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Complexity phase diagram for interacting and long-range bosonic Hamiltonians

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We classify phases of a bosonic lattice model based on the computational complexity of classically simulating the system. We show that the system transitions from being classically simulable to classically hard to simulate as it evolves in time, extending previous results to include on-site number-conserving interactions and long-range hopping. Specifically, we construct a complexity phase diagram with easy and hard “phases”, and derive analytic bounds on the location of the phase boundary with respect to the evolution time and the degree of locality. We find that the location of the phase transition is intimately related to upper bounds on the spread of quantum correlations and protocols to transfer quantum information. Remarkably, although the location of the transition point is unchanged by on-site interactions, the nature of the transition point does change. Specifically, we find that there are two kinds of transitions, sharp and coarse, broadly corresponding to interacting and noninteracting bosons, respectively. Our work motivates future studies of complexity in many-body systems and its interplay with the associated physical phenomena.

A major effort in quantum computing is to find examples of quantum speedups over classical algorithms, despite the absence of general principles characterizing such a speedup. The study of classical simulability of quantum systems evolving in time allows one to identify features underlying a quantum advantage. Studying the classical simulability of both quantum circuits [1–14] and Hamiltonians [15, 16], especially under restrictions such as spatial locality [17–21], allows one to understand the classical-quantum divide in terms of their respective computational complexity. Computational complexity has been closely linked to phases of matter in contexts such as dynamical phase transitions [20], measurement-based quantum computing [22], thermal phase transitions [23], and entanglement phase transitions [24]. Therefore, studying the complexity of simulating quantum dynamics is fruitful in understanding the nonclassical features of quantum many-body physics, both theoretically and experimentally.

In this work, we characterize the worst-case computational complexity of simulating time evolution under bosonic Hamiltonians and study a dynamical phase transition in approximate sampling complexity [20, 21]. Previous work [20] studied free bosons with nearest-neighbor hopping but did not consider the robustness of the transition to perturbations in the Hamiltonian, a crucial question in the study of any phase transition. In this work, we zoom into the physics of the dynamical phase transition. Among other things, we generalize Ref. [20] to include number-conserving interactions and long-range hops and conclude that the phase transition survives under perturbations in the Hamiltonian. The interactions we study are ubiquitous in experimental implementations of hopping Hamiltonians with ultracold atoms and superconducting circuits [25, 26]. Long-range hops that fall off as a power law are also native to several architectures [27–31]. We also study

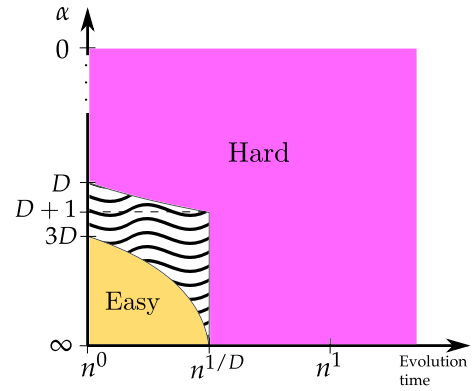


FIG. 1. (Color online). Slice of the complexity phase diagram for the long-range bosonic Hamiltonian in D -dimensions with n bosons when the number of sites is $m = \Theta(n^2)$. Colors represent whether the sampling problem is easy (yellow), hard (magenta), or not currently known (hatched). The X -axis parametrizes the evolution time as a polynomial function of n , and the Y -axis is α , the exponent characterizing the long-range nature of the hopping Hamiltonian (with scale $y = 1/\sqrt{\alpha}$ except for the point $\alpha = 0$).

the location of the phase transition and its dependence on various system parameters, constructing a *complexity phase diagram*, a slice of which is presented in Fig. 1.

