PRJ502: Thesis Research

Low temperature phases of interacting bosons in an optical lattice

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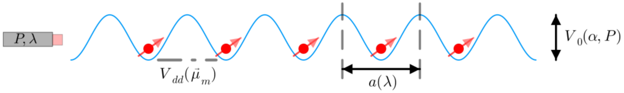
The Experiment

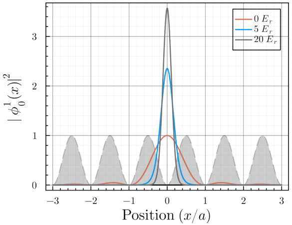
Dipolar gases trapped in an optical lattice creates a highly tunable quantum simulator setup.



Compute Bloch and Wannier wave-functions

$$\hat{H}_q u_q^n(x) = \left[\frac{\hbar^2}{2m}\left(-i\frac{d}{dx}+q\right)^2 + V(x)\right] u_q^n(x) = E_q^n u_q^n(x)$$

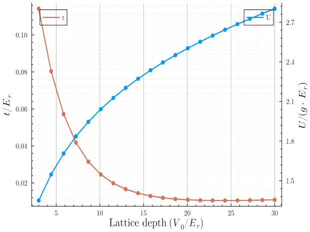
$$\phi_R^n(x) = \frac{1}{N}\sum_{q\in BZ} e^{iq(x-R)} u_q^n(x)$$



Compute BHM parameters

$$t_{i,j} = \langle w_i|\hat{H}|w_j\rangle$$

$$U_{i,j,k,l} = \langle w_i, w_j|\hat{V}|w_j, w_l\rangle$$



The Hamiltonian

Consider a system of spin-0 bosons with contact interaction:

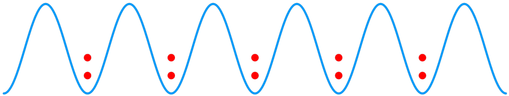
$$H = -t \sum_{\langle i,j \rangle} a_i^\dagger a_j + \frac{U}{2} \sum_i n_i (n_i - 1)$$

- t - hopping strength
- U - on-site interaction

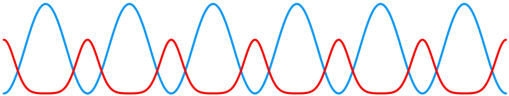
What quantum phases can be observed?

BHM: Expected phases

- Mott Insulator ($U >> t$) $\rightarrow$ $|\Psi_{MI}\rangle = \bigotimes_{i=1}^{M} |n\rangle$

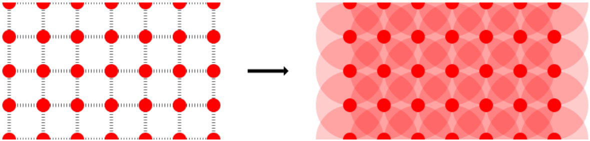


- Superfluid ($U << t$) $\rightarrow$ $|\Psi_{SF}\rangle = \frac{1}{N!}(\sum_{i=1}^{M} a_i^\dagger)^N |0\rangle$



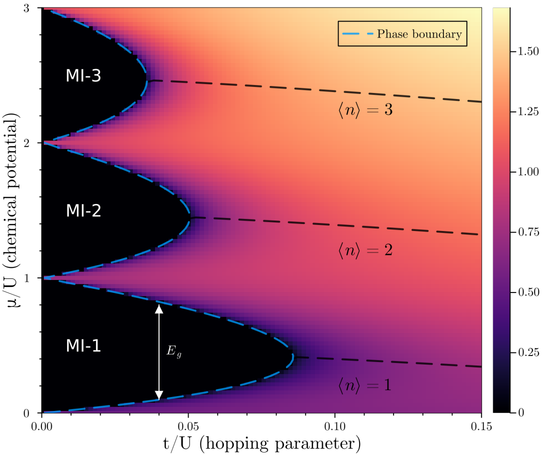
BHM: Mean Field Approximation

$$\hat{a}_i = \Psi_i + \delta\hat{a}_i \qquad \Big| \qquad \mathcal{O}(\delta a_i^2) \approx 0$$



