Tensor-network Study of Correlation-spreading Dynamics in the Two-dimensional Bose-Hubbard Model

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Article

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1 **Tensor-network study of correlation-spreading dynamics in the**
2 **two-dimensional Bose-Hubbard model**

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Abstract

Recent developments in analog quantum simulators based on cold atoms and trapped ions call for cross-validating the accuracy of quantum-simulation experiments with use of quantitative numerical methods; however, it is particularly challenging for dynamics of systems with more than one spatial dimension. Here we demonstrate that a tensor-network method running on classical computers is useful for this purpose. We specifically analyze real-time dynamics of the two-dimensional Bose-Hubbard model after a sudden quench starting from the Mott insulator by means of the infinite projected entangled pair state algorithm. Calculated single-particle correlation functions are found to be in good agreement with a recent experiment [Y. Takasu *et al.*, Sci. Adv. **6**, eaba9255 (2020)]. By estimating the phase and group velocities from the single-particle and density-density correlation functions, we predict how these velocities vary in the moderate interaction region, which serves as a quantitative benchmark for future experiments.

7 I. INTRODUCTION

State-of-art experimental platforms of cold atoms and trapped ions as analog quantum simulators have offered unique opportunities for studying far-from-equilibrium dynamics of isolated quantum many-body systems. Thanks to their high controllability and long coherence time, these platforms have already addressed a variety of intriguing phenomena that are in general difficult to simulate with classical computers, such as correlation spreading [1–3] and relaxation [4–6] after a quantum quench, many-body localization in a disorder potential [7–9], and quantum scar states [10, 11]. Nevertheless, accurate numerical methods using classical computers are highly demanded at the current stage of the studies of quantum many-body dynamics, since the classical computation still has complementary advantages over the quantum simulation in that it is free of noise and much more accessible owing to its wide dissemination. In this sense, it is important to cross-check the validity of quantum-simulation experiments and some numerical methods by comparing them with each other.

In particular, direct comparisons between experimental and numerical outputs have

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FIG. 1. (a) Schematic figure of iPEPS with a two-site unit cell. A rank-five tensor at each site is represented as a circle with four thin lines and one thick line. The former lines correspond to the virtual degrees of freedom with the bond dimension D , while the latter line corresponds to the physical degrees of freedom with the dimension of the local Hilbert space D_{phys} . The wave functions become more accurate as D increases. (b) Time dependence of the hopping J (a red solid line) and the onsite interaction U (a blue dashed line) with a finite-time quench. The parameter U/J is varied from ~ 99.4 to ~ 19.6 for $-\tau_Q < t < 0$. In the case of a sudden quench, we discard the region $-\tau_Q < t < 0$.

22 been made for dynamical spreading of two-point spatial correlations of the Bose-Hubbard
 23 model [1, 3, 12–15], which can be realized experimentally with ultracold bosons in optical
 24 lattices [16]. The correlation spreading has attracted much theoretical interest [12–15, 17–24]

25 in the sense that it is closely related to fundamental phenomena, including the propagation
 26 of quantum information and the thermalization. In one spatial dimension, quasi-exact nu-
 27 merical methods based on matrix product states (MPSs) have been used to validate the
 28 performance of the quantum simulators [1, 3, 12]. In two dimensions (2D), by contrast,
 29 accurate numerical simulations are challenging. Indeed, the comparisons with respect to
 30 a single-particle correlation have shown that a few types of the truncated Wigner approx-
 31 imation (TWA) fail to capture the real-time evolution accurately enough to extract the
 32 propagation velocity of the correlation [3, 14]. Moreover, while the propagation velocities
 33 obtained by a two-particle irreducible strong-coupling (2PISC) approach quantitatively agree
 34 with the experimental value, its applicability is limited to a strongly interacting regime, and
 35 it does not accurately give the value of the correlation itself [15].

