Phases of one-dimensional Bose-Hubbard model in optical lattices with dipole-dipole interactions

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Entanglement and Dynamics

Outline

1. Motivation
   - Bose-Hubbard models
   - EBH in optical lattices - theory
2. Generalized BHM
   - The model
   - Parameter values
3. Phases in one dimension
   - Phase diagram for $\rho = 1$
   - Phase diagram for fixed V/U

Bose-Hubbard Model

Basic model of bosons in an optical lattice:

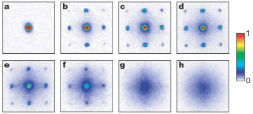
$$H = -t \sum_{\langle i,j \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i (n_i - 1) \quad (+ \sum_i \epsilon_i b_i^\dagger b_i)$$

Here, U is contact interaction between two bosons at the same lattice site, which we can parametrize using effective scattering length (a_s)

Two phases in limiting cases (for $\rho = 1$)

- $J \gg U$: superfluid (SF), delocalized wavefunctions
- $J \ll U$: Mott insulator (MI), localized wavefunctions

Experimentally realized in an optical lattice in 2002[1]:



Absorption images at time of flight at 15ms, pictures a-h correspond to V_0/E_R: 0, 3, 7, 10, 13, 14, 16 and 20

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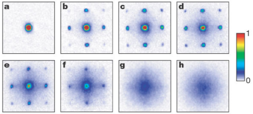

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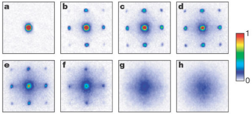

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Extended Bose-Hubbard Model

Addition of nearest-neighbour tunneling to previous hamiltonian:

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

V is mostly due to dipole-dipole interaction of bosonic particles:

$$V_{dip}(\mathbf{r} - \mathbf{r}') = \frac{C_{dd}}{4\pi} \frac{1 - 3\cos^2\theta}{|\mathbf{r} - \mathbf{r}'|^3}$$

For particles having magnetic dipole moment $C_{dd} = \mu_0 \mu^2$, and for particles having electric dipole moment $C_{dd} = d^2/\varepsilon_0$.

Additional phases with this extension to BHM

- density wave (DW) phase: $U \gg V$, $U \gg t$: "checkerboard" density distribution
- Haldane insulator: finite non-local string correlations: $C_{str}(r) = \langle \delta n_j e^{i\pi \sum_{j<k<j+r} \delta n_k} \delta n_{j+r} \rangle$.

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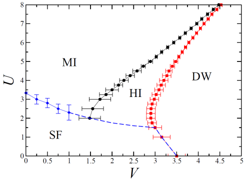
EBH phase diagram



The phase diagram of EBH for filling $\rho = 1$ has been calculated using density matrix renormalization group (DMRG) [2].

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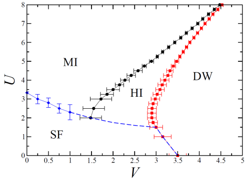

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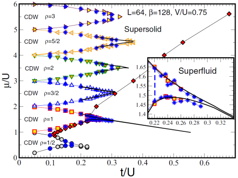

Different phases for $V/U = 3/4$ and varying filling (here measured by chemical potential μ) - calculated using DMRG (black lines) and Quantum Monte Carlo (symbols)[3].

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[3] GG Batrouni et al. "Competing phases, phase separation, and coexistence in the extended one-dimensional bosonic Hubbard model". In: *Physical Review B* 90.20 (2014), p. 205123

The model

We can extend our model even more by including next highest terms in our hamiltonian:[4]

$$H_{GBH} = -t \sum_{\langle i,j \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i(n_i - 1) + V \sum_{\langle i,j \rangle} n_i n_j + V_{nnn} \sum_{\langle\langle i,j \rangle\rangle} n_i n_j - T \sum_{\langle i,j \rangle} b_i^\dagger (n_i + n_j) b_j + \frac{P}{2} b_i^{\dagger 2} b_j^{\dagger 2}$$