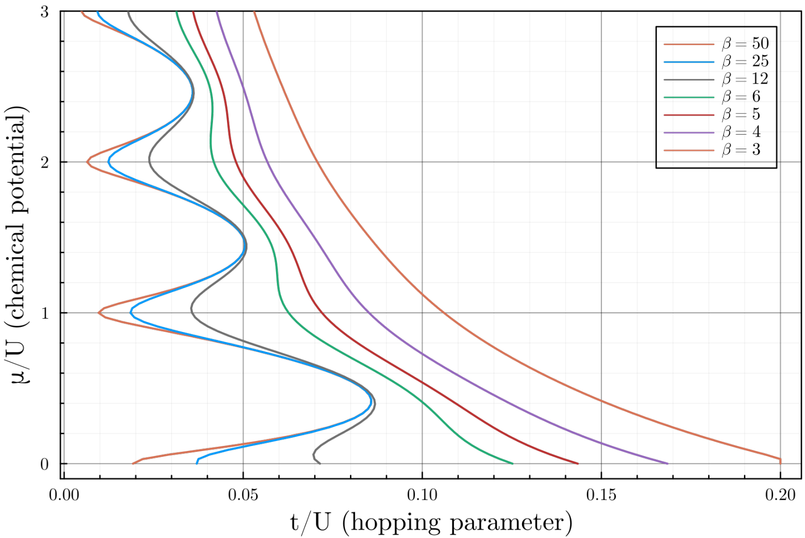
$$\underbrace{H = -t\sum_{\langle i,j\rangle} a_i^\dagger a_j + \frac{U}{2}\sum_i n_i(n_i - 1)}_{\text{coupled lattice sites}} \quad \rightarrow \quad \underbrace{H\{\Psi\} = \sum_i -zt\cdot(\Psi^* a_i + \Psi a_i^\dagger - |\Psi|^2) + \frac{U}{2} n_i(n_i - 1)}_{\text{de-coupled lattice sites}}$$

BHM: Mean Field Approximation, Phase Diagram

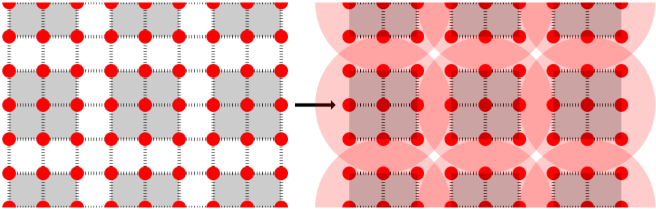


$$\text{ODLRO} \implies \lim_{|i-j|\to\infty} \langle a_i^\dagger a_j \rangle = |\Psi|^2 \neq 0$$

BHM: Mean Field Approximation, Finite temperature

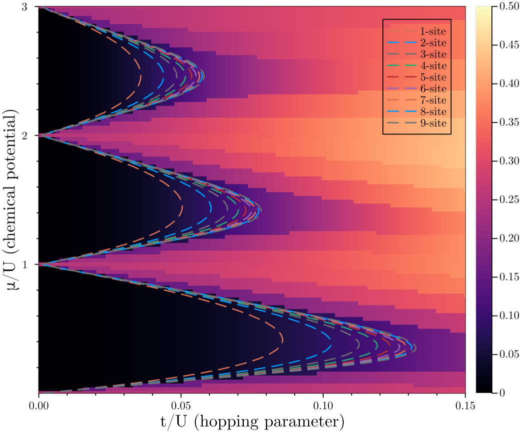


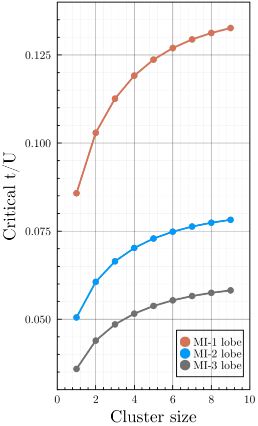
BHM: Cluster MFA



$$\underbrace{H = -t \sum_{\langle i,j \rangle} a_i^\dagger a_j + \frac{U}{2} \sum_i n_i(n_i - 1)}_{\text{coupled lattice sites}} \longrightarrow \underbrace{H\{\Psi_i\} = \sum_C H_{exact} + \sum_{C,C'} H_{MFT}\{\Psi_i\}}_{\text{de-coupled clusters of sites}}$$