36 In this paper, we present quantitative numerical analyses of the correlation-spreading
 37 dynamics of the 2D Bose-Hubbard model starting from a Mott insulating initial state with
 38 unit filling. To this end, we employ the tensor-network method based on the infinite pro-
 39 jected entangled pair state (iPEPS) [25–32] or the tensor product state [33–37], which is an
 40 extension of MPS to 2D systems [see Fig.1(a)]. The iPEPS studies on real-time dynamics of
 41 isolated [38–46] and open [38, 39, 47–49] quantum systems in 2D have begun very recently.
 42 Previous simulations suggest that iPEPS can represent relatively low-entangled states in
 43 short-time dynamics for simple spin 1/2 systems [38–41] and some itinerant electron sys-
 44 tems [43]. This observation may be valid for real-time dynamics in Bose-Hubbard systems;
 45 however, little is known about it until now. We find that the single-particle correlation com-
 46 puted with iPEPS, as well as the estimated propagation velocity of the correlation front,
 47 agrees very well with the experimental result [3], demonstrating that iPEPS can be useful for
 48 actual quantum-simulation experiments. We also conduct numerical simulations in a mod-
 49 erate interaction region, which has not been addressed by the previous experiments [1, 3].
 50 From the real-time evolution of the single-particle and density-density correlations, we show
 51 that the phase and group velocities approach each other when the interaction decreases.

52 II. RESULTS

53 A. Model

54 We consider the Bose-Hubbard model on a square lattice [50, 51]. The Hamiltonian is
 55 given as

$$\hat{H} = -J \sum_{\langle ij \rangle} (\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i, \quad (1)$$

56 where $\hat{a}_i^\dagger$ and $\hat{a}_i$ are the creation and annihilation operators at site i , $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ is the number
 57 operator, J is the strength of the hopping between nearest-neighbor sites, U is the strength
 58 of the onsite interaction, and μ is the chemical potential. The notation $\langle ij \rangle$ indicates that
 59 sites i and j are nearest neighbors. For simplicity, we ignore the effects of the trap potential
 60 and the Gaussian envelopes of optical lattice lasers, which do not affect short-time dynamics.
 61 We set the lattice spacing d_{lat} to be unity. The ground state at the commensurate filling is
 62 the Mott insulating (superfluid) state for $U \gg J$ ($U \ll J$). Hereafter, we will consider a
 63 sudden quench and a quench with a short time [see Fig. 1(b)].

64 B. Quench starting from the Mott insulator: Comparison with the exact diago- 65 nalization and the experiment

66 Let us first focus on the case of a sudden quench. We compare our results of iPEPS with
 67 those of the exact diagonalization (ED) method and obtain consistent results in a short time.
 68 In the ED simulations using the QuSpin library [52, 53], we choose the system sizes $L_x \times L_y$
 69 up to 5×4 and use the periodic-periodic boundary condition. We examine to what extent
 70 the energy is conserved in the iPEPS simulations. The grand potential density $\langle \hat{H} \rangle$ at $T = 0$
 71 starting from the Mott insulator $\otimes_i |n_i = 1\rangle$ should remain constant. They well converge
 72 for $D \geq 6$ and remain nearly constant up to $t \sim 0.4\hbar/J$ [54]. We also investigate how
 73 the single-particle correlations converge with increasing bond dimensions. The equal-time
 74 single-particle correlation function at a distance $\mathbf{r} = (x, y)$ for the system size N_s is defined
 75 as

$$C_{\mathbf{r}}^{\text{sp}}(t) = \frac{1}{2N_s} \sum'_{i,j} \langle \hat{a}_i^\dagger(t) \hat{a}_j(t) + \hat{a}_j^\dagger(t) \hat{a}_i(t) \rangle. \quad (2)$$

FIG. 2. Comparison of the single-particle correlation functions in the case of a sudden quench between iPEPS (blue lines with symbols) and ED (gray lines). The correlations at distances (a) $|\mathbf{r}| = 1$ and (b) $|\mathbf{r}| = \sqrt{2}$ are shown. Both results overlap perfectly in a short time.

Here $\sum'_{i,j}$ denotes the summation over (i, j) that satisfies $|x_j - x_i| = x$ and $|y_j - y_i| = y$. In the iPEPS simulations, $1/N_s \times \sum'_{i,j}$ is replaced by $1/2 \times \sum_{i=A,B} \sum'_{j}$ with A and B being sublattice sites because of the translational invariance. As shown in Fig. 2, $C^{\text{sp}}_{|\mathbf{r}|=1}(t) := [C^{\text{sp}}_{\mathbf{r}=(1,0)}(t) + C^{\text{sp}}_{\mathbf{r}=(0,1)}(t)]/2$ exhibits a peak at $t \sim 0.15\hbar/J$ in both results, and they overlap perfectly in this short time. For $t \gtrsim 0.15\hbar/J$, the correlation functions of ED start to exhibit a significant finite-size effect, whereas those of iPEPS converge for $D \geq 6$. We observe similar behavior for $C^{\text{sp}}_{|\mathbf{r}|=\sqrt{2}}(t) := C^{\text{sp}}_{\mathbf{r}=(1,1)}(t)$. The iPEPS results are better simulated up to a longer time.

