Mean-Field Theory for Extended Bose-Hubbard Model with Hard-Core Bosons

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Abstract. Here we analyze the extended Bose-Hubbard model for hard-core bosons in both a quadratic and a triangular lattice within a mean-field approximation. Especially interesting is the appearance of the supersolid phase for certain parameter values of the triangular lattice. We find analytical results for energies, condensate densities as well as phase boundaries except for the supersolid phase, for which just the density wave to supersolid boundary is derived analytically. The resulting quantum phase diagram for the triangular lattice coincides with a mathematically equivalent fermion model and agrees qualitatively with a recent Monte Carlo simulation.

Keywords: extended Bose-Hubbard model, hard-core bosons, Mott insulator, density wave, superfluid, supersolid

1 Introduction

Ultracold bosons in optical lattices are highly controllable and accurately observable quantum systems, which can be used as ideal quantum simulators to investigate open questions such as about intricate macroscopic quantum phenomena [1]. One prominent example is the elusive phenomenon of supersolidity, which amounts to a spontaneous breaking of both $U(1)$ and translational symmetry. Although initial experiments to observe supersolidity in helium turned out to be unsuccessful [2, 3], it has recently been proposed to realize a supersolid with dipolar bosons in a triangular optical lattice (see, for instance, Ref. [4] and references therein).

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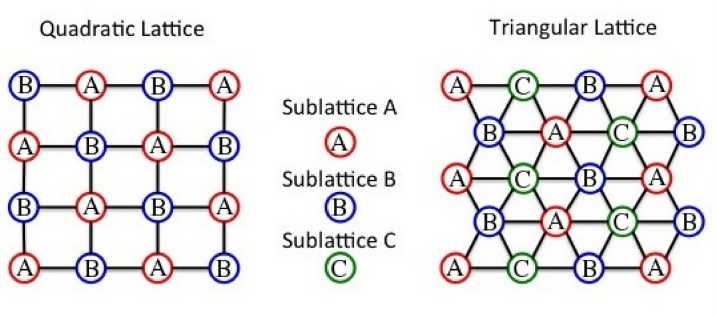


Fig. 1. The checkerboard pattern on the quadratic lattice (*left*) and a pattern with three sites in the unit cell on the triangular lattice (*right*).

Therefore, we analyze in the following a lattice potential close to absolute zero filled with bosons, where the dipoles are either of magnetic atomic or electric molecular origin. We consider hard-core bosons, i.e. bosons with such a strong contact interaction that two or more of them can not be at the same place at the same time. This is experimentally achieved by increasing the scattering length to a high value close to a Feshbach resonance using an external magnetic field [5]. Due to the additional dipolar interaction the interaction between next-neighbor bosons can be attractive or repulsive.

The Hamiltonian for the resulting extended Bose-Hubbard model reads:

$$\hat{H} = -J \sum_{<i,j>} \hat{a}_i^\dagger \hat{a}_j + \frac{V}{2} \sum_{<i,j>} \hat{n}_i \hat{n}_j - \mu \sum_i \hat{n}_i \,, \tag{1}$$

where $\hat{a}_i$ and $\hat{a}_i^\dagger$ are the bosonic annihilation and creation operators, whereas $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ denotes the bosonic number operator on the lattice site i. The symbol $< i, j >$ stands for next-neighbor combinations of sites i and j. The first term in Eq. (1) describes the hopping of bosons from site to site with the hopping energy J, the second describes the next-neighbor interaction with its strength V, and the third describes the dependency on the chemical potential μ within a grand-canonical description.

In this model we determine the ground-state quantum phase diagram by analyzing the mean-field approximation of the Hamiltonian (1) for a periodic distribution of bosons on the lattice like the checkerboard pattern and a pattern with three sites in the unit cell, which are both illustrated in Fig. 1. The quadratic lattice is not frustrated, i.e. the lattice geometry allows a density distribution, in which sites with density 1 have only sites with density 0 as next neighbors and vice versa. In the triangular lattice this is not possible, so it is called frustrated. In the following it will turn out that this frustration seems to be correlated to the appearance of the supersolid phase.

