Effects of extended correlated hopping in a bose-bose mixture

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(Dated: January 1, 2020)

We study the effects of assisted tunneling or correlated hopping between next nearest neighbours in a two species Bose-Hubbard system. The system is the bosonic analog of the fermionic system studied in Phys. Rev. Lett. 116, 225303 (2016). Using a combination of cluster mean field theory, exact diagonalization and analytical results, a rich phase diagram is determined including a pair superfluid phase as well as a superfluid quantum droplet phase. The former is the result of the interplay between single particle and correlated hopping, while the latter is the effect of large correlated hopping.

I. INTRODUCTION

The interplay of kinetic energies and various kinds of interactions between particles is the central theme of condensed matter physics. The simplest model effectively describing interacting bosons moving on a lattice is arguably the Bose-Hubbard model (BHM). In a translationally invariant system (without disorder) for generic filling densities of the lattice the system is superfluid for repulsive on-site interactions, while an interaction induced Mott insulator appears for sufficiently strong repulsion at integer fillings. While the early motivation for the BHM came from the desire to understand the effects of repulsive interactions on the superfluid phase [1], this model has been of central interest in the physics of Josephson-junction arrays and effective theories of quantum magnets. Renewed theoretical interest has been driven by highly tunable experimental realizations of close-to-ideal generalized BHMs in systems of ultra-cold atoms trapped in optical lattices, where other terms such as long range interactions, or higher order hopping processes are important (apart from the usually dominant on-site interactions and hopping processes) and lead to richer phases [2]. Among the plethora of different phenomena possible in generalized BHMs are supersolids [3], paired superfluids, (artificial) magnetic flux generated bosonic topological phases, various kinds of gapped phases where the interplay between lattice commensurability and interactions lead to devil’s staircase filling patterns [4] [5], so-called twisted superfluids with time-reversal symmetry breaking [6]. Bosonic Haldane insulators in one dimensional lattices [7], exotic gapless Mott insulators or so-called Bose metal phases induced by ring exchange interactions [8] etc.

Correlated hopping, i.e. a hopping process dependent on particle density, is one particular relevant term generalizing standard many body models that has been studied in various contexts. While initially considered for fermion systems, valence solids and organic conductors, such terms have also been studied in relation to pairing phenomena of fermions and mechanisms of high-temperature superconductivity [9] [10]. In relation to boson systems, correlated hopping has been of interest as it may lead to the formation of stable condensates of boson pairs [3] [11] [12] without direct attractive interactions (note that attractively interacting bosons are prone to collapse making the possibility of creating boson pairs quite intriguing [13]).

In an earlier paper [21], we introduced a 1-dimensional lattice construction (of two lattices with sites shifted so as to be maximally non-overlapping) for which contact interaction actually leads to extended correlated hopping that is strong and intriguingly destructively interferes with single-particle hopping and determined the quantum phase diagram for the lattice loaded with fermions, or equivalently hard-core bosons. In this article, we consider the effects of extended correlated hopping on a system with loosened on-site constraints, i.e. soft-core bosons, instead. We discuss the interplay of Mott physics, pair and single-particle/ hole superfluids, as well as other ground state phases when the lattice is loaded with bosons.
A. The model

Mechanisms leading to the appearance of such terms are manifold (independent of particle statistics, i.e. for both bosonic and fermionic systems): (i) they stem directly from the second quantized form of two particle interactions as corrections to the strongest on-site terms diagonal in the number basis [14], e.g., in Hubbard-like models, (ii) appear in strong coupling expansions around symmetry points, for instance corresponding to situations where motion is kinetically constrained (e.g., around double occupancy conservation associated with large on-site repulsion U in Hubbard models) [15–17], and (iii) can be engineered by periodic driving as has recently been shown in relation to the physics of ultra cold gases trapped in optical lattices [18–20].

Unlike in the fermionic case, where the correlated hopping has mostly been considered as an additional nearest neighbour process, the case of bosons has been considered mostly with correlated hopping extending beyond nearest neighbour sites (see however [15] for a more involved form of nearest neighbour correlated hopping treated for bosons). The case of the BHM in the strongly interacting regime, i.e. the hard-core limit, was studied in [3, 11] on the square and triangular lattices respectively.

