Criticality without Frustration for Quantum Spin-1 Chains

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Frustration-free (FF) spin chains have a property that their ground state minimizes all individual terms in the chain Hamiltonian. We ask how entangled the ground state of a FF quantum spin-s chain with nearest-neighbor interactions can be for small values of s. While FF spin-$1/2$ chains are known to have unentangled ground states, the case $s = 1$ remains less explored. We propose the first example of a FF translation-invariant spin-1 chain that has a unique highly entangled ground state and exhibits some signatures of a critical behavior. The ground state can be viewed as the uniform superposition of balanced strings of left and right brackets separated by empty spaces. Entanglement entropy of one half of the chain scales as $\frac{1}{2}\log n + O(1)$, where n is the number of spins. We prove that the energy gap above the ground state is polynomial in $1/n$. The proof relies on a new result concerning statistics of Dyck paths which might be of independent interest.

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The presence of long-range entanglement in the ground states of critical spin chains with only short-range interactions is one of the most fascinating discoveries in the theory of quantum phase transitions [1]. It can be quantified by the scaling law $S(L) \sim \log L$, where $S(L)$ is the entanglement entropy of a block of L spins. In contrast, noncritical spin chains characterized by a nonvanishing energy gap obey an area law [2] asserting that $S(L)$ has a constant upper bound independent of L.

One can ask how stable is the long-range ground state entanglement against small variations of Hamiltonian parameters? The scaling theory predicts [1,2] that a chain whose Hamiltonian is controlled by some parameter g follows the law $S(L) \sim \log L$ only if L does not exceed the correlation length $\xi \sim |g - g_c|^{-\nu}$, where $\nu > 0$ is the critical exponent and g_c is the critical point. For larger L the entropy $S(L)$ saturates at a constant value. Hence, achieving the scaling $S(L) \sim \log L$ requires fine-tuning of the parameter g with precision scaling polynomially with $1/L$ posing a serious experimental challenge.

The stringent precision requirement described above can be partially avoided for spin chains described by *frustration-free* (FF) Hamiltonians. Well-known (noncritical) examples of such Hamiltonians are the Heisenberg ferromagnetic chain [3], the Affleck-Kennedy-Lieb-Tasaki model [4], and parent Hamiltonians of matrix product states [5]. More generally, we consider Hamiltonians of a form $H = \sum_j g_j \Pi_{j,j+1}$, where $\Pi_{j,j+1}$ is a projector acting on spins j, $j+1$, and $g_j > 0$ are some coefficients. The Hamiltonian is called frustration-free if the projectors $\Pi_{j,j+1}$ have a common zero eigenvector ψ. Such zero eigenvectors ψ span the ground subspace of H. Clearly, the ground subspace does not depend on the coefficients g_j as long as they remain positive. This inherent stability against variations of the Hamiltonian parameters motivates a question of whether FF Hamiltonians can describe critical spin chains.

In this Letter we propose a toy model describing a FF translation-invariant spin-1 chain with open boundary conditions that has a unique ground state with a logarithmic scaling of entanglement entropy and a polynomial energy gap. Thus our FF model reproduces some of the main signatures of critical spin chains. In contrast, it was recently shown by Chen *et al.* [6] that any FF spin-$1/2$ chain has an unentangled ground state. Our work may also offer valuable insights for the problem of realizing long-range entanglement in open quantum systems with an engineered dissipation. Indeed, it was shown by Kraus *et al.* [7] and Verstraete *et al.* [8] that the ground state of a FF Hamiltonian can be represented as a unique steady state of a dissipative process described by the Lindblad equation with local quantum jump operators. A proposal for realizing such dissipative processes in cold atom systems has been made by Diehl *et al.* [9]. Prior to our work, an example of a FF spin chain with 21-dimensional spins and a linear scaling of the entanglement entropy was found by Irani [10]; see also [11]. It was conjectured in [12] that generic FF chains with d-dimensional spins and projectors of rank r have only highly entangled ground states with probability 1 provided that $d \le r \le d^2/4$ (which requires $d \ge 4$).

