Lieb-Robinson-like bounds for the Mott phase of the Bose-Hubbard model in dimensions greater than one

Ali Mokhtari-Jazi, Matthew R. C. Fitzpatrick, and Malcolm P. Kennett
Department of Physics, Simon Fraser University,
8888 University Drive, Burnaby, British Columbia, V5A 1S6, Canada
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Lieb-Robinson and related bounds set an upper limit on the rate of spreading of information in non-relativistic quantum systems. Experimentally, they have been observed in the spreading of correlations in the Bose-Hubbard model after a quantum quench. Using a recently developed two particle irreducible (2PI) strong coupling approach to out-of-equilibrium dynamics in the Bose-Hubbard model we calculate both the group and phase velocities for the spreading of single-particle correlations in one, two and three dimensions as a function of interaction strength. Our results are in quantitative agreement with measurements of the velocities for the spreading of single particle correlations in both the one and two dimensional Bose-Hubbard model realized with ultra-cold atoms. They also agree with the claim that the phase velocity rather than the group velocity was observed in recent experiments in two dimensions. We demonstrate that there can be large differences between the phase and group velocities for the spreading of correlations and also explore the variation of the anisotropy in the velocity at which correlations spread across the phase diagram of the Bose-Hubbard model. Our results establish the 2PI strong coupling approach as a powerful tool to study out-of-equilibrium dynamics in the Bose-Hubbard model in dimensions greater than one.

Ultra-cold atoms in optical lattices provide a versatile setting to investigate out-of-equilibrium dynamics in interacting quantum systems [1–8]. Atomic realizations of the Bose Hubbard Model (BHM) [9], a minimal model describing interacting bosons in an optical lattice [10], have also been proposed as quantum simulators in dimensions higher than one [11, 12]. Hence it is important to understand how information propagates in these systems. Of particular interest is the dependence of the speed on dimensionality and model parameters. The existence of a bound on the group velocity of the spreading of correlations in non-relativistic quantum systems was demonstrated by Lieb and Robinson [13]. In-situ imaging techniques such as quantum gas microscopes [14, 15] have enabled the experimental demonstration of such light-cone-like spreading [16] of correlations for bosons in a one dimensional optical lattice simulating the BHM.

The arguments that lead to the prediction of Lieb-Robinson bounds in spin systems do not strictly apply to the Bose-Hubbard model, but analogous bounds have been derived for interacting bosons on a lattice [17]. Theoretically, there exist a number of tools that allow for the calculation of dynamical correlations in the BHM in one dimension, including exact diagonalization (ED) and time-dependent density-matrix renormalization group methods (t-DMRG) [16, 18–21]. However, these tools are not effective for calculating the spreading of correlations in higher dimensional systems. Theorists have responded to this challenge by using a variety of methods to study the spreading of correlations in the Bose-Hubbard model in two dimensions, including considering Gutzwiller mean field theory with perturbative corrections [22–25] and doublon-holon pair theories [26, 27]. We employ a two-particle irreducible (2PI) strong coupling approach to the BHM developed by two of us [22–25] that allows accurate calculation of the speed at which correlations spread in dimensions higher than one. This approach has the advantages that it is exact in both the weak and strong interaction limits, and is applicable for small average particle number per site, $\bar{n}$. In Ref. [26], two of us used this approach to obtain 2PI equations of motion for single-particle correlations. Taking a low-energy limit of these equations of motion yields an effective theory (ET) that gives predictions that match exact results in one dimension [27].

Our work is motivated by recent experiments reported by Takasu et al. [12]. In that work, the authors studied the spreading of single-particle correlations for bosonic atoms confined in an optical lattice in one, two and three dimensions after a quench in the optical lattice depth starting from a Mott insulating state. In terms of the BHM these quenches corresponded to different values of the ratio $U/J_f$, where $U$ is the characteristic interaction energy scale and $J_f$ is the final value of the characteristic hopping energy scale $J$. In one dimension they considered parameters well in the Mott phase $[U/J_f = 6.8$, compared to the critical value $(U/J_f)_{1d}^{\text{cr}} = 3.4]$, and in two dimensions they considered parameters close to the transition to a superfluid $[U/J_f = 19.6$ compared to the critical value $(U/J_f)_{2d}^{\text{cr}} = 16]$. Defining the correlation wavefront as the first peak in the time evolution of the single-particle correlation function at each particle separation distance, Takasu et al. found the wavefront to propagate in one dimension with a velocity of $v_{\text{peak}} = 5.5(7)Ja/h$, where $a$ is the lattice spacing. This result is in accord with previous experimental [16] and theoretical work [16, 23, 25, 34].

Takasu et al. [12] reported the first measurements
of propagation speeds in two dimensions, \( v_{\text{peak}} = 13.7(2.1)Ja/\hbar \) (obtained from the first peak in the single-particle correlations) and \( v_{\text{trough}} = 10.2(1.4)Ja/\hbar \) (obtained from the first trough in the single particle correlations after the first peak). These values, especially \( v_{\text{peak}} \), are considerably larger than the Lieb-Robinson-like bound of \( v_{\text{LR}} = 8.4Ja/\hbar \) that Takasu et al. expected based on doublon-holon effective theories \[16\]. Takasu et al. argued that they measured the phase rather than the group velocity; only the latter is subject to a Lieb-Robinson-like bound.