Setup and summary of results.— Consider a system of n bosons hopping on a cubic lattice of m sites in D dimensions with real-space bosonic operators a_j . We let $m = \Theta(n^\beta)$ (see [32]) and assume sparse filling: $\beta \geq 1$. The Hamiltonian $H = \sum_{i,j} J_{ij}(t) a_i^\dagger a_j + \text{h.c.} + \sum_i f(n_i)$ has on-site interactions $f(n_i)$ and time-dependent hopping terms bounded by a power-law in the distance $d(i, j)$ as $|J_{ij}(t)| \leq 1/d(i, j)^\alpha$. The parameter α governs the degree of locality. When $\alpha = 0$, the

system has all-to-all couplings, while $\alpha \rightarrow \infty$ corresponds to nearest-neighbor hops. The on-site terms $J_{ii}(t)$ can be large, and the interaction strength is parametrized by V . For concreteness, our hardness results are stated assuming a Bose-Hubbard interaction $f(n_i) = Vn_i(n_i - 1)/2$, but they hold for generic on-site interactions [33]. We assume the bosons are initially sparse and well-separated. Specifically, partition the lattice into K clusters C_1, \dots, C_K containing b_1, \dots, b_K initial bosons, respectively, such that $b := \max b_i = O(1)$ does not scale with lattice size. Define the width L_i of a cluster C_i as the minimum distance between a site outside the cluster and an initially occupied site inside the cluster and let $L = \min_i L_i$. Thus, our initial states are chosen so the typical cluster size is $L = (m/n)^{1/D} = \Theta(n^{(\beta-1)/D})$.

The computational task of approximate sampling is to simulate projective measurements of the time-evolved state in the local boson-number basis. The *approximate sampling complexity* measures the running time of a classical algorithm needed to produce samples from some distribution \mathcal{D} that is $\epsilon = O(1/\text{poly}(n))$ -close in total variation distance to a target distribution \mathcal{D} (see [34]). Sampling from a distribution \mathcal{D} takes runtime $T(n, t)$ on a classical computer, where t is the evolution time. Like thermodynamic quantities, the complexity is defined asymptotically as $n \rightarrow \infty$, so we consider the scaling of T along a curve $t(n)$. Along any curve $t(n) = cn^\gamma$, sampling is *easy* if there exists a polynomial-runtime classical algorithm for all n , or *hard* if such an algorithm cannot exist. Since the problem is either easy or hard for a particular function $t(n)$, there is always a transition in complexity as opposed to a smooth crossover. We prove upper and lower bounds on the transition timescale by presenting sampling algorithms on the easiness side, and performing reductions to quantum supremacy proposals on the hardness side. Specifically, we show that approximate sampling is easy for all times $t < c_{\text{easy}}n^{\gamma_{\text{easy}}}$ and hard for all times $t > c_{\text{hard}}n^{\gamma_{\text{hard}}}$.

We find that the transition comes in two types, which we call “sharp” and “coarse”. For sharp transitions, these bounds coincide in the exponent $\gamma_{\text{easy}} = \gamma_{\text{hard}}$ and the transition occurs in the coefficient $c_{\text{easy}} \leq c_{\text{hard}}$. For coarse transitions, however, the transition occurs in the exponent. In our results, we will show that sampling is easy for any time $t = O(n^{\gamma_{\text{easy}}})$, but hard along any curve with exponent $\gamma_{\text{hard}} > \gamma_{\text{easy}}$ (see [35–37] for more precise definitions). An example of a sharp transition is when the transition timescale is $t_* = 2n$, so sampling is easy for $t \leq 1.99n$ and hard for $t \geq 2.01n$. An example of a coarse transition is $t_* = \Theta(n \log n)$, so sampling is easy for $t \leq cn$ and hard for $t \geq cn^{1.01}$.

We summarize our main results in Table I. The easiness result comes from applying classical algorithms for quantum simulation, and depend on Lieb-Robinson bounds on information transport [38–42]. The hardness results come from reductions to families of quantum circuits for which efficient approximate samplers cannot exist, modulo widely believed conjectures in complexity theory [10, 17–19], and from fast protocols to transmit quantum information across long distances [43, 44].

