Optimal light cone and digital quantum simulation of interacting bosons

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I. MOTIVATION AND BACKGROUND

A fundamental principle of many-body physics is causality: a strict prohibition of information propagation outside the light cone. However, in non-relativistic systems, it is often unclear whether such a light cone can be well defined. In the famous work by Lieb and Robinson, the amount of information is proved to be restricted in the effective light cone, which is characterized by the so-called "Lieb-Robinson bound." So far, the Lieb-Robinson bound is a crucial concept in accessing the precision error of various quantum simulation algorithms and the mathematical structure of quantum entanglement at low (or zero) temperatures; to name a few, the area law of entanglement [Hastings, J. Stat. Mech. (2007)], quasi-adiabatic continuation [Hastings and Wen, PRB (2005)], clustering theorems for correlation functions [Hastings and Koma, CMP (2007)], [Kuwahara and Saito, PRX (2022), QIP2022], tensor-network based classical simulation of many-body systems [Osborne, PRL (2006)], optimal circuit complexity of quantum dynamics [Haah, et al., FOCS (2018), QIP2019], sample complexity of quantum Hamiltonian learning [Anshu, et al., Nature Physics (2021), QIP2021], and quantum information scrambling [Robert and Swingle, PRL (2016)], etc.

However, the original work by Lieb and Robinson and the followed generalizations are severely limited to systems with the two conditions, i.e., i) short-rangeness of the interactions and ii) finite bound of local energy. The breakdown of these conditions is ubiquitous in realistic experiments (e.g., cold atom setups). Nevertheless, the speed limit on information propagation is highly nontrivial in such cases. The breakdown of condition (i), i.e., the existence of long-range interactions, has been intensively studied in the past decade [Kuwahara and Saito, PRX (2020), TQC2019], [Tran, et al., PRX (2021), QIP2021]. These studies have significantly unraveled the forms of optimal light cones for long-range interacting systems.

On the other hand, the breakdown of the latter condition (i.e., finite bound of local energy) has still been elusive despite great efforts over the years. When the norm of the interactions is locally unbounded, all the mathematical tools to prove the Lieb-Robinson bound break down. The representative example to break the condition is the interacting boson systems, which typically appear in cold atom experiments [Cheneau, et al., Nature (2012)]. Then, can one prove the linear light cone for interacting boson systems in general? The answer is generally no as has been shown by Eisert and Gross [Eisert and Gross, PRL (2009), QIP2009], where the speed of information propagation exponentially increases with time. This point necessitates us to restrict ourselves to specific classes of interacting boson systems. Among them, the most important class is the Bose-Hubbard model, the well-known minimal model describing cold atoms in optical lattices. Over a decade, the Lieb-Robinson bound in the Bose-Hubbard model has been a challenging open problem in the fields of quantum information and quantum many-body physics.

We here report the solution to this long-standing problem. In detail, we identify the optimal light cone for the Bose-Hubbard type models and establish a gate complexity to simulate the dynamics with an efficiency guarantee.

II. SUMMARY OF MAIN RESULTS AND APPLICATIONS

Before going to our main result, we explain what has been clarified before our work. First of all, considering the Lieb-Robinson bound in the Bose-Hubbard type model, the primary difficulty stems from the fact that the standard approach for the Lieb-Robinson bound necessarily yields a Lieb-Robinson velocity proportional to the norm of the local energy. That is, when all the bosons (say N bosons) clump at a single site, the on-site energy can be as large as $\mathrm{Poly}(N)$, which induces an infinite Lieb-Robinson

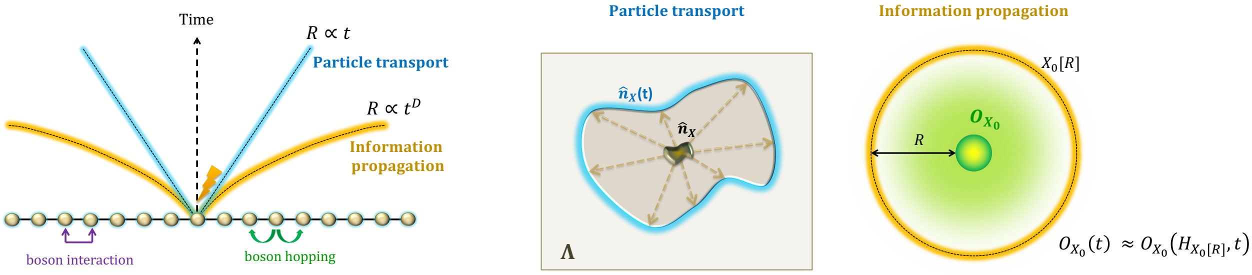

FIG. 1. Schematic pictures of the effective light cones.