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1.1 Mean-field approximation

It is not possible to determine the eigenvalues of the Hamiltonian in Eq. (1) exactly due to the presence of bilocal operators, i.e. a product of two operators at neighboring lattice sites. Using the mean-field (MF) approximation (see, for instance, Ref. [6]), however, we can rewrite the bilocal operators of the Hamiltonian approximately as

$$\hat{a}_i^\dagger \hat{a}_j \approx \psi_i^* \hat{a}_j + \psi_j \hat{a}_i^\dagger - \psi_i^* \psi_j \tag{2}$$

$$\hat{n}_i \hat{n}_j \approx \varrho_i \hat{n}_j + \varrho_j \hat{n}_i - \varrho_i \varrho_j \ , \tag{3}$$

where $\psi_i := \langle \hat{a}_i \rangle$ denotes the condensate density and $\varrho_i := \langle \hat{n}_i \rangle$ represents the boson density at lattice site i.

With Eqs. (2) and (3) the extended Bose-Hubbard Hamiltonian (1) is approximated according to

$$\hat{H} \overset{\text{MF}}{\approx} \sum_i \hat{h}_{\text{MF},i} \ , \tag{4}$$

where the local Hamiltonian reads

$$\hat{h}_{\text{MF},i} := -J \left(\hat{a}_i \Psi_i^* + \hat{a}_i^\dagger \Psi_i - \psi_i^* \Psi_i \right) + \frac{V}{2} \left(2 \hat{n}_i R_i - \varrho_i R_i \right) - \mu \hat{n}_i \ . \tag{5}$$

Here the mean fields

$$\Psi_i := \sum_{j \in NN_i} \psi_j, \qquad R_i := \sum_{j \in NN_i} \varrho_j \tag{6}$$

represent sums over expectation values on nearest neighboring sites, which have to be determined self-consistently. To this end we consider now periodic patterns in the distribution of ψ_i and ϱ_i over the lattice like the checkerboard pattern for the quadratic lattice or the pattern with three sites in the unit cell for the triangular lattice (see Fig. 1). Such a symmetry reduces the mean-field Hamiltonian for the whole lattice to the following Hamiltonian for one unit cell (UC):

$$\hat{h}_{\text{MF,UC}} = \left(J\Psi - \frac{V}{2} R \right) - J \sum_X \left(\hat{a}_X \Psi_X^* + \hat{a}_X^\dagger \Psi_X \right) + 2 \sum_X \hat{n}_X \left(\frac{V}{2} R_X - \frac{\mu}{2} \right) \tag{7}$$

with the abbreviation

$$\Psi := \sum_X \psi_X^* \Psi_X, \qquad R := \sum_X \varrho_X R_X \ , \tag{8}$$

where the sum has a finite number of summands $X \in \{A, B, \ldots\}$ named by capital letters corresponding to Fig. 1.

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1.2 Finding the ground state

After having calculated the energy eigenvalues E_i of the Hamiltonian (7) for different patterns, we have to describe the ground state at zero temperature for this system. Therefore the values of the mean-field parameters on each sublattice are determined by extremizing the energy eigenvalues:

$$\partial_{\varrho_X} E_i = 0 \quad \forall X\,, \qquad \partial_{\psi_X} E_i = 0 \quad \forall X\,. \tag{9}$$

In principle we have to consider each pattern and find out, which has the lowest ground-state energy. But here we will just discuss the special patterns shown in Fig. 1. An example for a pattern, which we do not describe, is a stripe pattern with $\Psi_A = \Psi_B = 2\psi_A + 2\psi_B$ on the quadratic lattice, which is not a special case of the checkerboard. Its energies can be calculated, but it turns out not to appear in the ground state.

1.3 Possible phases

The simplest non-superfluid phase, which occurs, is the Mott insulator (MI). All bosons are localized at lattice sites, i.e. the condensate density vanishes at all sites according to $\psi_X = \psi_Y = 0 \quad \forall X, Y$, and all are distributed homogeneously, thus $\varrho_X = \varrho_Y \quad \forall X, Y$. There are just two cases for hard-core bosons - the empty lattice with $\varrho_X = \varrho_Y = 0 \quad \forall X, Y$ and the full lattice with $\varrho_X = \varrho_Y = 1 \quad \forall X, Y$. In the second non-superfluid class of phases - the density wave phase (DW) - all bosons are localized, too, but the density distribution is not homogeneous, i.e. $\exists X, Y \quad \varrho_X \neq \varrho_Y$.

