Correlation length versus gap in frustration-free systems

David Gosset* Yichen Huang (黄溢辰)†

Abstract

Hastings established exponential decay of correlations for ground states of gapped quantum many-body systems. A ground state of a (geometrically) local Hamiltonian with spectral gap ϵ has correlation length ξ upper bounded as $\xi = O(1/\epsilon)$. In general this bound cannot be improved. Here we study the scaling of the correlation length as a function of the spectral gap in *frustration-free* local Hamiltonians, and we prove a tight bound $\xi = O(1/\sqrt{\epsilon})$ in this setting. This highlights a fundamental difference between frustration-free and frustrated systems near criticality. The result is obtained using an improved version of the combinatorial proof of correlation decay due to Aharonov et al.

Exponential decay of correlations is a basic feature of the ground space in gapped quantum many-body systems. The setting is as follows. We consider a geometrically local Hamiltonian H which acts on particles of constant dimension s, i.e., the Hilbert space is $(\mathbb{C}^s)^{\otimes n}$ where n is the total number of particles. The particles are located at the sites of a finite lattice (of some arbitrary dimension). We write the Hamiltonian as

$$H = \sum_i H_i,$$

where distinct terms H_i, H_j are supported on distinct subsets of particles. Here the support of a term H_i is the set of particles on which it acts nontrivially. We assume that H has constant range r with respect to the usual distance function d on the lattice, the shortest path metric. This means that the diameter of the support of each term H_i is upper bounded by r (e.g., $r = 2$ for nearest-neighbor interactions). Without loss of generality we assume that the smallest eigenvalue of each term H_i is equal to zero, and that $\|H_i\| \leq 1$.

If H has a unique ground state $|\psi\rangle$ and spectral gap ϵ, connected correlation functions decay exponentially as a function of distance [13, 22, 16]. In particular

$$|\langle\psi|AB|\psi\rangle - \langle\psi|A|\psi\rangle\langle\psi|B|\psi\rangle| \leq C\|A\|\|B\|e^{-d(A,B)/\xi}, \qquad \xi = O(1/\epsilon) \tag{1}$$

where $d(A, B)$ denotes the distance between the supports of two (arbitrary) local observables A, B, and C is a positive constant which depends on r and the lattice. In the transverse field

*Walter Burke Institute for Theoretical Physics and Institute for Quantum Information and Matter, California Institute of Technology. dngosset@gmail.com

†Institute for Quantum Information and Matter, California Institute of Technology. ychuang@caltech.edu

Ising chain the scaling $\xi = \Theta(1/\epsilon)$ is achieved [26, 9], which shows that the upper bound on ξ in (1) cannot be improved.

In gapped systems with (exactly) degenerate ground states, a modification of (1)

$$|\langle\psi|AB|\psi\rangle - \langle\psi|AGB|\psi\rangle| \leq C\|A\|\|B\|e^{-d(A,B)/\xi} \tag{2}$$

holds with $\xi = O(1/\epsilon)$ for any ground state $|\psi\rangle$ [14], where G is the projector onto the ground space. An overview of these results and the proof techniques used to obtain them is given in [15].

Here we specialize to *frustration-free* geometrically local Hamiltonians. Frustration-freeness means that any ground state of H is also in the ground space of each term H_i. Since we assume that H_i has smallest eigenvalue zero, this means that any ground state $|\psi\rangle$ of H satisfies $H_i|\psi\rangle = 0$ for all i. The ground energy of H is therefore zero and in general the ground space may be degenerate. The spectral gap ϵ of H is defined to be its smallest nonzero eigenvalue. Henceforth we assume (without loss of generality) that each term H_i in the Hamiltonian is a projector, i.e., $H_i^2 = H_i$.

There is a close connection between tensor network states and frustration-free Hamiltonians: for matrix product states or projected entangled pair states one can construct a frustration-free parent Hamiltonian as a sum of local projectors, where each projector annihilates the local reduced density matrix of the state [10, 24, 25].

