Energy redistribution and spatio-temporal evolution of correlations after a sudden quench of the Bose-Hubbard model

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An optical-lattice quantum simulator is an ideal experimental platform to investigate non-equilibrium dynamics of a quantum many-body system, which is in general hard to simulate with classical computers. Here, we use our quantum simulator of the Bose-Hubbard model to study dynamics far from equilibrium after a quantum quench. We successfully demonstrate the energy conservation law in the one- and three-dimensional systems and extract the propagation velocity of the single-particle correlation in the one- and two-dimensional systems. We corroborate the validity of our quantum simulator through quantitative comparisons between the experiments and the exact numerical calculations in one dimension. In the computationally hard cases of two or three dimensions, by using the quantum-simulation results as references, we examine the performance of a numerical method, namely the truncated Wigner approximation, revealing its usefulness and limitation. This work constitutes an exemplary case for the usage of analog quantum simulators.

Rapid advances in analog quantum simulation using highly controllable systems with long coherence time, such as ultracold gases in optical lattices (for example, see ref. [1–2]), Rydberg atoms in an optical tweezer array (for example, see ref. [3–5]), and trapped ions (for example, see ref. [6, 7]), have significantly expanded possibilities for studying dynamics of quantum many-body systems. One of the recent targets of optical-lattice quantum simulators has been the investigation of the non-equilibrium dynamics arising after a quantum quench [8–13], where a parameter of the system is varied rapidly and substantially. In the case of one dimension (1D) for a short time scale, quantum quench dynamics can be exactly computed with classical computers by means of the matrix product state (MPS) method [8–10]. In pioneering works of quantum-simulation research, the outputs of experiments were directly compared with those of exact numerical simulation with classical computers in order to examine the performance of the quantum simulators [8–10]. A two-point spatial correlation as a function of the distance of the two points has been the intense theoretical interest [11–24], and in fact, in one-dimensional systems, it has been shown that access to such a correlation function allows for exploring the dynamical spreading of quantum information, which is of great interest in connection with the Lieb-Robinson bound [9]. Such an exact computation is, however, generally intractable for a long time scale or in higher dimensions. While a more recent work has utilized outputs from a quantum simulator built with ultracold fermions in a Floquet-engineered optical lattice in three dimensions (3D) as a reference for examining the performance of an approximate numerical method, namely, the non-equilibrium dynamical mean-field theory [25], a direct comparison with quantitative theoretical approaches in the quench dynamics in higher dimensions is still lacking.

In this paper, we investigate the energy redistribution dynamics and the spatio-temporal evolution of the single-particle correlation function, the simplest two-point spatial correlations, in quantum quench dynamics starting with a Mott insulating state by using an optical-lattice quantum simulator of the Bose-Hubbard model (BHM) in two dimension (2D) and 3D as well as 1D. The kinetic- and interaction-energy redistribution dynamics turns out to be the demonstration of the energy conservation in the quench dynamics of a Bose-Hubbard quantum simulator. Further, we successfully observe the correlation spreading after a rapid quench from a Mott insulating state towards the quantum critical region in 2D as well as towards the Mott region in 1D. Especially interesting is the fact that we find that the measured propagation speed of the correlation in the dynamics in the quantum critical region exceeds the Lieb-Robinson-like bound set by the maximum velocity of the quasi-particles. This happens because the single-particle correlation spreads with two typical velocities, namely the group velocity and the phase velocity, as was pointed out in the recent theoretical work [24], and the observed velocity corresponds to the latter one.

In addition to these experimental findings, in order to corroborate the quantitative performance of our quantum simulator, we present a thorough comparison between the quantum-simulation results and state-of-the-arts theoretical calculations. We apply the exact numerical results of the MPS method in 1D, finding the excellent agreement with the observations. As for the case of the quench towards a deep superfluid phase in 3D, the time evolution of the kinetic and interaction energies is directly compared with numerical results obtained with use of the truncated Wigner approximation (TWA) based on
the Gross-Pitaevskii mean-field theory [23]. The good agreement between the experiment and the theory establishes the predictive power of the TWA for this type of quench. In contrast, in the case of the quench towards the quantum critical region in 2D, the TWA fails to capture quantitatively the experimental results. This indicates that our quantum simulation goes beyond current classical computation and the data serves as a useful reference for pushing out its boundary.