We consider the following 1-dimensional lattice Hamiltonian:

\[
H = \sum_i \left[ -t (b_i^\dagger b_{i+2} + h.c.) + X (b_i^\dagger n_{i+1} b_{i+2} + h.c.) + U n_i (n_i - 1) + V n_i n_{i+1} - \mu n_i \right],
\]

where \(b_i^\dagger\) is the bosonic creation operator at site \(i\) and \(n_i = b_i^\dagger b_i\) the corresponding density. The first term in the Hamiltonian describes direct hopping to next nearest neighbours with amplitude \(t\), while the second term, proportional to \(X\), is the density dependent or correlated hopping to next nearest neighbours conditioned on the occupancy of the intervening sites. The remaining terms describe the on-site repulsion \(U\) and the nearest-neighbour repulsion \(V\). There is no nearest-neighbour tunneling and hence no mixing between even and odd sites. Therefore, the model represents two bosonic species residing on two sublattices constituting a “zigzag” lattice. In our work we consider sublattices to be of equal lengths \(L/2\), and the total number of particles in the system to be \(N_{\text{total}} = N_{\text{even}} + N_{\text{odd}}\). Note that we do not a priori presume equal occupation of both sublattices.

The model describes two bosonic species confined in a one-dimensional optical lattice potential opposite for each species, i.e. one is trapped at the nodes and the other at the antinodes of the standing wave. Therefore, the distance between the nearest neighbours is half the lattice constant \(a/2\) leading to strong density dependent hopping and nearest neighbour repulsion. It is derived by analogy to the fermionic Hamiltonian studied in [21], also known as the Bariev model [22], and reproduces it in the limit of hard-core bosons. A bosonic model in a similar system is also studied in [23], where the two bosonic species are coupled by a laser-induced transition leading to node-antinode tunneling, however a rather weak interaction considered in this work makes the correlated hopping term negligible. A model with extended correlated hopping was also derived in [17], where bosons with internal spin are loaded to a single optical lattice and the different spin states are coupled by a Raman beam. The effective model obtained by the authors in the limit of strong repulsive density-density interactions and Raman coupling is precisely the one studied in [21], however with some constraints on available parameter ranges.

We recall here that the fermionic model [21] is analytically diagonalizable for a specific set of parameters \((X/t = 1)\) without interactions and arbitrary filling. For this parameter choice, a fermion on one sublattice cannot hop over a nearest neighbour fermion on the other sublattice (the matrix element \(-t + X n_{i+1} = 0\) vanishes for \(n_{i+1} = 1\) ). This strong additional symmetry constraint facilitates the analytical solution. For the same parameters, this symmetry is generally broken for a bosonic system since sites can be populated by more than one particle. Hence we rely heavily on numerical analysis, in particular small system exact diagonalization and cluster mean-field to produce the phase diagram.

We distinguish five basic phases: the Mott insulator phase, which is stabilized by positive correlated hopping \(X > 0\); the paired-holes superfluid, which occurs around the hard-core boson limit and is analogous to the ground state obtained in the fermionic case; the single particle superfluid phase; the phase-separated superfluid phase, where in order to minimize the energy it is preferable that the particles belonging to each sublattice concentrate in spatially disjoint regions. In analogy with the results of [17], the last phase may be identified as supersolid–like phase of soft-core bosons. Finally, in the limit of large \(X/t\) and weak interaction \(U\) (in particular in the case \(t = 0, U = 0, X > 0\)) we observe the formation of lattice analogs of superfluid droplets, i.e. spatial clustering of particles with superfluidity. The major contribution to the ground state in this phases comes from high-density clusters of type \(|\ldots 0 N N 0 \ldots,|\ldots 1 N N \ldots\rangle,|\ldots 0 1 N N \ldots\rangle,|\ldots 0 1 1 N N \ldots\rangle|\ldots 0 1 N N \ldots\rangle|\ldots 0 1 N \ldots\rangle|\ldots 1 1 0 \ldots\rangle\ldots (N = N_{\text{even}} = N_{\text{odd}})\).

II. RESULTS

A. Exact diagonalization

To gain exact insight into the ground state properties of the many body Hamiltonian Eq. (1), we first present an analysis based on exact diagonalization data. The ground state of the system is studied for a total system length of \(L = 12\) sites and particles \(N_i = 2N\) (where \(N\) is the number of particles on one of the sublattices) with periodic boundary conditions. We consider the system at
exactly unit filling \( N = L/2 \) as well as under the simplest deviations from this filling, i.e. \( N = L/2 - 1, L/2 + 1 \). The local bosonic Hilbert space is not truncated, i.e. we choose the maximal on site occupation to be \( n_{\text{max}} = N \).

