

Extended Bose-Hubbard model on small grids: Exact diagonalization and Monte Carlo studies

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The superfluid-insulator transition in systems of lattice bosons is usually analyzed in the framework of the Bose-Hubbard model, and has been extensively studied by theory and simulations. Less attention has been paid to the remnants of the transition in truncated lattices, with or without periodic boundary conditions. Here we consider the hard-core limit of the extended Bose-Hubbard model on small square and triangular grids—i.e., sections of the square and triangular lattices containing up to 13 sites. By mapping out the zero-temperature phase diagram through exact diagonalization, we find ground-state characteristics that are markedly different from those emerging in the thermodynamic limit, together with similarities. The dichotomy between superfluidlike and insulatinglike behavior is then investigated in two-dimensional systems of a few interacting bosons in the continuum, subject to confining and optical-lattice potentials mimicking the 3×3 square grid. Using path-integral Monte Carlo simulations, we compute kinetic and potential energies, as well as superfluidity and exchange-cycle statistics, finding hints of Bose-Hubbard behavior even in systems of just five particles.

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I. INTRODUCTION

A better knowledge of the mechanisms underlying the onset of emergent behavior in complex many-particle systems will make it easier to design materials with prescribed properties. Yet, a hallmark of complexity is that macroscale properties are often hard to predict from microscale features. In addition, the challenge of characterizing phase equilibria becomes increasingly more difficult when moving from classical to quantum many-body systems, for which analytic methods are limited and numerical simulations are considerably more expensive. From a theoretical point of view, it would be appropriate to work at zero temperature ($T = 0$), where the relevant quantum phases are already visible and their features stand out more clearly, since free from thermal noise. At $T = 0$, phase transitions may still occur in the ground state of a many-body system as functions of nonthermal parameters such as pressure, magnetic-field strength, or particle mass. Such “quantum phase transitions” [1,2] typically arise from the competition between various terms in

the Hamiltonian, each prompting a different kind of system self-organization.

A paradigmatic case is the Bose-Hubbard (BH) model [3], probably the simplest model of interacting bosonic particles on a lattice with a nontrivial phase diagram. Here, each particle experiences two competing forces: One pushes it to jump to neighboring sites, while the other pushes it away from neighboring particles. The interplay between these opposing tendencies is further regulated by the chemical potential, which decides how many particles the lattice is to contain. The ground state of this system is either insulating or superfluid, depending on the ratio between the hopping amplitude and the strength of repulsion. A large repulsion favors insulating (solidlike) behavior, characterized by integer boson densities and a gapped spectrum. Instead, highly mobile particles develop overall phase coherence and a nonzero superfluid response.

The BH model describes the behavior of an ultracold gas of bosonic atoms in an optical lattice [4–6]. At very low temperature, a gas of bosons is condensed. Turning on the lattice potential, the system remains in the condensed phase as long as the potential wells are shallow. In this regime, the kinetic energy is dominant and a delocalized wave function minimizes the total energy. In the opposite limit where the lattice potential is strong, the interatomic repulsion overcomes kinetic energy and the total energy is minimized by filling each lattice site with the same number of atoms.

The phase diagram of the BH model at $T = 0$ has been worked out numerically in both three [7] and two dimensions [8], and is well reproduced by a number of theories [9–13].

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Other phases appear when the range of interparticle repulsion is extended to further neighbors. In this case, supersolid phases (combining a nonuniform density with superfluidity) can also become stable [14–19]. Extended BH models provide a more realistic approximation than the original model to condensates of dipolar bosonic atoms in optical lattices [20–24]. Other generalizations of the BH model are possible [25–27], leading to a wealth of spatially modulated phases.

However, genuine phase transitions only occur when the lattice is infinite in every direction. In large samples, sharp crossover behaviors occur in place of proper, nonanalytic transitions. In turn, such crossovers do not arise from nowhere, but rather would be the continuation of trends that are present even in much smaller systems. In this paper, we put this expectation to the test on the simplest extended BH model (i.e., the original BH model with the addition of first-neighbor repulsion), which will be examined on two-dimensional grids (i.e., truncated lattices) small enough that diagonalization of the model can be done exactly. To accomplish this task, we must assume an infinite on-site repulsion, i.e., single site occupancy—despite this simplification, the gross features of the model stay unaltered. We shall see that BH behavior is quite different on small grids, whereby the structure of insulating “phases” deviates from the infinite-size limit, but the superfluid-insulator interplay nevertheless remains. Exact diagonalization studies have been carried out for the Bose-Hubbard model by various authors (see, e.g., Refs. [28–31]).

The rivalry between BH phases on a grid can also be analyzed in simulation, using the “language” of bosonic particles in continuous space. In this case we must apply an external field having the same symmetry of the grid and employ a box-shaped potential to prevent particles from exiting the grid region. At low but nonzero temperature, this system will be studied by path-integral Monte Carlo (PIMC) simulations, which provide reliable indications on the structure and energy of the sample, as well as on its superfluid response.

The paper is organized as follows: After presenting the model and the method in Sec. II, we discuss exact-diagonalization results in Sec. III, where the model is examined on various grids, with and without periodic boundary conditions. Then, in Sec. IV we comment on the results of boson simulations, and compare them with the ascertained behavior of the discrete model. Section V is devoted to conclusions.

II. MODEL AND METHOD

On a regular lattice, the (grand) Hamiltonian of the extended BH model reads

$$H = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + \frac{U}{2} \sum_i n_i(n_i - 1) + V \sum_{\langle i,j \rangle} n_i n_j - \mu \sum_i n_i, \quad (1)$$

where the first and third sums run over all pairs (each counted once) of nearest-neighbor (NN) sites, a_i and $a_i^\dagger$ are bosonic field operators, and $n_i = a_i^\dagger a_i$. Furthermore, $t > 0$ is the hopping parameter, $U > 0$ is the interaction energy between two particles on the same site, $V > 0$ is the interaction energy between two NN particles, and μ is the chemical potential.

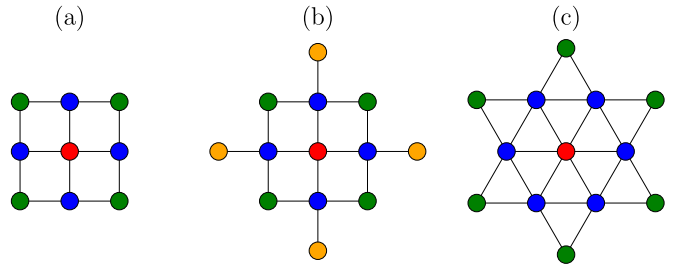


FIG. 1. The three grids on which we map out the phase diagram of the model by exact diagonalization: (a) Square, (b) Diamond, and (c) Star. We use different colors to mark first, second, and third neighbors of the central site. All these grids can be periodically replicated without overlaps or gaps.

As discussed in the Introduction, in order to make the dimension of state space finite, we must truncate the lattice *and* apply an upper cutoff n_{cut} on site occupancy. A finite n_{cut} will substantially affect the phase diagram only at low U/V and high μ/V (see Sec. III). The simplest choice is taking $U \rightarrow \infty$ in Eq. (1), corresponding to $n_{\text{cut}} = 1$ (hard-core limit). This is the model version we consider from now onward.

Focusing on the two-dimensional case, the phase diagram of hard-core bosons at $T = 0$ is known on the square [32,33] and the triangular lattice [34,35] (in the latter case there is also a supersolid region). On the square lattice, the only nontrivial insulating phase (i.e., other than the empty and fully occupied lattices) has checkerboard structure. This phase is stable in a lobe-shaped region of the t - μ plane. On the triangular lattice, two insulating phases (and lobes) instead exist, where either one or two triangular sublattices out of three are filled and the other(s) are empty. On a small-sized grid, homogeneity is lost and we expect (besides the removal of every singularity and sharp distinction between the phases) some more changes in the “insulating” sector, which will be especially evident at $t = 0$ [36–38]. Other differences will result from the application of periodic boundary conditions (PBC).

In Fig. 1 we show the grids considered in our study: Two different sections of the square lattice (“Square” and “Diamond”), with 9 and 13 sites, respectively, and a small fragment of the triangular lattice (“Star”) containing 13 sites. All such grids show discrete rotational symmetry around the central site. We have thus used different colors in Fig. 1 to identify shells of neighbors at the same distance from the central site. However, we cannot exclude that rotational symmetry is spontaneously broken in the actual ground state of the system, which will then be multiple (i.e., associated with a degenerate eigenvalue), making it impossible to describe, e.g., the local density just in terms of shell values (we shall give examples in Sec. III). We point out that the infinite lattice can be covered without overlaps or gaps with each tile in Fig. 1 (see Appendix A), meaning that for all such tiles we can contrast the effects of periodic and open boundary conditions on the system behavior.

For our model, the dimension of the Hilbert space on a grid of M sites is 2^M (with M equal to 9 or 13), i.e., small enough that we can compute a few exact energy eigenvalues and eigenstates in reasonable time. To this aim, we represent the Hamiltonian on the Fock basis $\{|x_1, \dots, x_M\rangle\}$ (with

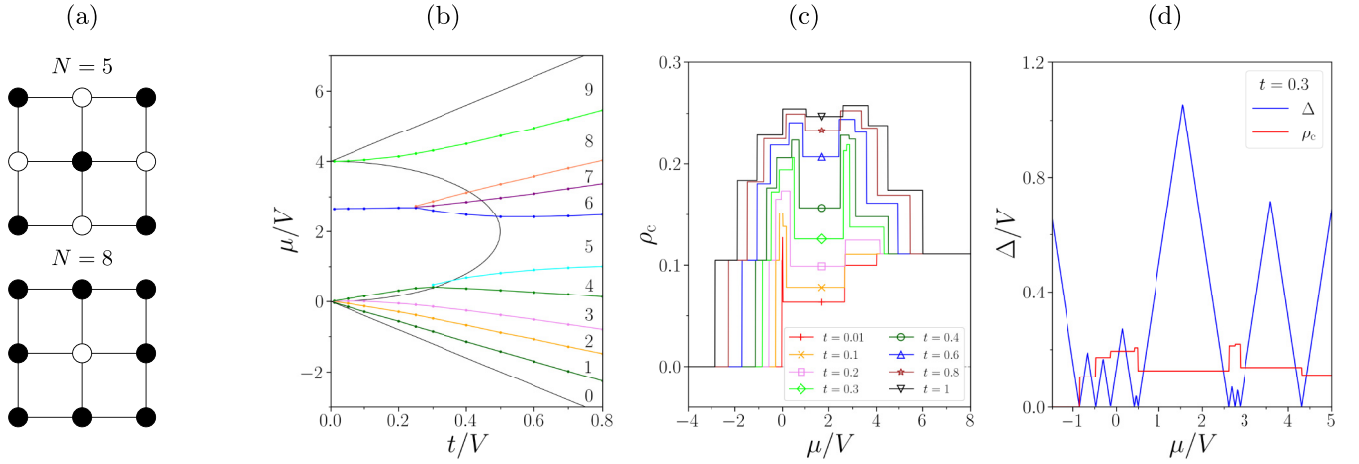


FIG. 2. Square. (a) Ground states of the system for $t = 0$ and $0 < \mu < 4V$. (b) Exact phase diagram at $T = 0$. The broken lines through the points are boundary lines of sectors. The black thin lines are mean-field phase boundaries [42]. (c) Condensate fraction $\rho_c(\mu)$ for various t . As t grows, the condensate fraction grows as well and the central dip becomes more shallow. (d) Energy gap $\Delta(\mu)$ for $t = 0.3$ (blue line). Also shown is the condensate fraction for the same t (red line).

