2\pi i \tilde{\theta} \tilde{A}_p} \; m_p\rangle, \tag{2}$$

where the sum is over all Motzkin walks, M_{2n} is the total number of Motzkin walks on $2n$ steps, $\tilde{A}_p$ is the area under the Motzkin walk m_p and $\tilde{\theta}$ is a constant to be determined by the condition of a small constant overlap with the ground state. The overlap with the ground state is defined by $\langle \mathcal{M}_{2n}|\phi\rangle = (1/M_{2n}) \sum_{m_p} e^{2\pi i \tilde{\theta} \tilde{A}_p}$. As $n \to \infty$, the random walk converges to a Wiener process [26] and a random Motzkin walk converges to a Brownian excursion [27]. We scale the walks such that they take place on the unit interval. The scaled area is denoted by A and $\tilde{\theta} \to \theta$. In this limit, the overlap becomes (see Fig. 3)[1]

$$\lim_{n\to\infty} \langle \mathcal{M}_{2n}|\phi\rangle \approx F_A(\theta) \equiv \int_0^\infty f_A(x)\, e^{2\pi i x \theta} dx \quad , \tag{3}$$

where $f_A(x)$ is the probability density function for the area of the Brownian excursion [28] shown in Fig. 3. In Eq. 3, taking $\theta \ll \mathcal{O}(1)$, gives $\lim_{n\to\infty} \langle \mathcal{M}_{2n}|\phi\rangle \approx 1$ because it becomes the integral of a probability distribution. However, taking $\theta \gg \mathcal{O}(1)$ gives a highly oscillatory integrand that nearly vanishes. To have a small constant overlap with the ground state, we take θ to be the standard of deviation of $f_A(x)$. Direct calculation then gives $\langle\phi|H|\phi\rangle = \mathcal{O}\left(n^{-2}\right)$. This upper bound decisively excludes the possibility of the model being describable by a conformal field theory [29].

Using various ideas in perturbation theory, computer science, and mixing times of Markov chains we obtain a lower bound on the gap that scales as n^{-c}, where $c \gg 1$. The lower bound on the gap is essentially an extension of the previous work [22]. Since it might be of independent interest in other contexts, we present a combinatorial and self-contained exposition of the proof in the SI, different in some aspects from that given in [22].

The model above has a unique ground state because the boundary terms select out the Motzkin state among all other walks with different fixed initial and final heights. Without the boundary projectors, all walks that start at height m_1 and end at height m_2 with $-2n \leq m_1, m_2 \leq 2n$ are ground states. For example, when $s = 1$, the ground state degeneracy grows quadratically with the

[1] $F_A(\theta)$ is the Fourier transform of the probability density function which is called the characteristic function.

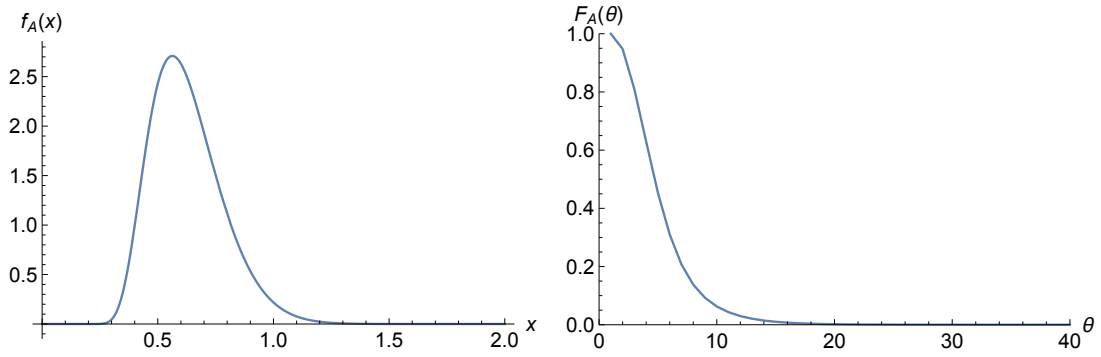

Figure 3: Left: Plot of the probability density of the area of a Brownian excursion $f_A(x)$ on $[0,1]$. Right: Fourier transform of $f_A(x)$ as defined by Eq. 3.

system's size $2n$ and exponentially when $s > 1$.