RESULTS

INVESTIGATING NON-EQUILIBRIUM DYNAMICS OF THE BOSE-HUBBARD MODEL

We consider a system of ultracold bosonic atoms confined in an optical lattice. When an optical lattice potential is deep, the system is quantitatively described by the BHM [26, 27],

\[
\hat{H} = -J \sum_{\langle j,l \rangle} (\hat{a}^\dagger_j \hat{a}^\dagger_l + h.c.) + \frac{U}{2} \sum_j \hat{a}^\dagger_j \hat{a}^\dagger_j \hat{a}_j \hat{a}_j + \sum_j (V_j - \mu) \hat{a}^\dagger_j \hat{a}_j,
\]  

where \( \hat{a}_j^\dagger \) and \( \hat{a}_j \) are the creation and annihilation operators at the site \( j \), \( J \) is the tunneling-matrix element between nearest-neighbor sites, \( U \) is the on-site interaction energy, \( \mu \) is the chemical potential, and \( V_j \) is the local potential offset at the site \( j \), which originates from the trap potential and the gaussian envelopes of optical lattice lasers. \( \sum_{\langle j,l \rangle} \) represents the summation over all neighboring sites.

When the atom number per site, namely the filling factor, is integer and the ratio \( U/J \) is varied, the BHM exhibits a continuous quantum phase transition between the Mott insulator and the superfluid. The system favors the superfluid phase for a relatively small \( U/J \) while it does the Mott insulator phase for a relatively large \( U/J \). For the unit filling case \( (\bar{n} = 1) \), the quantum critical point has been determined with exact numerical methods as \( (U/J)_c = 3.4 \) (1D) [28], 16 (2D) [29], and 29.3 (3D) [30], respectively.

Our analog simulator of the BHM is built with an ultracold Bose gas of \( ^{174}\text{Yb} \) atoms confined in a 3D optical lattice. We use this \( ^{174}\text{Yb} \)-atom-BHM quantum simulator in order to analyze dynamics after a quench of the ratio \( U/J \) starting with a Mott-insulator state with unit filling. We convert a \( ^{174}\text{Yb} \) Bose-Einstein condensate (BEC) in a weakly confining harmonic trap into the initial Mott-insulator state by slowly ramping up the optical-lattice depth up to \( s \equiv V_0/E_R = 15 \) for all the three directions, where \( V_0 \) is the depth of the optical lattice and \( E_R \) is the recoil energy of the optical-lattice laser whose wavelength is 532 nm. See Methods for the preparation. The prepared state is deep in a Mott insulator regime \( (U/J = 102.6) \) and is well approximated as a product of local Fock states,

\[
|\Psi_{\text{MI}}\rangle = \prod_j \hat{a}_j^\dagger \langle 0 |.
\]  

To realize a quench of \( U/J \), we rapidly ramp down the lattice depth for some directions towards a final value. For instance, in the case of 1D quench we ramp down the lattice depth only for the \( x \) direction while in the 3D case we do it for all the three directions. The ramp-down speed is set to be 100 \( E_R/\text{ms} \). By using the band-mapping techniques, we check that there is no discernible amount of the atoms in excited bands with this quench speed. We use the numerical values of \( U \) and \( J \) as functions of lattice depth reported in ref. [31].

After the quench process, we keep the lattice depth constant and let the system evolve. In order to obtain the single-particle correlation function at a certain distance \( \Delta \) in unit of a lattice spacing \( d \) [22],

\[
K_\Delta = \sum_{|i-j|=\Delta} \langle \hat{a}_i^\dagger \hat{a}_j \rangle
\]

after a certain hold time, we release the gas from the trapping and optical-lattice potentials to measure the time-of-flight (TOF) image, from which we deduce the momentum distribution. By performing Fourier transform of the momentum distribution, we obtain \( K_\Delta \). The kinetic energy of the BHM is equal to \( -JK_{\Delta \rightarrow -1} \). Moreover, we measure the onsite-interaction energy of the BHM, \( \frac{U}{Z} \sum_j \langle \hat{a}_j^\dagger \hat{a}_j^\dagger \hat{a}_j \hat{a}_j \rangle \), by means of the atom-number-projection spectroscopy [32, 33] for the 3D case and photoassociation spectroscopy [34] for the 1D case where we confirm that there are almost no multiple occupancies larger than two. These methods are rather efficient, especially in higher dimensions, for our current purpose of obtaining the ensemble average of the two-point correlation functions and Hubbard energies, since they do not require many data-samplings as in quantum-gas microscope techniques [9]. The experimental procedure and set-up, and typical high-resolution spectra are summarized in Section I and II of the Supplementary Materials.

It is worth noting that the dynamical evolution of the phase correlation, which is similar to the single-particle correlation, has been measured for weakly interacting Bose gases in one-dimensional optical lattices by means of the Talbot interferometry in ref. [35]. In contrast, the present work investigates the single-particle correlation in strongly correlated regimes in higher dimensions.
FIG. 1. Energy redistribution after quench in one dimension. Time evolution of the kinetic-energy term (red), the onsite-interaction-energy term (blue), and sum of them (green) are shown as a function of hold time \( t \) after a rapid quench into a Mott insulator state with \( U/J = 6.8 \) in 1D optical lattice tubes. The solid lines show the results of the numerical calculation at zero temperature with the MPS calculation using the time-dependent variational principle and local density approximation (LDA). Error bars for the kinetic-energy and onsite-interaction-energy terms denote the standard error of 15 independent measurements.