$x_i = 0$ or 1) and diagonalize the ensuing matrix numerically. In particular, the ground state $|g\rangle$ and its eigenvalue, the zero-temperature grand potential Ω of the entire grid, are obtained as functions of t and μ (in particular, the chemical potential is typically increased in steps of $0.01V$). Once $|g\rangle$ has been determined, we calculate the average occupancies of all nodes and the condensate fraction ρ_c [12,39]:

$$\rho_c = \frac{1}{M} \langle g | \tilde{a}_0^\dagger \tilde{a}_0 | g \rangle, \quad (2)$$

where $\tilde{a}_0 = (1/\sqrt{M}) \sum_{i=1}^M a_i$ is the zero-momentum field operator. In the superfluid phase of an infinite two-dimensional lattice system $\rho_c > 0$, since a nonzero superfluid response (as measured, in a simulation with PBC, through the winding-number fluctuations [40]) also entails a nonzero condensate density, and vice versa. Since the Hamiltonian commutes with the total number of particles, $\sum_i n_i$, the (t, μ) plane is divided into sectors where the number of particles takes a constant value N , from 0 to M . Clearly, $N = 0$ is the empty grid and $N = M$ is the fully occupied grid. In the N sector, the only nonzero Fourier coefficients of $|g\rangle$ are those relative to basis states with $\sum_i x_i = N$.

A distinguishing feature of insulating phases is the nonzero energy gap, in contrast to the zero gap of a superfluid or a supersolid phase (see, e.g., Ref. [41]). A finite gap signals that low-energy excitations are rather costly, implying a substantial robustness of the ground state to thermal fluctuations. In order to see to what extent this is recovered in our finite system, in addition to the lowest eigenvalue Ω , we also compute the second smallest eigenvalue (Ω_2), which finally yields the gap as $\Delta = \Omega_2 - \Omega$.

III. ZERO-TEMPERATURE RESULTS

In this section, we present the results for the hard-core extended BH model on various two-dimensional grids. We fix $T = 0$ and thus consider only properties of the ground state as functions of t/V and μ/V . When we apply open boundary conditions the system is intrinsically inhomogeneous, due to

boundary sites having a smaller number of first neighbors. Since the NN interaction is repulsive ($V > 0$), we expect a general tendency of the dense system to gather particles at the boundary of the grid. Homogeneity is recovered when PBC are applied, but again peculiarities are expected on small grids.

A. Square

The 3×3 square grid in Fig. 1(a) consists of a central site, together with its first- and second-neighbor sites. At $t = 0$, the system ground state corresponds to the occupancies yielding the lowest value of

$$h(x_1, \dots, x_M) = V \sum_{\langle i,j \rangle} x_i x_j - \mu \sum_i x_i, \quad (3)$$

for $x_i = 0, 1$. Clearly, the minimum- h state depends on μ : Aside from the trivial cases of the empty grid ($\mu < 0$) and the fully occupied grid ($\mu > 4V$), the only other possibilities are depicted in Fig. 2(a). While for $0 < \mu < (8/3)V$ the ground state (“chessboard”) mirrors the infinite-size structure of minimum energy on a smaller scale (though with an average occupation of $5/9$, instead of $1/2$), in the ground state for $(8/3)V < \mu < 4V$ (“ring”) the central site is empty and the boundary sites are all filled. The stability of the ring is a finite-size effect: The ring provides a smaller h than the chessboard when

$$8V - 8\mu < -5\mu \Rightarrow \mu > \frac{8}{3}V. \quad (4)$$

The full “phase diagram” at $T = 0$, obtained by exact diagonalization, is plotted in Fig. 2(b). In stark contrast with the mean-field phase boundaries [15,42] (reported in the same figure as black thin lines), there are no sharp phases in Fig. 2(b); rather, the t - μ plane is divided into sectors (see Sec. II) which, with the relevant exception of the line separating the 5 sector from the 8 sector, are vaguely indicative of the location of iso-density lines (constant-density profiles) in the thermodynamic limit (see, e.g., Ref. [43]).

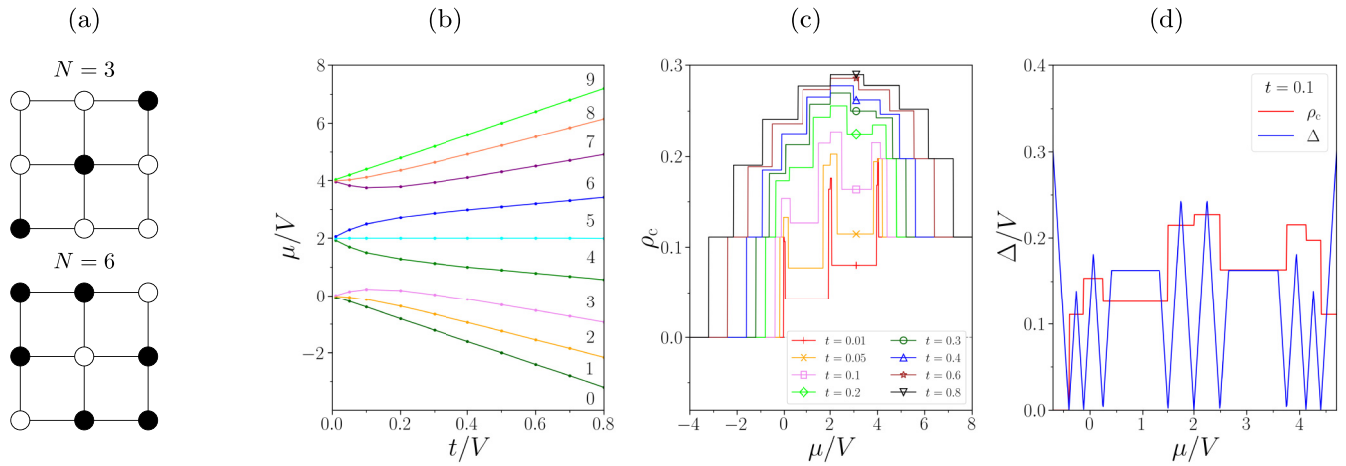


FIG. 3. Square with PBC. (a) Ground states of the system for $t = 0$ and $0 < \mu < 4V$. (b) Exact phase diagram at $T = 0$. The broken lines through the points are boundary lines of sectors. (c) Condensate fraction $\rho_c(\mu)$ for various t . As t grows, the condensate fraction grows as well. (d) Energy gap $\Delta(\mu)$ for $t = 0.1$ (blue line). Also shown is the condensate fraction for the same t (red line).

A quantity that more clearly discriminates between superfluidlike and insulatinglike behavior is ρ_c , plotted in Fig. 2(c) as a function of μ along a few iso- t lines. Each jump discontinuity of ρ_c occurs in coincidence with one of N . ρ_c develops a peak when we cross the “superfluid” region, while it takes a smaller value (in relative terms) when crossing an “insulator” region. Eventually, when $N = M = 9$ and $|g\rangle = |1, 1, \dots, 1\rangle$, it is easy to obtain from Eq. (2) that ρ_c becomes $1/M$. As t grows, the condensate fraction gradually increases and flattens out. A feature of the superfluid phase of hard-core bosons is that the maximum possible value of ρ_c is definitely smaller than 1. For example, we have verified numerically for $t = 20$ that the maximum ρ_c is approximately 0.3 [see Fig. 11(b) below]. The same is found in mean-field theory, where in models similar to the present one the asymptotic, $t \rightarrow \infty$ value of ρ_c is 0.25 [36,37]. Alternatively, we may consider the tight-binding model for hard-core bosons, where the condensate fraction equals 0.285 on Square, regardless of μ .

All in all, a clear correlation exists between ρ_c on Square and the condensate fraction on the square lattice, demonstrating that signatures of condensation are present even in a rather small boson system.

Then, we plot in Fig. 2(d) the gap Δ as a function of μ for $t = 0.3$. Δ is larger in the insulating phases than in the superfluid region; as a rule, the gap is wider the larger the distance in chemical potential from the nearest adjacent sector. The nonmonotonic behavior of Δ with μ has a simple explanation: While the less-costly excitation is holelike on the low- μ side of a sector, it is particlelike on the high- μ side. Looking more closely at the data, we indeed realize that $\partial\Delta/\partial\mu = \pm 1$, meaning that the first excited state, which is generally nondegenerate, is a linear combination of basis states with one particle more or less than those composing the ground state.

Finally, we have looked at the same grid, but with periodic conditions applied at the boundary. New boundary conditions bring about a redefinition of neighbors for boundary sites, resulting in a new phase portrait. In Fig. 3(a) we show the minimum- h structures for $t = 0$; both these structures, which are negative images of one another, break rotational symme-

try, implying degeneracy (here, equal to 6 for both). However, the lowest energy eigenvalue for $t > 0$ is nondegenerate and all symmetry-breaking Fock states of same species appear in the ground state with identical weight. The overall phase diagram is illustrated in Fig. 3(b). Compared to Fig. 2(b), the “insulating” regions are seemingly less extended in the t - μ plane, suggesting that (unless t is very small) superfluidlike behavior is present in the whole range $0 < N < 9$. This is also apparent from the condensate fraction [Fig. 3(c)], which already for $t = 0.3$ shows the typical bell shape of a superfluid. We note that $\rho_c = 1/M = 1/9$ in the 1 sector, since the ground state for $t > 0$ is an equal-weight linear combination of Fock states with $\sum_i x_i = 1$. Lastly, we look at the gap as a function of μ . In Fig. 3(d) (which refers to $t = 0.1$) we see a flat region in both $N = 3$ and $N = 6$ sectors, which just indicates that for those values of t and μ the first excited state is, as the ground state, a linear combination of basis states having $\sum_i x_i = 3$ or 6.

