Mean-Field theory for the Extended Bose-Hubbard Model

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Introduction

We use mean-field theory on a quadratic and a triangular optical lattice to solve the Extended Bose-Hubbard model, of which the Hamiltonian is given by:

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

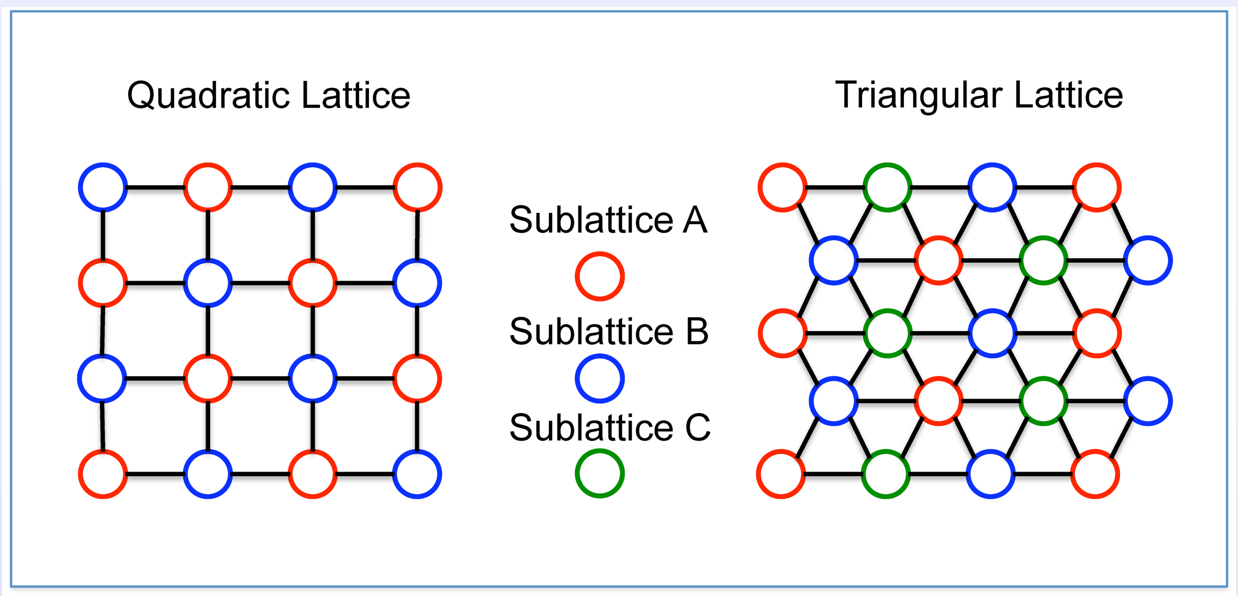
where $\hat{a}_i$ and $\hat{a}_i^\dagger$ are the bosonic annihilation and creation operators at site i, and $\hat{n}_i = \hat{a}_i^\dagger\hat{a}_i$. We consider the case of hard-core repulsion, where each site can only be occupied by at most 1 boson. For the triangular case our results show a supersolid phase and our general phase diagram is in qualitative agreement with recent Monte-Carlo simulation.

Derivation of the Mean-Field Hamiltonian on Sublattices

We first apply the mean-field theory approximation:

$$\hat{a}_i^\dagger\hat{a}_j = \langle\hat{a}_i^\dagger\rangle\hat{a}_j + \hat{a}_i^\dagger\langle\hat{a}_j\rangle - \langle\hat{a}_i^\dagger\rangle\langle\hat{a}_j\rangle$$
$$\hat{n}_i\hat{n}_j = \langle\hat{n}_i\rangle\hat{n}_j + \hat{n}_i\langle\hat{n}_j\rangle - \langle\hat{n}_i\rangle\langle\hat{n}_j\rangle$$

Next we divide the lattice into sublattices such that no two members of a sublattice are nearest neighbors.