Additional terms:

- V_{nnn} - next-nearest neighbour interaction
- T - density dependent tunneling
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Describing states of the bosons using Wannier functions ($w_i(\mathbf{r})$ describing state at i-th site), we can express above terms as:

$$t = -\int d\mathbf{r} w_i^*(\mathbf{r}) \left[\frac{-\hbar^2 \nabla^2}{2m} \right] w_j(\mathbf{r}) \tag{1}$$

$$U_{ijkl} = g \int d^3\mathbf{r_1} d^3\mathbf{r_2} w_i^*(\mathbf{r_1}) w_j^*(\mathbf{r_2}) U(\mathbf{r_1} - \mathbf{r_2}) w_k(\mathbf{r_1}) w_l(\mathbf{r_1}) \tag{2}$$

$$U = U_{1111}, \quad V = U_{1212}, \quad V_{nnn} = U_{1313}, \quad T = -U_{1112}, \quad P = U_{1122} \tag{3}$$

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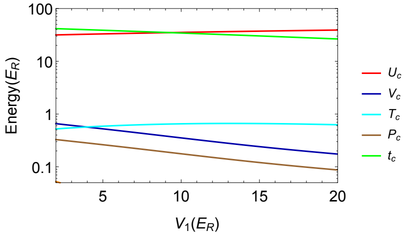
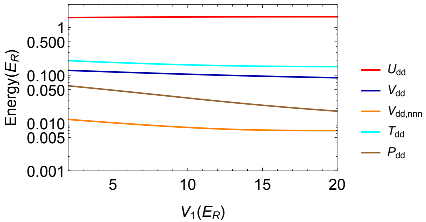
Parameter values

For one-dimensional lattice (lattice potentials $V_y = V_z = 50E_R$, $V_x = V_1$):





Total tunnelings and interactions are the sum of contact and dipole-dipole ones, $t = t_c + t_{dd}$, $U = U_c + U_{dd}$

Engineering U/t and V/t

3 parameters we can adjust

- V_1: here I used range from $2E_R$ to $20E_R$
- a_s: scattering length of contact interactions - adjustable by Feshbach resonance
- $d = \frac{C_{dd}}{4\pi E_R}$, can be changed by adjusting the orientation of magnetic dipoles

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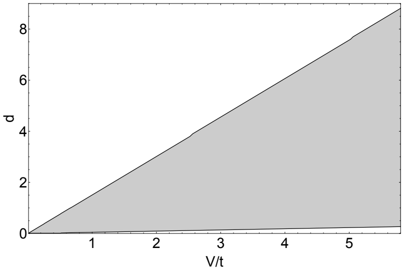
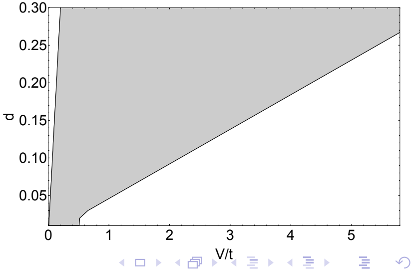
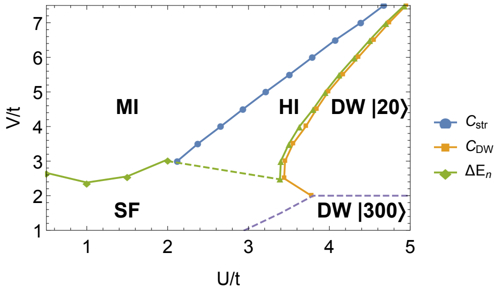
For aforementioned lattice depths and set value of d, there is a specific range of V/t values we can get by modifying V_1 and a_s, which is marked here as a shaded region:





Phase diagram for $\rho = 1$

For $d = 0.25$, $V2 = 50E_R$ and varying V_1 and a_s phase diagram was calculated with open boundary conditions DMRG for sizes up to 400 sites (using itensor library):