The more widespread stability of the superfluid phase under PBC seems to contradict the common belief that, when the system is periodically replicated, finite-size effects are reduced and the behavior is more similar to the infinite system. In fact, this cannot happen for Square because the number of sites on its edges is odd, and checkerboard ordering is thus excluded. A small grid where the chessboard ground state is not frustrated under PBC is the 4×2 rectangle (see Appendix A). As is seen in Fig. 4(a), the topology of the phase diagram is indeed similar to the mean-field (MF) phase diagram. Another example is the 4×3 rectangle, where, however, the periodic images of the grid in the y direction are shifted horizontally by one site to avoid frustration [Fig. 16(b)]. Also in this case, as illustrated in Fig. 4(b), the $T = 0$ phase diagram closely matches the MF one. Interestingly, for both rectangles the boundaries of the 0 and M sectors predicted by exact diagonalization perfectly coincide with those obtained from MF theory.

B. Diamond

We obtain Diamond from Square by also including the third neighbors of the central site [see Fig. 1(b)]. With four

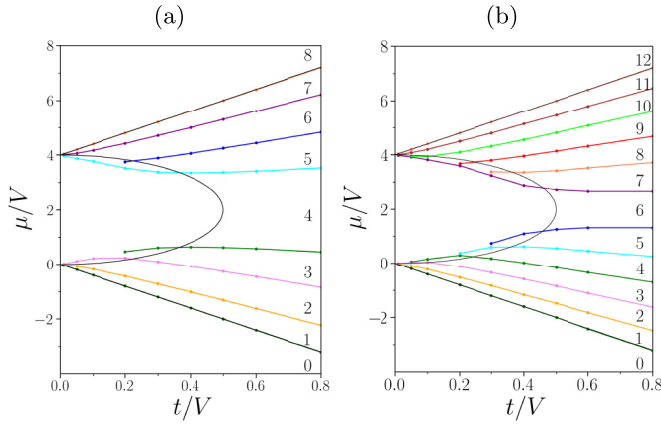


FIG. 4. Exact phase diagram at $T = 0$ of the 4×2 (a) and the 4×3 (b) rectangles with PBC. The broken lines through the points are boundary lines of sectors. The black thin lines are mean-field phase boundaries [42].

sites more, the phase diagram of the hard-core extended BH model results in better agreement with the phase diagram on the square lattice: At $t = 0$ the only nontrivial ground state has the checkerboard structure illustrated in Fig. 5(a). The $T = 0$ phase diagram, reported in Fig. 5(b), has the same topology of the mean-field phase diagram [15,42], in turn pretty similar to the actual one. Actually, the stability of the insulating ($N = 9$) “phase” on Diamond is greatly enhanced relative to the square lattice, where the superfluid phase takes over the insulating phase at $t \approx 0.5V$. Also for Square the stability of the insulatinglike phase for $N = 5$ overcomes $t = 0.5$, but this effect is more pronounced for Diamond. This is confirmed by the condensate fraction as a function of μ [Fig. 5(c)], where the hollow centered at $\mu = 2V$ is still clearly visible for $t = 1$. Also the energy gap is particularly large in the middle of the $N = 9$ region, even at t as large as 0.5 [Fig. 5(d)].

When Diamond is replicated periodically (which can be done in either of two ways; see Fig. 17) things change considerably. At $t = 0$ checkerboard order is ruled out and, in

its place, the nontrivial ground states are four [see Fig. 6(a)], with two of them being negative images of the other two. What is unusual in this case is the high degree of degeneracy of these phases, namely, 13 and 26 for the $N = 4$ and the $N = 6$ phase, respectively. This multiplicity just reflects the freedom of translating (and, for $N = 6$, also rotating) the filled sites rigidly on the grid without affecting the energy. As already commented for Square with PBC, the boundary lines of sectors are distributed rather uniformly in the $0 < N < 13$ region, suggesting superfluidlike behavior for all not too small t .

C. Star

The Star grid in Fig. 1(c) has the same number of sites as Diamond, but the underlying symmetry is now triangular. We have reported in Fig. 7(a) the nontrivial ground states for $t = 0$. While the former two are reminiscent of the $1/3$ and $2/3$ “solids” of the triangular-lattice model [34,42], the $N = 12$ state is totally new, and analogous to the ring of Fig. 2(a). Moreover, the $N = 7$ and $N = 12$ ground states are unique, whereas the energy for $N = 10$ is twofold degenerate. For these three phases, the h function reads

$$\begin{aligned} N = 7 : \quad h &= -7\mu, \\ N = 10 : \quad h &= 9V - 10\mu, \\ N = 12 : \quad h &= 18V - 12\mu. \end{aligned} \quad (5)$$

This implies that the transitions between them occur at $\mu = 3V$ and $\mu = (9/2)V$. The full $T = 0$ phase diagram is depicted in Fig. 7(b). Were it not for the “spurious” $N = 12$ phase, this phase diagram would match the infinite-size one almost perfectly. Like for Square and Diamond, also for Star $\rho_c(\mu)$ behaves as expected for a system traversing insulating and superfluid regions [Fig. 7(c)]. The same applies for the energy gap, which at $t = 0.2$ takes larger values in the middle of “insulating” regions [Fig. 7(d)].

Finally, moving to Star with PBC (which, again, can be applied in two equivalent ways; see Fig. 18), we plot in Fig. 8(a) the nontrivial ground states for $t = 0$. The degree

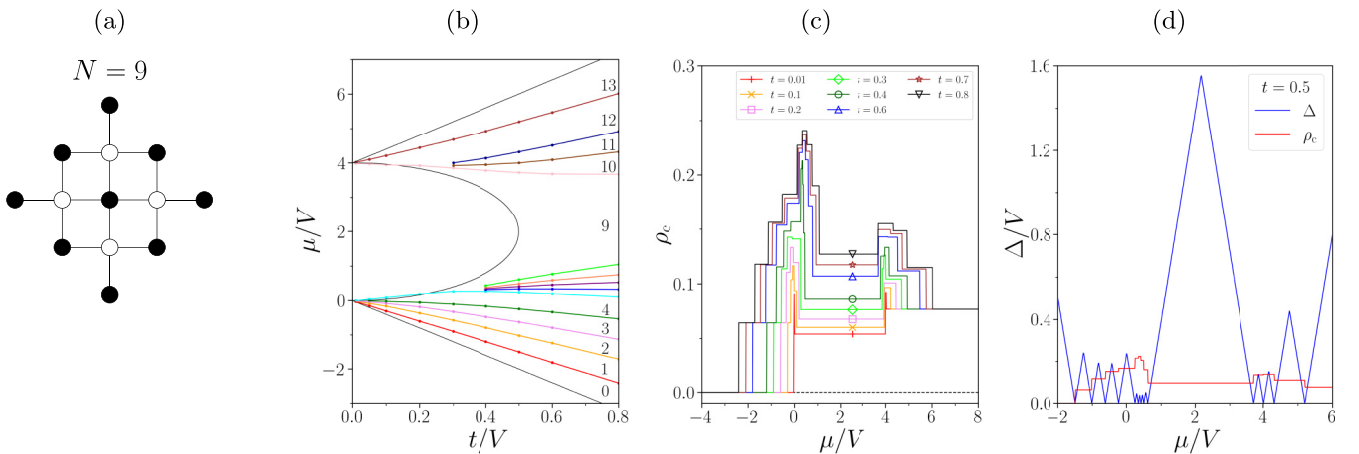


FIG. 5. Diamond. (a) Ground state of the system for $t = 0$ and $0 < \mu < 4V$. (b) Exact phase diagram at $T = 0$. The broken lines through the points are boundary lines of sectors. The black thin lines are mean-field phase boundaries [42]. (c) Condensate fraction $\rho_c(\mu)$ for various t . As t grows, the condensate fraction grows as well. (d) Energy gap $\Delta(\mu)$ for $t = 0.5$ (blue line). Also shown is the condensate fraction for the same t (red line).

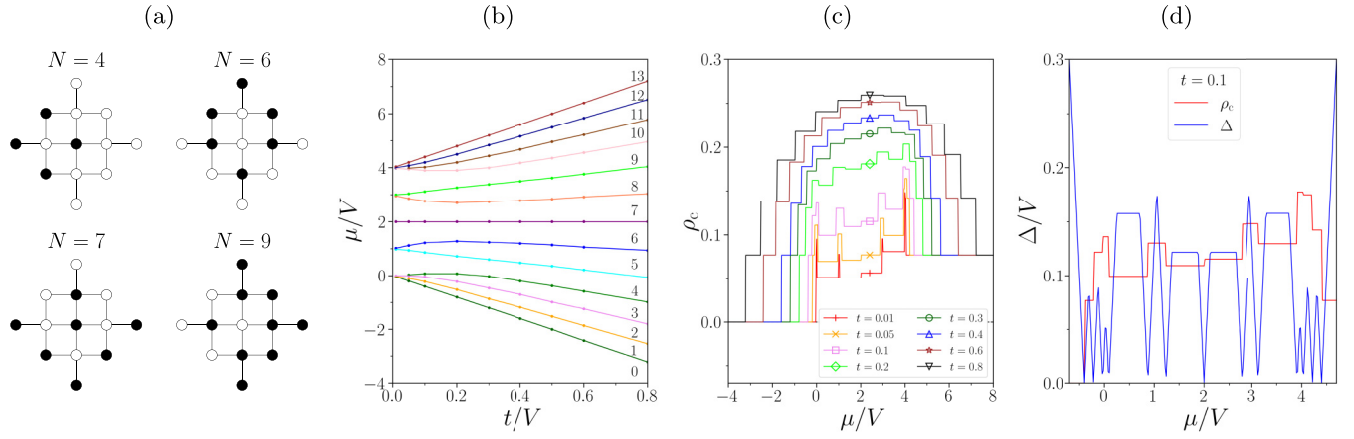


FIG. 6. Diamond with PBC. (a) Ground states of the system for $t = 0$ and $0 < \mu < 4V$. (b) Exact phase diagram at $T = 0$. The broken lines through the points are boundary lines of sectors. (c) Condensate fraction $\rho_c(\mu)$ for various t . As t grows, the condensate fraction grows as well. (d) Energy gap $\Delta(\mu)$ for $t = 0.1$ (blue line). Also shown is the condensate fraction for the same t (red line).

of degeneracy is 26 for the ground-state energy for $N = 3$ and 39 for $N = 4$ and $N = 6$. The other three phases are the negative images of the first three. The phase diagram in Fig. 8(b) is similar to the other two cases with PBC: The insulating regions are rather limited in extent, and the behavior is thus predominantly superfluidlike. Similar to the other grids, none of the ground states in Fig. 7(a) survive periodic replication of the grid; this greatly enhances the stability of the superfluidlike phase, while insulatinglike behavior is confined to $t \lesssim 0.1$.