Gapped frustration-free systems include widely studied spin chains such as the AKLT model [1] and the spin-1/2 ferromagnetic XXZ chain (with kink boundary conditions) [12, 3, 19]. A prevalent strategy to study topological phases in two and higher spatial dimensions is to construct exactly solvable models, such as the toric code [18] and more generally the quantum double [18] and string net [20] models. Almost all such models are gapped and frustration-free (commuting, even). Gapless frustration-free systems include the spin-1/2 ferromagnetic Heisenberg chain and the Rokhsar-Kivelson quantum dimer model [27]. Two recent papers construct gapless frustration-free spin chains in which the half-chain entanglement entropy diverges in the thermodynamic limit $n \to \infty$: a spin-1 example based on parenthesized expressions (with $\log(n)$ divergence) [7] and a higher spin generalization ($\sqrt{n}$ divergence) [21]. The classification of spin-1/2 chains in [8] provides many further examples of gapped and gapless frustration-free systems.

We establish the following tight upper bound on correlation length in frustration-free systems near criticality (i.e., in the limit $\epsilon \to 0$).

Theorem 1. *Suppose H is a frustration-free geometrically local Hamiltonian with spectral gap ϵ. Then decay of correlations* (2) *holds with $\xi = O(1/\sqrt{\epsilon})$ for any ground state $|\psi\rangle$ of H.*

In this theorem C in the bound (2) is an absolute constant, while the constant hidden in the big-O notation depends only on the interaction range r and a parameter g defined by

$$g = \max_i |\{H_j : [H_i, H_j] \neq 0\}|. \tag{3}$$

(g itself only depends on r and the geometry of the lattice.)

Theorem 1 may be of interest for at least two reasons. (i) For matrix product states or projected entangled pair states, it implies an upper bound on the energy gap of the parent

Hamiltonian in terms of the correlation length of the state. (ii) While frustration-free models such as those discussed above seem to be representative of many gapped phases of matter, our result states that gapless frustration-free systems cannot exhibit critical phenomena with, e.g., $\xi = \Theta(1/\epsilon)$. This may be relevant to understanding possible scaling limits of critical frustration-free systems, an issue which has been raised in references [7, 21, 8].

Reference [2] gives a combinatorial proof of correlation decay for frustration-free Hamiltonians. That proof gives an upper bound $\xi = O(1/\epsilon)$. To prove Theorem 1, we modify the argument from [2] using Chebyshev polynomials. In the field of Hamiltonian complexity [23, 11], Chebyshev polynomials have been used to prove area laws for the entanglement entropy in the ground states of one-dimensional gapped systems [6, 5, 17]. It is thus not surprising that they are useful in the present context.[1]

Proof. The first part of the proof follows reference [2]. For completeness we review the necessary material from that paper; we indicate below where this proof differs. Here we use a slightly different version of the detectability lemma [2] due to Arad [4].

Detectability Lemma ([2, 4])**.** *Let $H = \sum_i H_i$ be a frustration-free local Hamiltonian with ground space projector G and spectral gap ϵ. Choose some ordering of the terms H_i and let $P = \prod_i (1 - H_i)$ where the product is taken with respect to this ordering. Then*

$$\|P - G\| \leq 1/\sqrt{1 + \epsilon/g^2} \tag{4}$$

where g is given by (3)*.*

The result (4) holds for any order of the projectors $(1 - H_i)$ in the definition of P. Following [2], we fix a particular order as follows. It will be useful to define an "interaction graph" with a vertex for each term H_i and an edge between two vertices if the corresponding terms do not commute. Note that g is the maximum degree of this interaction graph.

We first partition the projectors $(1 - H_i)$ into a constant number c of layers (sets) such that any two projectors within a given layer commute. This partition can be obtained from a proper vertex coloring of the interaction graph using c colors (no two vertices with the same color share an edge). Since any graph with maximum degree Δ has such a coloring with $\Delta + 1$ colors we get $c \leq g + 1$. For example, for nearest-neighbor interactions in one dimension, each projector H_i has support on particles $i, i + 1$, and we may take $c = 2$ (with one layer consisting of all projectors with even values of i, and the other layer corresponding to odd values of i). After fixing the layers, we then choose some (arbitrary) ordering of them, e.g., in one dimension we might take the odd layer to be first and the even layer to be second. Finally, we take $P = L_c \cdots L_2 L_1$ where L_j is the product of all projectors $(1 - H_i)$ in layer j. Choosing P in this way we have [2]

$$\langle\psi|A(P^\dagger P)^m B|\psi\rangle = \langle\psi|AB|\psi\rangle \quad \text{for } m < \frac{d(A, B)}{(2c - 1)(r - 1)}. \tag{5}$$

[1] As in those previous works, below we make use of an operator (denoted $Q_m(P^\dagger P)$) which is an approximate ground space projector (AGSP). However the AGSP used here is different from those used in references [6, 5, 17]. In our proof we do not need an AGSP with small entanglement rank, which gives us greater freedom.