α	Easiness exponent γ_{easy}	Hardness exponent ^a γ_{hard}
$\alpha < \frac{D}{2}$?	$\frac{\beta}{D} \left(\alpha - \frac{D}{2} \right)$
$\frac{D}{2} \leq \alpha \leq D$		0
$D \leq \alpha \leq D + 1$		$\frac{\beta-1}{D} (\alpha - D)$
$D + 1 \leq \alpha \leq 2D + \frac{D}{\beta-1}$	0 ^b	$\frac{\beta-1}{D}$
$2D + \frac{D}{\beta-1} \leq \alpha < \infty$	$\frac{\beta-1}{D} \left(\frac{\alpha-2D}{\alpha-D} \right) - \frac{1}{\alpha-D}$	
$\alpha \rightarrow \infty$	$\frac{\beta-1}{D}$	$\frac{\beta-1}{D}$ if $D \geq 2$ or $V < \infty$ ∞ otherwise.

^a Up to an additive constant $\delta > 0$ that is present for $\alpha < D/2$, $D = 1$, or weak interactions $V = o(1)$.

^b The easiness timescale for this case is $t_{\text{easy}} = \log n$.

TABLE I. Exponents γ_{easy} and γ_{hard} in the easiness and hardness timescales for various regimes of α .

Note that the hardness exponents in Table I sometimes come with an infinitesimal $\delta > 0$ whenever at least one of the following cases holds: $\alpha < D/2$, $D = 1$, or weak interactions $V = o(1)$. When the easiness and hardness timescales coincide, we interpret this term δ as signifying a coarse transition, since it ensures $\gamma_{\text{hard}} > \gamma_{\text{easy}}$. In the $D = 1$ nearest-neighbor limit, we show the δ is optimal proving the transition is coarse.

We examine the various limits: $\alpha \rightarrow \infty$ (nearest-neighbor), $\alpha \rightarrow 0$ (all-to-all connectivity), $V \rightarrow 0$ (free bosons), and $V \rightarrow \infty$ (hardcore bosons). First, when $\alpha \rightarrow \infty$, the hardness timescale upper bound is $O(L)$ in all cases except when $V \rightarrow \infty$ and $D = 1$, which we discuss later. This matches the easiness timescale $t = \Omega(L)$, which corresponds to the distance L between clusters. This pins down t_* to $\Theta(L)$, which is when interference between clusters become relevant [20]. In the opposite limit when the model is sufficiently long-range ($\alpha < D/2$), the role of the dimension is unimportant, giving $\gamma_{\text{hard}} < 0$ in all cases, showing the immediate onset of hardness.

Next, we observe that the location of the transition t_* is generally independent of the interaction strength V . The only exception is the limit of hardcore interactions and nearest-neighbor hops ($V, \alpha \rightarrow \infty$) in 1D. There, $t_* \rightarrow \infty$, as the model maps to free fermions, or equivalently, matchgate circuits, which are easy to simulate at all times [1, 2].

The results for constant density $\beta = 1$, or $m = \Theta(n)$, are perhaps most experimentally relevant and are shown in Table II. In this case, the separation between clusters is a constant, and when $\alpha \geq D + 1$, the classical sampling algorithm works only for time $t = O(n^{-1/(\alpha-D)})$, so the easiness exponent asymptotes to 0 as $\alpha \rightarrow \infty$; in other words, sampling becomes hard after constant time, consistent with recent related results [45]. Nevertheless, for $\alpha \rightarrow \infty$, the easiness and hardness exponents still match, up to an irremovable $\delta > 0$ in 1D. We now outline the proofs of our results, whose details may be found in the Supplemental Material [46].