In closing this section, we discuss how the zero-temperature phase behavior of the extended BH model on a small grid changes when the U parameter in Eq. (1) is finite. For simplicity, only the case of $t = 0$ and $n_{\text{cut}} = 2$ is considered below, which already gives a taste of the much higher complexity of the finite- U case. We report in Fig. 9 the exact ground states at $t = 0$, as functions of U/V and μ/V , for the three grids in Fig. 1 (the hard-core limit is situated on the far right of each panel). Clearly, the phases are now many more, with an intricate interplay between several of them in

the star case. It is Curious how, for very small U/V , singly occupied sites disappear and only double occupancy becomes a possibility. Moreover, the sequence of low- U phases with increasing μ is almost identical to that for $U \rightarrow \infty$, but for the replacement of any $x_i = 1$ with $x_i = 2$.

IV. QUANTUM SIMULATIONS

In this section our aim is to show that the same oddities of the hard-core extended BH model on a small grid are seen in a system of bosonic particles in a convenient external field, designed to mimic the discrete system. For this investigation, we employ the PIMC method [40] in the canonical ensemble, which samples the equilibrium distribution at fixed N and T by leveraging on the isomorphism between quantum particles and imaginary-time paths (worldlines). Furthermore, we use the worm algorithm [44] for an efficient sampling of permutations. This study demonstrates that, under appropriate conditions, even the behavior of a few-body system can be

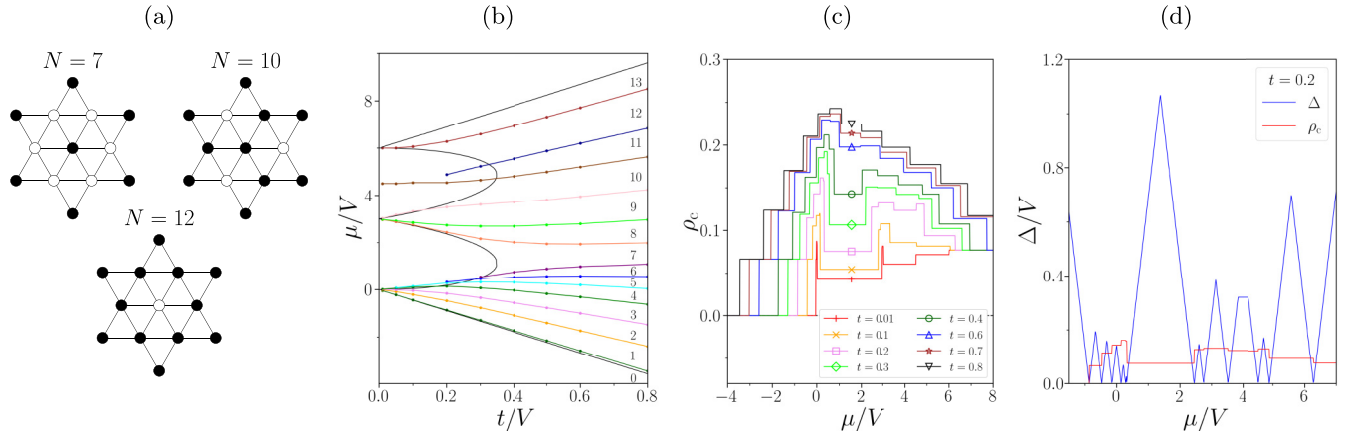


FIG. 7. Star. (a) Ground states of the system for $t = 0$ and $0 < \mu < 6V$ (see text). (b) Exact phase diagram at $T = 0$. The broken lines through the points are boundary lines of sectors. The black thin lines are the transition boundaries according to mean-field theory (see Appendix B). (c) Condensate fraction $\rho_c(\mu)$ for various t . As t grows, the condensate fraction grows as well. (d) Energy gap $\Delta(\mu)$ for $t = 0.2$ (blue line). Also shown is the condensate fraction for the same t (red line).

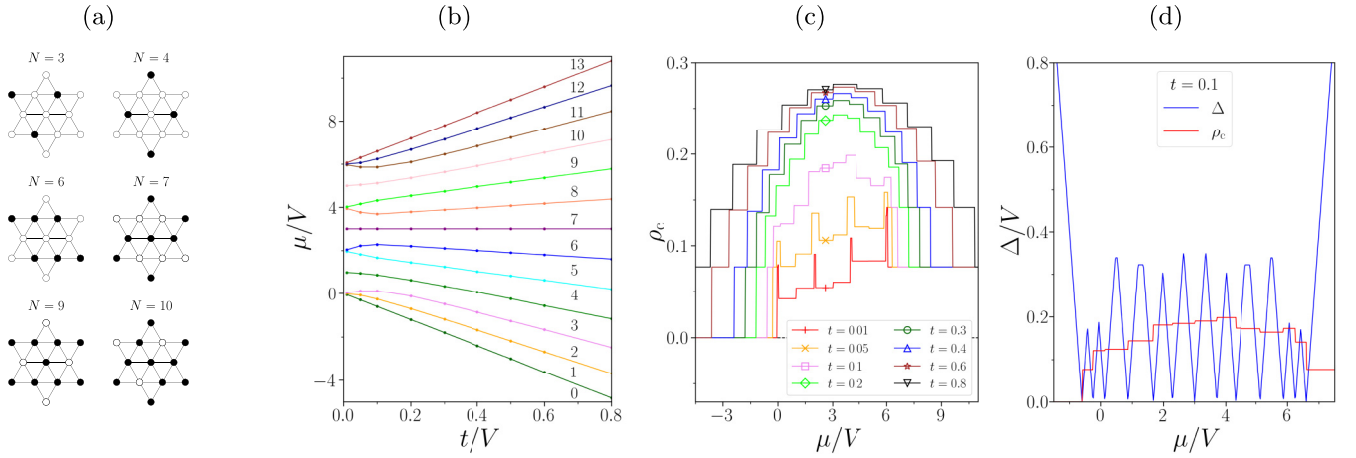


FIG. 8. Star with PBC. (a) Ground states of the system for $t = 0$ and $0 < \mu < 6V$. (b) Exact phase diagram at $T = 0$. The broken lines through the points are boundary lines of sectors. (c) Condensate fraction $\rho_c(\mu)$ for various t . As t grows, the condensate fraction grows as well. (d) Energy gap $\Delta(\mu)$ for $t = 0.1$ (blue line). Also shown is the condensate fraction for the same t (red line).

analyzed in terms of the interplay between superfluidlike and insulatinglike properties.

We investigate a two-dimensional system of spinless bosons with an inverse-power, $\epsilon(\sigma/r)^{12}$ interaction (with $\epsilon = 1$ and $\sigma = 1$). Classical particles interacting with this potential behave similarly to hard disks [45]. The r^{-12} law serves a twofold purpose: First, a potential taking large positive values for distances below ≈ 1 replicates the hard-core condition of the model studied in the previous section. Second, the inverse-power potential features a unit strength at $r \approx 1$, followed by a rapid extinction at larger distances, thereby mimicking a “contact” repulsion between hard-core particles of unit diameter.

To enforce the preference of particle positions for discrete values we use an optical-lattice potential. For square-lattice

order, this is given by

$$u_{\text{opt}}(x, y) = \frac{1}{4}V_0[2 - \cos(2\pi x) - \cos(2\pi y)] \quad (6)$$

with $V_0 > 0$ [notice that the minimum and maximum values of (6) are 0 and V_0 , respectively]. With this potential, x and y coordinates are pushed to take integer values. Finally, in order to confine particles to, e.g., a 3×3 square box centered at the origin, encompassing a total of nine sites, we add the potential

$$u_{\text{box}}(x, y) = \left(\frac{x}{1.5}\right)^{20} + \left(\frac{y}{1.5}\right)^{20}. \quad (7)$$

Under the action of u_{box} , the boson system “acquires” a definite area of 9 (units of σ^2). The combination of (6) and (7) will force particle worldlines to stay close to the sites of a grid

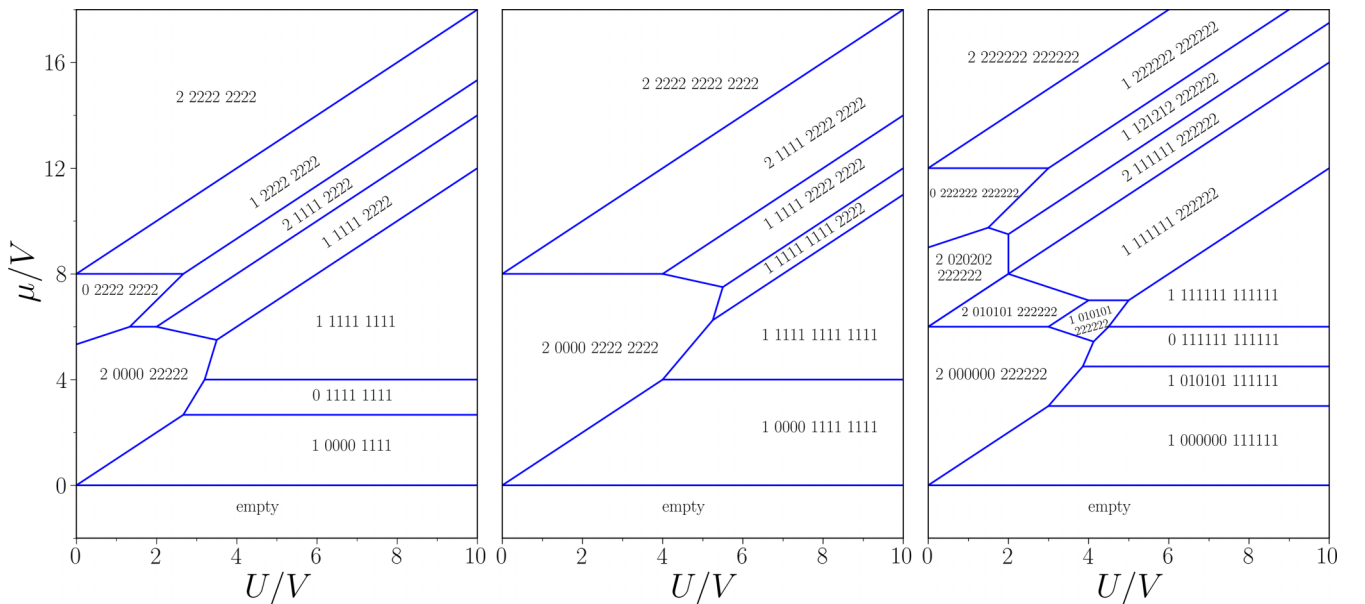


FIG. 9. Exact $t = 0$ ground states for finite U and $n_{\text{cut}} = 2$. Square (left). Diamond (middle). Star (right). Each ground state is labeled by a sequence of numbers, representing the occupancies of the central site, first-neighbor sites, second-neighbor sites, and (where relevant) third-neighbor sites.

