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Complexity phase transitions generated by entanglement

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Entanglement is one of the physical properties of quantum systems responsible for the computational hardness of simulating quantum systems. But while the runtime of specific algorithms, notably tensor network algorithms, explicitly depends on the amount of entanglement in the system, it is unknown whether this connection runs deeper and entanglement can also cause inherent, algorithm-independent complexity. In this work, we quantitatively connect the entanglement present in certain quantum systems to the computational complexity of simulating those systems. Moreover, we completely characterize the entanglement and complexity as a function of a system parameter. Specifically, we consider the task of simulating single-qubit measurements of k–regular graph states on n qubits. We show that, as the regularity parameter is increased from 1 to $n-1$, there is a sharp transition from an easy regime with low entanglement to a hard regime with high entanglement at $k=3$, and a transition back to easy and low entanglement at $k=n-3$. As a key technical result, we prove a duality for the simulation complexity of regular graph states between low and high regularity.

A fundamental question since the inception of quantum computing has been to understand the physical mechanisms underlying the computational speedup of quantum computers. One of the most widely studied resources for quantum speedups is entanglement [1, 2]. However, understanding precisely *how much* entanglement is necessary *and* sufficient for a quantum system to be intractable to arbitrary classical simulation techniques has remained elusive. Quantum computations involving next to no entanglement can be hard to simulate classically [3–5] and relatively little entanglement can be universal for quantum computation [6–8], while states with very high entanglement can be useless for quantum computation [9, 10].

One way the relation between entanglement and hardness has been studied is by considering the performance of specific simulation methods, like tensor networks [11–14]. The runtime of tensor-network algorithms depends exponentially on the amount of a certain type of entanglement [1, 11, 12], as it determines how efficiently we can contract the tensor network. However, it is an open problem to characterize the situations where tensor network algorithms are optimal. When can we find another algorithm that could do better in situations where tensor networks are inefficient? Moreover, when does the failure of tensor networks coincide with an inherent hardness of the problem itself? This essentially is the content of the second of Aaronson's "Ten Semi-Grand Challenges for Quantum Computing Theory" [15].

The effect of the presence of entanglement on hardness of classical simulation has been considered in various settings including measurement-based quantum computing (MBQC) [9, 10, 16, 17], the one-clean-qubit model [18], and more recently in a line of research considering the time evolution under certain classes of Hamiltonians [19, 20]. However, we lack a *quantitative connection* between the entanglement present in certain quantum states and the inherent computational complexity of simulating them.

In this paper, we answer Aaronson's question quantitatively with respect to the entanglement of regular graph states. For a simple graph $G=(V,E)$ given by vertex set V and edge set E, the corresponding graph state $|G\rangle$ is defined as

$$|G\rangle = \prod_{(i,j)\in E} (\mathsf{CZ})_{i,j} |+\rangle^{\otimes n}, \tag{1}$$

where $\mathsf{CZ}_{i,j}$ is the controlled-Z operator acting on vertices i and j. The action of the $\mathsf{CZ}_{i,j}$ gate is invariant to changing the control and target qubits. Graph states [21] are a very well-motivated class to investigate the interplay of classical simulability and entanglement. On one hand, a graph state directly maps to a tensor network, and one can invoke the measurement-based model of quantum computing [6, 22, 23] to argue that certain graph states are not efficiently simulable and are, moreover, universal resources for quantum computations. On the other hand, their entanglement can be conveniently analyzed using graph theory [7].

Examples of universal resource states are graph states on hexagonal, square, or triangular lattices [24, 25]. Under closed boundary conditions these resource states correspond to 3–, 4–, and 6–regular graphs, respectively. Conversely, graph states on a 2–regular graph, i.e., a one-dimensional cluster state, and the graph state on an $(n-1)$–regular graph on n qubits, i.e., the complete graph, are also well studied: both are efficiently simulable and at the same time have low entanglement [7, 25, 26]. However, for all other values of the regularity parameter k, it is unknown exactly when, if at all, classical simulation is intractable, and how the regularity parameter relates to the entanglement of the