Easy-sampling timescale.— To derive t_{easy} , we give an efficient sampling algorithm. The algorithm performs

α	Easiness exponent γ_{easy}	Hardness exponent γ_{hard}
$\alpha < \frac{D}{2}$?	$\frac{1}{D} (\alpha - \frac{D}{2})$
$\frac{D}{2} \leq \alpha \leq D + 1$		0
$D + 1 \leq \alpha < \infty$	$\frac{-1}{\alpha - D}$	0 if $D \geq 2$ or $V < \infty$ ∞ otherwise.
$\alpha \rightarrow \infty$	0	

TABLE II. Easiness and hardness timescale exponents when $\beta = 1$.

time evolution on each cluster C_i separately. This takes polynomial time in the number of basis states, which is $\binom{|C_i|+b_i-1}{b_i} = O(|C_i|^{b_i})$ and hence polynomial in n when $b_i = O(1)$. This product-state approximation of the exact time-evolved state $|\psi(t)\rangle = U_t |\psi(0)\rangle$ is achieved by decomposing the propagator U_t via a spatial decomposition scheme for quantum simulation [42, 47] that we call the HHKL decomposition. We complete the derivation of the easiness timescale by showing that the approximation is good for times $t < O(t_{\text{easy}})$.

We briefly present the HHKL decomposition. Let H_R be the sum over all terms in the Hamiltonian supported completely in region R and implicitly let $XY = X \cup Y$ represent the union of regions. The decomposition scheme approximates the time evolution unitary acting on region XYZ (where Y separates regions X and Z) by forward evolution on YZ , backward evolution on Y , and forward evolution on XY : $U_{XYZ} \approx U_{XY}(U_Y)^\dagger U_{YZ}$. The operator norm error made by this approximation is [42] $O((e^{vt} - 1)\Phi(X)(\ell^{-\alpha+D+1} + e^{-\ell}))$, where $v > 0$ is a characteristic velocity, $\Phi(X)$ is the area of the boundary of X , and ℓ is the minimum distance between any pair of sites in X and Z . The error is small for times t shorter than the time it takes for information to propagate from X to Z .

The velocity v of information propagation is also known as a Lieb-Robinson velocity and is determined by the operator norm of terms in the Hamiltonian which couple different sites [39]. Since bosonic operators have unbounded operator norm, this could result in an unbounded velocity [48]. However, because of boson number conservation under the Hamiltonian, the dynamics is fully contained in the n -boson subspace, within which the operator norm of each term is $O(n)$. While free bosons ($V = 0$) behave as in the single-particle subspace, implying the Lieb-Robinson velocity is $O(1)$, in the interacting case, an $O(n)$ Lieb-Robinson velocity would cause the asymptotic easiness timescale to vanish ($t_{\text{easy}} \rightarrow 0$).

Nevertheless, we can derive an easiness timescale independent of V for a clustered initial state, a key technical result detailed in [46]. Intuitively, at short times each boson is well-localized within its original cluster. Therefore, the relevant subspace has at most b bosons in each cluster C_i . Truncating the Hilbert space to allow only $b + 1$ bosons per cluster is therefore a good approximation at short times [46, 49], and the truncation error vanishes in the asymptotic limit.

The modified Hamiltonian H' after truncation has terms with norm only $O(b)$, giving an effective Lieb-Robinson velocity $v = O(b) = O(1)$ for states close to the initial state [50]. For this modified Hamiltonian, we apply the HHKL decomposition to bound the error caused by simulating each cluster separately. Once the error has been calculated, the timescale immediately follows by solving $\epsilon(t) = O(1)$ for $t = t_{\text{easy}}$, which is a lower bound on the transition timescale t_* . In Ref. [46], we give the full dependence of t_{easy} on various system parameters, including the filling fraction of bosons.

Sampling hardness timescale.— To derive t_{hard} , we give protocols to simulate universal quantum circuits by setting the time dependent parameters $J_{ij}(t)$ of the long-range bosonic Hamiltonian. This implies sampling is worst-case hard after time t_{hard} . Specifically, if a general sampling algorithm exists for times $t \geq t_{\text{hard}}$, we prove this algorithm can also simulate hard quantum circuits [17] when interactions are strong, and boson sampling [10] when interactions are weak.