We note that there are three known solutions for limiting cases of the model. (i) In particular, for unit filling in the hard-core boson limit \( U \gg t \) and small \( X/t \) ratios the system is a Mott insulator \( |\psi_{\text{Mott}}\rangle \). This is a simple extension of the known result for the standard Bose-Hubbard model to \( X \neq 0 \). The large energy penalty \( U \) associated with creating a doubly occupied site that allows for particle motion cannot be offset by the correlated hopping process. (ii) In the absence of correlated hopping \( X = 0 \), for generic fillings and arbitrary \( t/U \), the system is in a standard superfluid phase, which we denote as \( |\psi_{\text{bf}}\rangle \). (iii) Finally, for \( X = t \), and the hard core limit \( t/U \to 0 \) in which a site is occupied by at most one boson, the system is effectively fermionic and hence supports the so-called paired-hole superfluid state discussed in Ref. [21]. In this state \( \psi_{\text{ph}} \), any consecutive pair of bosons on the lattice is separated by an even number of empty (hole) sites. For such values of \( X \), the motion of particles allowed by the Hamiltonian is constrained so that effectively pairs of nearest neighbour holes move whenever an allowed single hopping event of a particle occurs.

In order to identify possible phases of the system, we calculate various order correlation functions as well as two specifically tailored properties of the exact wave functions.

1. The single particle superfluid phase: this is characterized by the off-diagonal part of the one-body density matrix \( \rho_{ij} = \langle b_i^\dagger b_j \rangle \). Since we are dealing with finite size chains, the superfluid is identified via the correlation function \( \phi_i = \sum_{j \neq i} \rho_{ij} \).

2. Paired hole superfluid: the model state for this phase is the ground state of the system in the hard-core limit \( |\psi_{\text{ph}}\rangle \), hence the best quantity to identify it for finite \( t/U \) is the fidelity \( F(\psi, \psi_{\text{ph}}) = |\langle \psi_{\text{ph}} | \psi \rangle|^2 \).

3. To gain an understanding of the structure of the ground state, we define two quantities: the contribution (weight) in the ground state of configurations (a) with certain maximal on-site occupations, and (b) for which the maximal sequence of occupied sites (called maximal cluster) has a specific length. For illustration consider the following vector in occupation number representation \( |1100101\rangle \). The maximal on-site occupation is 3. The maximal cluster is \([13111] \) and has length 5.

4. To identify how the ground state changes as one varies model parameters and track similarities to the limiting cases we compute fidelities \( F(\psi, \psi_{\text{ref}}) = |\langle \psi_{\text{ref}} | \psi \rangle|^2 \) of the calculated ground state \( |\psi\rangle \) with various reference states \( |\psi_{\text{ref}}\rangle \): (i) the Mott insulator \( |\psi_{\text{Mott}}\rangle \), (ii) the standard superfluid phase \( |\psi_{\text{bf}}\rangle \), (iii) the paired-hole superfluid \( |\psi_{\text{ph}}\rangle \), (iv) the paired-particles superfluid phase \( |\psi_{\text{pp}}\rangle \), which is analogous to the paired-holes superfluid for fillings larger than one, (v) the superfluid droplet state \( |\psi_{\text{ph}}\rangle \) for fillings larger than one, (vi) the superfluid droplet state \( |\psi_{\text{ph}}\rangle \) for fillings larger than one.
FIG. 3: Fidelity with ideal ph-superfluid state $|\psi_{\text{ph}}\rangle$ for small $t/U$ at several values of $X/t$ for $L = 12, 2N = 10$.

For strong interactions, up to $t/U \approx 0.1$, the contribution to the ground state is almost one for large CH ($X/t > 0.8$), however it is significant, i.e. larger than 0.5 even for CH as low as $X/t = 0.5$.

We begin by briefly discussing the regimes of the model at unit filling in which its properties coincide with the phases of the standard model for interacting spinless bosons on a lattice. This is best seen through fidelity with known limiting cases depicted in Fig. 2. In the limit of strong onsite interactions the Mott insulator known from the standard Bose-Hubbard model is additionally stabilized by the CH term, which effectively decreases the hopping rate. This is especially visible close to $X = t$, for which the insulating phase extends up to $t/U \approx 0.3$ ($t/U \approx 0.2$ for the standard Bose-Hubbard model). When the onsite interaction between particles goes to zero, the density fluctuations are no longer suppressed and the system at weak CH becomes superfluid, similar to the standard Bose-Hubbard model.

In what follows we will describe in more detail the results for filling $1 - 1/N$ and only later point out the similarities and differences between this case and fillings 1 and $1 + 1/N$. The properties we discuss are summarized in Fig. 4.

In the hard-core limit and at $X = t$ we have the known paired-holes superfluid solution, which significantly contributes to the ground state of the system well beyond the strong interaction limit and even at relatively small values of $X/t$. In Fig. 5 we plot the fidelity between the ph-superfluid state $|\psi_{\text{ph}}\rangle$ and the state of the system away from the hard-core and $X = t$ limit. This phase is characterized by almost null one- and two-particle correlation functions, and maximal contribution to the wave function from states characterized by cluster length $L_{\text{cluster}} = N_t$ and maximal occupation $n_{\text{max}} = 1$.

