Ultracold Atomic Gases in 1D Optical Lattices

DMRG Method in Inhomogeneous Lattice Topologies

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Summary

- cold atomic gases on optical lattices are a perfect experimental realization of the Hubbard Modell [1,2]
- all relevant parameters can be precisely controlled in the experiment allowing for unique comparison with theory throughout the whole phase-diagram [8]
- the Hubbard Hamiltonian facilitates a straight forward growing of the system, which makes this an ideal case for DMRG calculations [6,7]
- nevertheless DMRG involves a truncation procedure, which should be tested in all different regimes of the phase-diagram
- investigate how DMRG performs in spatially inhomogeneous lattices
- append lattice sites with different on-site energies, e.g. apply a superlattice, to check for the effect of localization or disorder on the spectrum of the reduced density-matrix and thus on the target state

Bose-Hubbard Model

- 1D optical lattice with I lattice sites and N bosonic particles
- restriction to the first energy-band, $T=0$, nearest neighbor tunneling, and an on-site two-particle contact interaction
- additional on-site potential can map arbitrary lattice topologies

$$\hat{H} = -J\sum_{i=1}^{I}\left(\hat{a}_{i+1}^{\dagger}\hat{a}_i + \hat{a}_i^{\dagger}\hat{a}_{i+1}\right) \quad \text{tunneling}$$
$$+\frac{V}{2}\sum_{i=1}^{I}\hat{n}_i(\hat{n}_i-1) \quad \text{interaction}$$
$$+\Delta\sum_{i=1}^{I}\epsilon_i\,\hat{n}_i \quad \text{superlattice potential}$$

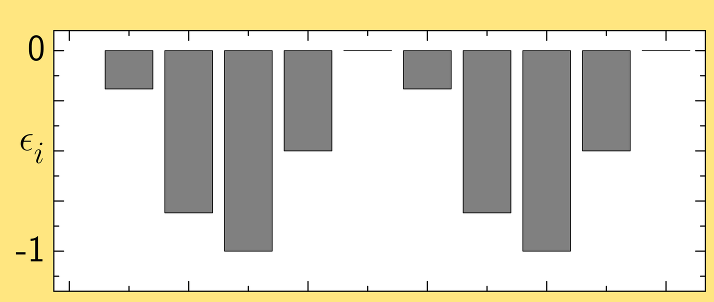
$\hat{a}_i^{\dagger},\ \hat{a}_i,\ \hat{n}_i$	creation, annihilation, occupation-number operators
J	tunneling matrix element
V	two particle interaction energy
Δ	strength of the superlattice potential
ϵ_i	topology of the superlattice potential

- use an occupation-number representation spanning the Fock-space $\mathcal{H}$ to formulate a matrix representation of the Hamiltonian

$$\mathcal{H} = \text{span}\{\,|\,\{n_1,\ldots,n_I\}_\alpha\,\rangle\}$$

Two-Color Superlattice

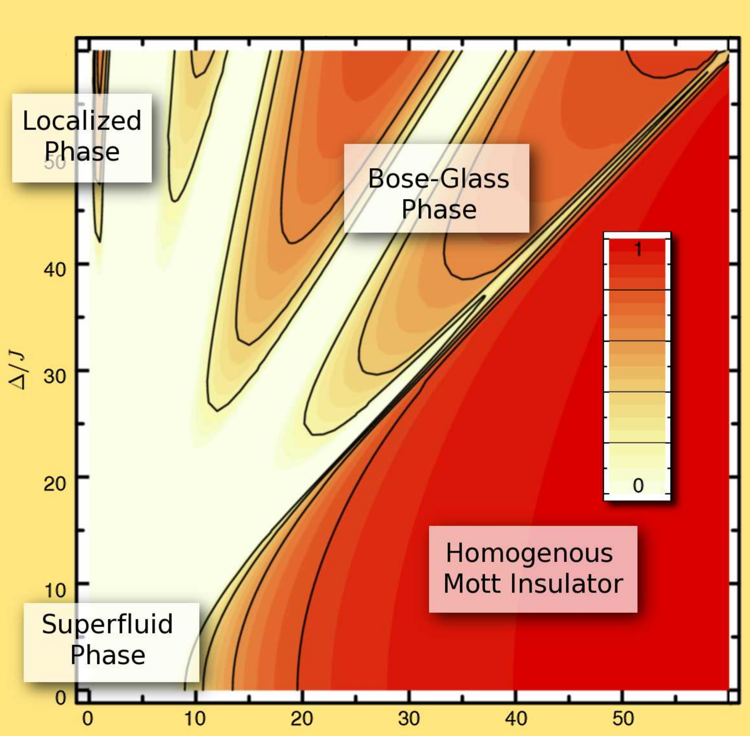
- superposition of two laser beams with slightly different wavelengths [5] form a superlattice potential
- Δ/J is the on-site energy of the deepest superlattice well



