Supercritical entanglement in local systems: Counterexample to the area law for quantum matter

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Quantum entanglement is the most surprising feature of quantum mechanics. Entanglement is simultaneously responsible for the difficulty of simulating quantum matter on a classical computer and the exponential speedups afforded by quantum computers. Ground states of quantum many-body systems typically satisfy an "area law": The amount of entanglement between a subsystem and the rest of the system is proportional to the area of the boundary. A system that obeys an area law has less entanglement and can be simulated more efficiently than a generic quantum state whose entanglement could be proportional to the total system's size. Moreover, an area law provides useful information about the low-energy physics of the system. It is widely believed that for physically reasonable quantum systems, the area law cannot be violated by more than a logarithmic factor in the system's size. We introduce a class of exactly solvable one-dimensional physical models which we can prove have exponentially more entanglement than suggested by the area law, and violate the area law by a square-root factor. This work suggests that simple quantum matter is richer and can provide much more quantum resources (i.e., entanglement) than expected. In addition to using recent advances in quantum information and condensed matter theory, we have drawn upon various branches of mathematics such as combinatorics of random walks, Brownian excursions, and fractional matching theory. We hope that the techniques developed herein may be useful for other problems in physics as well.

quantum matter | local Hamiltonians entanglement entropy | area law | spin chains | Hamiltonian gap

Study of quantum many-body systems (QMBSs) is the study of quantum properties of matter and quantum resources (e.g., entanglement) provided by matter for building revolutionary new technologies such as a quantum computer. One of the properties of the QMBS is the amount of entanglement among parts of the system (1, 2). Entanglement can be used as a resource for quantum technologies and information processing (2–5); however, at a fundamental level it provides information about the quantum state of matter, such as near-criticality (6, 7). Moreover, systems with high entanglement are usually hard to simulate on a classical computer (8). How much entanglement do natural QMBSs possess? What are the fundamental limits on simulation of physical systems?

The area law says that entanglement entropy between two subsystems of a system is proportional to the area of the boundary between them. A generic state does not obey an area law (9); therefore, obeying an area law implies that a QMBS contains much less quantum correlation than generically expected. One can imagine that any given system has inherent constraints such as underlying symmetries and locality of interaction that restrict the states to reside on special submanifolds rendering their simulation efficient (10).

Since the discovery that the Affleck–Kennedy–Lieb–Tasaki (AKLT) model (11) is exactly solvable, and that the density matrix renormalization group method (DMRG) (12) works extremely well on 1D systems, we have come to believe that 1D systems are typically easy to simulate. The DMRG and its natural representation by matrix product states (MPS) (13) gave systematic recipes for truncating the 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 matter in physics and chemistry (14, 15). We now know that generic local Hamiltonians, unlike the AKLT model, are gapless (16). One wonders about the limitations of DMRG.

The rigorous proof of a general area law does not exist; however, it holds for gapped systems in 1D (17). In the condensed matter community it is a common belief that gapped local Hamiltonians of QMBS on a D-dimensional lattice fulfill the area-law conjecture (8). That is, the entanglement entropy of a region of diameter L should scale as the area of the boundary $\mathcal{O}(L^{D-1})$ rather than its volume $\mathcal{O}(L^D)$. In the more general case, when the ground state is unique but the gap vanishes in the thermodynamical limit, it is expected that the area-law conjecture still holds, but now with a possible logarithmic correction, i.e., $S=\mathcal{O}(L^{D-1}\log L)$ (8). In other words, one expects that as long as the ground state is unique, the area law can be violated by at most a logarithmic factor. In particular, in 1D, it is expected that if we cut a chain of n interacting spins in the middle, the entanglement entropy should scale at most like $\log n$. This is based mostly on calculations done in $1+1$ conformal field theories (CFTs) (7, 18), as well as in the Fermi liquid theory (19).