To see why (5) holds, we view $(P^\dagger P)^m$ as consisting of $(2c-1)m$ layers. The reader may find it helpful to look at Figure 4 in [2]. Note that $(1-H_i)|\psi\rangle = |\psi\rangle$, i.e., any projector $(1-H_i)$ acts as the identity on a ground state $|\psi\rangle$. Likewise, for any term H_i with support disjoint from that of A we have $(1-H_i)A|\psi\rangle = |\psi\rangle$. More generally, in the expression $\langle\psi|A(P^\dagger P)^m$ we may replace many of the projectors with the identity; the ones which remain are said to be in the causal cone of A. Each layer reduces the distance between B and the causal cone of A by at most $(r-1)$. So if $m(2c-1)(r-1) < d(A,B)$ then every projector in the causal cone of A acts trivially on $B|\psi\rangle$ and (5) follows.

At this point we depart from the proof given in reference [2], using ideas from [5]. Equation (5) directly implies that for any degree-m polynomial $Q_m(x)$ with $Q_m(1) = 1$ and $m < \frac{d(A,B)}{(2c-1)(r-1)}$ we have

$$\langle\psi|AQ_m\big(P^\dagger P\big)B|\psi\rangle = \langle\psi|AB|\psi\rangle. \tag{6}$$

We choose Q_m to be a rescaled and shifted Chebyshev polynomial defined by

$$Q_m(x) = \frac{T_m\big(\frac{2x}{1-\delta}-1\big)}{T_m\big(\frac{2}{1-\delta}-1\big)}, \quad \text{where} \quad \delta = \frac{\epsilon}{g^2+\epsilon}, \tag{7}$$

and $T_m = \cos(m \arccos x) = \cosh(m \operatorname{arccosh} x)$ is the standard (degree-m) Chebyshev polynomial of the first kind. The function Q_m is a degree-m polynomial with $Q_m(1) = 1$ and [5]

$$|Q_m(x)| \le 2e^{-2m\sqrt{\delta}} \qquad \text{for} \quad 0 \le x \le 1-\delta. \tag{8}$$

Equation (8) follows from (7) and the facts that $|T_m(x)| \le 1$ for $|x| \le 1$ and $T_m(x) > \frac{1}{2}e^{2m\sqrt{\frac{x-1}{x+1}}}$ for $x > 1$ [5].

Since G projects onto the $+1$ eigenspace of the positive semidefinite operator $P^\dagger P$ we have $P^\dagger P - G \ge 0$. Using the Detectability Lemma we get

$$\|P^\dagger P - G\| = \|P - G\|^2 \le \frac{1}{1+\epsilon/g^2} = 1-\delta$$

and therefore we have the operator inequality

$$0 \le P^\dagger P - G \le (1-\delta)\cdot 1. \tag{9}$$

Again using the fact that G projects onto the $+1$ eigenspace of $P^\dagger P$ and the fact that $Q_m(1) = 1$ we have

$$Q_m(P^\dagger P) - G = Q_m(P^\dagger P - G). \tag{10}$$

Using (6) and then (10) we have, for all $m < \frac{d(A,B)}{(2c-1)(r-1)}$,

$$\begin{aligned} |\langle\psi|AB|\psi\rangle - \langle\psi|AGB|\psi\rangle| &= |\langle\psi|A\left(Q_m(P^\dagger P) - G\right)B|\psi\rangle| \\ &= |\langle\psi|AQ_m(P^\dagger P - G)B|\psi\rangle| \\ &\le \|A\|\|B\|\|Q_m(P^\dagger P - G)\| \\ &\le 2\|A\|\|B\|\exp\left(-2m\sqrt{\frac{\epsilon}{g^2+\epsilon}}\right) \end{aligned} \tag{11}$$

where in the last inequality we used (8) and (9). We now choose m to be the largest integer less than $\frac{d(A,B)}{(2c-1)(r-1)}$. Substituting the bound $m \geq \frac{d(A,B)}{(2c-1)(r-1)} - 1$ in (11) and using the fact that $\epsilon/(g^2+\epsilon) \leq 1$, we arrive at the desired bound (2) with $C = 2e^2$ and

$$\xi = \frac{(2c-1)(r-1)}{2}\sqrt{\frac{g^2+\epsilon}{\epsilon}} = O(1/\sqrt{\epsilon}).$$

