PRJ501: Thesis Research

Low temperature phases of Dipolar gas in an optical lattice

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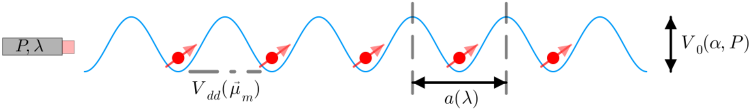
The Experiment

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



Such a system is also a physical realization of the Bose Hubbard Hamiltonian. This gives us a direct mapping of a theoretical toy model and an experimental setup.

The Hamiltonian

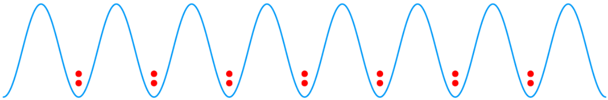
$$H = \underbrace{-t \sum_{\langle i,j \rangle} a_i^\dagger a_j + \frac{U}{2} \sum_i n_i(n_i - 1)}_{\text{Bose Hubbard Model}} + V \sum_{\langle i,j \rangle} n_i n_j + \dots$$

- t - hopping strength
- U - on-site interaction
- V - nearest-neighbour interaction

What (quantum) phases can be exhibited?

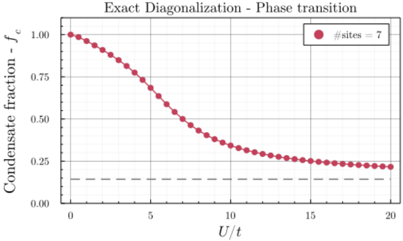
BHM: Expected phases

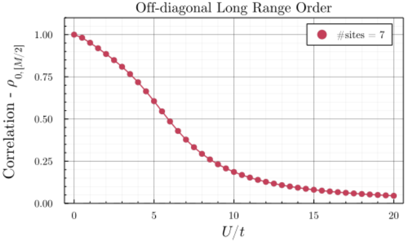
- Mott Insulator ($U >> t$) $\quad \rightarrow \quad |\Psi_{MI}\rangle = \bigotimes_{i=1}^{M} |n\rangle$



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

BHM: Exact Diagonalization (1D)



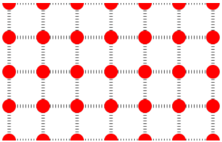
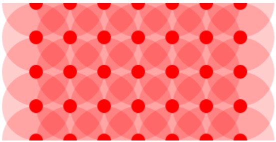


Condensate fraction $\implies ||a_i^\dagger a_j||_\infty / N \sim \mathcal{O}(1)$

Off-diagonal long-range order (ODLRO) $\implies \lim_{|i-j|\to\infty} \langle a_i^\dagger a_j \rangle \neq 0$

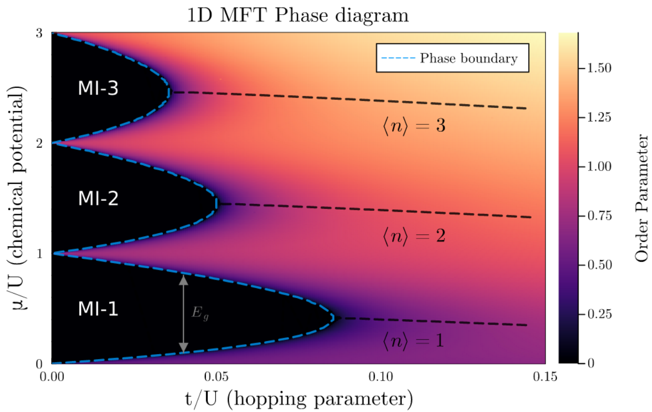
BHM: Mean Field Approximation

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

 → 

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

BHM: Mean Field Approximation, Phase Diagram



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

BHM: Mean Field Approximation, Phase Diagram, contd.

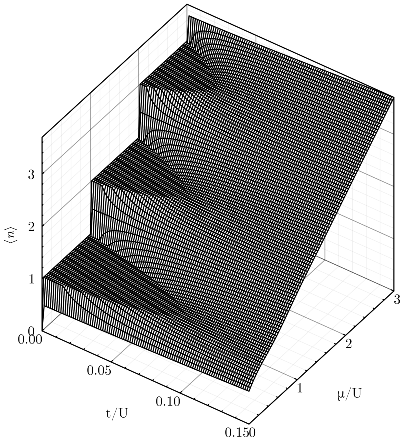
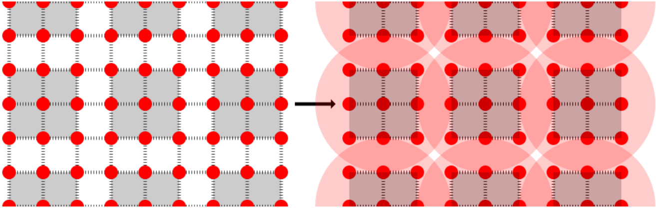