Main results.—We begin by describing the ground state of our model. The three basis states of a single spin will be identified with a left bracket $l \equiv [$, right bracket $r \equiv]$, and an empty space represented by 0. Hence a state of a single spin can be written as $\alpha|0\rangle + \beta|l\rangle + \gamma|r\rangle$ for some complex coefficients α, β, γ. For a chain of n spins, basis states $|s\rangle$ correspond to strings $s \in \{0, l, r\}^n$. A string s is called a *Motzkin path* [13] if and only if (i) any initial segment of s contains at least as many l's as r's and (ii) the total number of l's is equal to the total number of r's. For example, a string $lllr0rl0rr$ is a Motzkin path while $l0lrrrllr$ is not since its initial segment $l0lrrr$ has more r's than l's. By ignoring all 0's one can view Motzkin paths as balanced strings of left and right brackets. We are interested in the *Motzkin state* $|\mathcal{M}_n\rangle$, which is the uniform superposition of all Motzkin paths of length n. For example, $|\mathcal{M}_2\rangle \sim |00\rangle + |lr\rangle$ and $|\mathcal{M}_3\rangle \sim |000\rangle + |lr0\rangle + |l0r\rangle + |0lr\rangle$, and

$$|\mathcal{M}_4\rangle \sim |0000\rangle + |00lr\rangle + |0l0r\rangle + |l00r\rangle + |0lr0\rangle + |l0r0\rangle + |lr00\rangle + |llrr\rangle + |lrlr\rangle.$$

Let us first ask how entangled is the Motzkin state. For a contiguous block of spins A, let $\rho_A = \mathrm{Tr}_{j\notin A}|\mathcal{M}_n\rangle\langle\mathcal{M}_n|$ be the reduced density matrix of A. Two important measures of entanglement are the Schmidt rank $\chi(A)$, equal to the number of nonzero eigenvalues of ρ_A, and the entanglement entropy $S(A) = -\mathrm{Tr}\rho_A \log_2 \rho_A$. We will choose A as the left half of the chain, $A = \{1, \ldots, n/2\}$. We will show that

$$\chi(A) = 1 + n/2 \quad \text{and} \quad S(A) = \frac{1}{2}\log_2 n + c_n, \tag{1}$$

where $\lim_{n\to\infty} c_n = 0.14(5)$. The linear scaling of the Schmidt rank stems from the presence of locally unmatched left brackets in A whose matching right brackets belong to the complementary region $B = [1, n]\backslash A$. The number of the locally unmatched brackets m can vary from 0 to $n/2$ and must be the same in A and B leading to long-range entanglement between the two halves of the chain. In the Supplemental Material [14], we prove that the Schmidt decomposition of the Motzkin state can be written as

$$|\mathcal{M}_n\rangle = \sum_{m=0}^{n/2} \sqrt{p_m}\, |C_{0,m}\rangle_A \otimes |C_{m,0}\rangle_B, \tag{2}$$

where $|C_{0,m}\rangle$ and $|C_{m,0}\rangle$ are normalized uniform superpositions of all strings $s \in \{0, l, r\}^{n/2}$ with exactly m unmatched left and right brackets, respectively, while p_m is some probability distribution. The scaling of $S(A) = -\sum_m p_m \log_2 p_m$ can be understood by identifying Motzkin paths with trajectories of a particle hopping on a semi-infinite 1D lattice that start and end at the boundary. The Motzkin state $|\mathcal{M}_n\rangle$ then represents the uniform superposition of all such trajectories, while m is the coordinate of the particle after $n/2$ steps. Using the standard Brownian motion picture as a crude approximation, one should expect that the distribution of m has a width roughly $\sqrt{n}$ which explains the scaling $S(A) \approx (1/2)\log_2(n)$. A formal analysis performed in the Supplemental Material [14] shows that $p_m \sim m^2 \exp(-3m^2/n)$ for $n \gg 1$.

Although the definition of Motzkin paths may seem very nonlocal, we will show that the state $|\mathcal{M}_n\rangle$ can be specified by imposing local constraints on nearest-neighbor spins. Let Π be a projector onto the three-dimensional subspace of $\mathbb{C}^3 \otimes \mathbb{C}^3$ spanned by states $|0l\rangle - |l0\rangle$, $|0r\rangle - |r0\rangle$, and $|00\rangle - |lr\rangle$. Our main result is the following.

Theorem 1: The Motzkin state $|\mathcal{M}_n\rangle$ is a unique ground state with zero energy of a frustration-free Hamiltonian

$$H = |r\rangle\langle r|_1 + |l\rangle\langle l|_n + \sum_{j=1}^{n-1} \Pi_{j,j+1}, \tag{3}$$

where subscripts indicate spins acted upon by a projector. The spectral gap of H scales polynomially with $1/n$.