This belief has been seriously challenged by both quantum information and condensed matter theorists in recent years. Motivated by hardness results in quantum complexity theory, there are various interesting examples of 1D Hamiltonian constructions (20–22) that can have larger, even linear, scaling of entanglement entropy with the system's size. In condensed matter physics, nontranslationally invariant models have been proposed and argued to violate the area law maximally (i.e., linearly for a chain) (23); Huijse and Swingle gave a supersymmetric model with some degree of fine-tuning that violates the

Significance

We introduce a class of exactly solvable models with surprising properties. We show that even simple quantum matter is much more entangled than previously believed possible. One then expects more complex systems to be substantially more entangled. For over two decades it was believed that the area law is violated by at most a logarithm in the system's size for quantum matter (i.e., interactions satisfying physical reasonability criteria clearly stated in the article). In this work we introduce a class of physically reasonable models that we can prove violate the area law by a square root, i.e., exponentially more than the logarithm.

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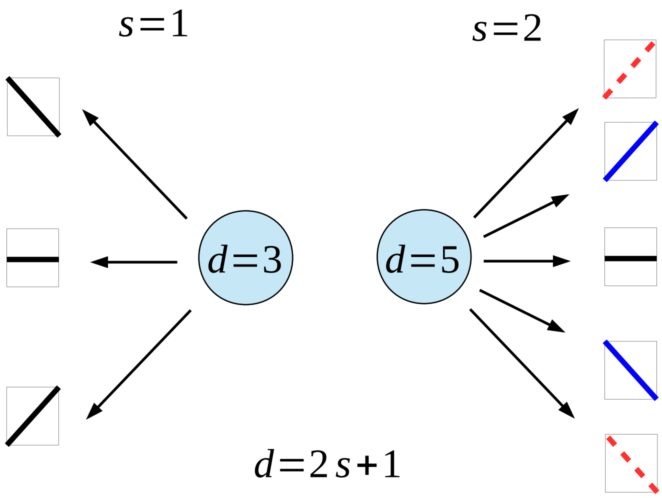

Fig. 1. Labeling the states for $s=1$ and $s=2$.

area law (24). More recently, Gori et al. (25) argued that in translationally invariant models a fractal structure of the Fermi surface is necessary for maximum violation of entanglement entropy, and using nonlocal field theories volume-law scaling was argued using simple constructions (26). Independently from ref. 20, chap. 6, Ramirez et al. constructed mirror symmetric models satisfying the volume law, i.e., maximum scaling with the system's size possible (27). The models described above are all interesting for the intended purposes but either have very large spins (e.g., $s\geq 10$) or involve some degree of fine-tuning. In particular, Irani proposed an $s=10$ spin-chain model with linear scaling of the entanglement entropy. This model is translationally invariant, but the local terms depend on the systems' size. This is a fine-tuning, and the spin dimension is quite high (21).

As noted previously, a generic state violates the area law maximally (9). It was largely believed that the ground state of "physically reasonable" models would violate the area law by at most a $\log(n)$ factor, where n is the number of particles (see ref. 28 for a review). Physically reasonable models need to have Hamiltonians that are (*i*) local, (*ii*) translationally invariant, and (*iii*) have a unique ground state. These requirements, among other things, eliminate highly fine-tuned models. This implies that $\log(n)$ is the maximum expected entanglement entropy in realistic physical spin chains.

In an earlier work, Bravyi et al. (29) proposed a spin-1 model with the ground-state half-chain entanglement entropy $S=(1/2)\log n+c$, which is logarithmic factor violation of the area law as expected during a phase transition. This model is not truly local as it depends crucially on boundary conditions. The scaling of the entanglement is exactly what one expects for critical systems.

We have found an infinite class of exactly solvable integer spin-s chain models with $s\geq 2$ that are physically reasonable and exact calculation of the entanglement entropy shows that they violate the area law to the leading order by $\sqrt{n}$ (Eq. **1**). The proposed Hamiltonian is local and translationally invariant in the bulk but the entanglement of the ground state depends on boundary projectors. We prove that it has a unique ground state and give a technique for proving the gap that uses universal convergence of random walks to a Brownian motion. We prove that the energy gap scales as n^{-c}, where using the theory of Brownian excursions we show that the constant $c\geq 2$. This bound rules out the possibility of these models being describable by a CFT. The Schmidt rank of the ground state grows exponentially with n.