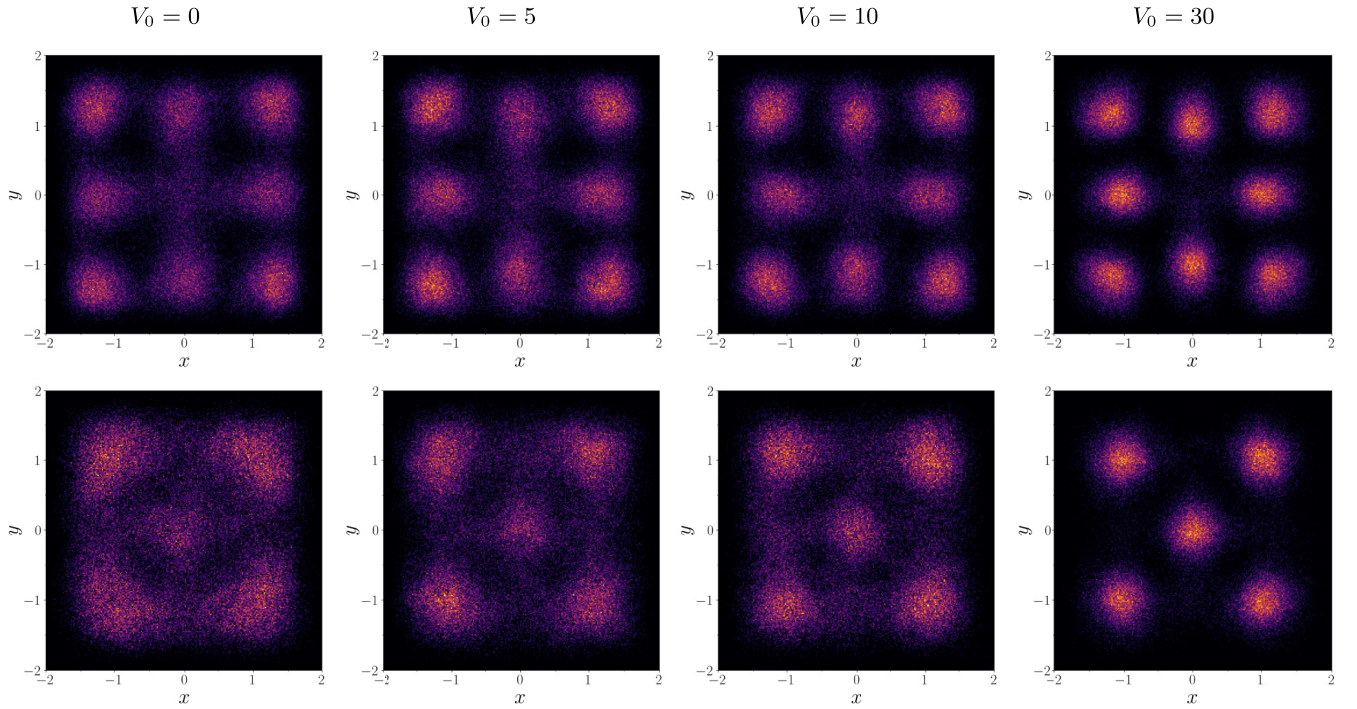


FIG. 10. Density of beads for $N = 8$ (top row) and $N = 5$ (bottom row), for $\lambda = 1$ and several values of V_0 .

identical to Square. Finally, the total Hamiltonian reads

$$H = \sum_{i=1}^N (-\lambda \nabla_i^2 + u_{\text{ext}}(\mathbf{r}_i)) + \sum_{i < j} u_{\text{int}}(|\mathbf{r}_i - \mathbf{r}_j|), \quad (8)$$

where $\lambda = \hbar^2/(2m)$ (m being the particle mass) and

$$u_{\text{int}}(|\mathbf{r} - \mathbf{r}'|) = \frac{1}{|\mathbf{r} - \mathbf{r}'|^{12}}, \quad u_{\text{ext}}(\mathbf{r}) = u_{\text{opt}}(\mathbf{r}) + u_{\text{box}}(\mathbf{r}). \quad (9)$$

In this system, the parameter λ plays a role analogous to t in the BH model: The larger λ , the stronger quantum fluctuations (i.e., the more dispersed are particle worldlines).

For a few selected N , and fixed λ and V_0 , we run our PIMC code for long times, measuring the equilibrium averages of the various terms in the Hamiltonian, the pressure Π , the superfluid fraction f_s , and the distribution $P(L)$ of the length of permutation cycles (with L from 1 to N). In particular, calling A the area of the box and $\mathcal{M} \gg 1$ the number of time slices (beads per particle), Π and f_s are computed as [46,47]

$$\begin{aligned} \Pi = & \frac{N\mathcal{M}}{\beta A} - \left\langle \frac{\mathcal{M}}{4A\lambda\beta^2} \sum_{i=1}^N \sum_{k=1}^{\mathcal{M}} (\mathbf{r}_i^k - \mathbf{r}_i^{k+1})^2 \right. \\ & + \frac{1}{2A\mathcal{M}} \sum_{i < j} \sum_{k=1}^{\mathcal{M}} r_{ij}^k u'_{\text{int}}(r_{ij}^k) \\ & \left. + \frac{1}{2A\mathcal{M}} \sum_{i=1}^N \sum_{k=1}^{\mathcal{M}} \mathbf{r}_i^k \cdot \nabla u_{\text{ext}}(\mathbf{r}_i) \right\rangle \end{aligned} \quad (10)$$

and

$$f_s = \frac{2m}{\lambda\beta} \frac{\langle A_z^2 \rangle - \langle A_z \rangle^2}{I_{\text{cl}}}. \quad (11)$$

In the above formulas, $\mathbf{r}_i^k$ is the vector radius of the k th bead in worldline no. i , $r_{ij}^k = |\mathbf{r}_i^k - \mathbf{r}_j^k|$, I_{cl} is the classical moment of inertia,

$$I_{\text{cl}} = m \sum_{i=1}^N \sum_{k=1}^{\mathcal{M}} (x_i^k x_i^{k+1} + y_i^k y_i^{k+1}), \quad (12)$$

and A_z is the total area enclosed by particle paths,

$$A_z = \frac{1}{2} \sum_{i=1}^N \sum_{k=1}^{\mathcal{M}} (x_i^k y_i^{k+1} - y_i^k x_i^{k+1}). \quad (13)$$

For systems with PBC the formula for f_s is different and uses the winding-number estimator [40]:

$$f_s = \frac{\langle W^2 \rangle}{2\lambda\beta N}. \quad (14)$$

Finally, $P(L)$ is precisely defined as the probability that a particle chosen at random belongs to a cycle of length L : Calling $\mathcal{N}_L(C)$ the number of L cycles in configuration C , with $\sum_L L \mathcal{N}_L(C) = N$, it follows $P(L) = L \langle \mathcal{N}_L(C) \rangle / N$, where $\langle \dots \rangle$ denotes the equilibrium average and $\sum_L P(L) = 1$. A flattened $P(L)$ is suggestive of superfluidlike behavior (see, e.g., Refs. [48–50]). In all our runs, the temperature stays fixed at $T = 0.5$, a low value.

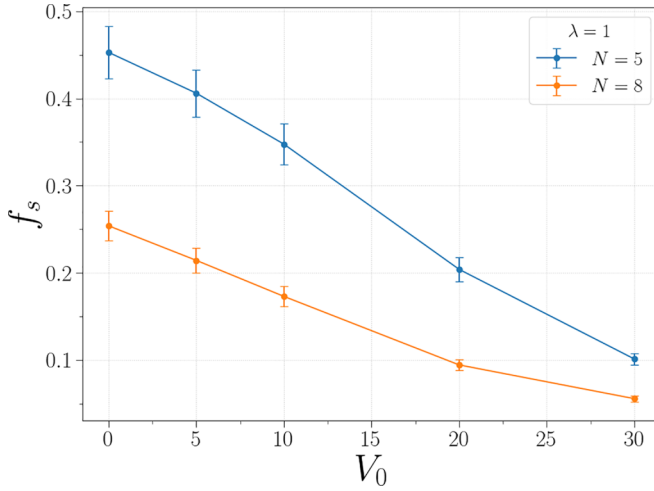


FIG. 11. Superfluid fraction for $N = 5$ and $N = 8$, for $\lambda = 1$ and several values of V_0 .