$\square$

A simple example shows that the upper bound on ξ in Theorem 1 cannot be improved. Consider the spin-1/2 ferromagnetic XXZ chain with kink boundary conditions [12, 3, 19]. The Hamiltonian for the chain of length n can be written as a sum of projectors

$$H(q) = \sum_{i=1}^{n-1} |\phi(q)\rangle\langle\phi(q)|_{i,i+1}, \qquad |\phi(q)\rangle = \frac{1}{\sqrt{q^2+1}}\big(q|10\rangle - |01\rangle\big) \tag{12}$$

where $0 < q < 1$ and $|0\rangle, |1\rangle$ are spin up/down respectively. The spectral gap of $H(q)$ is given by $\epsilon = 1 - \frac{2}{q+q^{-1}}\cos(\pi/n)$ [19] and vanishes as $q \to 1$ and $n \to \infty$.

The total magnetization $M = \sum_{i=1}^{n} \frac{1}{2}(1-\sigma_i^z)$ is conserved. It can be verified by a direct computation that

$$|\psi_1\rangle = \left(\frac{1-q^2}{1-q^{2n}}\right)^{1/2} \sum_{j=1}^{n} q^{j-1}\sigma_j^x|00\ldots0\rangle$$

satisfies $H(q)|\psi_1\rangle = 0$ and is the unique ground state in the symmetry sector where M has eigenvalue 1. Let $A = \frac{1}{2}(1-\sigma_1^z)$ and $B = \frac{1}{2}(1-\sigma_j^z)$ for some $j > 1$, so that $d(A,B) = j-1$. Then $\langle\psi_1|AB|\psi_1\rangle = 0$ and so

$$|\langle\psi_1|AB|\psi_1\rangle - \langle\psi_1|AGB|\psi_1\rangle| = |\langle\psi_1|A|\psi_1\rangle\langle\psi_1|B|\psi_1\rangle| = \left(\frac{1-q^2}{1-q^{2n}}\right)^2 q^{2d(A,B)}. \tag{13}$$

where in the first equality we used the fact that A and B commute with M. For simplicity we now take the limit $n \to \infty$. If we suppose (2) holds for some C and ξ, then (13) implies

$$\left(1-q^2\right)^2 q^{2d(A,B)} \leq Ce^{-d(A,B)/\xi}$$

Taking logs on both sides and using the fact that ξ does not depend on $d(A,B)$ gives the desired lower bound

$$\xi \geq \frac{1}{-2\ln q} = \frac{1}{-2\ln(1-O(\sqrt{\epsilon}))} = \Omega(1/\sqrt{\epsilon}).$$

where in the second step we used the fact that $\epsilon = 1 - \frac{2}{q+q^{-1}}$ (in the limit $n \to \infty$).

Remark. The XXZ chain also seems to nicely illustrate the optimality of the bound (4) in the Detectability Lemma. The bound states that $1 - \|P - G\| = \Omega(\epsilon)$, while we found using numerical diagonalization that for the XXZ chain (12) $1 - \|P - G\|$ is exactly equal to ϵ, for all choices of q and n that we tried (we used the aforementioned two-layer ordering of projectors in the definition of P). Presumably this equality holds for all $0 < q \leq 1$ and $n \geq 2$.

Acknowledgments

We thank Spiros Michalakis and John Preskill for interesting discussions. We acknowledge funding provided by the Institute for Quantum Information and Matter, an NSF Physics Frontiers Center (NFS Grant PHY-1125565) with support of the Gordon and Betty Moore Foundation (GBMF-12500028). Both authors contributed equally to this work; the author ordering is alphabetical.