We then introduce an external field. In the presence of the external field the boundary projectors are no longer needed. The model has a frustrated ground state, and its gap and entanglement are solvable. This makes the model truly local (Eq. **6**). We remark that the particle-spins can be as low as $s=2$ for $\sqrt{n}$ violation. We now describe this class of models and detail the proofs and further discussions in the *SI Appendix*. Let us consider an integer spin$-s$ chain of length $2n$. It is convenient to label the $d=2s+1$ spin states by $\{/,/,\cdots,/,0,\backslash,\backslash,\cdots,\backslash\}$ as shown in Fig. 1. Equivalently, and for better readability, we instead use the labels $\{u^1,u^2,\cdots,u^s,0,d^1,d^2,\cdots,d^s\}$ where u means a step up and d a step down. We distinguish each type of step by associating a color from the s colors shown as superscripts on u and d.

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 at the midpoint 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 are the source of the mutual information between the two halves and the large entanglement entropy of the half-chain (Fig. 3).

The Schmidt rank is $(s^{n+1}-1)/s-1\approx(s^{n+1})/s-1$, and using a 2D saddle-point method, the half-chain entanglement entropy asymptotically is (see *SI Appendix* for derivation)

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

where $\sigma=\sqrt{s}/(2\sqrt{s}+1)$ is constant and γ is the Euler constant. The ground state is a pure state (which we call the Motzkin state), whose von Neumann 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 correlation between the two halves.

Consider the following local operations to any Motzkin walk: interchanging zero with a nonflat step (i.e., $0d^k\leftrightarrow d^k0$ or $0u^k\leftrightarrow u^k0$) or interchanging a consecutive pair of zeros with a peak of a given color (i.e., $00\leftrightarrow u^kd^k$). 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 (30). This is important from a practical point of view and experimental realizations.

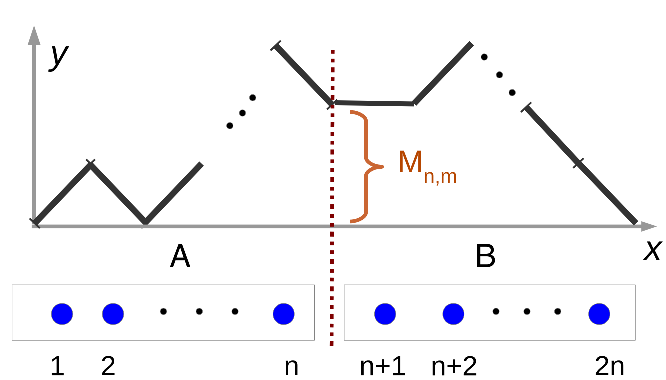

Fig. 2. Motzkin walk of length $2n$ with $s=1$. There are $M_{n,m}^2$ such walks with height m in the middle and coordinates (x,y):$(0,0)$, (n,m), $(2n,0)$.

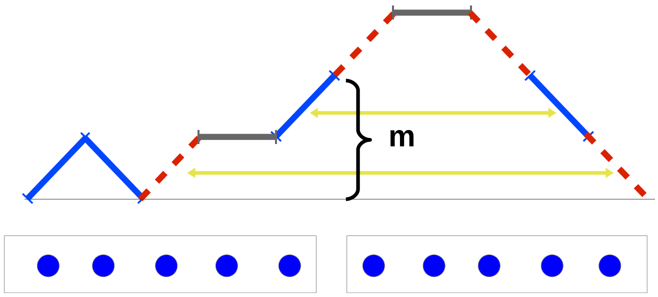

Fig. 3. Motzkin walk with $s=2$ colors of length $2n=10$. The height m quantifies the degree of correlation between the two halves.