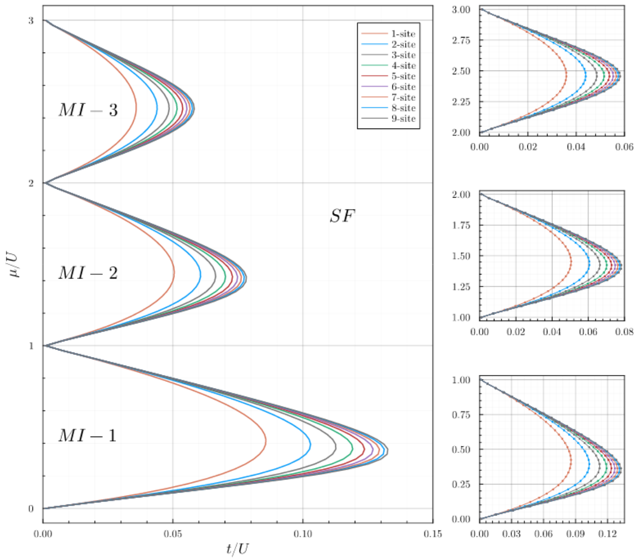
Figure 1: Average occupation number

BHM: Cluster MFA

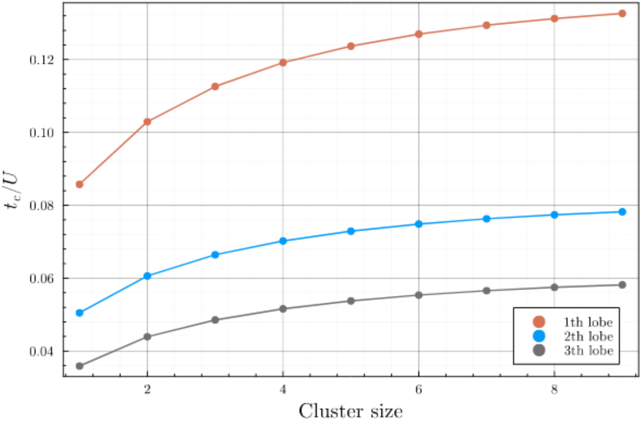


$$\underbrace{H = -t\sum_{\langle i,j\rangle} a_i^\dagger a_j + \frac{U}{2}\sum_i n_i(n_i - 1)}_{\text{coupled lattice sites}} \longrightarrow \underbrace{H\{\Psi_i\} = \sum_C H_{exact} + \sum_{C,C'} H_{MFT}\{\Psi_i\}}_{\text{de-coupled clusters of sites}}$$

BHM: Cluster MFA, Phase Diagram



BHM: Cluster MFA, Mott lobe critical points



eBHM: Expected Phases

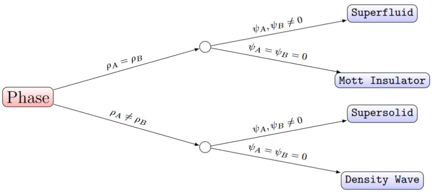
$$H = -t \sum_{\langle i,j \rangle} a_i^\dagger a_j + \frac{U}{2} \sum_i n_i(n_i - 1) + V \sum_{\langle i,j \rangle} n_i n_j$$

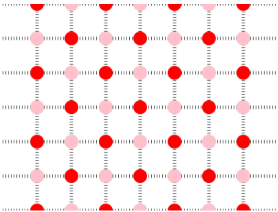
V vs. U terms introduces density modulations in the lattice giving rise to two more phases, analogous to the BHM phases.

- Mott Insulator $\longrightarrow$ Density Wave
- Superfluid $\longrightarrow$ Supersolid

eBHM: Mean Field Approximation

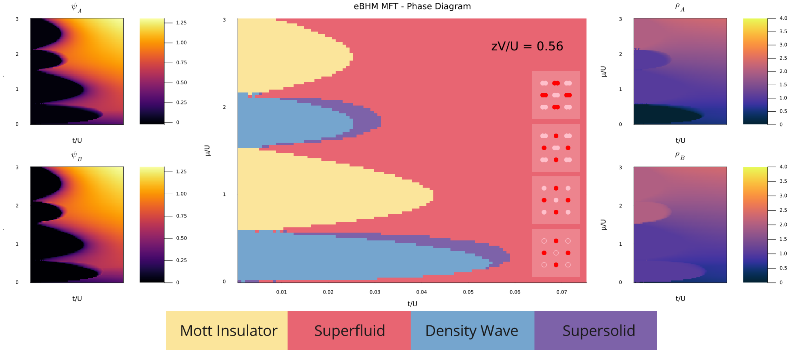
$$\hat{a}_i = \Psi_i + \delta\hat{a}_i \qquad \hat{n}_i = \rho_i + \delta\hat{n}_i$$