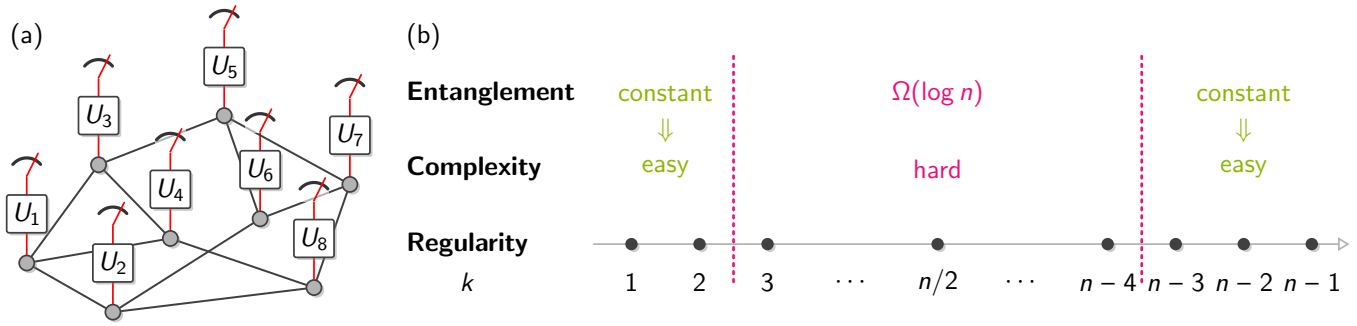

Figure 1. (a) The family of quantum states we consider are graph states on a k–regular graph G on n qubits with arbitrary single qubit rotations $U_1, U_2, \ldots, U_n$. The measurements are done in the standard basis. (b) Phase transitions of the entanglement (as measured by entanglement width) and computational complexity—whether classical simulation is easy or hard—as a function of the regularity parameter k. For both the entanglement width and the computational complexity, we take the worst case over all k–regular graphs G as well as $U_1, U_2, \ldots, U_n$.

corresponding graph state.

Our contributions.—In this work, we completely characterize the computational complexity of simulating k–regular graph states in arbitrary product bases and their entanglement as a function of the regularity parameter k; see Fig. 1. We also identify new resource states for MBQC: a result of independent interest. Our constructions reach all the way to almost fully connected graphs that may be more natural for some experimental architectures such as ion traps [27] or cavity quantum electrodynamics [28] than low-degree lattices.

Our two main results are summarized as follows and are illustrated in Fig. 1(b).

- As the regularity parameter k is increased from its minimal value of 1 to its maximal value of $n-1$, the simulation complexity first sharply changes from easy to provably hard precisely at $k=3$, but then changes sharply back to easy again at $k=n-3$.
- The entanglement scaling, measured by *entanglement width* [25], one-to-one correspond one-to-one with simulation complexity, changing from constant to at least logarithmic to constant at *the same values of* k at which the simulation complexity changes from easy to hard and back to easy.

Qualitatively, entanglement width measures the entanglement of "tree-like" bipartitions of the state: this directly determines the runtime of tensor-network algorithms. It is also an LOCC (Local Operations and Classical Communication) monotone and hence a meaningful measure of entanglement [6].

We consider simulation of quantum states in terms of both sampling from their output distributions *and* computing output probabilities up to constant multiplicative error in an arbitrary local product basis. Indeed, in the case where simulation is hard, the two notions of simulation are intricately linked: given that computing output probabilities to constant multiplicative error is harder than any problem in the complexity class GapP, the sampling task cannot be efficiently solved. This can be shown by a standard reduction due to Stockmeyer [29].

No general tool exists to pinpoint when entanglement produces simulation hardness. What we can say is something weaker: there is no known class of circuits such that computing output probabilities is GapP-hard but the circuit does not produce entanglement.

However, even for those instances, it is not clear that entanglement is what is producing the hardness, as there are other quantum resources present. Our work provides one of the first examples where entanglement can justifiably be said to produce simulation hardness.

We do this by appending single-qubit rotations at the end to perform the measurement in arbitrary local bases. This ensures all known classical simulation algorithms for quantum circuits that exploit specific quantum resources—in particular, low stabilizer rank or T-count [30, 31] and low negativity in quasiprobability representations [32–36]—are rendered inefficient. But, the last layer of local rotations does not affect the entanglement of the quantum state. So, local rotations enable us to understand to what extent entanglement present in a state serves as a necessary and sufficient criterion characterizing simulation complexity.

We have thus identified a setup where all known easy cases are efficiently simulable precisely *because* of the state having little entanglement. Additionally, all other cases are provably hard to simulate *because* the entanglement present in the system facilitates universal measurement-based quantum computation, as we detail below. To the best of our knowledge, this is the first setup where both features are simultaneously demonstrated; moreover, the entanglement and complexity transitions, as a function of a natural system parameter, are sharp.