FIG. 2. Spatio-temporal evolution of the single-particle correlation after quench in one dimension. a,b The single-particle correlations for distance in units of a lattice constant \( \Delta \) up to 4 are shown as a function of hold time \( t \). Note that the displayed correlations are normalized by the maximum value of the correlation \( C^{\text{1D}}(\Delta) \) during \( 0 < t < 1.6J/\hbar \) for each distance \( \Delta \); a, Experiment; b, numerical calculation. c-f, Time evolution of the single-particle correlation \( K_\Delta \) after quench. Solid blue lines show the results of numerical calculation. c, \( \Delta = 1 \); d, \( \Delta = 2 \); e, \( \Delta = 3 \); f, \( \Delta = 4 \). Error bars denote the standard error of 5 independent measurements. g, Time of first peak of single-particle correlation is plotted as a function of distance \( \Delta \). A fit with a linear function with a non-zero offset is shown as a solid line. Error bars denote the standard error of 5 independent measurements.

Experimental confirmation of our methods: dynamics of the 1D Bose Hubbard model after a sudden quench

First, we investigate the behaviors of atoms after a sudden quench in 1D. The results for Hubbard energy redistribution dynamics and the spatio-temporal evolution of the atom correlations are shown in Figs. 1 and 2 respectively. Specifically, we ramp the lattice depth in the \( z \) direction down to \( s = 5 \) implying \( U/J = 6.8 \), at which the ground state is a Mott insulator state close to the quantum critical point. Figure 1 shows the time evolution of the kinetic energy, the onsite-interaction energy, and the sum of the two energies. In a short time scale, while the sum of the two remains almost constant, the kinetic energy decreases and the interaction energy increases. After making a small overshoot, both energies end up with an almost steady value, i.e., the energies are redistributed. This is expected for an isolated system but has never been observed experimentally before.

Figure 2(a)-(d) shows the time evolution of the single-particle correlation function for several values of \( \Delta \). As the time evolves, the correlations first grow and each of them takes the first peak at a certain time. We extract the peak time for each \( \Delta \) by numerically fitting to the experimental data, which is plotted against \( \Delta \) in Fig. 2(e). The peak time increases linearly with the distance, i.e., the correlation exhibits a light-cone-like propagation. From the peak time versus \( \Delta \), we extract the propagation velocity as \( v = 5.5(7)Jd/\hbar \). The maximum velocity of a particle-hole excitation is given as[9][15]

\[
v_{\text{max}} \approx \frac{5Jd\sqrt{D}}{\hbar} \left[ 1 - \frac{16J^2}{9U^2} \right],
\]

which can be interpreted as a Lieb-Robinson-like bound. Here \( D \) denotes the spatial dimension. At \( U/J = 6.8 \), \( v_{\text{max}} = 5.8Jd/\hbar \) such that the condition \( v < v_{\text{max}} \) is satisfied, as expected. A similar propagation behavior has been also observed in the case of the density-density correlation [9]. However, we will see later an apparent breaking of \( v < v_{\text{max}} \) in the 2D case.

While these observations reveal important features of the non-equilibrium dynamics of BHM, this 1D study is also important from another aspect. Since our BHM quantum simulator is analog, it is imperative to examine its accuracy through a direct comparison with exact numerical calculations in 1D before applying it to the
cases of higher dimensions, in which exact computation on classical computers is currently unavailable. In Figs. 1 and 2 we compare the experimental results in 1D with the exact numerical ones at zero temperature obtained with the MPS method. For details of the MPS calculations, see Sec. IV of the Supplementary Materials. We see that the experimental observations are in good agreement with the exact numerical calculations with no fitting parameters.

**DYNAMICS OF BHM AFTER SUDDEN QUENCH IN HIGHER DIMENSIONS**

Having corroborated the quantitative validity of our BHM quantum simulator by the comparison between the theory and experiment in 1D, we now discuss the main result of this work of the quench dynamics in higher dimensions. Figure 3 shows the energy redistribution dynamics for the 3D case after the ramp-down of the lattice depth to $s = 5$ ($U/J = 3.4$), at which the ground state is deep in the superfluid phase. The general tendency of the time evolution is similar to the 1D case: the two energies are redistributed in a time scale smaller than $\hbar/J$ and the sum of the two remains almost constant within the displayed time window $t \lesssim \hbar/J$.