For the $s = 1$ case, if we impose periodic boundary conditions, then the the superposition of all walks with an excess of k left (right) parentheses is a ground state. This gives $4n + 1$ degeneracy of the ground state, which include unentangled product states.

When $s > 1$, each one of the walks with k excess left (right) parenthesis can be colored exponentially many ways; however, they will not be product states. Consider an infinite chain $(-\infty, \infty)$ and take $s > 1$. There is a ground state of this system that corresponds to the balanced state, where on average for each of the types of parentheses, the state contains as many ℓ^i as r^i. Suppose we restrict our attention to any block of n consecutive spins. This block contains the sites $j, j+1, \ldots, j+n-1$, which is a section of a random walk. Let us assume that it has initial height m_j and final height m_{j+n-1}. Further, let us assume that the minimum height of this section is m_k with $j \leq k \leq j+n-1$. From the theory of random walks, the expected values of $m_j - m_k$ and of $m_{j+n-1} - m_k$ are $\Theta(\sqrt{n})$. The color and number of any unmatched left parentheses in this block of n spins can be deduced from the remainder of the infinite walk. Thus a consecutive block of n spins has an expected entanglement entropy of $\Theta(\sqrt{n})$ with the rest of the chain. A similar argument shows that any block of n spins has an expected half-block entanglement entropy of $\Theta(\sqrt{n})$.

If we take $s = 1$, where the ground state can be a product state, the $\sqrt{n}$ unmatched parentheses just mentioned can be matched anywhere on the remaining left and right part of the chain. Two consecutive blocks of n spins can be unentangled because the number of parentheses that are matched in the next block is uncorrelated with the number of unmatched parentheses in the first block. However, when $s > 1$ the ordering has to match. Even though the number of unmatched parentheses in two consecutive blocks is uncorrelated, the order of the types of unmatched parentheses in them agrees.

The Hamiltonian without the boundary terms is truly translationally invariant, yet has a degenerate ground state. We now propose a model with a unique ground state and other desirable properties, such as the gap and entanglement entropy scalings. To do so, we put the system in an external field, where the model is described by the new Hamiltonian

$$\begin{aligned} \tilde{H} &\equiv H + \epsilon_0 F \\ F &\equiv \sum_{i=1}^{2n} \{r\rangle_i\langle r \ + \ \ell\rangle_i\langle \ell\} \end{aligned}$$

where, H is as before but without the boundary projectors and $0 < \epsilon_0 \ll 1$. It is clear that F treats ℓ and r symmetrically; therefore, the change in the energy as a result of applying an external field depends only on the total number of unmatched parentheses denoted by m. We denote the change

in the energy of m unmatched parenthesis by ΔE_m. When $s = 1$, the degeneracy after applying the external field will be, one for the Motzkin state, two-fold when there is a single imbalance, three-fold for two imbalances, etc. Since the energies are equal for all m imbalance states, it is enough to calculate the energy for an excited state with m imbalances resulting only from excess left parentheses. We denote these states by $g_m\rangle$, where $0 \leq m \leq 2n$.

The first order energy corrections, obtained from first order degenerate perturbation theory, are analytical shown to be

$$\frac{\epsilon_0}{2n}\langle g_m|F|g_m\rangle \approx 2\sigma n\epsilon_0 + \frac{\epsilon_0 m}{16\sqrt{s}}\left(\frac{m}{n}\right). \tag{4}$$

The physical conclusion is that the Hamiltonian without the boundary projectors, in the presence of an external field, F, has the Motzkin state as its unique ground state with energy $2\sigma n\epsilon_0$. Moreover, what used to be the rest of the degenerate zero energy states, acquire energies above $2\sigma n\epsilon_0$ that for first elementary excitations scales as $1/n$. Based on numerical work, we believe that the gap in the balanced space scales as $1/n^2$.

The energy corrections just derived do not mean that the states with m imbalances will make up for all of the the low energy excitations. For example, when $s > 1$, in the presence of an external field, the energy of states with a single crossed term will be lower than those with large m imbalances and no crossings.