Main results.—In the hard regime, our proofs also rely on showing GapP-hardness of estimating probabilities—of a specific family of k–regular graphs in a specific family of local bases—implying the hardness of sampling. Conversely, easiness of sampling and computing output probabilities up to constant multiplicative error are independent properties and not implied by one another. However, our proofs in the easy regimes show that *both* tasks are efficiently possible for our particular setup. Specifically, we prove the following results.

Theorem 1 (The easy regime)**.** *In the regimes of very low ($k \leq 2$) and very high ($k \geq n-3$) regularity, locally rotated k–regular graph states (a) have constant entanglement width, and (b) can be simulated by a polynomial time classical algorithm.*

For all other values of k, we show that classical simulations are not efficiently possible:

Theorem 2 (The hard regime)**.** *For every $3 \leq k \leq n-4$, there exist locally rotated k–regular graph states such that (a) these states cannot be simulated classically in polynomial time, assuming the* PH *is infinite, (b) the entanglement width scales at least logarithmically.*

We also get the following corollary.

Corollary 3. *For every $3 \leq k \leq n-4$, assuming $\mathsf{BPP} \subsetneq \mathsf{P}^{\#\mathsf{P}}$, there exist k–regular graph states satisfying Theorem 2(a) such that their entanglement width is superlogarithmic.*

Assuming stronger hardness conjectures, the lower bounds on the entanglement width can be sharpened to $\Omega(n^{\delta})$ for some constant $\delta > 0$ (assuming the exponential time hypothesis) and to $\Omega(n^{1/2})$ (assuming the strong exponential time hypothesis.)

The complexity class $\mathsf{P}^{\#\mathsf{P}}$ is as defined in [38]. Let us note that our hardness results—while stated for the worst case—are in fact also valid on average over the local rotations via worst-to-average case reductions [41, 75] (see Section 5 of the Supplemental Material [39] for details.) Together, our results completely characterize the classical simulability of locally rotated regular graph states as a function of the regularity parameter in terms of both sampling and computing probabilities.

Proof of easiness results.—In order to prove our easiness results, we utilize connections between entanglement width and classical simulations of graph states. Let the entanglement width of a graph G be $\mathsf{ew}(|G\rangle)$; see Refs. [25, 39] for the precise definition.

First, note that for $k \in \{1, 2, n-3, n-2, n-1\}$, $\mathsf{ew}(|G\rangle)$ is a constant for every $G \in \mathcal{G}_k$, where $\mathcal{G}_k$ is the set of all k–regular graphs. To see this, we make use of relations between entanglement width of a graph state $|G\rangle$ and width measures of the underlying graph G. Particularly, entanglement width is equal to the rank width of the underlying graph for graph states. Furthermore it can be related to the tree width and clique width of G [25]. All these width measures express how "tree-like" the graph is from different perspectives [43]. 1– and 2–regular graphs have bounded tree width, which implies they have bounded rank width and therefore bounded entanglement width. Additionally, rank width, and hence, entanglement width, satisfy a duality property: if it is bounded for a graph G, it is also bounded for the complement $\overline{G}$ of G [44, 45]. This fact allows us to argue that $(n-3)$– and $(n-2)$–regular graphs have bounded entanglement width.

Qualitatively, graph states with low entanglement width are efficiently simulable via tensor network simulation methods by the technique of Ref. [17]. For a graph G, the idea is to construct a tree-tensor-network decomposition of a graph state $|G\rangle$. This takes time $\mathrm{poly}(n, 2^{\mathsf{ew}(|G\rangle)})$. Given this decomposition, and using techniques of Refs. [11, 12, 17], one can compute any output probability under any set of local rotations. Additionally, one can also sample from the resulting output distributions.

Hamming weight symmetry for the complete graph. For the complete graph—i.e, the $(n-1)$–regular graph—we construct a new recursive algorithm that allow us to simulate arbitrary single-qubit product measurements.

Specifically, our approach requires an inherent symmetry of the complete graph: the fact that any output probability of the complete graph on n vertices has a Hamming weight symmetry—it can be written as a linear combination of $n+1$ many terms, one for each Hamming weight, such that each of them is efficiently computable. See the Supplemental Material [39] for details.

While it is known that output probabilities of the complete graph can be computed efficiently [7, 25, 26], to the best of our knowledge, our approach is novel and might have applications elsewhere to prove easiness, especially in problems having a Hamming weight symmetry. Some recent works have used this symmetry to devise classical algorithms for quantum simulation [46, 47].