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

$$H=\Pi_{boundary}+\sum_{j=1}^{2n-1}\Pi_{j,j+1}+\sum_{j=1}^{2n-1}\Pi_{j,j+1}^{cross}, \quad [2]$$

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

$$\Pi_{j,j+1}\equiv\sum_{k=1}^{s}\Big[|D^k\rangle_{j,j+1}\langle D^k|+|U^k\rangle_{j,j+1}\langle U^k|+|\varphi^k\rangle_{j,j+1}\langle\varphi^k|\Big], \quad [3]$$

with $|D^k\rangle\sim[|0d^k\rangle-|d^k0\rangle]$, $|U^k\rangle\sim[|0u^k\rangle-|u^k0\rangle]$, and $|\varphi^k\rangle\sim[|00\rangle-|u^kd^k\rangle]$. The projectors $\Pi_{boundary}\equiv\sum_{k=1}^{s}[|d^k\rangle_1\langle d^k|+|u^k\rangle_{2n}\langle u^k|]$ select out the Motzkin state by excluding all walks that start and end at nonzero heights. Lastly, $\Pi_{j,j+1}^{cross}\equiv\sum_{k\neq i}|u^kd^i\rangle_{j,j+1}\langle u^kd^i|$ ensures that balancing is well ordered. For example, we want to ensure that the unbalanced sequence of steps $u^3u^1u^2$ is balanced by $d^2d^1d^3$ and not, say, $d^1d^3d^2$. $\Pi_{j,j+1}^{cross}$ penalizes wrong ordering by prohibiting $00\leftrightarrow u^kd^i$ when $k\neq i$. These projectors are required only when $s>1$ and do not appear in ref. 29.

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 has important implications for its physics. When it is gapless, the scaling by which the gap vanishes as a function of the system's size has important consequences for its physics. For example, gapped systems have exponentially decaying correlation functions (22), and quantum critical systems are necessarily gapless (31). Moreover, systems that obey a CFT are gapless but the gap must vanish as $1/n$ (32). 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 functions, 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 use techniques from mathematics such as Brownian excursions and universal convergence of random walks to a Brownian motion, as well as other ideas from computer science such as linear programming and fractional matching theory. We describe the ideas and leave the details of the proofs for *SI Appendix*.

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 $\langle\phi|H|\phi\rangle\geq\mathcal{O}(n^{-2})$. Take

$$|\phi\rangle=\frac{1}{\sqrt{M_{2n}}}\sum_{m_p}e^{2\pi i\tilde{\theta}\tilde{A}_p}|m_p\rangle, \quad [4]$$

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 (33) and a random Motzkin walk converges to a Brownian excursion (34). 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. 4 for the density and Fig. 5 for its Fourier transform; $F_A(\theta)$ is the Fourier transform of the probability density function, which is called the characteristic function.)

$$\lim_{n\to\infty}\langle\mathcal{M}_{2n}|\phi\rangle\approx F_A(\theta)\equiv\int_0^\infty f_A(x)e^{2\pi ix\theta}dx, \quad [5]$$

where $f_A(x)$ is the probability density function for the area of the Brownian excursion (35) shown in Fig. 4. In Eq. **5**, 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 $\langle\phi|H|\phi\rangle=\mathcal{O}(n^{-2})$. This upper bound decisively excludes the possibility of the model being describable by a conformal field theory (18).

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 $c\gg 1$. Because it might be of independent interest in other contexts, we present a combinatorial and self-contained exposition of the proof in the *SI Appendix*, different in some aspects from that given in ref. 29.

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

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

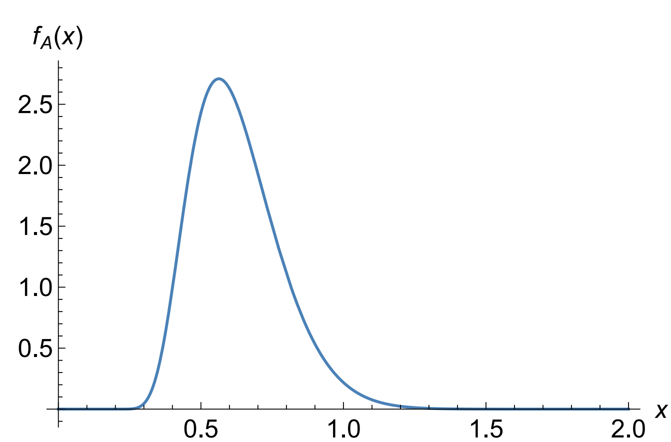

Fig. 4. Plot of the probability density of the area under a Brownian excursion $f_A(x)$ on $[0,1]$.