For non-vanishing condensate densities two classes of phases are defined. When the density distribution is homogeneous, i.e. $\varrho_X = \varrho_Y \quad \forall X, Y$, but the bosons are not localized, i.e. $\psi_X = \psi_Y \neq 0 \quad \forall X, Y$, then the phase is called superfluid (SF). The remaining possible phases are called supersolid (SS), i.e. the density distribution is not homogeneous, thus $\exists X, Y \quad \varrho_X \neq \varrho_Y$ and at least two condensate densities are unequal, so $\exists X, Y \quad \psi_X \neq \psi_Y$.

2 Quadratic lattice

The checkerboard pattern is described by the two sites A, B in the unit cell. To find the Hamiltonian for this pattern, we have to express Ψ_A, Ψ_B, R_A, and R_B in terms of ψ_A, ψ_B, ϱ_A, and ϱ_B according to Eq. (6), which is $\Psi_A = 4\psi_B$, $\Psi_B = 4\psi_A$, $R_A = 4\varrho_B$ and $R_B = 4\varrho_A$, since the next neighbors of every site are always four of the other kind (see Fig. 1).

We can now write the Hamiltonian in the two-site basis

$$\mathcal{B} = \{|0,0\rangle\,, |1,0\rangle\,, |0,1\rangle\,, |1,1\rangle\}\ , \tag{10}$$

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where $|n_A, n_B\rangle$ denotes the state of the unit cell with n_X bosons on site X. Thus the Hamiltonian becomes

$$\left(\hat{h}_{\mathrm{MF,UC}}\right)_{\mathcal{B}} = \\ = \begin{pmatrix} E_0 & -4J\psi_A^* & -4J\psi_B^* & 0 \\ -4J\psi_A & E_0 + 4V\varrho_A - \mu & 0 & -4J\psi_B^* \\ -4J\psi_B & 0 & E_0 + 4V\varrho_B - \mu & -4J\psi_A^* \\ 0 & -4J\psi_B & -4J\psi_A & E_0 + 4V\left(\varrho_A + \varrho_B\right) - 2\mu \end{pmatrix} \quad (11)$$

with the abbreviation $E_0 := J\Psi - VR/2 = 4J\left(\psi_A^*\psi_B + \psi_B^*\psi_A\right) - 4V\varrho_A\varrho_B$.

Determining the mean-field parameters via (9) leads to simple solutions for $\psi_A = \psi_B = 0$, which are the non-superfluid phases - Mott insulator (MI) and density wave (DW):

ϱ_A	ϱ_B	$\psi_A = \psi_B$	$\frac{E}{V}$	domain of J, μ	phase
0		0	0	$\mathbb{R}$	MI
0	1		$-\frac{\mu}{V}$		DW
1	0				
1			$4 - 2\frac{\mu}{V}$		MI

So in the density wave phase we find a checkerboard density distribution with zero or one boson localized at the respective lattice sites.

For the superfluid phase, i.e. $\psi_X = \psi_Y \neq 0 \quad \forall X, Y$, the Hamiltonian is not diagonal, but the energy eigenvalues and the mean-field parameters can be calculated analytically:

$\varrho_A = \varrho_B$	$\psi_A = \psi_B$	$\frac{E}{V}$	domain of J, μ	phase
$\frac{\frac{\mu}{V}+4\frac{J}{V}}{4+8\frac{J}{V}}$	$\frac{\sqrt{\frac{\mu}{V}+4\frac{J}{V}}\sqrt{4+4\frac{J}{V}-\frac{\mu}{V}}}{\left\lvert 4+8\frac{J}{V}\right\rvert}$	$-\frac{\left(\frac{\mu}{V}+4\frac{J}{V}\right)^2}{4+8\frac{J}{V}}$	$0 \leq \frac{\mu}{V} + 4\frac{J}{V}$ $0 \leq 4 + 4\frac{J}{V} - \frac{\mu}{V}$	SF

We find conditions here, under which these formulas are valid, because outside of the domain for J and μ (see previous table) the density $\varrho_A = \varrho_B$ could not be between 0 and 1, which is a necessary condition for hard-core bosons. Note that the self-consistency equations (9) turn out to not allow a supersolid phase in the quadratic lattice.

Since we know now the energies of all phases, we can calculate, which energy becomes the smallest one for certain parameter values J and μ, yielding the quantum phase diagram shown in Fig. 2. The phase boundaries can be expressed analytically in the following way:

DW-MI	$\frac{\mu}{V} = -4\frac{J}{V}$	second-order transition
DW-MI	$\frac{\mu}{V} = 4\frac{J}{V} + 4$	second-order transition
DW-SF	$2 < \frac{\mu}{V}: \quad \frac{\mu}{V} = 2 + 2\sqrt{1 - 4\left(\frac{J}{V}\right)^2}$ $\frac{\mu}{V} < 2: \quad \frac{\mu}{V} = 2 - 2\sqrt{1 - 4\left(\frac{J}{V}\right)^2}$	first-order transition

The order of the phase transitions describes, whether the order parameters ψ and ϱ change continuously or discontinuously with J and μ (see Fig. 3).