In this paper we solve the equations of motion for our 2PI effective theory, and calculate the group and phase velocities for the spreading of single particle correlations in the Bose-Hubbard model after a quench in one, two and three dimensions.

Our main results can be summarized as follows: i) We obtain the group and phase velocities for correlation spreading throughout the Mott phase for the BHM in one, two and three dimensions; ii) We obtain quantitative agreement between the phase velocity of single-particle correlations in the one and two dimensional BHM calculated using our ET and the speeds measured experimentally in Refs. \[12\] \[10\]; iii) We confirm that Takasu et al. measure the phase rather than the group velocity for the spreading of correlations; and iv) We track the evolution of anisotropy in the phase and group velocities in the BHM in both two and three dimensions.

We study the Bose Hubbard model on a \( d \)-dimensional cubic lattice, with \( d = 1, 2, \) and \( 3 \), for which the Hamiltonian is

\[
\hat{H}_{\text{BHM}} = - \sum_{\langle i,j \rangle} J(t) \left( \hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i \right) - \mu \sum_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1),
\]

where \( \hat{a}^\dagger \) and \( \hat{a}_i \) are creation and annihilation operators, respectively, for a boson on site \( i \), \( \hat{n}_i \) is the number operator on site \( i \), \( U \) is the interaction strength and \( \mu \) the chemical potential. We restrict the hopping to be between nearest neighbour sites, and allow the magnitude \( J(t) \) to be time dependent, as required for a quench protocol. The details of the derivation of our effective theory and the equations of motion for the single particle correlations are presented in Refs. \[33\] and \[34\]. The quantity we calculate is the single particle density matrix

\[
\rho_1(\Delta \mathbf{r}, t) = \frac{1}{N_s} \sum_{\mathbf{k}} \cos (\mathbf{k} \cdot \Delta \mathbf{r}) \, n_{\mathbf{k}}(t),
\]

where \( N_s \) is the number of sites and \( n_{\mathbf{k}}(t) \) is the particle distribution over the quasi-momentum \( \mathbf{k} \) and \( \Delta \mathbf{r} \) is the particle separation distance. \( n_{\mathbf{k}}(t) \) is related to the density, \( n(t) \), via

\[
n(t) = \frac{1}{N_s} \sum_{\mathbf{k}} n_{\mathbf{k}}(t).
\]

In addition to single-particle correlations, density-density correlations have also been considered in the literature \[23\] \[26\]. Such correlations are not as easily accessible with our approach, but in the strong coupling limit, the single-particle correlations contain the same information \[23\] \[44\].

The protocol we follow is to start with \( J/U = 0 \) for a \( \tilde{n} = 1 \) Mott phase and then ramp \( J \) to a final value \( J_f \) over a timescale \( \tau_Q \) after waiting a time \( t_c \) \[31\] \[36\]. We then solve the ET equations of motion to obtain \( \rho_1(\Delta \mathbf{r}, t) \), from which we extract the group and phase velocities for the spreading of single-particle correlations. More details on the procedure we used can be found in the supplementary materials \[36\]. We now discuss our results for one, two and three dimensions in turn.

**One dimension:** We consider one-dimensional chains with 50 sites and periodic boundary conditions. In previous work \[34\] we showed that the spreading of correlations calculated with our effective theory matches well with exact diagonalization results in small systems and exact results for larger systems in one dimension. For a given \( U/J_f \), we calculate \( \rho_1(\Delta \mathbf{r}, t) \) and for each value of \( \Delta \mathbf{r} \) we obtain the timewise positions of the wave packet, and the largest peak [i.e. the point in time where \( \rho_1(\Delta \mathbf{r}, t) \) takes its maximum value]. To obtain the position of the wave packet, we estimate the upper and lower envelopes of \( \rho_1(\Delta \mathbf{r}, t) \) using an interpolation based on a cubic spline and then find the center of the envelope, which we identify as the position of the wave packet. By tracking the propagation of the wave packet, we can extract the group velocity for the spreading of single-particle correlations \[34\].

![FIG. 1. Dynamics of \( \rho_1(\Delta \mathbf{r}, t) \) calculated from the ET for \( \Delta r/a = 10 \) with the envelope of the wavepacket shown in red and the position of the wave packet marked by the dashed black vertical line. The parameters used are \( \beta U = 1000 \), \( U/J_f = 18.2 \), \( \mu/U = 0.4116 \), \( t_c/U^{-1} = 5 \), \( t_Q/U^{-1} = 0.1 \) and \( N_s = 50 \).](image)
peak of the \( \rho_1(\Delta r, t) \) time series to extract the phase velocity. An example of the envelope tracing of \( \rho_1(\Delta r, t) \) is given in Fig. 1 for \( \Delta r/a = 10 \) and \( U/J_f = 18.2 \), with the timewise position of the wave packet marked by a vertical dashed black line. Figure 2 plots the time \( t/U \) for the maximum peak and the wave packet to travel a distance \( \Delta r/a \) for the same parameters used in Fig. 1. By performing linear fits to the data in Fig. 2, we extract estimates for the phase and group velocities.