Discussion.—Our result raises several questions. First, one can ask what is the upper bound on the ground state entanglement of FF spin-1 chains and whether the Motzkin state achieves this bound. For example, if the Schmidt rank $\chi(L)$ for a block of L spins can only grow polynomially with L, as it is the case for the Motzkin state, ground states of FF spin-1 chains could be efficiently represented by matrix product states [15] (although finding such representation might be a computationally hard problem [15]). We conjecture that for spin-2 chains one can achieve a power law scaling of $S(A)$ in Eq. (1) by introducing two types of brackets, say, $l \equiv [$, $r \equiv]$, $l' \equiv \{$, and $r' \equiv \}$, such that bracket pairs lr and $l'r'$ are created from the "vacuum" 00 in a maximally entangled state $(|lr\rangle + |l'r'\rangle)/\sqrt{2}$. We expect the modified model with two types of brackets to obey a scaling $S(A) \sim \sqrt{n}$, while its gap will remain lower bounded by an inverse polynomial. One drawback of the model based on Motzkin paths is the need for boundary conditions and the lack of the thermodynamic limit. It would be interesting to find examples of FF spin-1 chains with highly entangled ground states that are free from this drawback. Finally, an intriguing open question is whether long-range ground state entanglement (or steady-state entanglement in the case of dissipative processes) in 1D spin chains can be stable against general local perturbations, such as external magnetic fields.

Proof of Theorem 1. To prove the first part of the theorem we shall need a more local description of Motzkin paths. Let $\Sigma = \{0, l, r\}$. We will say that a pair of strings $s, t \in \Sigma^n$ is equivalent, $s \sim t$, if s can be obtained from t by a sequence of local moves

$$00 \leftrightarrow lr, \qquad 0l \leftrightarrow l0, \qquad 0r \leftrightarrow r0. \tag{4}$$

These moves can be applied to any consecutive pair of letters. For any integers $p, q \geq 0$ such that $p + q \leq n$ defines a string

$$c_{p,q} \equiv \underbrace{r \ldots r}_{p}\underbrace{0 \ldots 0}_{n-p-q}\underbrace{l \ldots l}_{q}. \tag{5}$$

In the Supplemental Material [14] we prove the following simple fact.

Lemma 1. Any string $s \in \Sigma^n$ is equivalent to one and only one string $c_{p,q}$. A string $s \in \Sigma^n$ is a Motzkin path if and only if it is equivalent to the all-zeros string, $s \sim c_{0,0}$.

This shows that the set of all strings Σ^n can be partitioned into equivalence classes $C_{p,q}$, such that $C_{p,q}$ includes all strings equivalent to $c_{p,q}$. In other words, $s \in C_{p,q}$ if and only if s has p unmatched right brackets and q unmatched left brackets. Accordingly, the set of Motzkin paths $\mathcal{M}_n$ coincides with the equivalence class $C_{0,0}$.

Let us now define projectors "implementing" the local moves in Eq. (4). Define normalized states

$$|\phi\rangle \sim |00\rangle - |lr\rangle, \qquad |\psi^l\rangle \sim |0l\rangle - |l0\rangle, \qquad |\psi^r\rangle \sim |0r\rangle - |r0\rangle$$

and a projector $\Pi = |\phi\rangle\langle\phi| + |\psi^l\rangle\langle\psi^l| + |\psi^r\rangle\langle\psi^r|$. Application of Π to a pair of spins j, $j+1$ will be denoted $\Pi_{j,j+1}$. If some state ψ is annihilated by every projector $\Pi_{j,j+1}$, it must have the same amplitude on any pair of equivalent strings; that is, $\langle s|\psi\rangle = \langle t|\psi\rangle$ whenever $s \sim t$. It follows that a Hamiltonian $H_\sim = \sum_{j=1}^{n-1} \Pi_{j,j+1}$ is FF and the ground subspace of $H_\sim$ is spanned by pairwise orthogonal states $|C_{p,q}\rangle$, where $|C_{p,q}\rangle$ is the uniform superposition of all strings in $C_{p,q}$. The desired Motzkin state $|\mathcal{M}_n\rangle = |C_{0,0}\rangle$ is thus a ground state of $H_\sim$. (It is worth mentioning that not all states $|C_{p,q}\rangle$ are highly entangled. For example, $|C_{n,0}\rangle = |r\rangle^{\otimes n}$ is a product state.) How can we exclude the unwanted ground states $|C_{p,q}\rangle$ with $p \neq 0$ or $q \neq 0$? We note that $C_{0,0}$ is the only class in which strings never start from r and never end with l. Hence a modified Hamiltonian $H = |r\rangle\langle r|_1 + |l\rangle\langle l|_n + H_\sim$ that penalizes strings starting from r or ending with l has a unique ground state $|C_{0,0}\rangle$. This proves the first part of theorem 1.