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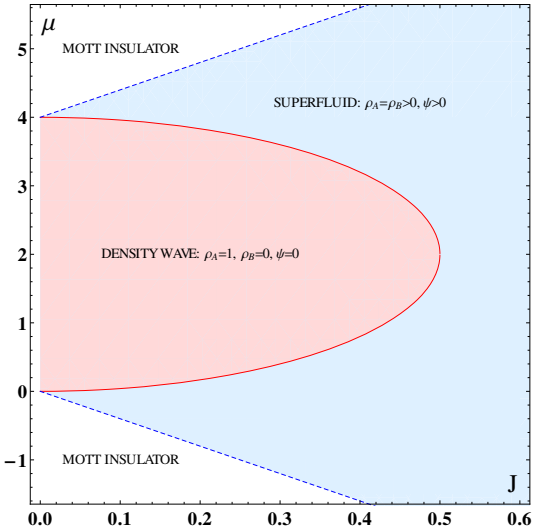


Fig. 2. Phase diagram of the quadratic lattice with continuous (*dashed*) and discontinuous (*solid*) phase transitions (J and μ in units of V).

3 Triangular lattice

The considered pattern from Fig. 1 for the triangular lattice of three sites A, B, C in the unit cell yields according to Eq. (6) the mean fields $\Psi_A = 3\psi_B + 3\psi_C$, $\Psi_B = 3\psi_A + 3\psi_C$, $\Psi_C = 3\psi_A + 3\psi_B$, $R_A = 3\varrho_B + 3\varrho_C$, $R_B = 3\varrho_A + 3\varrho_C$ and $R_C = 3\varrho_A + 3\varrho_B$. The Hamiltonian for one unit cell turns out to be a 8×8-matrix, which we omit here for the sake of simplicity. Analyzing the corresponding self-consistency equations (9), we find the non-superfluid states, i.e. $\psi_X = \psi_Y = 0 \quad \forall X, Y$, which are the empty lattice (MI), the full lattice (MI) and, additionally, two density wave phases with average densities of $1/3$ and $2/3$ and degenerated energies:

ϱ_A	ϱ_B	ϱ_C	$\psi_A = \psi_B = \psi_C$	$\frac{E}{V}$	domain of J, μ	phases
0			0	0	$\mathbb{R}$	MI
0	0	1		$-\frac{\mu}{V}$		DW
0	1	0				
1	0	0				
1	1	0		$3 - 2\frac{\mu}{V}$		
1	0	1				
0	1	1				
1				$9 - 3\frac{\mu}{V}$		MI

The superfluid phase with $\psi_X = \psi_Y \neq 0 \quad \forall X, Y$ is here quite similar to the quadratic lattice, just a few constants have changed, and again, we find certain conditions for the domain of J and μ:

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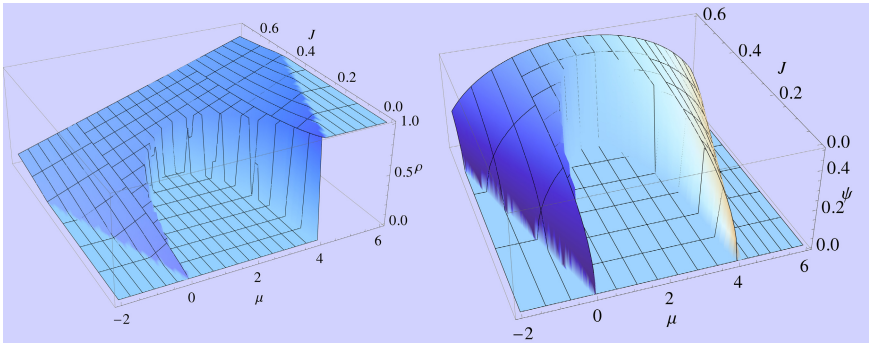


Fig. 3. Order parameters ϱ (*left*) and ψ (*right*) over J and μ. In the density wave region ϱ is chosen to be zero. In the other regions we have $\varrho_A = \varrho_B = \varrho$ (J and μ in units of V).