BHM: Cluster MFA, Phase Diagram





Extended Bose Hubbard Model

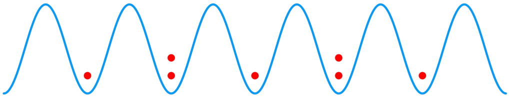
Consider a system of spin-0 bosons with nearest neighbour interactions:

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

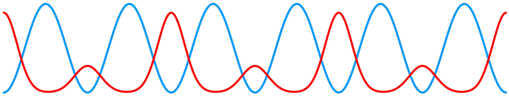
V vs. U terms introduces density modulations in the lattice giving rise to two more phases, analogous to the BHM phases.

eBHM: Expected phases

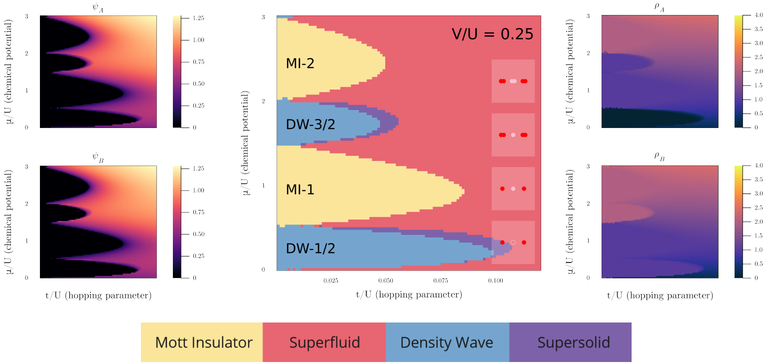
- Density Wave ($U, V >> t,\ V \sim U$)



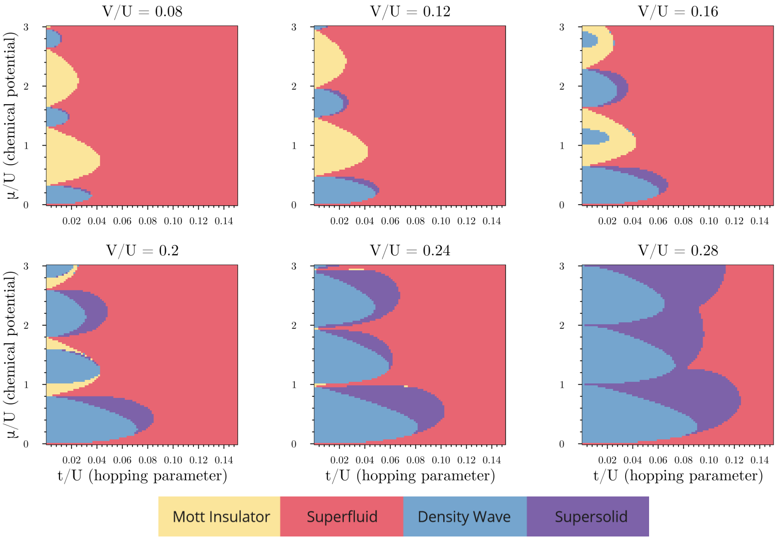
- Supersolid ($U, V << t,\ V \sim U$)



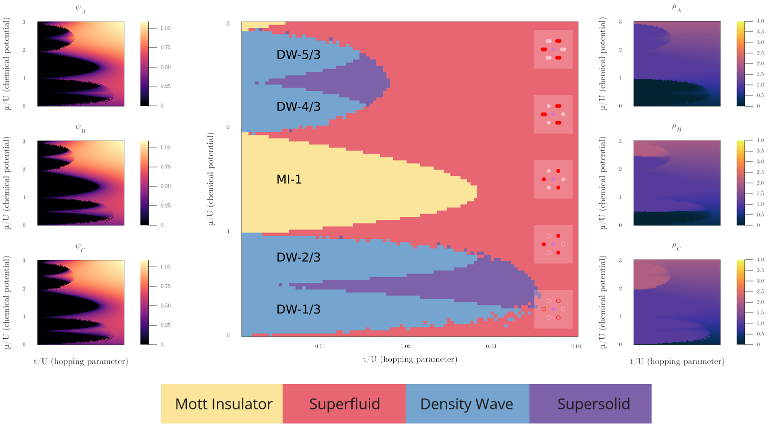
eBHM: MFA Phase Diagram



eBHM: MFA Phase Diagram (Left to Right, Top to Bottom)



eBHM: MFA, Triangular Lattice



Spin-1 Bose Hubbard model

Consider a system of spin-1 bosons with contact interactions:

$$H = -t \sum_{\langle i,j \rangle \sigma} a^{\dagger}_{i\sigma} a_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma}(n_{i\sigma} - 1) + U_s \sum_{i} (\mathrm{S_i}^2 - 2n_i)$$

We do not expect any fundamentally new phases besides Mott insulator and superfluid. However, the nature of these phases can be influenced by the spin degree of freedom.