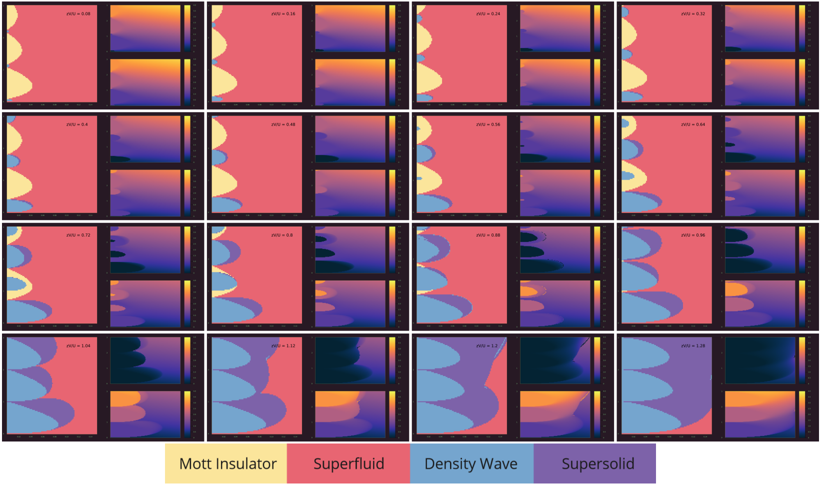


Mean-field parameters: $\{\Psi_A, \Psi_B, \rho_A, \rho_B\}$

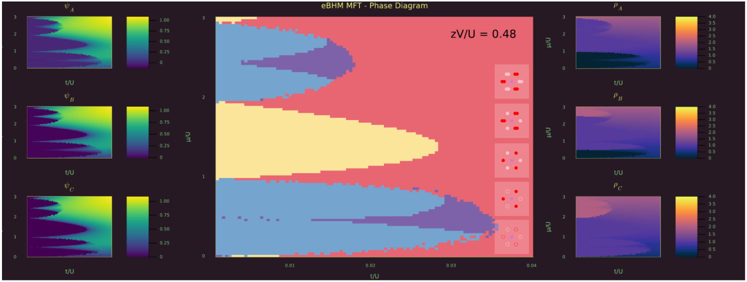
eBHM: MFA Phase Diagram



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



eBHM: MFA, Triangular Lattice



Mott Insulator	Superfluid	Density Wave	Supersolid

Moving beyond mean field; QMC

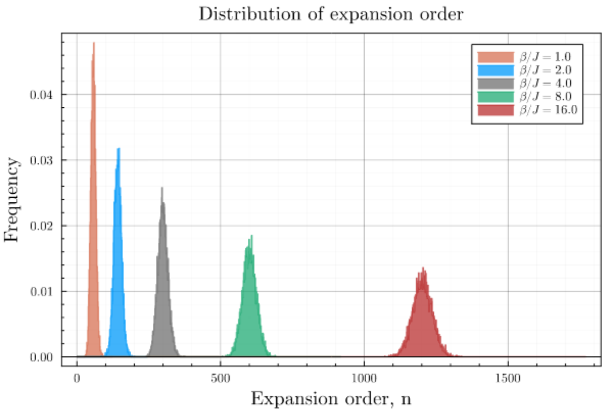
$$Z = Tr(\exp(-\beta H))$$

$$Z = Tr\left[\sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \cdot \left(\sum_b H_{b,1} + H_{b,2}\right)^n\right]$$

$$Z = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \cdot \sum_{|\alpha\rangle} \sum_{S_n} \langle\alpha| \left(\prod_{\{b,i\}\in S_n} H_{b,i}\right) |\alpha\rangle = \sum_{C_i \in \mathcal{C}} w(C_i)$$

Define configuration of the system, $C_i \equiv [|\alpha\rangle, S_n]$. Sample these $C_i \in \mathcal{C}$ ergodically to compute diagonal observables.

Stochastic Series Expansion



We can maintain a cut-off n_{max} dynamically as the simulation progresses and introduce negligible error.