In the interval $0.25 \lesssim t/U \lesssim 0.5$ we observe a change of sign of one-particle correlation function $\phi$ as well as a small growth of two-particle correlation function $\Phi$. The latter is associated with the appearance of bosonic pairs, which is also confirmed by the fact that maximal contribution to the wave function comes from states with maximal occupation 2 or 3. Yet, the pair character of the superfluid in this region is rather weak. Moreover, at $t/U \approx 0.31$ we observe a significant change in the structure of states contributing to the wave function: the states with long clusters no longer dominate, instead the states of cluster lengths 3 or 4 account for about 70% of the wave function. This can be associated with the appearance of superfluid droplets in the system, however of different kind (fragmented and with lower onsite density) as the fidelity with the superfluid droplet phase $|\psi_{\infty}\rangle$ is zero.

The true superfluid quantum droplet phase starts to appear at $t/U \approx 0.5$, where it is linked to a significant growth of the absolute value of the correlation functions $\phi$ and $\Phi$. We also notice the change in the structure of the wave function indicated by the growing contribution from states having clusters of length 4 and 5 (3, 4 in the limit of large $t/U$) and maximal onsite occupation 3, 4 or 5, e.g., states with high-density clusters of type $|...01540\rangle, |...014410\rangle...$. The overlap with the model superfluid quantum droplet state $|\psi_{\infty}\rangle$ (Fig. 3) increases to reach 0.8 around $t/U = 1$.

Note that the one-particle correlation function becomes negative, which signals the change of the character of the superfluid. In this regime the BEC occurs in the $k = \pi$ momentum state, rather than the standard $k = 0$ state.

Let us now explore the case of $t/U \to \infty$ and varied $X/t$. The properties of the system in this limit are summarized in Fig. 4b. At weak correlated hopping $X/t \lesssim 0.2$ the ground state of the system is the standard superfluid which is confirmed by large value of the correlation functions and almost unit fidelity with $|\psi_0\rangle$.

In the interval $0.2 \lesssim X/t \lesssim 0.67$ the one- and two-particle correlation functions decrease slightly and the fidelity with $|\psi_0\rangle$ drops to zero. At the same time the predominant contribution to the wave function comes from states with short one- and two-site clusters with maximal on-site occupation of 3 and 4. This is due to phase separation, i.e. the particles belonging to each sublattice concentrate in spatially disjoint regions of length $L/2$ in which they are effectively described by the standard Bose-Hubbard model:

$$H_{\text{BH}} = \sum_{i=1}^{L/2} \left[ -t (b_i^+ b_{i+2} + h.c.) + \frac{U}{2} n_i (n_i - 1) \right]$$

(and similarly for even sites) and form a superfluid. In the bulk of each such region only even/odd sites are occupied leading to 1-site clusters, however at their interface two consecutive even-odd sites can be occupied, hence the 2-site clusters are present. An exemplary state, which may contribute to the ground state is $|103010020201\rangle$.

For even larger values of the correlated hopping $X/t \gtrsim 0.67$ the one-particle correlation function becomes negative and the two-particle correlation function drops slightly. We also observe sudden clustering of particles in clusters of length 3 and 4 with maximal occupation being 5, 4 or 3, which signals the transition to the superfluid droplet phase. This is confirmed by the fast increase of fidelity with $|\psi_{\infty}\rangle$, which reaches 0.5 around $X/t \approx 0.7$ and 0.8 for $X/t \approx 1$.
In Fig. 5 we show the results for filling $1 + 1/N$. They are similar to the case of filling $1 - 1/N$, which we discussed in more detail. The most important difference is the nature of the ground state for $X = t$ and strong interactions. While for fillings below 1 the bosonic system behaves similarly to the fermionic case and its ground state is the paired-hole superfluid, for fillings above 1 we have a completely new situation. Exact diagonalization data show that the system with two additional particles above the unit filling becomes a paired-particles superfluid (pp-superfluid), in which doubly-occupied sites are paired and particles belonging to such pair can only hop in a leapfrog manner, i.e. a particle hops over a doubly-occupied site as hopping over a single particle is suppressed by the correlated hopping term. The effective tunneling parameter associated with such hopping process is positive, i.e. $-t + 2X = +t$, hence to minimize the energy we need the ground state of the form $|\psi\rangle \propto \sum_i (-1)^i b_i b_{i+1}^\dagger |1 \ldots \rangle$.