velocity as $N \to \infty$. Although it is unlikely that many bosons will clump together in realistic experiments, we must take the theoretical possibility of such situations into account. Therefore, to estimate the Lieb-Robinson velocity, we at least need to estimate the speed for bosons to clump together. Such analysis is essential in truncating the boson number with an error guarantee.

Based on the above discussion, we have to tackle the following primary targets separately: i) the speed of boson particle transport, ii) propagation of total information. Relevant to the first issue i), Schuch, Harrison, Osborne, and Eisert brought the first breakthrough by considering the diffusion of the initially concentrated bosons in the vacuum and ensured that the bosons have a finite propagation speed [Schuch, et al., PRA (2011), QIP2011]. Very recently, the initial setup has been relaxed to general states while assuming a macroscopic number[*1] of boson transport [Faupin, et al., PRL (2022)]. On the second issue ii), Wang and Hazzard derived the Lieb-Robinson velocity that was proportional to the square root of the total number of bosons [Wang and Hazzard, PRX Quantum (2020)], which is qualitatively better than the previous one. However, the velocity is still infinitely large in the thermodynamic limit. The first meaningful Lieb-Robinson bound has been derived by Kuwahara and Saito, where the linear light cone was proved under the assumptions that the initial state is steady and has a small number of bosons in each site [Kuwahara and Saito, PRL (2021), TQC2021], which has been improved in the subsequent work [Yin and Lucas, PRX (2022)]. Thus, the remaining problems are the following:

1. Proving the finite speed of boson particle transport for arbitrary initial states

2. Identifying the optimal light cone of information propagation for arbitrary non-steady initial states with low-boson density[*2].

In summary, we have solved the above problems in general setups [see also Fig. 1]. Our results are applicable to arbitrary time-dependent Bose-Hubbard-type Hamiltonians in arbitrary dimensions starting from a non-steady initial state. Such a setup is most natural in practice and crucial in estimating the gate complexity of digital quantum simulation of interacting boson systems.

As a critical difference between bosons and fermions (or spin models), we have clarified that the acceleration of information propagation can occur in high dimensions. Furthermore, as a practical application, we develop a gate complexity for efficiency-guaranteed digital quantum simulations of interacting bosons based on the Haah-Hastings-Kohtari-Low (HHKL) algorithm [Haah, et al., FOCS (2018), QIP2019].

1. *Boson particle transport*

We consider a quantum system on a D-dimensional lattice (graph) with Λ set for all sites. We focus on the Bose-Hubbard type Hamiltonian in the form of

$$H = \sum_{\langle i,j \rangle} J_{i,j}(b_i b_j^\dagger + \mathrm{h.c.}) + f\left(\{\hat{n}_i\}_{i\in\Lambda}\right) \tag{1}$$

[*1] Macroscopic number means $\Omega(N_{\mathrm{total}})$ with N_{total} the number of all the bosons in the system.

[*2] Without low-boson density condition [i.e., Eq. (4)], it has been already known that the Lieb-Robinson velocity can be arbitrarily large [Barmettler, et al., PRA (2012)]

with $|J_{i,j}| \le \bar{J}$, where $\sum_{\langle i,j\rangle}$ is the summation for all pairs of the adjacent sites $\{i,j\}$ on the lattice and $f(\{\hat{n}_i\}_{i\in\Lambda})$ is an arbitrary function of the boson number operators $\{\hat{n}_i\}_{i\in\Lambda}$ with $\hat{n}_i = b_i^\dagger b_i$. The function $f(\{\hat{n}_i\}_{i\in\Lambda})$ includes arbitrary long-range boson-boson couplings. Moreover, all results are applied to the time-dependent Hamiltonians.