Spin-1/2 chain $\longleftrightarrow$ Hard-core bosons

XXZ spin-1/2 model:

$$H = \frac{J_x}{2} \sum_{\langle i,j \rangle} (S_i^+ S_j^- + S_j^+ S_i^-) + J_z \sum_{\langle i,j \rangle} S_i^z S_j^z + h_z \sum_i S_i^z$$

eBHM w/ hard-core bosons:

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

Map the operators like so:

$$S_i^+ \equiv a_i^\dagger \qquad S_i^z \equiv (n_i - 1/2)$$

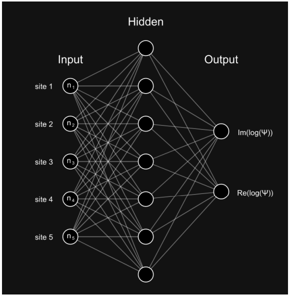
Analogous quantities:

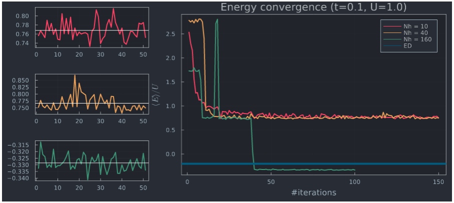
$$t \equiv \frac{J_x}{2} \qquad V \equiv J_z \qquad \mu = J_z - h_z$$


to be continued

Supplement 0: Neural Network ansatz

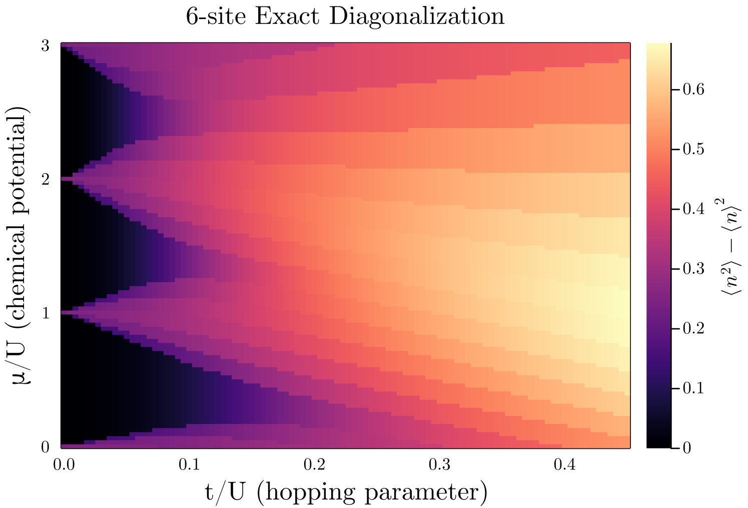
Ansatz for the wave-function: $\Psi = \sum_n \Psi(n)|n\rangle$ such that $\Psi(n)$ is captured by a neural network.



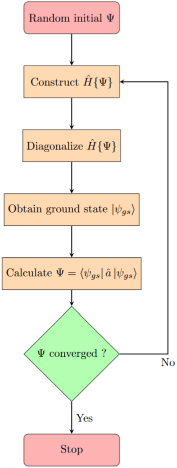


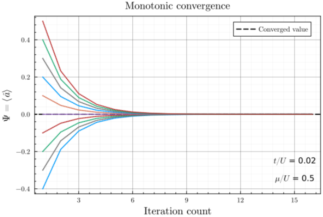
Train the network weights to minimize $\langle \hat{H} \rangle$.

Supplement 1: Exact Diagonalization, Phase Diagram



Supplement 2: BHM Mean Field





Supplement 3: eBHM Mean Field

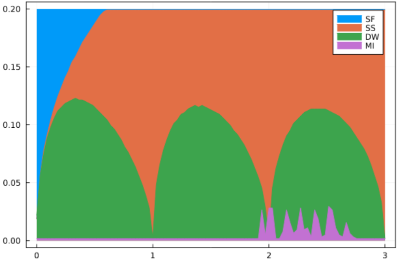
$$H_A\{\Psi_A, \Psi_B, \rho_A, \rho_B\} = -zt \cdot (\Psi_B^* a_A + \Psi_B a_A^\dagger - \Psi_A^* \Psi_B) + zV \cdot (\rho_B n_A - \rho_A \rho_B) + \frac{U}{2} n_A(n_A - 1)$$

$$H_B\{\Psi_A, \Psi_B, \rho_A, \rho_B\} = -zt \cdot (\Psi_A^* a_B + \Psi_A a_B^\dagger - \Psi_B^* \Psi_A) + zV \cdot (\rho_A n_B - \rho_B \rho_A) + \frac{U}{2} n_B(n_B - 1)$$

$$H\{\Psi_A, \Psi_B, \rho_A, \rho_B\} = \sum_{i \in A} H_i + \sum_{j \in B} H_j$$

Supplement 4: 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 5: Local minima