FIG. 3. Comparison of the single-particle correlation functions in the case of a finite-time quench between iPEPS (blue lines with symbols) and the experiment (red circles). The correlations at distances (a) $|\mathbf{r}| = 1$, (b) $|\mathbf{r}| = 2$, and (c) $|\mathbf{r}| = 3$ are shown. Both results are in good agreement.

Next, we compare the correlations of iPEPS with those of the experiment [3] for a finite quench time. Figures 3(a–c) show the time evolution of correlations at distances $|\mathbf{r}| = 1, 2$, and 3, respectively. Qualitative behavior is essentially equivalent to the case of the sudden quench, although the correlation function shifts to an earlier time. For $|\mathbf{r}| = 1$, both data show a peak at $t \sim 0.12\hbar/J_{\text{final}}$. Similarly, the first-peak times are consistent with each other for $|\mathbf{r}| = 2$ and 3, and they become longer with increasing distances. When the energy is approximately conserved (namely, for $t \lesssim 0.4\hbar/J_{\text{final}}$ [54]), the intensities of correlations also overlap very well. They are also consistent with those obtained by TWA [3, 13, 14], while the iPEPS simulations can deal with a slightly longer time and capture the correlation peaks more clearly [54].

C. Estimates of group and phase velocities in the moderate interaction region

Having confirmed the applicability of iPEPS simulations to real-time evolution of the Bose-Hubbard model, we study how information propagates by a sudden quench in the moderate interaction region. There are two kinds of velocity that are relevant to the correlation spreading. One is the group velocity v_{gr} , which corresponds to the propagation of the envelope of the wave packet and is a suitable quantity to characterize the spreading of correlations. In non-relativistic quantum many-body systems, v_{gr} is bounded above, and the upper bound is known as the Lieb-Robinson bound [23, 24, 55, 56]. Notice that the Lieb-Robinson bound for the Bose-Hubbard model has not been rigorously derived with a few exceptions for limited situations [18, 23, 24]. The phase velocity v_{ph} is the other characteristic quantity, which corresponds to the propagation of the first peak of the wave packet, and does not have to obey the Lieb-Robinson bound.

To estimate the group velocity from the single-particle correlations, long-time simulations are required in general. However, it is challenging in the iPEPS simulations. To circumvent the difficulty, we estimate the group velocity by the density-density correlation. It is known that the propagation velocity of the first peak of this correlation agrees very well with the group velocity [1, 12]. The equal-time density-density correlation function at a distance $\mathbf{r} = (x, y)$ for the system size N_s is defined as

$$C_{\mathbf{r}}^{\text{dd}}(t) = \frac{1}{N_s} \sum'_{i,j} \langle \hat{n}_i(t) \hat{n}_j(t) \rangle_c, \quad (3)$$

FIG. 4. (a) Single-particle and (b) density-density correlation functions per bond at $U/J = 5$ for the bond dimension $D = 8$. The normalization factor at a distance $\mathbf{r} = (x, y)$ is given as $N_{\text{bond}} = 2$ for $x \neq y$ ($|\mathbf{r}| = 1, 2$, and 3), while it is $N_{\text{bond}} = 4$ for $x = y$ ($|\mathbf{r}| = \sqrt{2}$). The black symbol corresponds to the first peak in the correlation function obtained by cubic spline interpolation of data points. The propagation velocities along the horizontal or vertical axis are extracted by the data at $|\mathbf{r}| = 1, 2$, and 3 . The velocity estimated from the density-density correlation functions is slower than that from the single-particle correlation functions.

where $\langle \cdots \rangle_c$ denotes a connected correlation function. In our simulations, $\langle \hat{n}_i(t) \hat{n}_j(t) \rangle_c = \langle \hat{n}_i(t) \hat{n}_j(t) \rangle - 1$ because $\langle \hat{n}_i(t) \rangle = 1$ for all sites and time steps. As in $C_{\mathbf{r}}^{\text{sp}}(t)$, the summation is replaced by that within sublattice sites in the iPEPS simulations. The parity-parity correlation closely related to the density-density one can be measured in experiments by using the quantum-gas microscope techniques [1].

