Pair Superfluidity of Three-Body Constrained Bosons in Two Dimensions

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We examine the equilibrium properties of lattice bosons with attractive on-site interactions in the presence of a three-body hard-core constraint that stabilizes the system against collapse and gives rise to a dimer superfluid phase formed by virtual hopping processes of boson pairs. Employing quantum Monte Carlo simulations, the ground state phase diagram of this system on the square lattice is analyzed. In particular, we study the quantum phase transition between the atomic and dimer superfluid regime and analyze the nature of the superfluid-insulator transitions. Evidence is provided for the existence of a tricritical point along the saturation transition line, where the transition changes from being first-order to a continuous transition of the dilute bose gas of holes. The Berzinskii-Kosterlitz-Thouless transition from the dimer superfluid to the normal fluid is found to be consistent with an anomalous stiffness jump, as expected from the unbinding of half-vortices.

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Due to their remarkable versatility, cold-atom systems are ideally suited to realize quantum simulators for the physics of strong correlations [1]. A fascinating approach towards enhancing correlations in atomic systems stems from the fact that they can emerge via dissipative processes. In fact, dissipation-induced correlation effects were observed in an experiment with Feshbach molecules subject to strong inelastic collisions [2]. More recently, it was found that three-body loss processes for bosons in an optical lattice give rise to an effective Bose-Hubbard model description with a local three-body hardcore constraint [3]. Such a constraint stabilizes the system in the presence of strong attractive interactions, where dimer bound states proliferate. The effective lattice model describing this situation is the Bose-Hubbard Hamiltonian

$$H = -t \sum_{\langle ij \rangle} \left( b_i^\dagger b_j + \text{h.c.} \right) + \frac{U}{2} \sum_i n_i (n_i - 1) - \mu \sum_i n_i$$

(1)

where $t$ denotes the tunneling matrix element for nearest neighbor sites $\langle ij \rangle$ and $U < 0$ an attractive on-site interaction [2]. The filling $n$ is controlled by varying the chemical potential $\mu$, $b_i$ ($b_i^\dagger$) denote bosonic annihilation (creation) operators and $n_i$ the number operator for bosons on lattice site $i$. In contrast to the usual Bose-Hubbard model, the Hilbert space is now restricted by the constraint $\langle b_i^3 \rangle = 0$ to a maximum of two bosons on each lattice site. In recent proposal [4], a similar effective lattice model of bosons with a three-body constraint was derived for spin-1 atoms, which in addition includes an explicit correlated hopping term $H' = -t' \sum_{\langle ij \rangle} \left( b_i^\dagger b_j^\dagger b_j b_i + \text{h.c.} \right)$ of the dimer bound states.

The model in Eq. (1) exhibits an intriguing phase diagram, shown in Fig. 1 for the case of a two-dimensional square lattice. Recent analytical calculations [5] and numerical works for the one-dimension case [6,7,8] exhibited that besides the trivially insulating phases at $n = 0$ and $n = 2$, the system stabilizes two kinds of superfluid phases. The atomic superfluid (ASF) is characterized by a finite atomic condensate with $\langle b_i \rangle \neq 0$ and a finite superfluid response $\rho_s$. For strong interactions $|U| \gg t$ however, a dimer (pair) superfluid phase (DSF) [8] is stabilized, which is characterized by a vanishing atomic condensate and $\langle b_i \rangle = 0$, but a finite dimer condensate density with an order parameter $\langle |b_i|^2 \rangle \neq 0$. Such single-component DSF phases have been observed before in models with explicit correlated or pair hopping processes [4,9]. In the DSF phase, the $U(1)$ symmetry of the Hamiltonian is partially broken down to $\mathbb{Z}_2$, and at the DSF to ASF transition, this remaining $\mathbb{Z}_2$ symmetry gets broken. With respect to this partial internal symmetry breaking, DSF are thus related to spin nematic states [11]. Within Ginzburg-Landau theory, a Feshbach resonance term couples the ASF and DSF order parameter fields, which implies an effective $U(1) \times \mathbb{Z}_2$ symmetry similar as in the boson Feshbach resonance.
problem [12, 13]. From such analysis, the ASF-DSF transition was found to be Ising-like at unit filling, \( n = 1 \), and driven first-order by fluctuations via the Coleman-Weinberg mechanism [14] for \( n \neq 1 \).

Here, we study the ground state and thermal phase diagram of the three-body constrained Bose-Hubbard model in Eq. (1) using quantum Monte Carlo (QMC) simulations. We focus on a two-dimensional square lattice geometry, on which true off-diagonal long-range order (ODLRO) within the ASF and DSF regimes emerges in the ground state. Besides establishing the presence of ODLRO, we assess the above mentioned theory for the ASF-DSF transition [5, 6] as well as a recent effective Hamiltonian approach that allows for efficient updates of correlated hopping terms [23]. We can now measure the probabilities \( \langle C^2 \rangle = 1 \) (related to \( H \)) and \( \langle H \rangle \) denoting all correlated hopping terms in the original Hamiltonian that allow for efficient updates of the Hamiltonian, such that \( \langle H \rangle = \langle C \rangle \rho_s \). We indeed obtain evidence for a trapping point at one of the transition lines. The thermal Berzinskii-Kosterlitz-Thouless (BKT) transition out of the DSF phase is found to be consistent with an unbinding of half-vortices [15].