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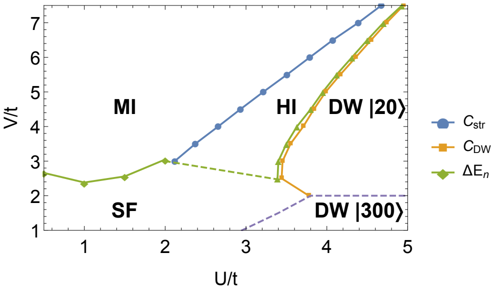

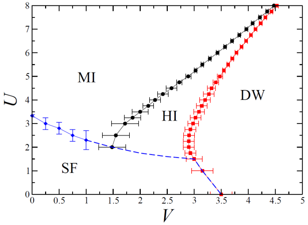

Figure: Simple EBH phase diagram.

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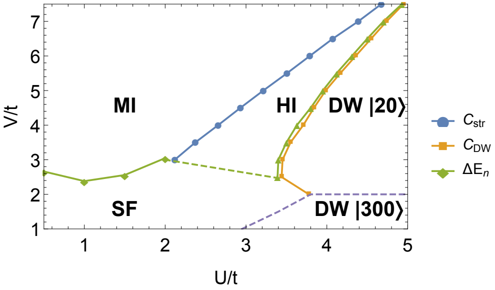

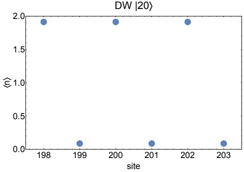

Figure: particle density for $U/t = 1.5$, $V/t = 3.8$

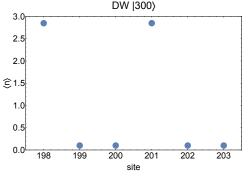

Figure: particle density for $U/t = 4$, $V/t = 4.5$

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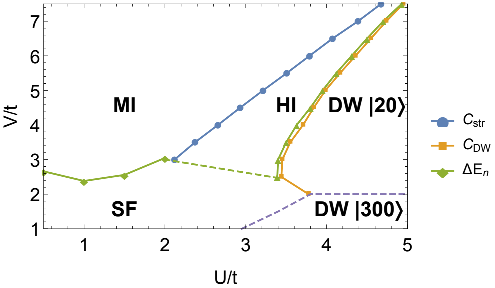

SF - MI transition:

$$\Delta E_n = \lim_{L\to\infty} E_L^{(1)} - E_L^{(0)}$$

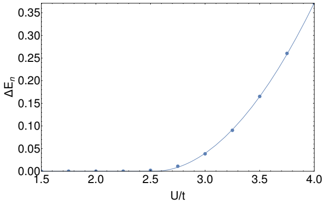

Figure: $V/t = 1.5$

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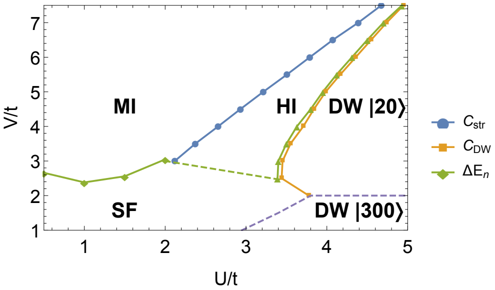

MI - HI transition:

$$C_{str} = \lim_{r\to\infty} \langle \delta n_j e^{i\pi \sum_{j<k<j+r} \delta n_k} \delta n_{j+r} \rangle$$