We repeat the process illustrated in Figs. 1 and 2 throughout the Mott insulating phase and determine the group and phase velocity at each value of \( U/J_f \). The results of these calculations and a comparison to the velocities determined experimentally in Refs. 12 and 16 are presented in Fig. 3. Note that the velocities obtained in Ref. 16 are actually for density-density correlations rather than single-particle correlations, but at strong coupling, these two correlations should spread with similar velocities. Deep in the Mott insulating phase, the phase velocity is much larger than than the group velocity but the two velocities converge in the vicinity of the critical point. The results we obtain here are consistent with those recently obtained using matrix product states by Despres et al. and experiments 12, 16. Having established that our effective theory reproduces existing experimental results and theoretical results obtained using essentially exact methods in one dimension, we now turn to two dimensions, where there has been no previous theoretical study of the phase velocity of the spreading of single-particle correlations.

**Two dimensions:** We consider a 50 \( \times \) 50 lattice with periodic boundary conditions and follow the same procedure as outlined for one dimension to calculate \( \rho_1(\Delta r, t) \). As noted by previous authors, the spreading of correlations in two dimensions is anisotropic in both the Mott insulating and superfluid regimes. We calculate the phase and group velocities as a function of \( U/J_f \) along both the crystal axes and the diagonals using the same protocol as for one dimension and present the results in Fig. 4. We consider parameters \( \beta U = 1000, \mu/U = 0.4116, \mu_c/U = 5 \), and \( v_Q/U^{-1} = 0.1 \).

Takasu et al. 12 identified propagation velocities for single-particle correlations by fitting to the peak and the following trough in \( \rho_1(\Delta r, t) \) at each \( \Delta r \). These values were \( v_{\text{peak}} = 13.7(2.1)J_f a/h \) and \( v_{\text{trough}} = 10.2(1.4)J_f a/h \) for \( U/J_f = 19.6 \). In Fig. 4 we show the group and phase velocities, evaluated along both the diagonals and the crystal axes in two dimensions. We used the peaks in \( \rho_1(\Delta r, t) \) to calculate the phase velocity and accordingly plot Takasu et al.’s \( v_{\text{peak}} \) value in Fig. 4. For \( U/J_f = 19.6 \) we find the group velocity and phase velocity (determined using the peak in \( \rho_1(\Delta r, t) \)) along the diagonals to be \( v_g^d \approx 8.8J_f a/h \) and \( v_{\text{ph}}^d \approx 11.5J_f a/h \) and along the crystal axes \( v_g^c \approx 8.2J_f a/h \) and \( v_{\text{ph}}^c \approx 11.9J_f a/h \). We also determined the phase velocity using the first trough after the peak in \( \rho_1(\Delta r, t) \) and obtained...
The degree of anisotropy of both the phase and group velocities in two dimensions is a function of $U/J_f$ and close to isotropic spreading as $U/J_f$ approaches the critical value of $(U/J_f)^2d = 16$. Theoretical calculations for the group velocity in the superfluid regime [37] indicate that the superfluid also displays anisotropic spreading of correlations, with the opposite sense to that in the Mott insulator regime. In Fig. 5 we show the spreading of $\rho_1(\Delta \mathbf{r}, t)$ at four times after the quench, for Euclidean distances $\Delta \leq 4$, as measured by Takasu et al. (we display the correlations at the same times as those shown in Ref. [12]).

**Discussion:** We have applied our 2PI strong coupling approach to the BHM to calculate the spreading of single-particle correlations and have found excellent agreement with experiments in one [12, 16] and two [12] dimensions. This establishes our 2PI strong coupling approach as a powerful tool to study out-of-equilibrium dynamics in the BHM in dimensions greater than one. Given that the method gives more accurate results for equilibrium properties, such as phase boundaries, with increasing dimension [33], we expect the same to be true for out of equilibrium dynamics. Hence, as it reproduces exact results in one dimension, the 2PI method is complementary to numerical methods that give essentially exact results for out of equilibrium dynamics only in one dimension. In addition, the 2PI method can be extended to disordered systems [35, 38] and multi-component boson...
systems. We have also demonstrated anisotropy in the spreading of correlations on the lattice in both two and three dimensions. This anisotropy persists throughout the entire Mott phase, apparently vanishing only around the critical point. Our results for the phase velocity and group velocity as a function of $U/J$ demonstrate that while they are relatively similar in the vicinity of the transition to the superfluid, deeper in the Mott phase there can be very significant differences, with the phase velocity being much larger than the group velocity. Differentiating between these two velocities is important for understanding the rate of information spreading in the BHM since Lieb-Robinson-like bounds apply to the group rather than the phase velocity. At the present time there have been only a few measurements of the velocities at which correlations spread in the BHM, we hope that our results give an incentive to further experimental measurements of correlation spreading in the BHM.

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