Nature of Mott insulator

Consider the limit $U, U_s \gg t$.

$$H_i = \frac{U_s}{2}(S_i^2 - 2n_i) + \frac{U}{2} n_i(n_i - 1) - \mu n_i$$

The ground state can be described as a fock state with well-defined net spin like so $|n_i; S_i, m_i\rangle$, such that $n_i + S_i =$ even.

As a result, we have:

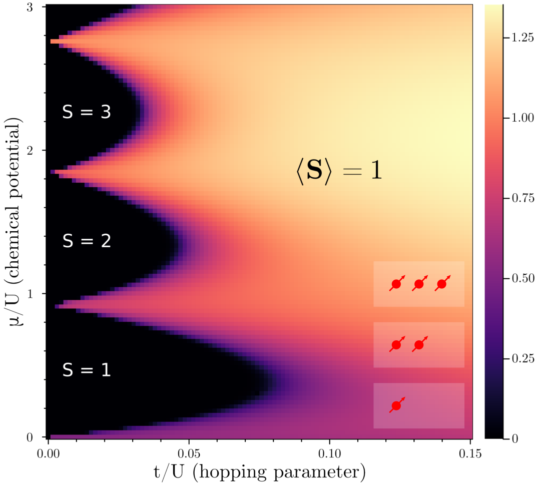
$$S_i \in \begin{cases} \{0, 2, 4, \dots, n_i\} \text{ if } n \text{ is even} \\ \{1, 3, 5, \dots, n_i\} \text{ if } n \text{ is odd} \end{cases}$$

sBHM: Observables

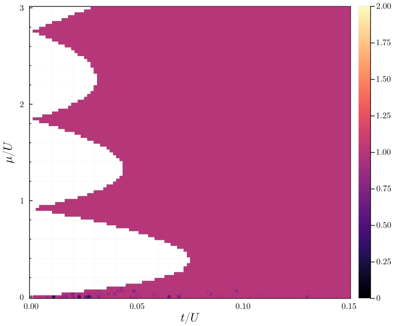
In order to study the ground state phases, we track the following quantities:

1. SF order parameter: $\Psi = (\Psi_1, \Psi_0, \Psi_{\bar{1}}) = \sqrt{n_s} \cdot (\eta_1, \eta_0, \eta_{\bar{1}})$
2. Net spin: $\langle \vec{S}^2 \rangle \sim S(S+1)$
3. Average spin: $|\langle \vec{S} \rangle| = \sum_{\alpha\beta} \eta^*_\alpha J_{\alpha\beta} \eta_\beta$

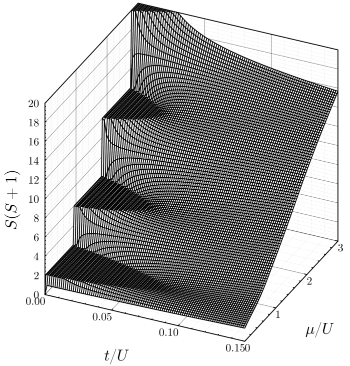
Ferromagnetic interaction ($U_s = -0.08$)



Ferromagnetic interaction ($U_s = -0.08$)