We now specialize to the quadratic case, while the triangular case is derived similarly. Decomposing the Hamiltonian for each sublattice:

$$\hat{H} \simeq \hat{H}_{\mathrm{MF}} = \sum_{i_A}\Big[-4J\left(\psi_B(\hat{a}_{i_A}+\hat{a}_{i_A}^\dagger)-\psi_A\psi_B\right)-\mu\hat{n}_{i_A}+2V(2\rho_B\hat{n}_{i_A}-\rho_A\rho_B)\Big]$$
$$+\sum_{i_B}\Big[-4J\left(\psi_A(\hat{a}_{i_B}+\hat{a}_{i_B}^\dagger)-\psi_A\psi_B\right)-\mu\hat{n}_{i_B}+2V(2\rho_A\hat{n}_{i_B}-\rho_A\rho_B)\Big]$$

where $\langle\hat{a}_i\rangle = \langle\hat{a}_i^\dagger\rangle = \psi_A$, if $i \in A$ $\quad\langle\hat{a}_i\rangle = \langle\hat{a}_i^\dagger\rangle = \psi_B$, if $i \in B$

$\langle\hat{n}_i\rangle = \rho_A$, if $i \in A$ $\quad\langle\hat{n}_i\rangle = \rho_B$, if $i \in B$

Since both parts of the Hamiltonian are local and the lattices are homogenous, we can consider a simpler two-site system corresponding to two adjacent sites each pertaining to a different sublattice [1]:

$$\hat{h}_{\mathrm{MF}} = -4J\left[\psi_B(\hat{a}_A+\hat{a}_A^\dagger)+\psi_A(\hat{a}_B+\hat{a}_B^\dagger)\right]+\hat{n}_A(-\mu+4V\rho_B)$$
$$+\hat{n}_B(-\mu+4V\rho_A)+8J\psi_A\psi_B-4V\rho_A\rho_B$$

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References

[1] J. Links *et al.*, Ann. Henri Poinc. **7**, 1591 (2006)

[2] X.-F. Zhang *et al.*, Phys. Rev. B **84**, 174515 (2011)

Quadratic Lattice

- **In the two-site basis, the matrix form of the Hamiltonian is:**

$$\begin{pmatrix} E_0 & -4J\psi_B & -4J\psi_A & 0 \\ -4J\psi_B & E_0-\mu+4\rho_B & 0 & -4J\psi_A \\ -4J\psi_A & 0 & E_0-\mu+4\rho_A & -4J\psi_B \\ 0 & -4J\psi_A & -4J\psi_B & E_0-2\mu+4(\rho_A+\rho_B) \end{pmatrix}$$

with $E_0 = 4J(\psi_B\psi_A+\psi_A\psi_B)-4\rho_A\rho_B$ and $V=1$

- **Mott Insulator (MI) and Density Wave (DW) Phases: $\psi = 0$**

$\psi_A = \psi_B = 0$, which makes the Hamiltonian diagonal. For these phases:

Energy	Densities	Region of minimality	Phase
0	$\rho_A = 0\ \rho_B = 0$	$\mu < 0$	Lower Mott Insulator (MI)
$-\mu$	$\rho_A = 0\ \rho_B = 1$	$0 < \mu < 4$	Density Wave (DW)
$-\mu$	$\rho_A = 1\ \rho_B = 0$	$0 < \mu < 4$	Density Wave (DW)
$-2\mu+4$	$\rho_A = 1\ \rho_B = 1$	$4 < \mu$	Upper Mott Insulator (MI)

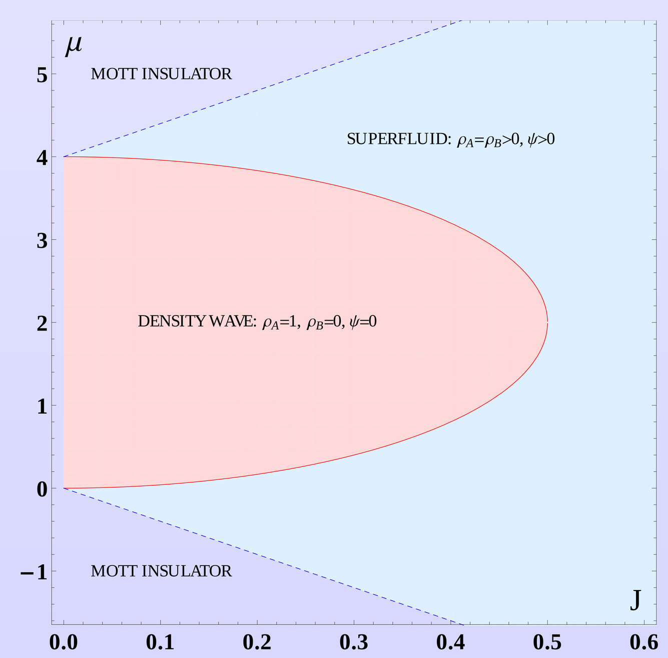
- **Superfluid (SF) Phase: $\psi \neq 0$**