The structure of the wave function can be also inferred from the unit contribution of the states with cluster of length $L_{\text{cluster}} = 12$ and maximal occupation $n_{\text{max}} = 2$, and the negative sign of the one-particle correlation function. Note that close to $t/U \approx 0.1$ there appear contributions from states with clusters of length 11 and maximal occupation 3, i.e. states of the type: $|0231\ldots\rangle$ in which the energy is lowered through formation of a low-density droplet.

**B. Analytical estimates**

To estimate the extent of the phases identified in the previous section we perform the strong coupling expansion up to the second order in $t/U$ [24]. We rewrite the model Hamiltonian [1] as:

$$H = H_0 - \frac{t}{U} \sum_{i=1}^L \left[ b_i^\dagger \left(1 - \frac{X}{t} n_{i+1}\right) b_{i+2} + \text{h.c.} \right],$$

where $H_0 = \sum_{i=1}^L \left[ \frac{1}{2} n_i (n_i - 1) - \frac{\mu}{U} n_i \right]$ is diagonal in the number basis and the term proportional to $t/U$ is a per-
We calculate the energies for the Mott insulator state of density \( n_0 \)

\[
|\psi_{\text{Mott}}(n_0)\rangle = |n_0n_0\ldots\rangle,
\]

obtaining up to the second order in \( t/U \):

\[
E_{\text{Mott}} = L \left[ \frac{1}{2} n_0(n_0 - 1) - \frac{\mu}{U} n_0 \right] - \frac{2t^2}{U} L n_0(1 + n_0) \left( 1 - \frac{X}{t} n_0 \right)^2 .
\]

In the standard superfluid-Mott insulator transition, the variation from the Mott state leading to superfluidity is an addition of one hole/particle, however in the present case we assume the symmetric occupation of the two sublattices, hence the superfluid ansatz of the form:

\[
|\psi_{\text{Holes}}\rangle = \frac{2}{n_0 L} \sum_{i \text{ odd}, j \text{ even}} b_i b_j |n_0n_0\ldots\rangle,
\]

\[
|\psi_{\text{Parts}}\rangle = \frac{2}{(n_0 + 1) L} \sum_{i \text{ odd}, j \text{ even}} b_i^\dagger b_j^\dagger |n_0n_0\ldots\rangle,
\]

where the two additional holes/particles are not spatially correlated. We compute the energies of both states obtaining:

\[
E_{\text{Holes}} = 2\frac{\mu}{U} - 2(n_0 - 1) + L \left[ \frac{1}{2} n_0(n_0 - 1) - \frac{\mu}{U} n_0 \right] - \frac{4t}{U} n_0 \left( 1 - \frac{X}{t} n_0 \right) - \frac{4t^2}{U^2} n_0(n_0 + 1) \left[ 1 - \frac{X}{t} (n_0 - 1) \right]^2 + \frac{2t^2}{U^2} (n_0 + 1)(3n_0 + 1) \left( 1 - \frac{X}{t} n_0 \right)^2 - \frac{2t^2}{U^2} L n_0(n_0 + 1) \left( 1 - \frac{X}{t} n_0 \right)^2 ,
\]

\[
E_{\text{Parts}} = -\frac{4t}{U} n_0 \left( 1 - \frac{X}{t} n_0 \right) - \frac{4t^2}{U^2} n_0(n_0 + 1) \left[ 1 - \frac{X}{t} (n_0 - 1) \right]^2 + \frac{2t^2}{U^2} (n_0 + 1)(3n_0 + 1) \left( 1 - \frac{X}{t} n_0 \right)^2 - \frac{2t^2}{U^2} L n_0(n_0 + 1) \left( 1 - \frac{X}{t} n_0 \right)^2 .
\]
for to uncorrelated holes, and
\[
E_{\text{Parts}} = -2\frac{\mu}{U} + 2n_0 + L \left[ \frac{1}{2} n_0(n_0 - 1) - \frac{\mu}{U} n_0 \right] - \frac{4t}{U} (n_0 + 1) \left( 1 - \frac{X}{t} n_0 \right) - \frac{4t^2}{U^2} n_0(n_0 + 1) \left[ 1 - \frac{X}{t} n_0 + 1 \right]^2 + \frac{2t^2}{U^2} n_0(3n_0 + 2) \left( 1 - \frac{X}{t} n_0 \right)^2 - \frac{2t^2}{U^2} n_0(n_0 - 1) \left( 1 - \frac{X}{t} n_0 \right)^2
\]
for two uncorrelated particles.