The first problem is to identify how the boson number distribution changes with time evolution. In detail, we need to know the upper bound of the moment function ($X \subseteq \Lambda$)

$$\mathrm{tr}\left[\rho_0(t)\hat{n}_X^s\right] = \mathrm{tr}\left[\rho_0 \hat{n}_X(t)^s\right] \quad (s\in\mathbb{N}), \quad \hat{n}_X := \sum_{i\in X}\hat{n}_X, \tag{2}$$

where ρ_0 is arbitrarily chosen. Our first result gives the following general upper bound:

Result 1. For $R \ge c_0 t\log t$, the time-evolution $\hat{n}_X(t)$ satisfies the operator inequality of

$$[\hat{n}_X(t)]^s \preceq \left[\hat{n}_{X[R]} + \delta\hat{n}_{X[R]} + c_2 ts\right]^s, \quad \delta\hat{n}_{X[R]} = e^{-c_1R/t}\sum_{j\in\Lambda} e^{-c_1' d_{j,X[R]}}\hat{n}_j \tag{3}$$

with $X[r]$ the extended subset by length r as $X[r] := \{i\in\Lambda | d_{i,X} \le r\}$, where $\{c_0, c_1, c_1', c_2\}$ are the constants of $\mathcal{O}(1)$. The operator $\delta\hat{n}_{X[R]}$ is as small as $e^{-\mathcal{O}(R/t)}$ if there are not many bosons around the region $X[R]$. We can apply this theorem to a wide range of setups. Interestingly, it holds for systems with arbitrary long-range boson-boson interactions, such as the Coulomb interaction.

2. Lieb-Robinson bound and gate complexity of quantum simulation

We here assume that the boson-boson interaction is finite unlike the setup for Result 1 and the initial state ρ_0 satisfies the following low-boson-density condition:

$$\mathrm{tr}(\rho_0\hat{n}_i^s) \le \frac{1}{e}\left(\frac{b_0}{e}s^\kappa\right)^s, \tag{4}$$

where b_0 and κ (≥ 1) are the constants of $\mathcal{O}(1)$. From this condition, the boson number distribution at each site decays (sub)-exponentially at the initial time. The simplest example is the Mott state, where a finite fixed number of bosons sit on each site.

In proving the Lieb-Robinson bound, we utilize the boson number truncation at each site after the time evolution. From Result 1, we can quantitatively estimate the truncation error, which allows us to derive the following result,

Result 2. For an arbitrary operator O_X and O_Y with unit norm[*3] ($\|O_X\| = \|O_Y\| = 1$), the time evolution $O_{X_0}(t)$ is well approximated by using the subset Hamiltonian on $X_0[R]$ with the error of

$$\left\|[O_X(t), O_Y]\,\rho_0\right\|_1 \le e^{-C(R/t^D)^{\frac{1}{\kappa D}}}, \tag{5}$$

for $R \ge t^D\mathrm{polylog}(t)$, where $\|\cdot\|_1$ is the trace norm and C is an $\mathcal{O}(1)$ constant.

From Result 2, the speed of information propagation is proportional to t^{D-1}. We can demonstrate that the obtained upper bound is qualitatively optimal by explicitly developing time evolution to achieve the bound [see Fig. 4 in the technical abstract].

By combining Result 1 and Result 2, we can finally estimate the sufficient number of quantum gates that implement the bosonic time evolution e^{-iHt} acting on an initial state ρ_0:

Result 3. For an arbitrary initial state ρ_0 with the condition (4), the number of elementary quantum gates for implementing $e^{-iHt}\rho_0 e^{iHt}$ up to an error ϵ is at most

$$|\Lambda| t^{D+1}\mathrm{polylog}(|\Lambda|t/\epsilon), \tag{6}$$

with the depth of the circuit $t^{D+1}\mathrm{polylog}(|\Lambda|t/\epsilon)$, where the error is given in terms of the trace norm. Remember that $|\Lambda|$ is the number of the sites in the total system.

[*3] The condition of the unit norm is not essential and can be removed as long as the operator O_X and O_Y are upper-bounded by $|O_X| \preceq \mathrm{poly}[(\hat{n}_i)_{i\in X}]$ and $|O_Y| \preceq \mathrm{poly}[(\hat{n}_i)_{i\in Y}]$