$\psi_A = \psi_B \neq 0$ and $\rho_A = \rho_B \neq 0$, thus Hamiltonian no longer diagonal, but can still be exactly diagonalized. Unlike $\psi = 0$ case, for all regions there is only one minimal eigenvalue, which can be exactly extremized:

$$\psi_{\mathrm{SF}} = \frac{\sqrt{4J-\mu+4}\sqrt{4J+\mu}}{4(2J+1)},\qquad \rho_{\mathrm{SF}} = \frac{4J+\mu}{4+8J},\qquad E_{\mathrm{SF}} = -\frac{(4J+\mu)^2}{8J+4}$$

- **Phase Transitions:**

For Superfluid-Density Wave (SF-DW) and Superfluid-Mott Insulator (SF-MI) phase transition curves, we simply equate the exact energies and solve for μ in terms of J:



Dashed → Continuous, Solid → Discontinuous

Upper Mott phase → Superfluid:

$$\mu = 4(J+1)$$

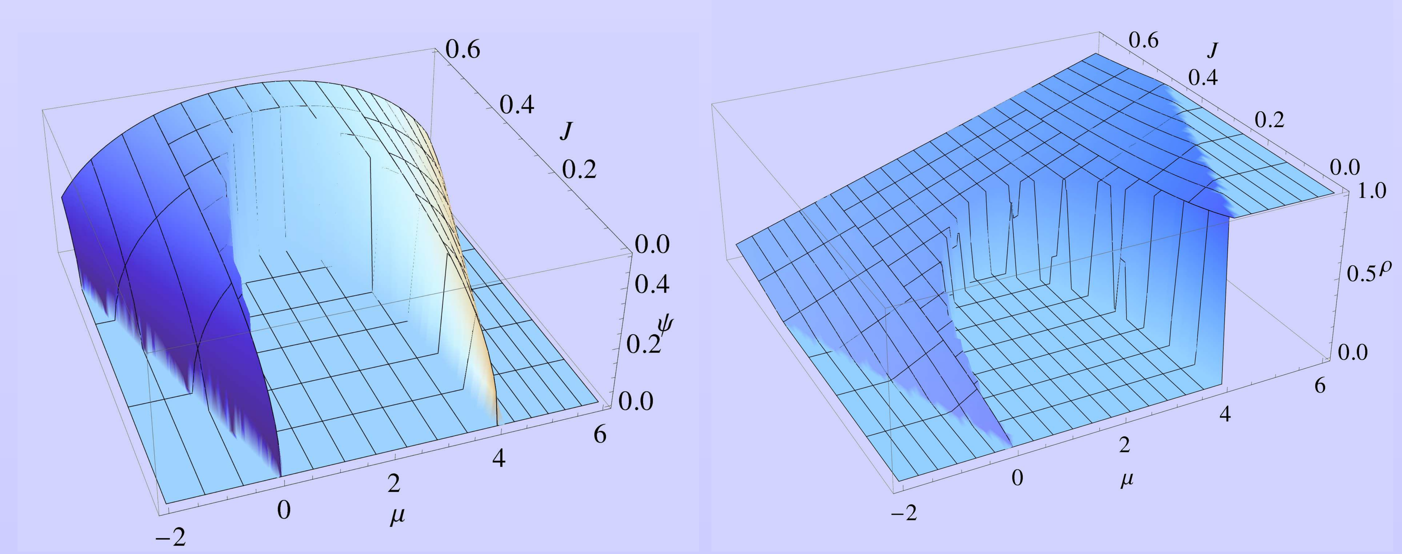
Lower Mott phase → Superfluid:

$$\mu = -4J$$

Density Wave phase → Superfluid:

$$\mu > 2:\quad \mu = 2+2\sqrt{1-4J^2}$$
$$\mu < 2:\quad \mu = 2-2\sqrt{1-4J^2}$$