In the system under consideration another possible variation from the Mott state is a superfluid with two paired holes/particles. To check which one, the standard or the paired-holes/particles superfluid, is energetically more favourable we take the following states (the origin of the phase factor in the pp-superfluid was explained in the previous section):
\[
|\psi_{\text{PHoles}}\rangle = \frac{1}{n_0\sqrt{L}} \sum_i a_i a_{i+1} |n_0 n_0 \ldots\rangle,
\]
\[
|\psi_{\text{Parts}}\rangle = \frac{1}{(n_0 + 1)\sqrt{L}} \sum_i a_i^\dagger a_{i+1} (-1)^i |n_0 n_0 \ldots\rangle
\]
and again compute the energies perturbatively up to the second order in \( t/U \).

\[
E_{\text{PHoles}} = 2\frac{\mu}{U} - 2(n_0 - 1) + L \left[ \frac{1}{2} n_0(n_0 - 1) - \frac{\mu}{U} n_0 \right] - \frac{2t}{U} n_0 \left[ 1 - \frac{X}{t} (n_0 - 1) \right] + \frac{t^2}{U^2} (n_0 + 1)(7n_0 + 1) \left( 1 - \frac{X}{t} n_0 \right)^2 - \frac{2t^2}{U^2} n_0(n_0 + 1) \left[ 1 - \frac{X}{t} n_0 - 1 \right]^2 - \frac{2t^2}{U^2} L n_0(1 + n_0) \left( 1 - \frac{X}{t} n_0 \right)^2,
\]
\[
E_{\text{Parts}} = -2\frac{\mu}{U} + 2n_0 + L \left[ \frac{1}{2} n_0(n_0 - 1) - \frac{\mu}{U} n_0 \right] - \frac{4t}{U} (n_0 + 1) \left( 1 - \frac{X}{t} n_0 + 1 \right) + \frac{t^2}{U^2} n_0(7n_0 + 6) \left( 1 - \frac{X}{t} n_0 \right)^2 - \frac{2t^2}{U^2} n_0(n_0 + 2) \left[ 1 - \frac{X}{t} (n_0 + 1) \right]^2 - \frac{2t^2}{U^2} L n_0(1 + n_0) \left( 1 - \frac{X}{t} n_0 \right)^2.
\]
In Fig[7] on top of the phase diagrams obtained by the cluster Gutzwiller method we show the boundaries between the Mott insulator and the two possible types of the superfluid obtained by putting to zero the energy difference \( E_{\text{Parts/Holes}} - E_{\text{Mott}} \) and \( E_{\text{Parts/Holes}} - E_{\text{Mott}} \). Moreover, in Fig[7] we plot the maximal value of \( t/U \) which supports the Mott insulator as obtained from the energy estimates.

Apart from the standard and ph/pp-superfluids, the system also supports the phase-separated superfluid phase, i.e. such that the particles belonging to each sublattice concentrate in spatially disjoint regions and form two separate superfluids on lattices of length \( L/2 \). Here we estimate the value of \( t/U \) for which such phase is energetically more favourable than the standard superfluid at fixed total density \( \rho = n_0/L \). Assuming that in the superfluid phase with weak interaction only the zero momentum mode is occupied, the kinetic energy is \(-2t/U\rho L\). Further, since only half of each sublattice is occupied, the average number of particles per site on occupied sites is \( 2\rho \), i.e. \( n_0 = \rho L \) distributed equally over \( L/2 \) sites (\( L/4 \) occupied sites on each sublattice). We obtain the following estimate for the energy of the superfluids cramped up on a half of each sublattice
\[
E_{\text{sep}} = -\frac{2t}{U} \rho L + \frac{1}{2}(2\rho)(2\rho - 1) \frac{L}{2} - \frac{\mu}{U} \rho L = \left[ -\frac{2t}{U} \rho + \frac{1}{2}(2\rho - 1) - \frac{\mu}{U} \rho \right] L.
\]

To estimate the energy of the standard superfluid in the presence of the correlated hopping, we assume to be in a regime of parameters in which the correlated hopping only modifies the tunneling rate but does not change the nature of the superfluid, as shown by the exact diagonalization data. We obtain the following
\[
E_{\text{SF}} = -\frac{2(t - X\rho)}{U} \rho L + \frac{1}{2}(2\rho - 1) \frac{L}{2} - \frac{\mu}{U} \rho L = \left[ \frac{2(t - X\rho)}{U} \rho + \frac{1}{2}(2\rho - 1) - \frac{\mu}{U} \rho \right] L.
\]
The system is in the standard superfluid phase whenever \( E_{\text{SF}} < E_{\text{sep}} \), which leads to a simple criterion for the extension of the standard superfluid
\[
\frac{t}{U} < \frac{1}{4\alpha},
\]
where we introduced a new parameter \( \alpha = X/t \).