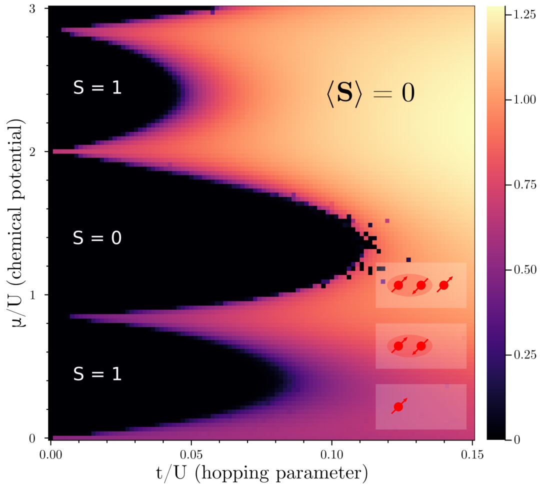


(a) Average spin, $\langle S \rangle$

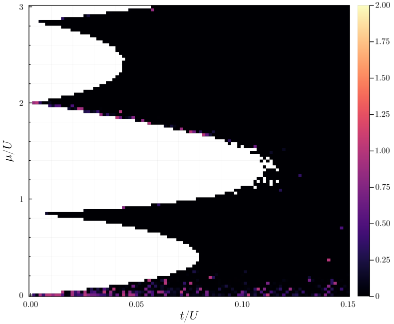


(b) Net spin eigenvalue, $\langle S^2 \rangle$

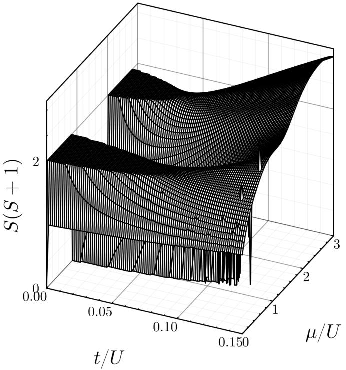
Anti-ferromagnetic interaction ($U_s = 0.08$)



Anti-ferromagnetic interaction ($U_s = 0.08$)



(a) Average spin, $\langle S \rangle$

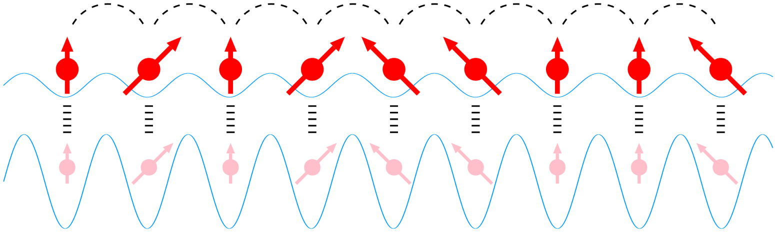


(b) Net spin eigenvalue, $\langle S^2 \rangle$

The setup

Consider a band of spin-1 conduction bosons interacting with a set of localized impurity bosons on a lattice:

$$H = -t \sum_{\langle i,j \rangle \sigma} a^{\dagger}_{i\sigma} a_{j\sigma} - J_h \sum_i \vec{S}_i \cdot \vec{s}_i$$



Re-aligning our basis

In the strong-coupling limit ($J_h \gg t$), we can rotate the conduction bosons to align with the impurities:

$$\begin{bmatrix} a_{i,1} \\ a_{i,0} \\ a_{i,\bar{1}} \end{bmatrix} = \begin{bmatrix} \cos^2\frac{\theta_i}{2} & -\frac{1}{\sqrt{2}}\sin\theta_i e^{-i\phi_i} & \sin^2\frac{\theta_i}{2} e^{-2i\phi_i} \\ \frac{1}{\sqrt{2}}\sin\theta_i e^{i\phi_i} & \cos\theta_i & -\frac{1}{\sqrt{2}}\sin\theta_i e^{-i\phi_i} \\ \sin^2\frac{\theta_i}{2} e^{2i\phi_i} & \frac{1}{\sqrt{2}}\sin\theta_i e^{i\phi_i} & \cos^2\frac{\theta_i}{2} \end{bmatrix} \begin{bmatrix} d_{i,1} \\ d_{i,0} \\ d_{i,\bar{1}} \end{bmatrix}$$

This gives us the following hamiltonian:

$$H = \underbrace{\sum_{\langle i,j\rangle\sigma\sigma'} g_{ij}^{\sigma\sigma'} d_{i\sigma}^\dagger d_{j\sigma'}}_{V} \underbrace{- J_H \sum_i (n_{i,1} - n_{i,\bar{1}})}_{H_0}$$

Computing the effective hamiltonian

Since we have a triply degenerate ground state:

$$|0,2\rangle = d^\dagger_{2,1} d^\dagger_{2,1} |0\rangle \qquad |2,0\rangle = d^\dagger_{1,1} d^\dagger_{1,1} |0\rangle \qquad |1,1\rangle = d^\dagger_{2,1} d^\dagger_{1,1} |0\rangle$$