- **Values of the order parameters: ψ and ρ**



Triangular Lattice

- **In the three-site basis, the matrix form of the Hamiltonian is:**

$$\begin{pmatrix}
E_0 & -3J(\psi_B+\psi_C) & -3J(\psi_A+\psi_C) & -3J(\psi_A+\psi_B) & 0 & 0 & 0 & 0 \\
-3J(\psi_B+\psi_C) & \substack{3(\rho_C+\rho_B)\\+E_0-\mu} & 0 & 0 & -3J(\psi_A+\psi_C) & -3J(\psi_A+\psi_B) & 0 & 0 \\
-3J(\psi_A+\psi_C) & 0 & \substack{3(\rho_A+\rho_C)\\+E_0-\mu} & 0 & -3J(\psi_B+\psi_C) & 0 & -3J(\psi_A+\psi_B) & 0 \\
-3J(\psi_A+\psi_B) & 0 & 0 & \substack{3(\rho_A+\rho_B)\\+E_0-\mu} & 0 & -3J(\psi_B+\psi_C) & -3J(\psi_A+\psi_C) & 0 \\
0 & -3J(\psi_A+\psi_C) & -3J(\psi_B+\psi_C) & 0 & \substack{3(\rho_A+\rho_B+2\rho_C)\\+E_0-2\mu} & 0 & 0 & -3J(\psi_A+\psi_b) \\
0 & -3J(\psi_A+\psi_B) & 0 & -3J(\psi_B+\psi_C) & 0 & \substack{3(\rho_A+2\rho_B+\rho_C)\\+E_0-2\mu} & 0 & -3J(\psi_A+\psi_c) \\
0 & 0 & -3J(\psi_A+\psi_B) & -3J(\psi_A+\psi_C) & 0 & 0 & \substack{3(2\rho_A+\rho_B+\rho_C)\\+E_0-2\mu} & -3J(\psi_B+\psi_c) \\
0 & 0 & 0 & 0 & -3J(\psi_A+\psi_B) & -3J(\psi_A+\psi_C) & -3J(\psi_B+\psi_C) & \substack{6(\rho_A+\rho_B+\rho_C)\\+E_0-3\mu}
\end{pmatrix}$$

with $E_0 = 6J(\psi_A\psi_B+\psi_A\psi_C+\psi_B\psi_C)-3(\rho_A\rho_B+\rho_A\rho_C+\rho_B\rho_C)$ and $V=1$

- **Mott Insulator and Density Wave Phases: $\psi = 0$**

$\psi_A = \psi_B = \psi_C = 0$, which makes the Hamiltonian diagonal. For these phases:

Energy	Minimal ρ	Region of Minimality	Phase
0	$\rho_A = \rho_B = \rho_C = 0$	$\mu < 0$	Lower MI
$-\mu$	$\rho_A = 1, \rho_B = \rho_C = 0$	$0 < \mu < 3$	Lower DW
$-\mu$	$\rho_A = \rho_B = 1, \rho_C = 0$	$0 < \mu < 3$	Lower DW
$-\mu$	$\rho_A = \rho_B = 0, \rho_C = 1$	$0 < \mu < 3$	Lower DW
$-2\mu+3$	$\rho_A = \rho_B = 1, \rho_C = 0$	$3 < \mu < 6$	Upper DW
$-2\mu+3$	$\rho_A = 0, \rho_B = \rho_C = 1$	$3 < \mu < 6$	Upper DW
$-2\mu+3$	$\rho_B = 0, \rho_A = \rho_C = 1$	$3 < \mu < 6$	Upper DW
$-3\mu+9$	$\rho_A = \rho_B = \rho_C = 1$	$6 < \mu$	Upper MI

- **Superfluid Phase: $\psi \neq 0$**

$\psi_A = \psi_B = \psi_C \neq 0$ and $\rho_A = \rho_B = \rho_C \neq 0$, thus Hamiltonian no longer diagonal, but can still be exactly diagonalized. Unlike $\psi = 0$ case, for all regions there is only one minimal eigenvalue, which can be exactly extremized:

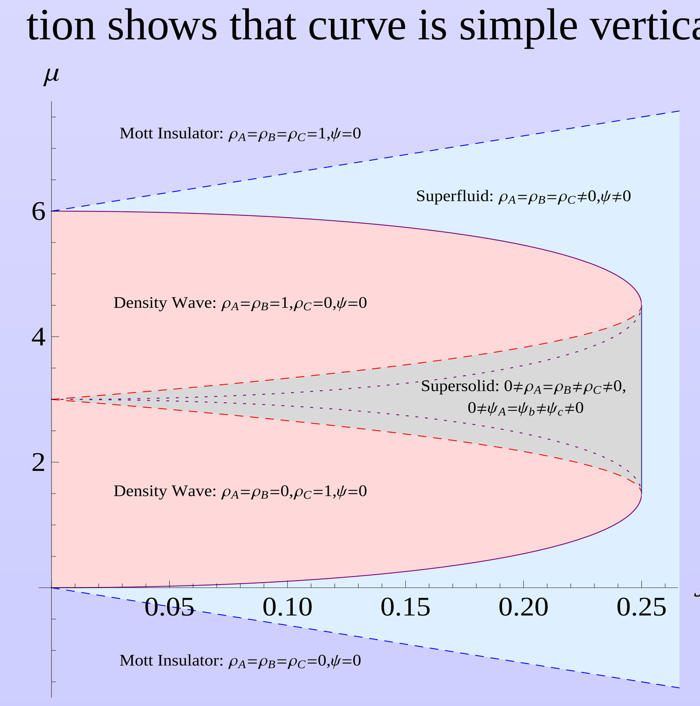
$$\psi_{\mathrm{SF}} = \frac{\sqrt{6J-\mu+6}\sqrt{6J+\mu}}{6(2J+1)},\quad \rho_{\mathrm{SF}} = \frac{6J+\mu}{6(2J+1)},\quad E_{\mathrm{SF}} = -\frac{(6J+\mu)^2}{8J+4}$$

- **Supersolid Phase: $0 \neq \psi_A = \psi_B \neq \psi_C \neq 0,\ \rho_A = \rho_B \neq \rho_C \neq 0$**

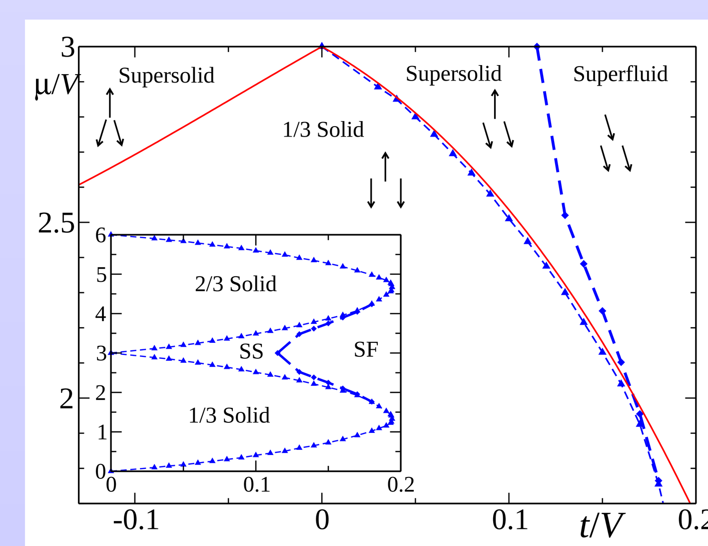
Hamiltonian can still be exactly diagonalized with one universally minimal eigenvalue (E_{SS}), which is too complicated for exact extremization.

- **Phase Transitions:**

For SF-DW and SF-MI transitions, equate exact energies to find transition curves. DW-SS is second order transition, thus apply DW parameters to SS extremization equation $\frac{\partial E_{\mathrm{SS}}}{\partial\psi_A} = 0$ to find transition curve. Similar method cannot be used for SS-SF because it is first order and exact energy for SS is unknown, thus no analytical curve has been found, even though numeric simulation shows that curve is simple vertical line.



Dashed → Continuous, Solid → Discontinuous, Dotted → contrast between DW-SS and DW-SF



Exact phase diagram found using Monte Carlo methods [2]. Note: J-axis is dilated by 2 here. Quantum fluctuations cause Superfluid to shrink, also SS-SF no longer vertical line.