C. Phase diagrams

We now turn to our main results, i.e. the full phase diagram obtained within a cluster mean-field (CM) approach. The mean-field decoupling of the single particle hopping yields a sufficient description of the Mott-insulator to superfluid transition in the standard BHM. However, given the additional correlations induced by occupation number dependent hopping, we need to use the multi-site extention (CM) of the standard Gutzwiller
The variational CM ansatz is a product state $|\Psi_G\rangle = \prod_i |\psi\rangle$, where each $|\psi\rangle$ is a linear combination of $d$-site Fock states $\{|n\}\rangle = \{|n_1, \ldots, n_d\}\rangle$ ($n_i = 1, 2, \ldots, n_{\text{max}}$)

$$|\psi\rangle = \sum_n f_n |n\rangle.$$  

The Hamiltonian for the $d$-site cluster is the same as in the case of on-site interaction terms and in the interior of the cluster $S = \{3, \ldots, d-2\}$. The boundary sites are coupled to the rest of the system via mean-field parameters $\langle b_0 \rangle$, $\langle b_{d+1} \rangle$, $\langle b_{-1} n_0 \rangle$, $\langle n_{d+1} b_{d+2} \rangle$:

$$H_{\text{cluster}}^{n} = \left\langle m \right| H_S + \frac{U}{2} \sum_{i=1}^{d} n_i (n_i - 1) |n\rangle 
$$

$$- t \left\langle m \right| \left( b_0^\dagger \right) \left( 1 - \frac{X}{t} n_1 \right) b_2 + \text{h.c.} |n\rangle 
$$

$$- t \left\langle m \right| \left( b_{d-1}^\dagger \right) \left( 1 - \frac{X}{t} n_d \right) \langle b_{d+1} \rangle + \text{h.c.} |n\rangle 
$$

$$- t \left\langle m \right| \left( b_{-1}^\dagger \right) \left( 1 - \frac{X}{t} n_0 \right) b_1 + \text{h.c.} |n\rangle 
$$

$$- t \left\langle m \right| \left( b_d^\dagger \right) \left( 1 - \frac{X}{t} n_{d+1} \right) b_{d+2} + \text{h.c.} |n\rangle.$$  

The $d$-site ground state wave function of $|G\rangle$ is computed self-consistently. First, a generic initial state of the cluster with $f_n^{0} = 1/|\{n\}|$ is used to compute the mean-field parameters. Subsequently, a new ground state is obtained and the mean-field parameters are updated. The convergence criterion to be fulfilled is $\sum_n |f_n^{t} - f_n^{t-1}| < \epsilon$.

FIG. 6: Color legend: superfluid parameter $\phi_i = \langle b_i^\dagger \rangle + \sum_j \langle b_i^\dagger b_j \rangle$ on central sites. Shaded areas depict specific phases, red: phase-separated, orange/pink: paired holes with two/four holes, blue/green: paired particles with two/four additional particles, yellow: Mott insulator. Strong coupling expansion results are depicted in black, dot-dashed: transition to ph/pp-superfluid, continuous: transition to standard superfluid. a) $X=0.0$, b) $X=0.6\ t$, c) $X=0.8\ t$, d) $X=1.0\ t$, e) $X=1.2\ t$. 

The Hamiltonian for the $d$-site cluster is the same as in the case of on-site interaction terms and in the interior of the cluster $S = \{3, \ldots, d-2\}$. The boundary sites are coupled to the rest of the system via mean-field parameters $\langle b_0 \rangle$, $\langle b_{d+1} \rangle$, $\langle b_{-1} n_0 \rangle$, $\langle n_{d+1} b_{d+2} \rangle$:

$$H_{\text{cluster}}^{n} = \left\langle m \right| H_S + \frac{U}{2} \sum_{i=1}^{d} n_i (n_i - 1) |n\rangle 
$$

$$- t \left\langle m \right| \left( b_0^\dagger \right) \left( 1 - \frac{X}{t} n_1 \right) b_2 + \text{h.c.} |n\rangle 
$$

$$- t \left\langle m \right| \left( b_{d-1}^\dagger \right) \left( 1 - \frac{X}{t} n_d \right) \langle b_{d+1} \rangle + \text{h.c.} |n\rangle 
$$

$$- t \left\langle m \right| \left( b_{-1}^\dagger \right) \left( 1 - \frac{X}{t} n_0 \right) b_1 + \text{h.c.} |n\rangle 
$$

$$- t \left\langle m \right| \left( b_d^\dagger \right) \left( 1 - \frac{X}{t} n_{d+1} \right) b_{d+2} + \text{h.c.} |n\rangle.$$  