Lastly for small ϵ_0 the ground state will deform away from the Motzkin state to prefer the terms with more zeros in the superposition. But as long as ϵ_0 is small, the universality of Brownian motion guarantees the scaling of the entanglement entropy. It is, however, not yet clear to us whether ϵ_0 can be tuned to a quantum critical point where the ground state has a sharp transition from highly entangled to nearly a product state. It is possible that the transition is smooth and that the entanglement continuously diminishes as ϵ_0 becomes larger. For example, in the limit where $\epsilon_0 \gg 1$, the effective unperturbed Hamiltonian is approximately F, whose ground state is simply the product state $0\rangle^{\otimes 2n}$.

Our model shows that simple 1D systems can possess high amount of quantum correlations (i.e., entanglement). From a fundamental physics perspective, it is surprising that a 1D translationally invariant quantum spin chain with a unique ground state has about $\sqrt{n}$ entanglement entropy. Moreover, this adds to the collection of exactly solvable models from which further physics can be extracted. Such a spin chain can in principle be experimentally realized, and the large amount of entanglement may serve as a resource for quantum technologies.

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[1] J. Eisert, M. Cramer, and M. Plenio, Reviews of Modern Physics **82**, 277 (2010).
[2] N. Schuch, M. M. Wolf, F. Verstraete, and J. I. Cirac, Physical review letters **100**, 030504 (2008).
[3] A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature **416**, 608 (2002).
[4] M. B. Hastings, Journal of Statistical Physics p. P08024 (2007).

[5] B. Swingle and T. Senthil, Phys. Rev. B **87**, 045123 (2013).
[6] I. Chuang and M. Nielson, *Quantum Computation and Quantum Information* (Cambridge University Press, 2000), 1st ed.
[7] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. **90**, 227902 (2003).
[8] P. Hayden, D. W. Leung, and A. Winter, Communications in Mathematical Physics **265**, 95 (2006).
[9] M. B. Hastings, lecture notes from Les Houches summer school (2010).
[10] M. M. Wolf, F. Verstraete, M. B. Hastings, and J. Cirac, Phys. Rev. Lett. **100**, 070502 (2008).
[11] F. G. S. L. Brandão and M. Horodecki, Nature Physics **9**, 721 (2013).
[12] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Comm. Math. Phys. **115**, 477 (1988).
[13] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
[14] D. Perez-Garcia, F. Verstraete, M. M. Wolf, and J. I. Cirac, Quantum Inf. Comput. 7 **401** (2007).
[15] G. Vidal, Phys. Rev. Lett. **93**, 040502 (2004).
[16] G. K.-L. Chan and S. Sharma, Ann. Rev. Phys. Chem. **62**, 465 (2011).
[17] S. R. White and D. J. Scalapino, Physical Review Letters **80**, 1272 (1998).
[18] S. R. White and R. L. Martin, J. Chem. Phys. **110**, 4127 (1999).
[19] A. Kolezhuk, H. Mikeska, and S. Yamamoto, Physical Review B **55**, 3336 (1997).
[20] S. Irani, J. Math. Phys. **51**, 022101 (2010).
[21] D. Gottesmann and M. B. Hastings, New J. Phys. **12**, 025002 (2010).
[22] S. Bravyi, L. Caha, R. Movassagh, D. Nagaj, and P. W. Shor, Phys. Rev. Lett. **109**, 207202 (2012).
[23] B. Kraus, H. P. Büchler, S. Diehl, A. Kantian, A. Micheli, and P. Zoller, Phys. Rev. A **78**, 042307 (2008), URL `http://link.aps.org/doi/10.1103/PhysRevA.78.042307`.
[24] S. Sachdev, *Quantum phase transitions* (Wiley Online Library, 2007).
[25] P. Mathieu and D. Sénéchal, *Conformal field theory* (Springer, 1997).
[26] Y. V. Prokhorov, Theory of Probability & Its Applications **1**, 157 (1956).
[27] R. T. Durrett, D. L. Iglehart, et al., The Annals of Probability **5**, 130 (1977).
[28] S. Janson et al., Probability Surveys **4**, 80 (2007).
[29] P. Calabrese and J. Cardy, J. Phys. A: Math. Theor. **42**, 504005 (2009).