Proof of hardness for $3 \leq k \leq n/2$. In order to prove hardness, we use the fact that certain graph states are resources for MBQC. Using Aaronson's result that $\mathsf{postBQP} = \mathsf{PP}$ [48], the output probabilities of a resource state for MBQC with local rotations are GapP-hard to compute [6, 49–51]. Then, using Stockmeyer's theorem, it is not possible to efficiently sample from their output distribution unless the polynomial hierarchy collapses [29]; see [52] for an overview of this argument. In particular, this is true for the square lattice and the hexagonal lattice [24].

Furthermore, we exploit the fact that certain single-qubit Clifford operations on a graph state $|G\rangle$, with classical communication and standard basis measurements, result in *vertex deletion* and *local complementation* of G

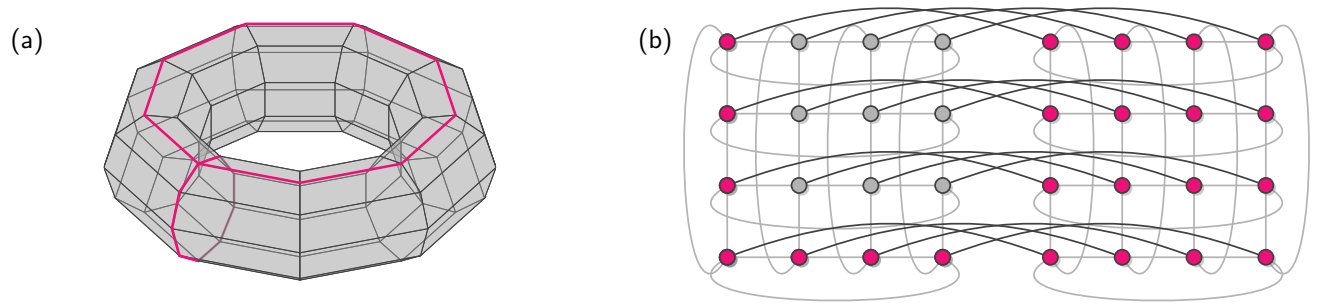

Figure 2. (a) A grid graph with closed boundary conditions is a torus, which is a 4–regular graph. This is a resource state for MBQC: "cutting open" the torus along the pink lines gives back a grid graph. (b) Two tori connected together to construct a 5–regular graph. The pink vertices are ones we delete to recover a grid graph, which proves that this is a valid resource state for MBQC.

[53]. Local complementation flips the neighborhood of a vertex: connected vertices in the neighborhood are disconnected, and any two disconnected vertices are joined by an edge. This is illustrated in Fig. 3. It is known that if we transform a parent graph G to a hexagonal or grid graph by vertex deletion and local complementation, then $|G\rangle$ is a universal resource for MBQC and hence hard to simulate [25, 50].

Our construction starts from the observation that hexagonal and square lattices with closed boundary conditions on the torus are, respectively, 3– and 4–regular graphs. These are universal resources for MBQC, since we can reach planar hexagonal and square lattices by vertex deletion: we "cut" the torus open, see Fig. 2(a). Consequently, computing the output probabilities of G in an arbitrary local basis is GapP-hard for 3– and 4–regular graphs.

For graphs with higher regularity, we need more involved constructions. We reverse-engineer k–regular resources by starting from the 4–regular resource state—the square lattice on a torus—and boost it up to k–regularity by adding gadgets, which can be removed by local complementation or vertex deletion.

In light of this, starting from a grid graph on a torus, i.e., an n vertex, 4–regular graph, we add just a single gadget, namely another grid graph on a torus, see Fig. 2(b). We then judiciously connect two grid graphs in a way such that every vertex is k–regular. It is nontrivial to argue that such a connection pattern even exists. We prove it does using the Gale-Ryser theorem [54–56], for every $4 < k \leq n/2$. The Gale-Ryser theorem is constructive. Thus, our constructions prove that there exists an explicit n–vertex, k–regular graph G such that computing the output probabilities of G in an arbitrary local basis is GapP-hard, for every $4 \leq k \leq n/2$.

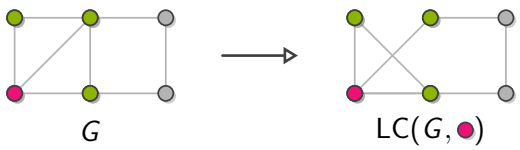

Figure 3. To perform local complementation $LC(G,a)$ of a graph G with respect to vertex a (pink), we take the complement of the subgraph comprising the neighbors of the pink vertex (green).