The $d$-site ground state wave function of $|G\rangle$ is computed self-consistently. First, a generic initial state of the cluster with $f_n^{0} = 1/|\{n\}|$ is used to compute the mean-field parameters. Subsequently, a new ground state is obtained and the mean-field parameters are updated. The convergence criterion to be fulfilled is $\sum_n |f_n^{t} - f_n^{t-1}| < \epsilon$.
\(10^{-7}\), where \(i\) is an index of the iteration. From the obtained wave vector we compute the average quantities \(\langle n_i \rangle\), \(\langle n_i^2 \rangle\), \(\langle b_i \rangle\), \(\langle b_i^2 \rangle\) on the most central sites, as being minimally coupled to the mean-field they should most accurately describe the properties of the system. However, we also examine the cluster as a whole in search of any spatial patterns and correlations of the local observables.

The results obtained by CM are depicted in Figure 6 for a cluster of size \(d = 6\) and \(n_{\text{max}} = 5\). Additionally, for the purpose of efficient self-consistent computation, we loose the constraint of equal occupation of sublattices and allow the number of particles in the even/odd lattice to differ by one. The results show, however, that only the vectors with equal number of particles in both sublattices contribute to the final wave function describing the cluster. The main information is represented by contour plots of the superfluid parameter. Additionally, we plot the boundaries of phases resulting from the analytical estimates (AE) of the previous section.

In Figure 7 we plot the maximum value of \(t/U\) vs. \(X/t\) for which the system is in the Mott insulator phase assuming that the transition can be either to the standard or ph/pp-superfluid.

The CM method reveals several qualitatively different phase diagrams for different values of \(X/t\). These phase diagrams are distinguished by the phases surrounding the Mott insulator and whether the preferable scenario in the limit of large \(t/U\) is phase separation or formation of superfluid droplets. As throughout this paper, we assume fillings around unit density. The main characteristics in different regimes are listed below:

\(X/t \leq 0.2\): AE show that the Mott insulating phase is surrounded by the standard superfluid phase; ED indicates that there is no phase separation in the limit of large \(t/U\), the correlated hopping is weak and it only modifies the tunneling rate but does not affect the system qualitatively.

\(0.2 \leq X/t \leq 0.5\): AE show that the Mott insulating phase is surrounded exclusively by the superfluid phase; ED indicates that in the limit of large \(t/U\) the system becomes phase-separated.

\(0.5 < X/t \leq 0.75\): AE show that the bottom of the lobe is partially surrounded by the paired-holes superfluid; in the limit of large \(t/U\) we observe clustering of particles in the ED results. This is confirmed by the CM calculation.

\(0.75 < X/t \leq 1.05\): AE show that the bottom and the top of the lobe are partially surrounded by the paired-holes/particles superfluids, respectively; both the CM and ED results show a possible direct transition from Mott insulator to a superfluid phase containing low-density droplets; ED indicates that in the limit of large \(t/U\) the system is in the superfluid droplet phase;

\(X/t \geq 1.05\): AE show there is no direct transition from the Mott insulating phase to the standard superfluid, it is either to the paired-holes superfluid at the bottom or to the paired-particles superfluid at the top; numerical ED and CM results suggest that there is also a direct transition from the Mott insulator to the superfluid droplet phase and indicate that in the limit of large \(t/U\) the system is in the superfluid droplet phase.

III. CONCLUDING REMARKS

In this paper, we have studied an extended Bose Hubbard model where two standard Bose-Hubbard chains are coupled by a correlated hopping term. This leads to a rich phase diagram with two non-standard types of the superfluid: the paired-holes/paired particles superfluid and the droplet superfluid. The phases of the system have been identified with complementary methods (finite size exact diagonalization, analytical perturbative expansions and cluster mean-field) which yield results consistent with each other in this 1-dimensional system. An interesting open question for further study is to engineer a broadly tunable Bose system of the form considered here.
We thank M. Gajda and T. Sowiński for discussion and valuable comments. JS acknowledges the National Science Center, Poland Grant No. 2015/16/S/ST2/00445. M.L. acknowledges the Spanish Ministry MINECO (National Plan 15 Grant: FISICATEAMO No. FIS2016-79508-P, FPI), European Social Fund, Fundaci Cellex, Generalitat de Catalunya (AGAUR Grant No. 2017 SGR 1341 and CERCA/Program), ERC AdG NOQIA, and the National Science Centre, Poland-Symfonia Grant No. 2016/20/W/ST4/00314.

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