A. Bosons in a 3×3 box

As a first example, we work in the same setup of Greiner's experiment [5]: Keeping N fixed and assuming a sufficiently large value of λ (i.e., 1), we increase V_0 progressively to see the system transitioning from superfluidlike to insulatinglike conditions. We point out that this is not the manner to look at this transition in the hard-core extended BH model; however, if the initial state is superfluid, enhancing the strength of the confining potential more and more will increasingly suppress the mobility of particles and thus reduce the superfluid fraction. The most interesting cases to probe are $N = 5$ and $N = 8$, corresponding to the states of Fig. 2(a). As is clear from Fig. 2(b), for either N we can make the entire journey from superfluid to insulator while keeping canonical conditions. We produce several hundred million Monte Carlo (MC) moves, using a number of beads per particle up to 1024; equilibrium averages are computed over the second half of the MC trajectory. In Fig. 10 we show the position-dependent density of beads as a function of V_0 . For both values of N , the expected insulating-phase structure eventually emerges, though shadows of it are already apparent for $V_0 = 0$, as an effect of pair repulsion only. However, with the lattice potential switched off, the density of beads is measurably nonzero in the whole box, pointing to a small superfluid response. This is confirmed by the evolution of f_s with V_0 : Starting from a nonzero value at $V_0 = 0$ ($\simeq 0.25$), f_s monotonically decreases with increasing V_0 (see Fig. 11). It must be considered that, for $\lambda = 1$ and $V_0 = 0$, a system of a few interacting bosons in a small box cannot be a full-fledged superfluid (i.e., phase coherent and uniform) and a much larger λ is needed to make the density more uniform in the box. After all, also in the extended BH model on Square the average density at $T = 0$ and, say, $t = 1$ is all but uniform (see Fig. 12), showing inhomogeneities analogous to those exhibited by the small- t system. As for the various energy terms in the Hamiltonian, we find that the averages of kinetic, confinement, and interaction contributions are roughly independent of V_0 , while the optical contribution grows almost linearly with V_0 (figure not shown). Finally, for $N = 8$ the pressure increases almost linearly with V_0 , as

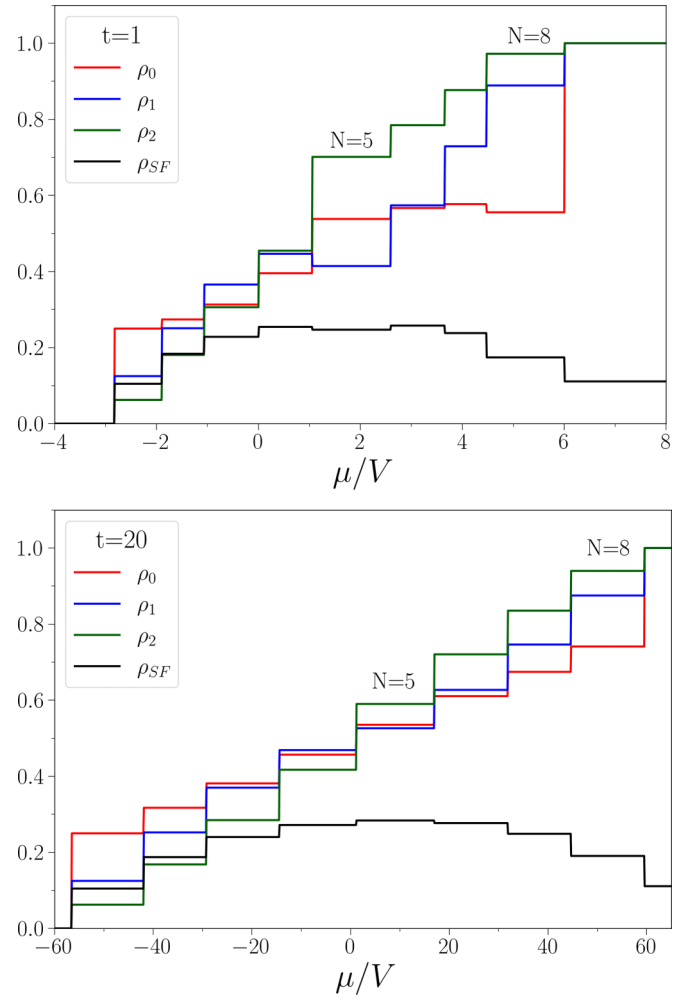


FIG. 12. Hard-core extended BH model on Square. Average site occupancies ρ_n ($n = 0$: central site; $n = 1$: first-neighbor sites; $n = 2$: second-neighbor sites) plotted as functions of μ , for $t = 1$ (top) and $t = 20$ (bottom). Also shown is the condensate fraction ρ_c (black line). Notice the difference in μ scale between the two panels.

expected for a system becoming increasingly more incompressible.

We observe a curious behavior for $N = 8$ and $V_0 = 0$. In Fig. 13 we plot the cycle-length distribution $P(L)$ for varying strength ϵ of the interparticle repulsion (the figure is for $\lambda = 1$, but the evidence is similar for $\lambda = 0.5$ or 0.1). We see that $P(L)$ oscillates, alternating maxima at odd values of L with minima at even values. When ϵ is decreased, the oscillations of $P(L)$ persist but they dampen progressively. An oscillatory $P(L)$ also exists for $V_0 > 0$, but the modulation is less evident. Instead, nothing similar is observed for $N = 5$ or other values of N . We have also verified that $P(L)$ flattens out when we remove the box potential and apply PBC. The non-monotonous decay of $P(L)$ is hard to interpret: Admittedly, it is an exclusive property of the $N = 8$ system ascribable to both interparticle forces and confinement.

Next, we consider the other setup where V_0 is kept fixed at, say, 5, while λ is progressively increased, starting from $\lambda = 0.1$. We expect to see a crossover from insulatinglike to superfluidlike behavior, akin to the transition occurring in the BH model for increasing t at fixed N . As λ grows,

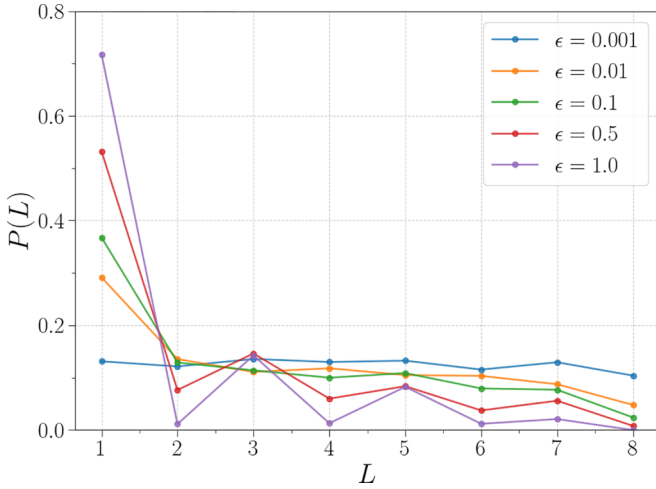


FIG. 13. Distribution $P(L)$ of exchange-cycle lengths for $\lambda = 1$, $N = 8$, and $V_0 = 0$, plotted as a function of ϵ .

we make the number of particle beads accordingly larger, in order to keep sampling efficiency high as the acceptance rate of exchange MC moves decreases. In Fig. 14 we show density maps for $N = 8$. Again, we see a smooth transition from a structure reminiscent of the BH ground state at $t = 0$ to a distribution of beads that is slightly more uniform in the box. In turn, the superfluid fraction grows monotonically from roughly zero at $\lambda = 0.1$ to $\simeq 0.3$ at $\lambda = 2$. Of the various energy contributions, only kinetic energy varies appreciably, growing substantially with increasing λ .

B. The box is removed and PBC are applied

The density of beads should become more uniform when confinement is removed and periodic conditions are applied at the boundary of the 3×3 square, much like the behavior reported in Fig. 3. With $\lambda = 1$, we find similar results for $N = 3$ and $N = 6$. As V_0 grows, we move from a roughly uniform density of beads for $V_0 = 10$ (where $f_s \simeq 1$) to a density function which, unlike the configurations in Fig. 3(a), exhibits pronounced maxima in all potential wells ($f_s \simeq 0.15$ at $V_0 = 100$). This happens because rotational symmetry around the center, which is broken in the $t = 0$ ground state of the BH model, is fully restored when hopping (no matter how small) is allowed.

C. Other box shapes

We have carried out a few simulations also for bosons subject to a confining potential with triangular symmetry (i.e., same as in the star-shaped grid), augmented with a box potential of hexagonal shape:

$$u_{\text{opt}}(x, y) = \frac{2}{9}V_0 \left[3 - \cos\left(2\pi x + \frac{2\pi y}{\sqrt{3}}\right) - \cos\left(\frac{4\pi y}{\sqrt{3}}\right) - \cos\left(2\pi x - \frac{2\pi y}{\sqrt{3}}\right) \right],$$

$$u_{\text{box}}(x, y) = \left(\frac{x}{1.75}\right)^{20} + \left(\frac{x + \sqrt{3}y}{3.5}\right)^{20} + \left(\frac{-x + \sqrt{3}y}{3.5}\right)^{20}. \quad (15)$$

In Fig. 15, top, we plot density maps for $N = 12$ and $\lambda = 1$, as functions of V_0 . Similarly to Fig. 10 we see a smooth transition from a superfluidlike to an insulatinglike structure. Contrary to expectation, $V_0 = 30$ is not large enough to fully recover the structure seen in Fig. 7(a). This happens because the hexagonal box is unfit for totally excluding particles from approaching the 6 minima of the optical-lattice potential at distance two from the center.

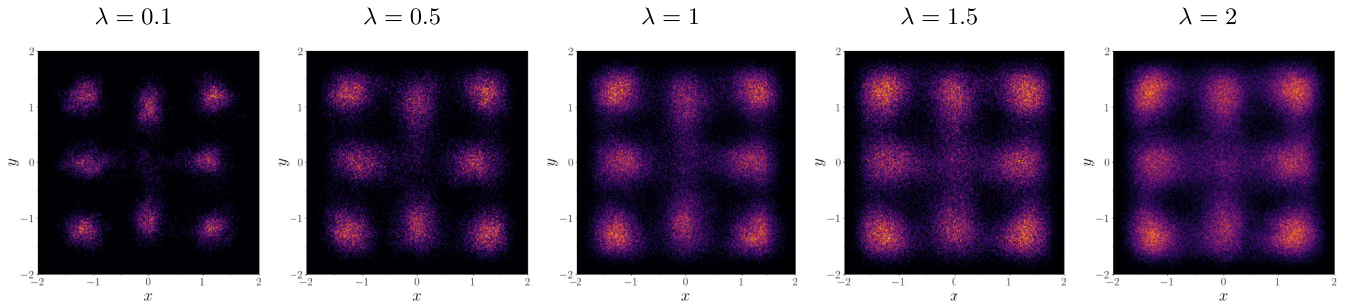
We have also tried to confine bosons in a circular box of radius 1.85, i.e., intermediate between the second-neighbor and the third-neighbor distance on the triangular grid. In Fig. 15, bottom, we report the results for $N = 7$ and $\lambda = 1$. For $V_0 = 0$, the structure is superfluid ($f_s = 0.22$). Upon increasing V_0 , six spots at second-neighbor positions eventually appear, and the superfluid fraction eventually drops to zero ($f_s \simeq 0.04$ at $V_0 = 30$). In this case, no spurious density maxima appear at distance two from the center because, with seven particles only, the interparticle repulsion is fully effective in excluding particles from these sites.