The duality property.—Finally, we show that the complexity of simulating graphs with low regularity and graphs with high regularity satisfies a duality. Specifically, we prove that the complement of an $n \times n$ hexagonal graph or grid graph is a resource state for MBQC. Hence, the corresponding $(n-4)$–regular graph state is universal under postselection, and simulating product measurements of it is classically intractable.

To see this, consider an $n \times n$ grid graph G, and mark three vertices—a corner vertex of degree 2, and its two neighbors, see Fig. 4. Denote these vertices by a (pink vertex), b, and c (green vertices). Now, in the complement graph $\overline{G}$, apply *local complementation* to vertex a, that is, we take the complement of the neighborhood of a. Then delete vertices a, b, c, and subsequently, delete all vertices in the same row and column as a in G. We are left with an $(n-1) \times (n-1)$ grid graph, which is a resource state for MBQC. An analogous strategy shows that the complement of an $n \times n$ hexagonal lattice is also a resource state for MBQC.

Proof of hardness for $n/2 < k \leq n-4$. We now extend our hardness proof to the regime of $n/2 < k \leq n-4$. The idea is to take the hard graphs we constructed for $4 \leq k \leq n/2$, comprising two copies of the grid graph on the torus, and then complement those hard graphs. If we started with a k–regular graph, after complementation, we are left with an $(n-k-1)$–regular graph. We then delete all vertices which were part of the second grid graph in the original graph and then apply local complementation to one of the vertices and vertex deletion in the column and row of that vertex.

As a consequence, we obtain an explicit duality of simulation complexity between regimes of high and low

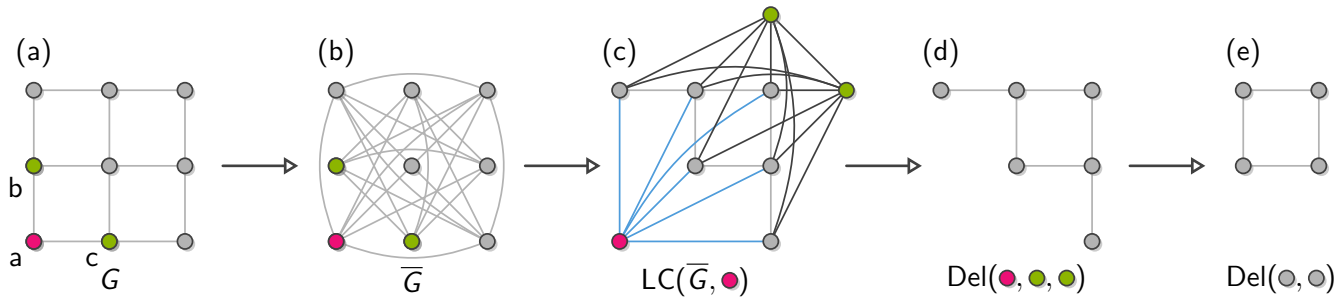

Figure 4. A visual proof that the complement of a grid graph is a resource state for MBQC. (a) A 3×3 grid graph G. Consider (b) $\overline{G}$—the complement of G. (c) Apply a local complementation to vertex a. (d) Delete vertices b and c. (e) Delete some of the gray vertices to finally reach a 2×2 grid graph.

regularity. That is, we find that there is an explicit n–vertex, k–regular graph G such that computing the output probabilities of G in an arbitrary local basis is GapP-hard, for every $n/2 < k \leq n-4$.

Finally, we obtain bounds on entanglement width of regular graphs in the easy regime using width measures from graph theory [44, 45, 57–65], specifically tree width, rank width, and clique width, which can be related to the entanglement width.

Outlook.—We have completely resolved Aaronson's question for regular graph states, going significantly beyond initial results on the interplay between simulability and entanglement in Refs. [16, 17, 25].

An immediate follow-up problem is to characterize the interplay between entanglement and simulation complexity of more restricted, physical families of graphs such as planar or bipartite graphs. Our gadgets do not obviously generalize to more restricted cases. Hence, we need new techniques to prove hardness.

Additionally, we can ask: can Aaronson's question of which systems are classically simulable be resolved generally, or even for slightly more general setups beyond graph states? Beyond graph states, entanglement width is not always related to classical simulation complexity: it remains open if there is a universal single *physical property* that fully determines simulation complexity.

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