Spectral gap.—Let $\lambda_2 > 0$ be the smallest nonzero eigenvalue of the Hamiltonian H defined in Eq. (3). An upper bound $\lambda_2 \leq O(1/\sqrt{n})$ can be easily derived by constructing a low-energy excited state as explained in the Supplemental Material [14]. The main technical contribution of this Letter is a lower bound $\lambda_2 \geq n^{-O(1)}$. Below we sketch the main ideas involved in the proof.

Recall that a string $s \in \{l, r\}^{2m}$ is called a *Dyck path* if and only if any initial segment of s contains at least as many l's as r's, and the total number of l's is equal to the total number of r's. For example, Dyck paths of length 6 are *lllrrr*, *llrlrr*, *llrrlr*, *lrlrlr*, and *lrllrr*. Let $\mathcal{D}_m$ be the set of all Dyck paths of length $2m$ and $\mathcal{D}$ be the union of all $\mathcal{D}_m$ with $2m \leq n$. We shall connect a pair of Dyck paths s, $t \in \mathcal{D}$ by an edge if and only if they are related by insertion or removal of a consecutive lr pair. This defines a graph $G = (\mathcal{D}, E)$ that we shall call a *Dyck graph*. Let $\mathcal{M}_n$ be the set of all Motzkin paths of length n.

The first step in the proof is to relate the gap of H to the gap of a stochastic matrix P describing a random walk on the Dyck graph. This step is accomplished by deforming the Hamiltonian H such that the terms responsible for creation and annihilation of pairs of brackets become a small perturbation. The FF property allows us to choose the deformation such that it does not change the ground state, while the spectral gap shrinks at most by a factor $n^{-O(1)}$. The analysis uses the projection lemma of [16] and the exact formula for the spectral gap of the Heisenberg chain found by Koma and Nachtergaele [3]. Finally, we use the standard gap-preserving reduction from stoquastic Hamiltonians [17] to stochastic matrices. It allows us to prove the following.

Lemma 2. The gap of H coincides up to a factor $n^{-O(1)}$ with the gap of a stochastic matrix P describing a random walk on the Dyck graph. For any edge (s, t) of the Dyck graph, the transition probability from s to t is $P(s,t) = \Omega(1/n^3)$ and $P(s,s) \geq 1/2$. The unique steady state is

$$\pi(s) = \frac{1}{|\mathcal{M}_n|}\binom{n}{2m} \quad \text{for } s \in \mathcal{D}_m. \tag{6}$$

Furthermore, $\pi(s)P(s,t) = \pi(t)P(t,s)$ for all $s, t \in \mathcal{D}$.

Since the proof involves a combination of well-known techniques, we defer it to the Supplemental Material [14]. Note that the gap of P refers to the difference $1 - \lambda_2(P)$, where $\lambda_2(P)$ is the second-largest eigenvalue of P.

To bound the spectral gap of P we shall connect any pair of Dyck paths s, $t \in \mathcal{D}$ by a *canonical path* $\gamma(s,t)$ on the Dyck graph $G = (\mathcal{D}, E)$, that is, a sequence $s_0, s_1, \ldots, s_l \in \mathcal{D}$ such that $s_0 = s$, $s_l = t$, and $(s_i, s_{i+1}) \in E$ for all i. The canonical paths theorem [18] shows that $1 - \lambda_2(P) \geq 1/(\rho l)$, where l is the maximum length of a canonical path and ρ is the maximum edge load defined as

$$\rho = \max_{(a,b)\in E} \frac{1}{\pi(a)P(a,b)} \sum_{s,t:\ (a,b)\in\gamma(s,t)} \pi(s)\pi(t). \tag{7}$$

The key new result that allows us to choose a good family of canonical paths is the following.

Lemma 3. Let $\mathcal{D}_k$ be the set of Dyck paths of length $2k$. For any $k \geq 1$ there exists a map $f\colon \mathcal{D}_k \to \mathcal{D}_{k-1}$ such that (i) the image of any path $s \in \mathcal{D}_k$ can be obtained from s by removing a single consecutive lr pair, (ii) any path $t \in \mathcal{D}_{k-1}$ has at least one preimage in $\mathcal{D}_k$, and (iii) any path $t \in \mathcal{D}_{k-1}$ has at most four preimages in $\mathcal{D}_k$.