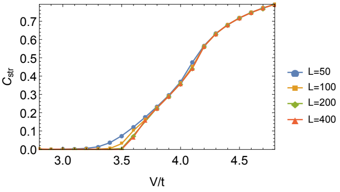

Figure: $U/t = 5.5$

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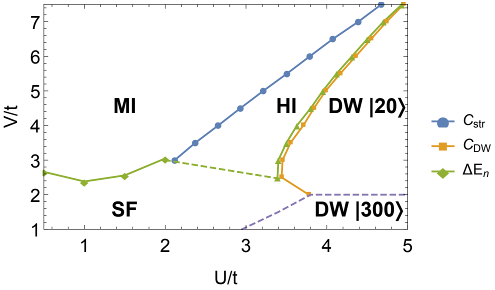


HI - DW transition:

$$C_{DW}(r) = \lim_{r\to\infty} (-1)^r \langle \delta n_j \delta n_{j+r} \rangle$$

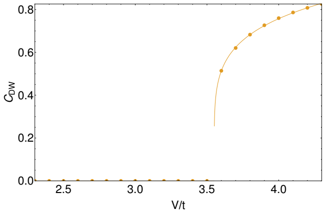
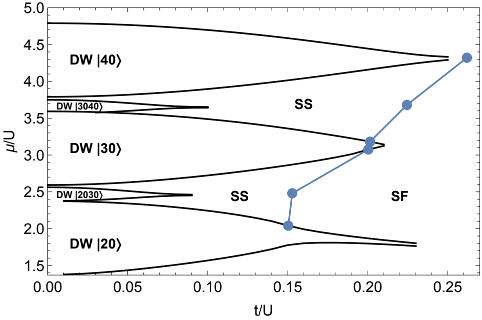


Figure: $U/t = 3.5$

Phase diagram for fixed V/U

Here $V/U = 0.75$, $V_{nnn} = V/8$, T and P are neglected. For various lattice fillings (from $\rho = 1$ to $\rho = 2$) phase diagram was calculated with open boundary conditions DMRG with 192 sites:



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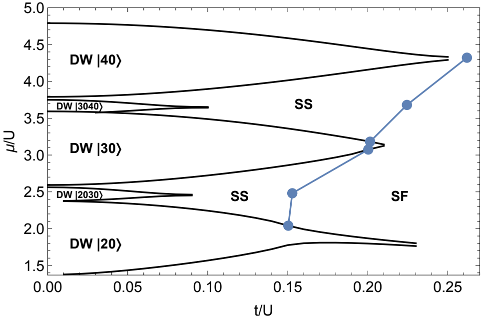

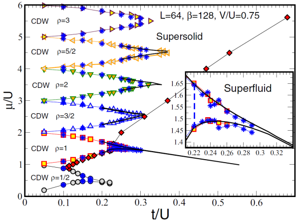

Figure: Simple EBH phase diagram.

Phase diagram for fixed V/U

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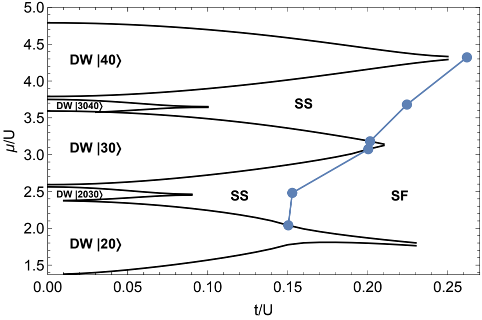


SF - SS (supersolid) and SF - DW transitions:

$$C_{DW}(r) = \lim_{r\to\infty} (-1)^r \langle \delta n_j \delta n_{j+r} \rangle$$

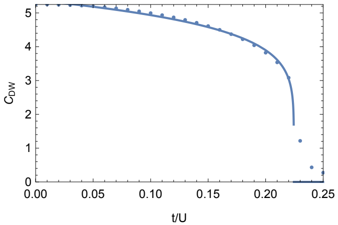
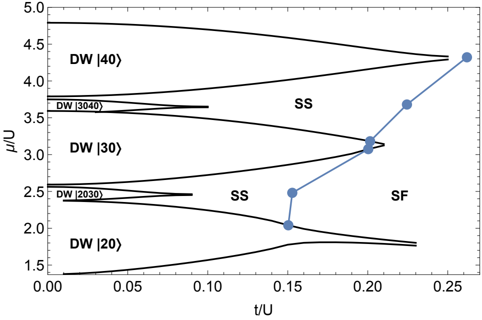