We proceed to perturbatively calculate the energy by diagonalizing V in this degenerate subspace. The first order correction is found to be $E_0^{(1)} = -4\sqrt{2}\,\mathrm{Re}\left\{ g^{1,1}_{1,2} \right\}$, giving us:

$$E_0^{(1)}(\theta_i, \phi_i, \theta_j, \phi_i) \sim \left[\cos^2\frac{\theta_i}{2}\cos^2\frac{\theta_j}{2} + \frac{1}{2}\cos(\phi_i - \phi_j)\sin\theta_i \sin\theta_j \right.$$
$$\left. + \cos(2(\phi_i - \phi_j))\sin^2\frac{\theta_i}{2}\sin^2\frac{\theta_j}{2} \right]$$

Computing the effective hamiltonian (contd.)

We can then view the following expression as an effective hamiltonian governing the magnetic order of the localized spins:

$$H_{\text{eff}}(\theta_i, \phi_i, \theta_j, \phi_j) = E_0^{(1)}(\theta_i, \phi_i, \theta_j, \phi_j) + E_0^{(0)}$$

Further, inverting the spin components from spherical polar to cartesian provides more insight into the nature of the effective interactions.

$$S_i^x = \cos\phi_i \sin\theta_i \qquad S_i^y = \sin\phi_i \sin\theta_i \qquad S_i^z = \cos\theta_i$$

Computing the effective hamiltonian (contd.)

It turns out that the first order correction cannot be neatly inverted in this manner. However, such a structure does emerge at the second order correction which roughly has the following form:

$$\sum_{\dots}(\dots)\cdot\frac{|g_{i,j}^{\sigma,\sigma'}|^2}{E-E_0}$$

Below is the matrix of these mod squared values that have been inverted in terms of the cartesian spin components.

$$|g_{ij}^{\sigma\sigma'}|^2=\frac{t_{i,j}^2}{4}\begin{bmatrix}(1+\vec{S}_i\cdot\vec{S}_j)^2 & 2(1-(\vec{S}_i\cdot\vec{S}_j)^2) & (1-\vec{S}_i\cdot\vec{S}_j)^2\\ 2(1-(\vec{S}_i\cdot\vec{S}_j)^2) & 4(\vec{S}_i\cdot\vec{S}_j)^2 & 2(1-(\vec{S}_i\cdot\vec{S}_j)^2)\\ (1-\vec{S}_i\cdot\vec{S}_j)^2 & 2(1-(\vec{S}_i\cdot\vec{S}_j)^2) & (1+\vec{S}_i\cdot\vec{S}_j)^2\end{bmatrix}$$

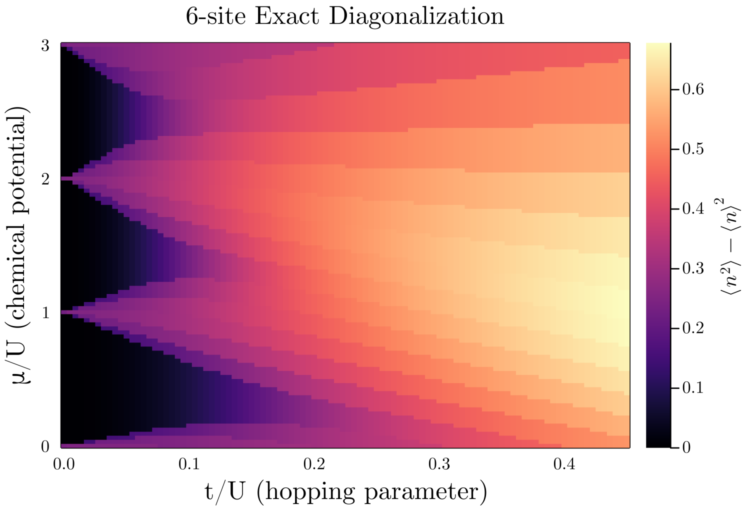
Conclusion & Future outlook

In this thesis, we have extensively studied the nature of phases exhibited by the Bose Hubbard model and documented the qualitative effect of various inter-particle interactions.