FIG. 5. Estimated group (red circles) and phase (blue squares) velocities from the density-density and single-particle correlation functions for the bond dimensions $D = 8$ and $D = 9$. The data for $D = 8$ and $D = 9$ overlap within the error bars. The velocities and their error bars are obtained by extrapolation of the distance dependence of the peak time. The results obtained by the 2PISC approach [15] (triangles), TWA [13] (diamonds), and the experiment [3] (a star) are also shown. Both velocities gradually merge with decreasing interaction.

117 We extract the propagation velocities from the first peak in both correlations for $|\mathbf{r}| = 1$,
 118 2, and 3. For simplicity, we consider the sudden quench hereafter. When the interaction
 119 becomes weaker, we have confirmed that the energy is conserved in a longer time frame;
 120 typically, $t \lesssim 0.9\hbar/J$ for $U/J \sim 5$ [54]. All the correlation peaks for $|\mathbf{r}| \leq 3$ appear in
 121 this time frame (see Fig. 4). The first peak of the single-particle correlation appears at
 122 $t \sim 0.35\hbar/J$ for $|\mathbf{r}| = 1$, while it appears at $t \sim 0.65\hbar/J$ for $|\mathbf{r}| = 3$. By contrast, the first
 123 peak of the density-density correlation appears at $t \sim 0.25\hbar/J$ for $|\mathbf{r}| = 1$, while it appears
 124 at $t \sim 0.7\hbar/J$ for $|\mathbf{r}| = 3$. It takes a long time for propagation in the latter case. The
 125 first-peak time is almost a linear function of the distance [54], and the system exhibits the
 126 light-cone-like spreading of correlations.

127 We summarize the interaction dependence of the group and phase velocities in Fig. 5. In
 128 the weak interaction region, the estimated group velocities are $v_{\text{gr}} \sim 4J/\hbar$. They are similar
 129 to those obtained by the TWA at filling factor $\nu = 10$ [13]. They are also consistent with the

group velocity $v_{\text{gr}}(U = 0) = 4J/\hbar$ of a single particle [13]. In the strong interaction region, the estimated group velocity $v_{\text{gr}} \sim (8 \pm 2)J/\hbar$ at $U/J = 19.6$ coincides with that obtained by the 2PISC approach [15] within the error bar of extrapolation. It is also comparable to the group velocity $v_{\text{gr}}(U \gg J) = 6J/\hbar \times [1 + \mathcal{O}(J^2/U^2)]$ of a quasi-particle in the large U limit [1, 3, 12]. Similarly, the estimated phase velocity agrees very well with the results of the 2PISC approach [15] and the experiment [3]. In the intermediate region, the estimated group velocity is closer to the single-particle group velocity in the superfluid region, whereas it is comparable to the 2PISC result near and above the critical point $U_c/J \sim 16.7$ [57–59]. Both group and phase velocities gradually converge to the same value as U/J is decreased.

III. CONCLUSION

We have studied real-time dynamics of the 2D Bose-Hubbard model after a sudden quench starting from the Mott insulator with unit filling. We have employed the 2D tensor-network method based on the infinite projected entangled pair states, which are the 2D extension of the well-known matrix product states in one dimension. Calculated single-particle correlation functions reproduce the recent experimental results very well. The iPEPS algorithm can simulate real-time dynamics long enough for extracting the propagation velocities from correlations. We have also estimated the group and phase velocities in the moderate interaction region, in which the 2PISC approach and the TWA are not applicable. Our findings would be useful in the future analog quantum simulation of Bose-Hubbard systems. The ability of the tensor-network method that accurately calculates the real-time dynamics of 2D quantum many-body systems opens up the possibility of applying it to other quantum-simulation platforms, such as Rydberg atoms, trapped ions, and superconducting circuits.

IV. METHODS

A. Real-time evolution by infinite projected entangled pair states

We prepare iPEPS with a two-site unit cell [see Fig. 1(a)]. The symbols D and D_{phys} denote the virtual bond dimension and the dimension of the local Hilbert space, respectively. The former improves the accuracy of the wave function, whereas the latter corresponds to the maximum particle number n_{max} as $D_{\text{phys}} = n_{\text{max}} + 1$. Although n_{max} can take infinity in