**Method.**— We employ a directed loop algorithm in the stochastic series expansion (SSE) representation [16, 17] at finite temperatures. The simulations are performed on square lattices of linear extent \( L \) (and \( N = L^2 \) sites), with periodic boundary conditions, such that the superfluid density is obtained from the winding number \( W \) fluctuations, \( \rho_s = T(W^2)/(2t) \) [18, 19]. Since ODLRO in our system is forbidden at finite temperature, we need to perform the simulations at sufficiently low \( T \) to probe ground state properties of the finite system, as detailed below. Using two kinds of directed loops, in which the worm heads carry either a single creation (annihilation) operator \( b^\dagger (b) \) or a pair operator \( (b^\dagger)^2 \), provides direct access to the equal-time Green’s function of the atoms \( G_1(i,j) = \langle b^\dagger_i b_j \rangle \) as well as the dimers \( G_2(i,j) = \langle (b^\dagger_i)^2(b_j)^2 \rangle \) [17, 21]. The atomic and dimer condensate densities are obtained as \( C_1 = 1/N^2 \sum_{ij} G_1(i,j) \) and \( C_2 = 1/N^2 \sum_{ij} G_2(i,j) \) respectively after extrapolations to the thermodynamic limit. A similar scheme with pair-worms was shown recently to be efficient for simulating two-component boson systems [22]. Here, we find that accessing the dimer condensate density based on \( G_2 \) still becomes problematic at the relevant low temperatures: Histograms are strongly peaked in the dimer condensate density on the lengths of the pair operator loops) exhibit fat-tailed distributions, i.e. the estimator of this quantity is dominated by rare events that make its sampling inefficient. A typical histogram within the DSF region is shown in Fig. 2. This behavior results from the fact that pairs of bosons proliferate at large \( |U| \) near \( n = 1 \). A worm head carrying a bosonic pair operator performs an off-diagonal move (corresponding to the hopping of a dimer) only if it encounters a bond that shares a dimer (or an empty site, if the worm either carries annihilation or creation operators) and a single atom. Such processes are thus strongly suppressed in the relevant parameter regime. Moreover, the fat tail of the histogram fits well to a Fréchet distribution. The exponent of the power-law decay in the tail is \( \alpha > -3 \) (\( \alpha \approx -2.2 \) for the histogram in Fig. 2), so that the variance does not exist, and the central limit theorem for the mean value does not hold.

Hence, we resign to alternative estimates of the dimer condensate density in the DSF region. We employ two different means of adding correlated hopping terms to the original Hamiltonian that allow for efficient updates of the boson pairs. The results from both approaches agree within error bars, and with results based on \( G_2 \) in cases, where the distribution of the loop lengths leads to a finite variance. In the first approach, we add to \( H \) the correlated hopping term \( H' \), such that \( H_1 = H + H' \). The other approach couples \( C_2 \) directly to the Hamiltonian, such that \( H_2 = H - h/N \sum_{ij} \left( (b^\dagger_i)^2 b_j \right)^2 + h.c. + 1 \) features correlated hopping terms between all sites of the system (the diagonal term allows the insertion of long-range vertices into the SSE operator string). The coupling \( h/N \) ensures an extensive energy. Besides the diagonal update of the short-range terms in \( H_2 \), we insert/remove long-range vertices using heat-bath probabilities [24]. We can now measure \( C_2 \) based on the estimator \( C_2 = (\sum_b (H_b)^2)/(Nt)^2 - (H_b)/(Nh) \), where \( H_b \) denotes all correlated hopping terms in \( H_2 \) and \( H_0 \) the atomic kinetic energy term on bond \( b \). This method remains robust down to very low values of \( h/|U| \sim 10^{-4} \), so that we extract the condensate density of the model \( H \) by fitting to a low-degree polynomial (the data is found to be essentially linear up to \( t'/|U|, h/|U| \sim 10^{-2} \), performing a bootstrap analysis for the error estimation. Such a scaling is shown in the right panel of Fig. 2, and extrap-
system sizes along $\mu/|U|$, which is absent in the ASF regime, correspondingly we observe in the DSF region a strong finite-temperature phase diagram along this line (cf. Fig. 2) exhibits the temperature scale at which the system undergoes a BKT transition, below which superfluidity is indeed first-order for attractive interactions. We find from our QMC simulations that such transitions are not able to discern whether the quantum phase transition indeed is first-order or not (histograms of various observables did not exhibit any two-peak structures on the accessible system sizes $L < 20$ at these low temperatures). Controlling $\mu$ as to fix $n = 1$ for all finite systems in order to directly address the $n = 1$ case also turned out unfeasible. Given the above estimate of $(t/|U|)_c$, the mean-field value $(t/|U|)_c \approx 0.044$ is found to underestimate the stability of the DSF phase by about 20%. The calculations of Ref. [2], while accounting for quantum fluctuations effects, still show a similar deviation.

ASF-insulator quantum phase transitions. Next, we address the quantum phase transitions between the ASF and the (trivially) insulating phases at $n = 0$ and $n = 2$. While SF to insulator transitions are often continuous, they can be driven first-order for attractive interactions. We find from our QMC simulations that the transition from the empty system ($n = 0$) to the ASF is indeed first-order over an extended parameter regime. This is evident from robust discontinuities in both the filling $n$ and superfluid density $\rho_s$, such as those shown in the left panel of Fig. 4 at $\mu/|U| = -1.2$. From Ref. [2], the transition is expected to turn continuous beyond a tricritical point near $\mu/|U| \approx -0.9$. Performing simulations down to $\mu/|U| = -1.5$, we did not obtain evidence for a continuous transition, indicating strong effects of the Feshbach resonance coupling for $\mu/|U| < -0.5$. The scenario of Ref. [2], including a tricritical point, is found.
we became aware of recent results [29] on the thermal phase transitions in an extended three-body constrained boson lattice model, consistent with our findings.

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