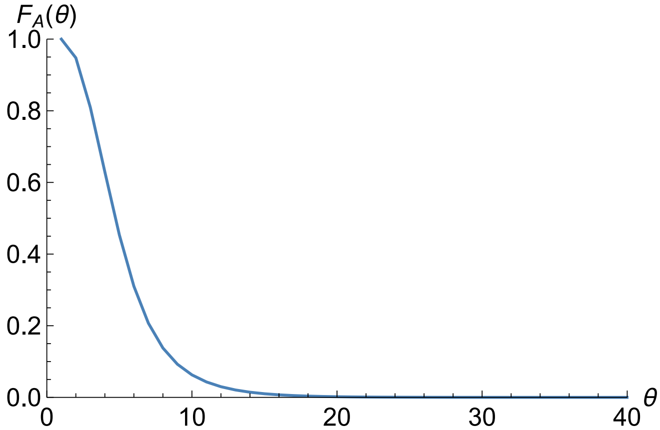

Fig. 5. Fourier transform of $f_A(x)$ as defined by Eq. **5**.

When $s>1$, each one of the walks with k excess up (down) steps can be colored exponentially many ways; however, generically 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 color, the state contains as many u^i as d^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 $j\le k\le j+n-1$. 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 step-ups 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 step-up 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 unbalanced steps that are matched in the next block is uncorrelated with the number of unbalanced steps in the first block. However, when $s>1$ the ordering has to match. Even though the number of unbalanced steps in two consecutive blocks is uncorrelated, the order of the types of unbalanced steps 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 that has the other desirable properties of the model with boundaries, such as the gap and entanglement entropy scalings as before. To do so, we put the system in an external field, where the model is described by the Hamiltonian

$$\tilde{H}\equiv H+\epsilon F$$
$$F\equiv\sum_{i=1}^{2n}\sum_{k=1}^{s}\left(|d^k\rangle_i\langle d^k|+|u^k\rangle_i\langle u^k|\right), \qquad [6]$$

where H is as before but without the boundary projectors and $\epsilon=\epsilon_0/n$ with ϵ_0 being a small positive constant. It is clear that F treats u and d symmetrically; therefore, the change in the energy as a result of applying an external field depends only on the total number of unbalanced steps denoted by m. We denote the change in the energy of m unbalanced steps by ΔE_m. When $s=1$, the degeneracy after applying the external field will be one for the Motzkin state, twofold when there is a single imbalance, threefold for two imbalances, etc. Because 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 step-ups. We denote these states by $|g_m\rangle$, where $0\le m\le 2n$.

The first-order energy corrections, obtained from first-order degenerate perturbation theory, are analytically calculated to be

$$\epsilon\langle g_m|F|g_m\rangle\approx 4\sigma\epsilon n+\frac{m\epsilon}{8\sqrt{s}}\left(\frac{m}{n}\right). \qquad [7]$$

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 $4\sigma\epsilon_0$. Moreover, what used to be the rest of the degenerate zero-energy states acquire energies above $4\sigma\epsilon_0$ that for first elementary excitations scale as $1/n^2$. Moreover, the numerical calculations indicate that the spin–spin correlation functions are flat (36). We leave further investigations for future work.

The energy corrections just derived do not mean that the states with m imbalances will make up for all of 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.

Because $\|\epsilon F\|\ll\|H\|$, 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 is small, the universality of Brownian motion guarantees the scaling of the entanglement entropy. It is, however, not yet clear to us whether ε 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 becomes larger. For example, in the limit where $|\epsilon|\gg\|H\|/\|F\|$, the effective unperturbed Hamiltonian is approximately F, whose ground state is simply the product state $|0\rangle^{\otimes 2n}$.

Our model shows that simple physical systems can be much more entangled than expected. 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 be used as a resource for quantum technologies and computation.

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