In the interacting case, our reduction from universal quantum computation to a long-range Hamiltonian hinges on implementing a universal gate set. Using a dual-rail encoding to encode a qubit in two modes of each cluster C_i , we show in Ref. [46] how to implement arbitrary single-qubit operations in $O(1)$ time and controlled-phase gates [51] between adjacent clusters in a time that depends on their spacing L . For hardcore bosons, the entangling gate is constructed slightly differently, and features an easiness result for the 1D nearest-neighbor case.

The two-qubit gate uses free particle state-transfer as a subroutine [43, 44] to bring adjacent logical qubits near each other. We implement the constant-depth circuit of Ref. [17], which consists only of onsite and nearest-neighbor gates between qubits in a 2D grid. The total time for hardness under this scheme takes time $O(\min[L, L^{\alpha-D}])$ when $\alpha > D$ and $O(1)$ when $\alpha \in [D/2, D]$. In 1D, simulating a 2D circuit introduces extra overhead. Nevertheless, we can recover the same timescale up to an infinitesimal $\delta > 0$ in the exponent by only encoding n^δ logical qubits.

Lastly, when $\alpha < D/2$, state transfer takes time $o(1)$ but the time for an entangling gate is $O(1)$. We can still achieve coarse hardness for time $o(1)$ by mapping the system onto free bosons, which we now come to.

In the noninteracting case, we implement the boson sampling scheme of Ref. [10], which showed that a Haar-random unitary applied to m sites containing n bosons gives a hard-to-sample state. It also gave an $O(n \log m)$ -depth decomposition of a linear-optical unitary in the circuit model without spatial locality. We give a faster implementation for the continuous-time Hamiltonian model, which can include simultaneous noncommuting terms but imposes spatial locality, a result of independent interest [46]. Specifically, we show that most linear-optical states of n bosons on m sites can be constructed in time $\min[O(nm^{1/D}), \tilde{O}(nm^{\alpha/D-1/2})]$, which is faster than the circuit model when $\alpha < D/2$. This result also uses free-particle state transfer as a subroutine. As in the 1D interacting case, we can implement the reduction on a polynomi-

ally growing number of bosons n^δ , resulting in the timescale of Table I for free bosons. This result resolves an important conceptual question posed by Ref. [20] for the noninteracting, nearest-neighbor case by closing the gap between t_{easy} and t_{hard} . In this limit, the transition timescale is at $\Theta(L/v)$, both with and without interactions, showing that the algorithm of Ref. [20] is optimal and that the presence of interactions does not change the phase diagram.

Sharp and coarse transitions— In the nearest-neighbor limit $\alpha \rightarrow \infty$, where the exponents on our hardness and easiness timescales match up to an infinitesimal (δ), we can make precise statements about the nature of the transition. In the presence of interactions and in two dimensions and above, the bounds on the timescale in the nearest-neighbor limit coincide up to a multiplicative constant at $t_{\text{easy}} = t_{\text{hard}} = \Theta(L)$, proving the transition is sharp. However, in 1D, the hardness timescale only matches up to an infinitesimal $\delta > 0$ in the exponent $c_{\text{hard}} = c_{\text{easy}} + \delta$. In this case, we show that c_{hard} cannot be improved any further, proving that this is a coarse transition.

To understand the physics behind the two kinds of transitions, it is illuminating to study the approach to the transition point from both sides. On the easiness side, the important quantity is the many-body entanglement. At short times, the wavefunction is approximately separable, implying easiness of classical simulation. The separable state is computed using an HHKL decomposition, whose errors grow in time until they become $O(1)$ at the transition timescale. These errors upper bound the amount of entanglement present across any cut, so the easy phase corresponds to states with no entanglement, and the complexity transition occurs as the entanglement grows from zero entanglement to area-law entanglement.

However, sampling complexity in one dimension is special because area-law entanglement is classically simulable using matrix product states [52, 53]. Specifically, in 1D, we prove an extended easiness timescale of $t_{\text{easy}} = cL$ for any constant c [46]. Thus, sampling is easy for all times $O(L)$, implying that the δ in the hardness exponent cannot be removed, and the transition is coarse. Further, our results suggest the sampling complexity increases smoothly as the entanglement grows from area-law to volume-law, as explained below. However, if $D \geq 2$, the argument based on entanglement breaks down because tensor-network contraction takes time exponential in the system size in both the worst case and average case [54, 55], and there are known examples of constant-depth 2D circuits that are hard to simulate [17].