V. CONCLUSIONS

Perfect ordering can only take place in an infinitely large system. In practice, already fairly small systems can anticipate some features of the ordered phase in an elementary form if the temperature is low enough. It is worth studying how this structuring builds up in a finite quantum system. We have chosen the BH model for a demonstration.

The BH model is a popular model of bosonic particles on a lattice, with hopping (αt) and on-site repulsion (αU) terms, describing the competition between tunneling (large t/U) and localization (large U/t) at low temperature. Including in the model a longer-range repulsion (“extended BH model”) is a common strategy to make more varied the crystalline structure of the insulator; in this case, also phases with mixed superfluid-crystalline nature (supersolids) may become stable. Further peculiarities arise from the application of a confining potential (e.g., from putting particles in a trap), which makes the system inhomogeneous and strongly affects the structure of all phases (see, e.g., Refs. [49,51]). A truncated lattice is a limiting case of confinement, corresponding to a trapping potential that blows up upon crossing the edge of the grid.

We have investigated the extended BH model on small two-dimensional grids, using exact diagonalization to reconstruct the zero-temperature phase diagram in the hard-core, $U \rightarrow \infty$ limit. Imposing single site occupancy leads to a drastic simplification, but nevertheless it is a valuable approximation when the chemical potential is not too large. For three different grids, we have traced the boundaries between regions (sectors) comprising ground states with the same number N of bosons. Some of these lines are in clear correspondence with the isodensity lines (and phase boundaries) of the infinite-size system, while others are unexpected and point to the existence of novel finite-size ground states (“phases”) where particles gather on the boundary of the grid. By computing the condensate fraction and the energy gap we can clearly distinguish between superfluidlike and insulatinglike phases. The same exercise has been repeated under PBC, finding that the superfluid region is now more extended.

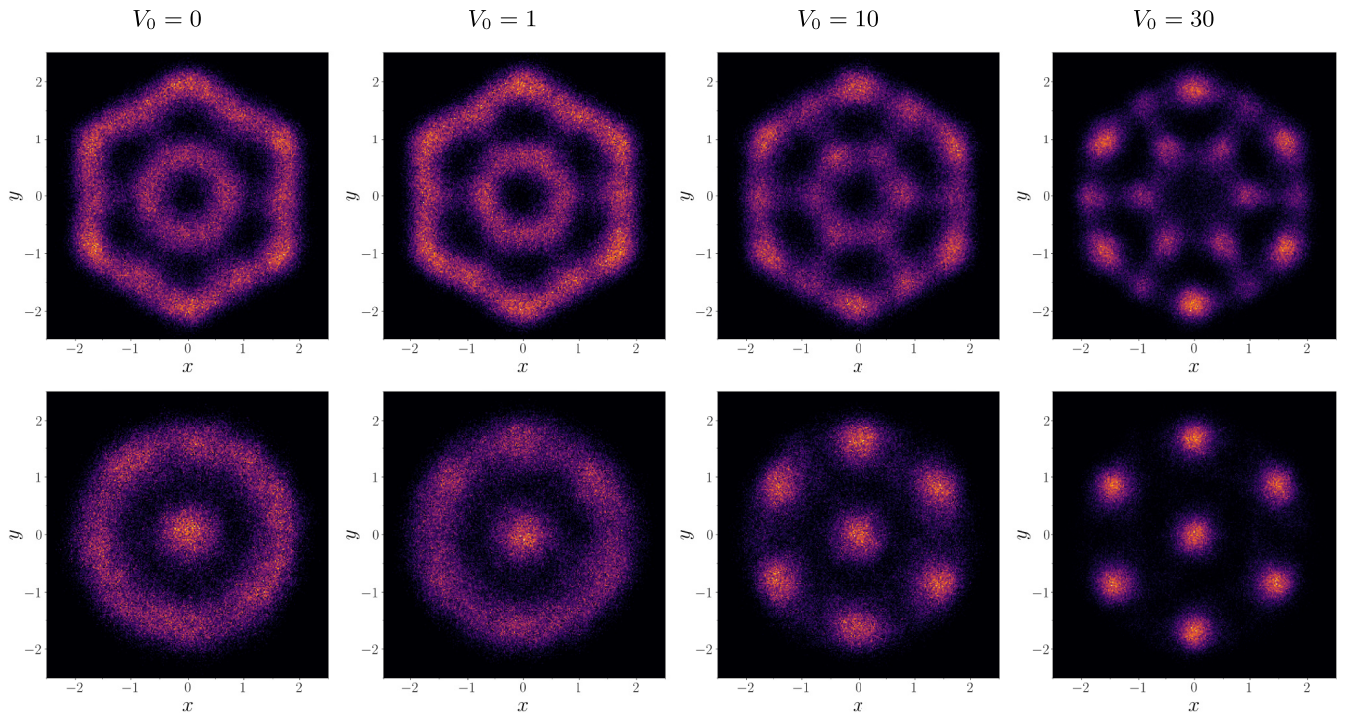
FIG. 14. Density of beads for $N = 8$ and $V_0 = 5$, for several values of λ .

Next, we have tried to reproduce some of the aforementioned unusual features in a few-boson system in continuous space, with the aim of exploring the connections between the low-temperature properties of confined bosonic particles and the physics of BH models. To this purpose, we consider bosons interacting through an inverse-power repulsion and expose them to suitable optical-lattice and box potentials, tailored to the geometry of the grid. Using PIMC simulations, we have recovered the same smooth crossover from superfluid to insulating behavior observed in the extended BH model on a small grid, including the structure of the insulating phase.

Broadening the perspective, our results provide a theoretical benchmark for several emerging experimental platforms. Specifically, the geometries analyzed here, such as the 3×3 tile and the 13-site star, can be faithfully realized using programmable optical tweezer arrays [52,53]. In these setups, the single-site resolution offered by quantum gas microscopy allows for a direct observation of the density profiles and insulatinglike patterns we investigated [54,55]. Furthermore, the

hard-core limit explored in our exact diagonalization study is naturally suited for implementation in superconducting qubit processors [56,57], where the interplay between hopping and interactions mimics the extended BH Hamiltonian.

Finally, our PIMC results in the continuum suggest that signatures of latticelike behavior and superfluidity are robust even in small traps, a finding that could be tested in experiments with few-body systems of dipolar atoms [58] or excitons in semiconductor nanostructures [59,60]. In particular, two examples of systems where the extended BH paradigm is at play, and where our constrained continuous-space simulations can fruitfully complement the experiments, are magnetic atoms confined in an optical lattice [23] and semiconductor excitons on a lattice imprinted by an array of electrodes [24]. In the former case, anisotropic long-range interactions can be distinctly tuned to originate a wealth of stripe-ordered states, both stable and metastable. Other insulating phases, with integer or fractional filling, can be realized with dipolar excitons confined in customizable lattice grids.

FIG. 15. Simulation results for box shapes different from square. Density of beads for $N = 12$ (top row) and $N = 7$ (bottom row), for $\lambda = 1$ and several values of V_0 .

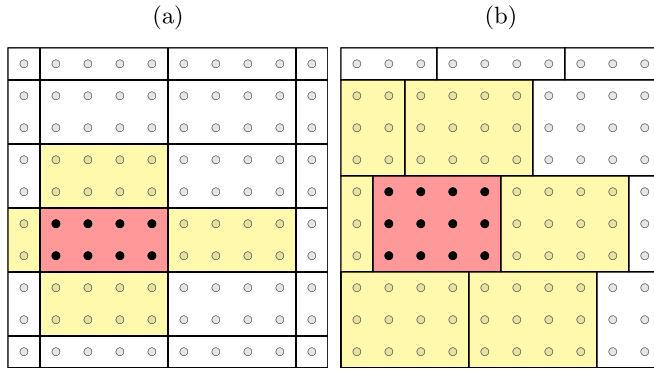


FIG. 16. The rectangular grids analyzed in this paper, drawn together with their periodic images.

In both these experiments, the grid contains 100–200 sites. These numbers of sites are still too large to observe deviations of the BH behavior from the thermodynamic limit. It would be intriguing if the same experiments could be replicated with even smaller grids, as this might reveal finite-size effects similar to those analyzed in the present paper.

By bridging the gap between discrete lattice models and continuous-space simulations [61,62], our study confirms that the fundamental competition between kinetic energy and repulsion, typical of Bose-Hubbard physics, emerges robustly even in systems composed of just a few particles [63,64]. This offers a clear path for the design and calibration of small-scale quantum simulators [65].

ACKNOWLEDGMENTS

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

APPENDIX A: TILING THE LATTICE WITH GRIDS

In this Appendix we report some figures that (to avoid text overloading) could not find a place in Sec. III.

In the two panels of Fig. 16 we show how the 4×2 and 4×3 rectangular grids mentioned in Sec. III A are repeated periodically. In either case, there is no *a priori* exclusion of checkerboard order in the model ground state. We note that on the 4×2 grid each vertical interaction has to be counted twice.

Figures 17 and 18 show how the infinite lattice can be covered with Diamond or Star tiles without overlaps or gaps. This can be done in two distinct ways, illustrated in the panels of each figure. Though different as for the association of

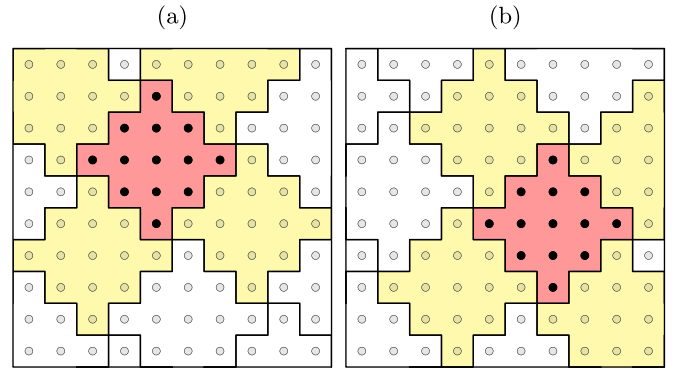


FIG. 17. Diamond and its periodic images, chosen in two different ways. Both choices exclude realizability of checkerboard order.

nearest neighbors to the boundary sites, the two choices are equivalent in terms of energy eigenvalues and eigenstates.