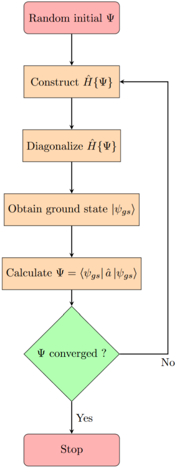
The next step would be to extend and validate results beyond the mean-field level, through techniques of Tensor Networks and/or Quantum Monte Carlo. While some attempts were made during the thesis, several roadblocks were faced which have not been resolved as of yet.

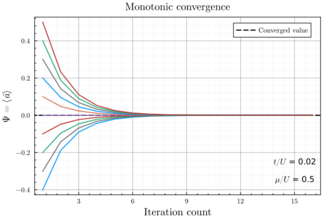
All figures and illustrations were made with **Julia 1.8** using the **Plots.jl** and **Luxor.jl** packages. All code written for the thesis can be found at `https://github.com/20akshay00/`.

Supplement 1: Exact Diagonalization, Phase Diagram



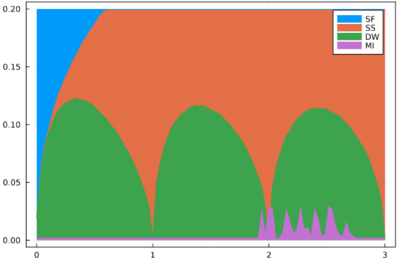
Supplement 2: BHM Mean Field





Supplement 3: Extracting Phase Boundaries

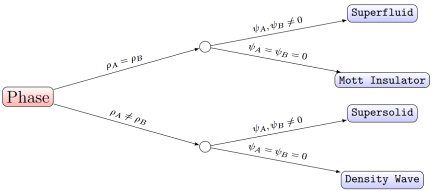
Naive method: Compute for a grid of parameter values and find the points where the order parameter jumps.

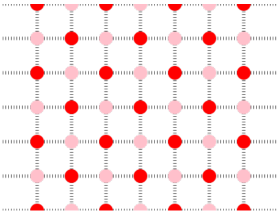


Precise method: Use a bisection algorithm. Precision scales as 2^{-n} for n iterations. But very sensitive to convergence issues.

Supplement 4: eBHM, Mean Field Approximation

$$\hat{a}_i = \Psi_i + \delta \hat{a}_i \qquad \hat{n}_i = \rho_i + \delta \hat{n}_i$$

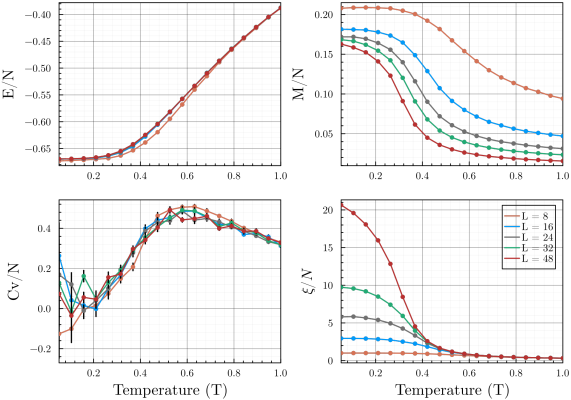




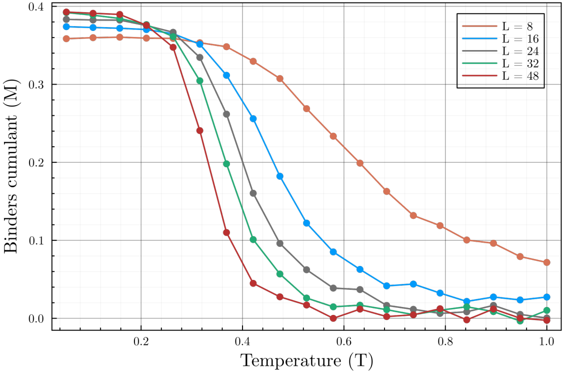
Mean-field parameters: $\{\Psi_A, \Psi_B, \rho_A, \rho_B\}$

Supplement 5: Stochastic Series Expansion

$$H = J \sum_{b=1}^{B} [S^z_{i(b)} S^z_{j(b)} + \frac{1}{2}(S^+_{i(b)} S^-_{j(b)} + S^-_{i(b)} S^+_{j(b)})]$$



Supplement 5: Stochastic Series Expansion (contd.)



Binder cumulant, $U_L = 1 - \frac{\langle M^4 \rangle_L}{3\langle M^2 \rangle_L^2}$.