158 Bose-Hubbard systems, it is practically bounded above in the presence of interaction [60, 61].
 159 We can choose finite D_{phys} in the simulations of real-time dynamics. In the case of a sudden
 160 quench to the Mott insulating region ($U/J > U_c/J \sim 16.7$ [57–59]), we set the dimension of
 161 the local Hilbert space as $D_{\text{phys}} = 3$ because the number of particles deviates only slightly
 162 from unity [60, 61]. For $U/J < U_c/J$, we choose $D_{\text{phys}} = 5$ so that the wave functions can
 163 further take into account the effect of particle fluctuations. When U is close to zero (at
 164 $U/J = 2$ in our simulations), we use slightly larger $D_{\text{phys}} = 7$. The initial Mott insulating
 165 state $\otimes_i |n_i = 1\rangle$ can be represented with the bond dimension $D = 1$. As for static properties,
 166 the Bose-Hubbard model was investigated by finite PEPS or iPEPS, and the phase transition
 167 between the Mott insulating and superfluid phases was reproduced [62–70].

168 The wave function at each time $|\Psi(t)\rangle = e^{-it\hat{H}/\hbar}|\Psi(0)\rangle$ is obtained by real-time evolving
 169 iPEPS [38–40]. The real-time evolution operator in a small time step dt can be approximated
 170 by the Suzuki-Trotter decomposition [71–73] as $e^{-idt\hat{H}/\hbar} \sim \prod_{\langle ij \rangle} e^{-idt\hat{H}_{ij}/\hbar}$, where $\hat{H}_{ij} =$
 171 $-J(\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i) + U[\hat{n}_i(\hat{n}_i - 1) + \hat{n}_j(\hat{n}_j - 1)]/(2z) - \mu(\hat{n}_i + \hat{n}_j)/z$ with the coordination
 172 number $z = 4$ is the local Hamiltonian satisfying $\hat{H} = \sum_{\langle ij \rangle} \hat{H}_{ij}$. After applying the two-
 173 site gate $e^{-idt\hat{H}_{ij}/\hbar}$ to neighboring tensors, we approximate the local tensors by the singular
 174 value decomposition in such a way that the virtual bond dimension of iPEPS remains D .
 175 In the actual simulations, the second-order Suzuki-Trotter decomposition is used for this
 176 simple update algorithm [29, 74], and the tensor-network library TeNeS [75, 76] is adopted.
 177 The wave functions are optimized up to the bond dimension $D = 9$. As we will see later,
 178 qualitative behavior of correlation functions is nearly the same for $D \geq 6$. When extracting
 179 the propagation velocities, we mainly use the data for $D = 8$ and $D = 9$ to ensure sufficient
 180 convergence of physical quantities. We have numerically found that at these values of D ,
 181 the number of particles is nearly conserved during the real-time evolution starting from the
 182 Mott insulator.

183 Physical quantities in the thermodynamic limit are calculated by the corner transfer
 184 matrix renormalization group (CTMRG) method [30–32, 34, 77–83]. The bond dimension
 185 of the environment tensors is chosen as $\chi = 2D^2$ to ensure that physical quantities are well
 186 converged.

187 To compare our results obtained by iPEPS with the experiment [3], we consider a quench
 188 with a short time $\tau_Q = 0.1\text{ms}$ [13, 14] [see Fig. 1(b)]. For $-\tau_Q < t < 0$, both J and U are
 189 controlled. The wave function is updated as $|\Psi(t + dt)\rangle \sim e^{-idt\hat{H}(t)/\hbar}|\Psi(t)\rangle$ with the time-

dependent Hamiltonian $\hat{H}(t)$ in this region. For $t > 0$, both parameters are fixed. We take $J_{\text{final}} = J(t = 0) \sim 0.0612\hbar/\tau_Q$ as the unit of energy. The discrete time step for the real-time evolution is set to be $dt/(\hbar/J_{\text{final}}) = \tau_Q/(\hbar/J_{\text{final}})/15 \sim 0.00408$ for all t . To compare the iPEPS results with the exact real-time dynamics in finite-size systems, we also consider a sudden parameter change and set the time step as $dt/(\hbar/J) = 0.005$. We have checked that the simulations with doubled and halved dt do not change the results significantly.

V. DATA AVAILABILITY

The data in this paper are available from the authors upon request.

VI. CODE AVAILABILITY

The codes in this paper are available from the authors upon request.

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VII. AUTHOR CONTRIBUTIONS

R.K. and I.D. designed and coordinated the studies. R.K. performed the numerical simulations. R.K. and I.D. contributed to the writing of the manuscript.

395 **VIII. COMPETING INTERESTS**

396 The authors declare no competing interests.

397 **IX. ADDITIONAL INFORMATION**

398 **Supplementary information** is available for this paper at XXXXXX.

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