$\varrho_A = \varrho_B = \varrho_C$	$\psi_A = \psi_B = \psi_C$	$\frac{E}{V}$	domain of J, μ	phases
$\frac{\frac{\mu}{V}+6\frac{J}{V}}{6+12\frac{J}{V}}$	$\frac{\sqrt{\frac{\mu}{V}+6\frac{J}{V}}\sqrt{6+6\frac{J}{V}-\frac{\mu}{V}}}{\left\vert 6+12\frac{J}{V}\right\vert}$	$-\frac{\left(6\frac{J}{V}+\frac{\mu}{V}\right)^2}{4+8\frac{J}{V}}$	$0 \leq \frac{\mu}{V}+6\frac{J}{V}$ $0 \leq 6+6\frac{J}{V}-\frac{\mu}{V}$	SF

For the supersolid case with $0 \neq \psi_A = \psi_B \neq \psi_C \neq 0$ we can still diagonalize the Hamiltonian and find a universal minimal energy E_{SS}, which turns out to be too complicated for an exact extremalization.

Finding the phase transitions is simple for the SF-DW and SF-MI transition using the above mentioned analytical expressions for the energies. The DW-SS transition is of second order, so we can insert the DW-parameters into the extremalization equation $\partial E_{\mathrm{SS}}/\partial\psi_A = 0$ to find it. The resulting phase boundary makes the density wave region asymmetric (see Fig. 4). For the SS-SF transition we can not use this method, because this transition is of first order and the analytic expression for the energy of the supersolid is unknown, thus no analytical curve has been found. However, a numeric simulation shows, that this curve is simply a straight line. That fits to the results found in Ref. [7] for a mathematically equivalent fermion model.

Furthermore we compare in Fig. 4 the mean-field results with the recent Monte Carlo simulations of Ref. [4], where the J-axis is dilated by a factor of 2. The comparison shows, that quantum fluctuations cause the superfluid to shrink or, equivalently, the density waves to grow and the SS-SF transition is no longer a straight line in the Monte Carlo simulation. Thus, we conclude, that the mean-field approximation produces qualitatively correct results, but quantitatively it is not that accurate. The mean-field approximation could, in principle, be improved by interpreting the mean fields as variational parameters and by taking into account quantum fluctuations systematically as has been shown for the Bose-Hubbard model in Ref. [8].

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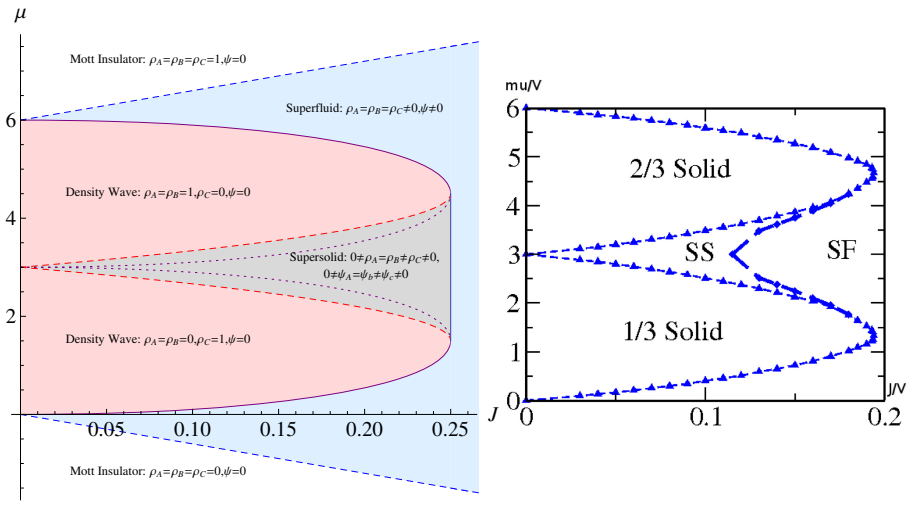


Fig. 4. *left*: Mean-field phase diagram of the triangular lattice with continuous (*dashed*) and discontinuous (*solid*) phase transitions. The *dotted* lines in comparison with the DW-SS transition illustrate the asymmetry of the DW region (J and μ in units of V). *right*: Exact phase diagram found using Monte Carlo methods [4]. Note that the J-axis is dilated by a factor of 2 in comparison with the mean-field results on the *left*.

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