Figure: $\rho = 7/4$

Phase diagram for fixed V/U

Here $V/U = 0.75$, $V_{nnn} = V/8$, T and P are neglected. For various lattice fillings (from $\rho = 1$ to $\rho = 2$) phase diagram was calculated with open boundary conditions DMRG with 192 sites:



Correlations in DW regime:

$$\langle b_i^\dagger b_{i+r} \rangle \sim e^{-\frac{r}{\xi}}$$

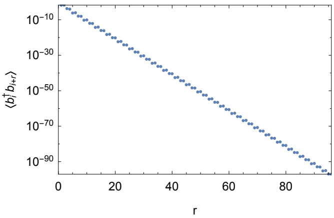
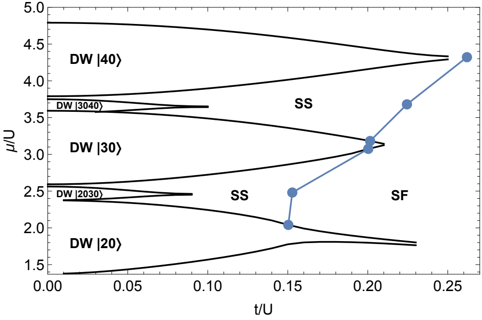


Figure: Log plot of correlations, $\rho = 7/4$, $t/U = 0.01$

Phase diagram for fixed V/U

Here $V/U = 0.75$, $V_{nnn} = V/8$, T and P are neglected. For various lattice fillings (from $\rho = 1$ to $\rho = 2$) phase diagram was calculated with open boundary conditions DMRG with 192 sites:



Correlations in SS regime:

$$\langle b_i^\dagger b_{i+r} \rangle \sim r^{-s}$$

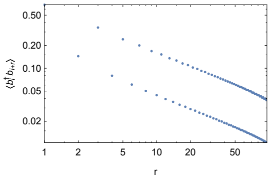
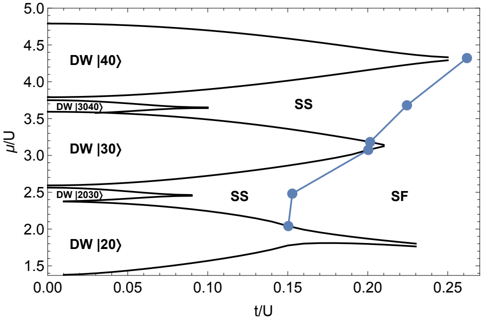


Figure: Log-log plot of correlations, $\rho = 7/4$, $t/U = 0.15$

Phase diagram for fixed V/U

Here $V/U = 0.75$, $V_{nnn} = V/8$, T and P are neglected. For various lattice fillings (from $\rho = 1$ to $\rho = 2$) phase diagram was calculated with open boundary conditions DMRG with 192 sites:



Correlations in SF regime:

$$\langle b_i^\dagger b_{i+r} \rangle \sim r^{-s}$$

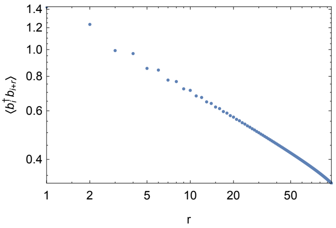


Figure: Log-log plot of correlations, $\rho = 7/4$, $t/U = 0.25$

Summary

- Bose-Hubbard model can be generalized with additional terms that can be calculated straightforwardly using Wannier functions
- Including those additional terms do not qualitatively change phase diagram, proving HI phase robustness
- Including next-nearest neighbour interactions influences SS regime extent for higher lattice fillings and creates additional DW patterns

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Acknowledgements

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