On the hardness side, many-body entanglement is necessary but not sufficient for sampling hardness [1, 2, 56]. Since our hardness results in the interacting case rely on mapping bosons to qubits via a dual-rail encoding, we understand the transition by counting the number of encoded logical qubits. For coarse transitions, as the evolution time approaches the transition timescale t^* from above, the number of encoded logical qubits shrinks as n^δ , where $\delta \rightarrow 0$ as $t \rightarrow t^*$. This illustrates that while the problem is still asymptotically hard as

$n \rightarrow \infty$, one needs to go to higher boson numbers n to achieve the same computational complexity. On the other hand, for sharp transitions, as we approach the transition from the hard side, the number of encoded logical qubits suddenly jumps from $\Omega(n^c)$ for some constant c to $O(\log n)$. In Ref. [46], we elaborate on how to use the number of effective logical qubits as an order parameter for the phase transition. Whether or not such an order parameter is a universal way to characterize complexity phase transitions deserves closer attention.

Finally, in the noninteracting case, we do not know the nature of the transition in $D \geq 2$. However, if the infinitesimal in the hardness timescale cannot be removed, it would indicate a coarse transition. Alternatively, there may exist a constant-depth boson sampling circuit on a nearest-neighbor architecture for which approximate sampling is classically hard. It has been proved by Brod [57] that exact sampling of constant-depth boson sampling is classically hard. Nevertheless, Brod points out that it is unclear if this exact sampling hardness can be extended to the approximate sampling hardness we consider in this paper. As such, in $D \geq 2$ without interactions, the type of transition is an open problem.

Lastly, we note that the transition can also be studied for the case when the bosons evolve under local random gates, as is done in Ref. [58]. The authors observe a seemingly coarse complexity transition as a function of depth, although the true nature of the transition is open in this case as well.

Outlook.— We have mapped out the complexity of the long-range Bose-Hubbard model as a function of the particle density β , the degree of locality α , the dimensionality D , and the evolution time t . An interesting open question concerns regions of the phase diagram at finite α without definitive easiness/hardness results. These gaps are closely related to finding state-transfer protocols which saturate Lieb-Robinson bounds. Stronger Lieb-Robinson bounds can increase t_{easy} , and faster state-transfer can reduce t_{hard} , as evidenced by the improvement over the first version of this manuscript [59] due to results from Ref. [44]. These observations show that studying complexity phase transitions provides a nice testbed for, and gives an alternative perspective on results pertaining to the locality of quantum systems.

Our results directly apply to a wide range of experimental platforms in quantum information, such as cold atoms and trapped ions, as their Hamiltonians are special cases of the one that we study, or straightforward extensions. Our model is also ideal for studying dynamics in long-range interacting systems and models of modular networks. We elaborate on these connections in Ref. [46].

If the qualitative features of the phase diagram we have derived for the Bose-Hubbard model hold more generally, our results may hint at a notion of universality present in transitions between complexity phases. In 1D, we have proved that the transition is always coarse. However, in 2D and higher, when there are interactions, the transition is sharp. In contrast, in 2D and higher for noninteracting transitions, the transition type is unknown. This dependence on the dimension and possible dependence on interaction type hints at classify-

ing complexity phases of matter, and the transitions between them, based on generic features such as connectivity, dimensionality, and kinds of interactions.

Along this line, it would be interesting to study whether similar features occur for different kinds of complexity phase transitions. In our work, the transition occurs in the dynamics of a many-body Hamiltonian. However, different approaches are possible. For example, one could consider open quantum systems, where decoherence might drive dynamical transitions from hard to easy. A particularly rich class is that of random quantum circuits with interspersed measurements [60–62], which have distinct non-equilibrium phases and entanglement phase transitions, and which may be promising models to study complexity phase transitions.

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