We next investigate the dynamical spreading of the single-particle correlation after a quantum quench in 2D. The final lattice depth in this case is $s = 9$ implying $U/J = 19.6$, at which the ground state is a Mott insulator phase near the quantum critical point. Figure 4(a)-(d) show the spatial distribution of the single-particle correlation at several hold times after a quench. We clearly observe that the correlation first grows between nearest-neighbor sites and then it propagates for larger distances at later times. More directly Fig. 4(e)-(g) shows the time evolution of the single-particle correlation function $K_{\Delta_x,\Delta_y}$ for several values of $(\Delta_x, \Delta_y)$, where $\Delta_x$ ($\Delta_y$) denotes the distance in the $x$ ($y$) direction in units of a lattice spacing $d$. The delay in the growth of the correlation for longer distance is clearly observed along the directions of $x$, $y$, and $x + y$, in Fig. 3(e), (f), and (g), respectively. In the same manner as the 1D case, we extract the position of the first peak in the time evolution of the correlation at each distance, which is plotted against the Euclidean distance $\sqrt{\Delta_x^2 + \Delta_y^2}$ in Fig. 4(h). We further extract the propagation velocity from the linear fitting to Fig. 4(h) as $v = 12.6(1.6)Jd/\hbar$. According to Eq. (3), the maximum velocity of the particle-hole excitation is $v_{\text{max}} = 8.4Jd/\hbar$, which is slower than the observed propagation velocity in Fig. 4. Similar analysis of the propagation velocity is also done for the minimum of the correlation after the first peak in Fig. 4(i) with essentially the same result.

**DISCUSSION**

The observed apparent breaking of the LB-like bound in 2D case shown in Fig. 4 can be interpreted along the line explained in ref. [24]. The correlation spatially propagates as a wave packet, whose width spreads in time. This means that the velocity of the front edge of the wave packet, namely the phase velocity, is faster than that of its center, namely the group velocity. The velocity extracted from the experimental data in the way described above corresponds to the phase velocity while the meaningful propagation velocity, which should be compared with the LB-like bound, does to the group velocity. In the case of the final lattice depth $s = 9$ at 2D, we cannot accurately extract the group velocity because of the unclear separation of the two velocities. Instead, In Sec. V of the Supplementary Materials, we show an example, in which the phase velocity is well separated from the group velocity.

Next, we discuss the usefulness and limitation of some numerical methods based on the quantum simulation results. Since there is no exact computation method applicable to the 3D case, it is meaningful to examine the accuracy of some approximate methods by using the quantum simulation results as a quantitative reference. In Fig. 4 we also show the numerical calculations as solid lines obtained with the TWA [23], which is supposed to be able to describe quantitatively non-equilibrium dynamics of Bose gases in optical lattices in a weakly interacting regime at least for a short time. In the TWA calculations, we take the Mott insulator state of Eq. (2) as the initial state.
and set the system size to be $30^3$ sites. We ignore the trapping potential because it is irrelevant to the dynamics within the time window $t \lesssim h/J$ as was discussed in the 1D case. The TWA results are in good agreement with the experimental observations. More details of the TWA calculations are written in ref. [23].

The solid lines in Fig. 4(e)-(g) represent the results obtained by using the TWA. While the TWA agrees with the experiment in a very short time scale ($t < 0.1 h/J$), it fails to capture important properties of the correlation dynamics, such as the locations of the correlation peak and dip, and the almost converged value of the correlation at a relatively long time ($t > 1 h/J$) in contrast to the 3D case. This disagreement is consistent with the general fact that the TWA is less accurate when $U/(DnJ)$ is larger. This failure of the TWA indicates that one needs to push out the boundary of currently available numerical techniques for quantitative description of the quantum simulation results.

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METHODS

Preparation of initial Fock state

The detail of our experimental setup is described in ref. [32]. We first prepare a BEC of $^{174}$Yb atoms confined in an optical far-off resonant trap (FORT) whose wavelength is 532 nm. The trap frequencies of the FORT are given by $(\omega_x, \omega_y, \omega_z) = 2\pi \times (28, 130, 160)$ Hz, where the $x$ and $y$ axes were tilted from the $x$ and $y$ axes, to which two of the optical lattices are directed, by 45°. Then we slowly ramp up the optical-lattice depth for all the three directions from $s = 0$ to 5 in 100 ms and from 5 to 10 in another 100 ms. A typical number of atoms is chosen to be $N = 1.3 \times 10^4$ such that the filling factor is unity.
Lattice quench

We perform the quench by sudden decrease of the optical lattice with depth of $s E_R$ in $0.01(15 - s)$ ms. See also Sec. I on Supplementary Materials. The excitation of the atoms into higher bands is negligible with this procedure. For the cases of 1D and 2D quench, we decrease the lattice depth along the one direction of $x$ and two directions of $x$ and $y$, respectively. It is to be noted that when lattice depth is $10.6 E_R$, $U/J$ is equal to 29.34, which is the critical lattice depth for the superfluid-Mott transition at $n = 1$. 

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