References

[1] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki. Rigorous results on valence-bond ground states in antiferromagnets. *Physical Review Letters*, 59:799–802, 1987.

[2] D. Aharonov, I. Arad, U. Vazirani, and Z. Landau. The detectability lemma and its applications to quantum Hamiltonian complexity. *New Journal of Physics*, 13(11):113043, 2011.

[3] F. C. Alcaraz, S. R. Salinas, and W. F. Wreszinski. Anisotropic ferromagnetic quantum domains. *Physical Review Letters*, 75(5):930–933, 1995.

[4] I. Arad. Private communication (to be published soon).

[5] I. Arad, A. Kitaev, Z. Landau, and U. Vazirani. An area law and sub-exponential algorithm for 1D systems. arXiv:1301.1162.

[6] I. Arad, Z. Landau, and U. Vazirani. Improved one-dimensional area law for frustration-free systems. *Physical Review B*, 85(19):195145, 2012.

[7] S. Bravyi, L. Caha, R. Movassagh, D. Nagaj, and P. W. Shor. Criticality without frustration for quantum spin-1 chains. *Physical Review Letters*, 109(20):207202, 2012.

[8] S. Bravyi and D. Gosset. Gapped and gapless phases of frustration-free spin-$\frac{1}{2}$ chains. *Journal of Mathematical Physics*, 56(6):061902, 2015.

[9] M. A. Continentino. Quantum scaling in many-body systems. *Physics Reports*, 239(3):179–213, 1994.

[10] M. Fannes, B. Nachtergaele, and R. F. Werner. Finitely correlated states on quantum spin chains. *Communications in Mathematical Physics*, 144(3):443–490, 1992.

[11] S. Gharibian, Y. Huang, Z. Landau, and S. W. Shin. Quantum Hamiltonian complexity. arXiv:1401.3916.

[12] C.-T. Gottstein and R. F. Werner. Ground states of the infinite q-deformed Heisenberg ferromagnet. arXiv:cond-mat/9501123.

[13] M. B. Hastings. Lieb-Schultz-Mattis in higher dimensions. *Physical Review B*, 69(10):104431, 2004.

[14] M. B. Hastings. Locality in quantum and Markov dynamics on lattices and networks. *Physical Review Letters*, 93(14):140402, 2004.

[15] M. B. Hastings. Locality in quantum systems, 2010. arXiv:1008.5137.

[16] M. B. Hastings and T. Koma. Spectral gap and exponential decay of correlations. *Communications in Mathematical Physics*, 265(3):781–804, 2006.

[17] Y. Huang. Area law in one dimension: Degenerate ground states and Renyi entanglement entropy. arXiv:1403.0327.

[18] A. Y. Kitaev. Fault-tolerant quantum computation by anyons. *Annals of Physics*, 303(1):2–30, 2003.

[19] T. Koma and B. Nachtergaele. The spectral gap of the ferromagnetic XXZ-chain. *Letters in Mathematical Physics*, 40(1):1–16, 1997.

[20] M. A. Levin and X.-G. Wen. String-net condensation: A physical mechanism for topological phases. *Physical Review B*, 71(4):045110, 2005.

[21] R. Movassagh and P. W. Shor. Power law violation of the area law in quantum spin chains. arXiv:1408.1657.

[22] B. Nachtergaele and R. Sims. Lieb-Robinson bounds and the exponential clustering theorem. *Communications in Mathematical Physics*, 265(1):119–130, 2006.

[23] T. J. Osborne. Hamiltonian complexity. *Reports on Progress in Physics*, 75(2):022001, 2012.

[24] D. Perez-Garcia, F. Verstraete, M. M. Wolf, and J. I. Cirac. Matrix product state representations. *Quantum Information and Computation*, 7(5-6):401–430, 2007.

[25] D. Perez-Garcia, F. Verstraete, M. M. Wolf, and J. I. Cirac. PEPS as unique ground states of local Hamiltonians. *Quantum Information and Computation*, 8(6):650–663, 2008.

[26] P. Pfeuty. The one-dimensional Ising model with a transverse field. *Annals of Physics*, 57(1):79–90, 1970.

[27] D. S. Rokhsar and S. A. Kivelson. Superconductivity and the quantum hard-core dimer gas. *Physical Review Letters*, 61(20):2376–2379, 1988.