APPENDIX B: MEAN-FIELD PHASE BOUNDARY ON THE TRIANGULAR LATTICE

In this Appendix, the classic mean-field treatment of the ordinary BH model at $T = 0$ [12] is adapted to the extended BH model on the triangular lattice, taking into account the tripartite nature of the lattice. The purpose of this calculation is to obtain approximate boundary lines separating the insulating phases from the superfluid phase in the thermodynamic limit.

Let A, B, and C be the three sublattices. The Hamiltonian of the model reads

$$H = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + H_0 \quad (\text{B1})$$

with

$$\begin{aligned} H_0 = & \frac{U}{2} \sum_{i \in A} n_i(n_i - 1) + \frac{U}{2} \sum_{i \in B} n_i(n_i - 1) \\ & + \frac{U}{2} \sum_{i \in C} n_i(n_i - 1) + \frac{V}{2} \sum_{i \in A} n_i \sum_{j \in \text{NN}_i} n_j \\ & + \frac{V}{2} \sum_{i \in B} n_i \sum_{j \in \text{NN}_i} n_j + \frac{V}{2} \sum_{i \in C} n_i \sum_{j \in \text{NN}_i} n_j \\ & - \mu \sum_{i \in A} n_i - \mu \sum_{i \in B} n_i - \mu \sum_{i \in C} n_i. \end{aligned} \quad (\text{B2})$$

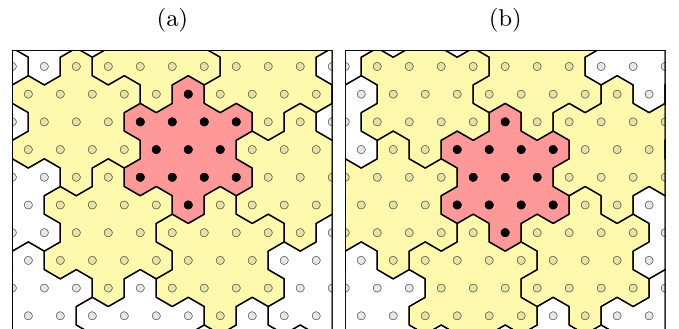


FIG. 18. Star and its periodic images, chosen in two different ways.

In a mean-field type of approach, all sites belonging to the same sublattice are given the same occupancy. This amounts to replacing the original Hamiltonian with an effective three-site Hamiltonian H' , written in terms of sublattice field operators:

$$\begin{aligned} H' &= -\frac{1}{2}t[a_A^\dagger(3a_B + 3a_C) + a_B^\dagger(3a_A + 3a_C) \\ &\quad + a_C^\dagger(3a_A + 3a_B) + \text{H.c.}] + H'_0 \\ &= -3t[a_A^\dagger(a_B + a_C) + a_B^\dagger(a_A + a_C) \\ &\quad + a_C^\dagger(a_A + a_B)] + H'_0, \end{aligned} \quad (\text{B3})$$

where

$$\begin{aligned} H'_0 &= \frac{U}{2}[n_A(n_A - 1) + n_B(n_B - 1) + n_C(n_C - 1)] \\ &\quad + \frac{V}{2}[n_A(3n_B + 3n_C) + n_B(3n_A + 3n_C) \\ &\quad + n_C(3n_A + 3n_B)] - \mu(n_A + n_B + n_C). \end{aligned} \quad (\text{B4})$$

Let $\{|x_A, x_B, x_C\rangle\}$ be the set of Fock states in this representation. These states are eigenstates of H'_0 with eigenvalue

$$\begin{aligned} \epsilon(x_A, x_B, x_C) &= \frac{U}{2}[x_A(x_A - 1) + x_B(x_B - 1) + x_C(x_C - 1)] \\ &\quad + 3V(x_A x_B + x_A x_C + x_B x_C) \\ &\quad - \mu(x_A + x_B + x_C). \end{aligned} \quad (\text{B5})$$

Using the decoupling approximation with $\langle a_\alpha \rangle = \phi_\alpha$ ($\alpha = A, B, C$), the hopping term in (B3) is linearized as

$$\begin{aligned} H'_1 &\equiv 3t(\phi_A^* \phi_B + \phi_B^* \phi_A + \phi_A^* \phi_C + \phi_C^* \phi_A + \phi_B^* \phi_C + \phi_C^* \phi_B) \\ &\quad - 3t[(\phi_B + \phi_C)a_A^\dagger + (\phi_B^* + \phi_C^*)a_A] \\ &\quad - 3t[(\phi_A + \phi_C)a_B^\dagger + (\phi_A^* + \phi_C^*)a_B] \\ &\quad - 3t[(\phi_A + \phi_B)a_C^\dagger + (\phi_A^* + \phi_B^*)a_C]. \end{aligned} \quad (\text{B6})$$

Now, let $|x_{0A}, x_{0B}, x_{0C}\rangle$ be the minimum-energy eigenstate of H'_0 , while H'_1 is treated as a small perturbation. Then, at first order in t the effect of H'_1 is

$$\begin{aligned} \langle x_{0A}, x_{0B}, x_{0C} | H'_1 | x_{0A}, x_{0B}, x_{0C} \rangle \\ = 3t(\phi_A^* \phi_B + \phi_B^* \phi_A + \phi_A^* \phi_C + \phi_C^* \phi_A + \phi_B^* \phi_C + \phi_C^* \phi_B). \end{aligned} \quad (\text{B7})$$

At second order in t , the energy correction due to H'_1 is instead

$$\sum_{(x_A, x_B, x_C) \neq (x_{0A}, x_{0B}, x_{0C})} \frac{|\langle x_{0A}, x_{0B}, x_{0C} | H'_1 | x_A, x_B, x_C \rangle|^2}{\epsilon(x_{0A}, x_{0B}, x_{0C}) - \epsilon(x_A, x_B, x_C)}. \quad (\text{B8})$$

In this sum, the only nonzero terms correspond to

$$\begin{aligned} (x_A, x_B, x_C) &= (x_{0A} \pm 1, x_{0B}, x_{0C}), (x_{0A}, x_{0B} \pm 1, x_{0C}), \\ &\quad (x_{0A}, x_{0B}, x_{0C} \pm 1), \end{aligned} \quad (\text{B9})$$

being, e.g.,

$$\begin{aligned} \langle x_{0A}, x_{0B}, x_{0C} | H'_1 | x_{0A} \pm 1, x_{0B}, x_{0C} \rangle \\ = \begin{cases} -3t(\phi_B^* + \phi_C^*)\sqrt{x_{0A} + 1} \\ -3t(\phi_B + \phi_C)\sqrt{x_{0A}}. \end{cases} \end{aligned} \quad (\text{B10})$$

Moreover,

$$\begin{aligned} \epsilon(x_{0A}, x_{0B}, x_{0C}) - \epsilon(x_{0A} + 1, x_{0B}, x_{0C}) \\ = \mu - Ux_{0A} - 3V(x_{0B} + x_{0C}); \\ \epsilon(x_{0A}, x_{0B}, x_{0C}) - \epsilon(x_{0A} - 1, x_{0B}, x_{0C}) \\ = -\mu + U(x_{0A} - 1) + 3V(x_{0B} + x_{0C}), \end{aligned} \quad (\text{B11})$$

etc. The perturbed energy is then

$$\begin{aligned} E &= \epsilon(x_{0A}, x_{0B}, x_{0C}) + 3t(\phi_A^* \phi_B + \phi_B^* \phi_A + \phi_A^* \phi_C + \phi_C^* \phi_A \\ &\quad + \phi_B^* \phi_C + \phi_C^* \phi_B) + 9t^2|\phi_B + \phi_C|^2[A] \\ &\quad + 9t^2|\phi_A + \phi_C|^2[B] + 9t^2|\phi_A + \phi_B|^2[C] \\ &\equiv \epsilon(x_{0A}, x_{0B}, x_{0C}) + \sum_{\alpha, \beta} \phi_\alpha^* A_{\alpha, \beta} \phi_\beta, \end{aligned} \quad (\text{B12})$$

where $A_{\alpha, \beta}$ is a real symmetric matrix and

$$\begin{aligned} [A] &= -\frac{x_{0A} + 1}{Ux_{0A} + 3V(x_{0B} + x_{0C}) - \mu} \\ &\quad + \frac{x_{0A}}{U(x_{0A} - 1) + 3V(x_{0B} + x_{0C}) - \mu}, \end{aligned} \quad (\text{B13})$$

$$\begin{aligned} [B] &= -\frac{x_{0B} + 1}{Ux_{0B} + 3V(x_{0A} + x_{0C}) - \mu} \\ &\quad + \frac{x_{0B}}{U(x_{0B} - 1) + 3V(x_{0A} + x_{0C}) - \mu}, \end{aligned} \quad (\text{B14})$$

and

$$\begin{aligned} [C] &= -\frac{x_{0C} + 1}{Ux_{0C} + 3V(x_{0A} + x_{0B}) - \mu} \\ &\quad + \frac{x_{0C}}{U(x_{0C} - 1) + 3V(x_{0A} + x_{0B}) - \mu}. \end{aligned} \quad (\text{B15})$$

If the Hermitian form in (B12) is of definite sign, then we are either in an insulating phase ($\phi^* A \phi > 0$ for any $\phi \neq 0$) or in the superfluid phase ($\phi^* A \phi < 0$, signaling an instability towards nonzero ϕ values). Hence, the phase boundary is given by the condition that the form is semidefinite:

$$\begin{vmatrix} 3t([B] + [C]) & 1 + 3t[C] & 1 + 3t[B] \\ 1 + 3t[C] & 3t([A] + [C]) & 1 + 3t[A] \\ 1 + 3t[B] & 1 + 3t[A] & 3t([A] + [B]) \end{vmatrix} = 0. \quad (\text{B16})$$

Equation (B16) defines the locus of (t, μ) points providing the upper limit of stability of the insulating phase for the given x_{0A} , etc. To treat the hard-core case, we took $U = 1000V$.

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