The lemma allows one to organize the set of all Dyck paths $\mathcal{D}$ into a *supertree* $\mathcal{T}$ such that the root of $\mathcal{T}$ represents the empty path and such that children of any node s are elements of $f^{-1}(s)$. The properties of f imply that Dyck paths of length $2m$ coincide with level-m nodes of $\mathcal{T}$, any step away from the root on $\mathcal{T}$ corresponds to insertion of a single consecutive lr pair, and any node of $\mathcal{T}$ has at most four children. The five lowest levels of the supertree $\mathcal{T}$ are shown in Fig. 1 in the Supplemental Material [14]. Hence the lemma provides a recipe for growing long Dyck paths from short ones without overusing any intermediate Dyck paths. It should be noted that restricting the maximum number of children to four is optimal since $|\mathcal{D}_k| = C_k \approx 4^k/\sqrt{\pi}k^{3/2}$, where C_k is the kth Catalan number. Our proof of lemma 3 based on the fractional matching method can be found in the Supplemental Material [14]. This method appears to be new and might be interesting in its own right.

We can now define the canonical path $\gamma(s,t)$ from $s \in \mathcal{D}_m$ to $t \in \mathcal{D}_k$. Any intermediate state in $\gamma(s,t)$ will be represented as uv where $u \in \mathcal{D}_{l'}$ is an ancestor of s in the supertree and $v \in \mathcal{D}_{l''}$ is an ancestor of t. The canonical path starts from $u = s$, $v = \emptyset$ and alternates between shrinking u and growing v by making steps towards the root (shrink) and away from the root (grow) on the supertree. The path terminates as soon as $u = \emptyset$ and $v = t$. The shrinking steps are skipped whenever $u = \emptyset$, while the growing steps are skipped whenever $v = t$. Note that any intermediate state uv obeys

$$\min(|s|,|t|) \le |u| + |v| \le \max(|s|,|t|). \qquad (8)$$

Since any path $\gamma(s,t)$ has length at most $2n$, it suffices to bound the maximum edge load ρ. Fix the edge $(a,b) \in E$ with the maximum load. Let $\rho(m,k,l',l'')$ be the contribution to ρ that comes from canonical paths $\gamma(s,t)$ such that $a = uv \in \mathcal{D}_{l'+l''}$, where

$$s \in \mathcal{D}_m, \qquad t \in \mathcal{D}_k, \qquad u \in \mathcal{D}_{l'}, \qquad v \in \mathcal{D}_{l''},$$

and such that b is obtained from a by growing v (the case when b is obtained from a by shrinking u is analogous). The number of possible source strings $s \in \mathcal{D}_m$ contributing to $\rho(m,k,l',l'')$ is at most $4^{m-l'}$ since s must be a descendant of u on the supertree. The number of possible target strings $t \in \mathcal{D}_k$ contributing to $\rho(m,k,l',l'')$ is at most $4^{k-l''}$ since t must be a descendant of v on the supertree. Taking into account that $\pi(s)$ and $\pi(t)$ are the same for all $s \in \mathcal{D}_m$ and $t \in \mathcal{D}_k$, we arrive at

$$\rho(m,k,l',l'') \le 4^{m+k-l'-l''} \frac{\pi(s)\pi(t)}{\pi(a)P(a,b)} = \frac{\pi_m \pi_k}{\pi_{l'+l''} P(a,b)},$$

with

$$\pi_l = 4^l \binom{n}{2l} \Big/ |\mathcal{M}_n|.$$

Here we used Eq. (6). lemma 2 implies that $1/P(a,b) \le n^{O(1)}$. Furthermore, the fraction of Motzkin paths of length n that have exactly $2l$ brackets is

$$\sigma_l = C_l \binom{n}{2l} \Big/ |\mathcal{M}_n|.$$

However $C_l \approx 4^l/\sqrt{\pi} l^{3/2}$ coincides with 4^l modulo factors polynomial in $1/n$. Hence

$$\rho(m,k,l',l'') \le n^{O(1)} \frac{\sigma_m \sigma_k}{\sigma_{l'+l''}}.$$

By definition, $\sigma_l \le 1$ for all l. Also, one can easily check that σ_l as a function of l has a unique maximum at $l \approx n/3$ and decays monotonically away from the maximum. Consider two cases. Case (1): $l' + l''$ is on the left from the maximum of σ_l. From Eq. (8) one gets $\min(m,k) \le l' + l''$ and thus $\sigma_m \sigma_k \le \sigma_{\min(m,k)} \le \sigma_{l'+l''}$. Case (2): $l' + l''$ is on the right from the maximum of σ_l. From Eq. (8) one gets $\max(m,k) \ge l' + l''$ and thus $\sigma_m \sigma_k \le \sigma_{\max(m,k)} \le \sigma_{l'+l''}$. In both cases we get a bound $\rho(m,k,l',l'') \le n^{O(1)}$. Since the number of choices for m, k, l', l'' is at most $n^{O(1)}$, we conclude that $\rho \le n^{O(1)}$ and thus $1 - \lambda_2(P) \ge n^{-O(1)}$. lemma 2 now gives the desired lower bound on the gap of H.

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