Phase Diagram

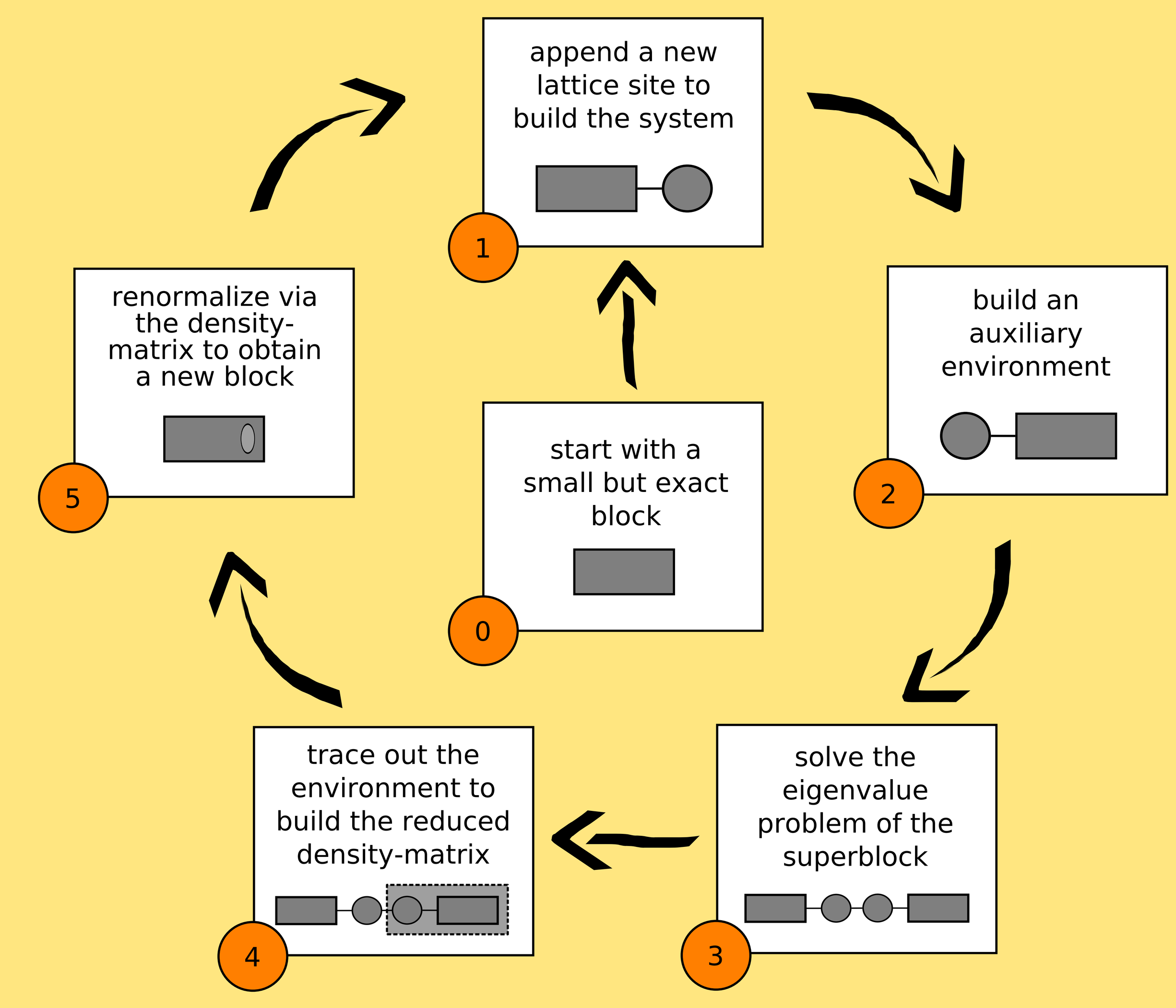
- exact diagonalization for a moderate system size $(I=N=10)$ with periodic boundary conditions yields ground states

$$|\,\psi^{(0)}\,\rangle = \sum_{\alpha=1}^{D} C_\alpha^{(0)}\,|\,\{n_1,\ldots,n_I\}_\alpha\,\rangle \qquad \hat{H}\,|\,\psi^{(0)}\,\rangle = E_0\,|\,\psi^{(0)}\,\rangle$$



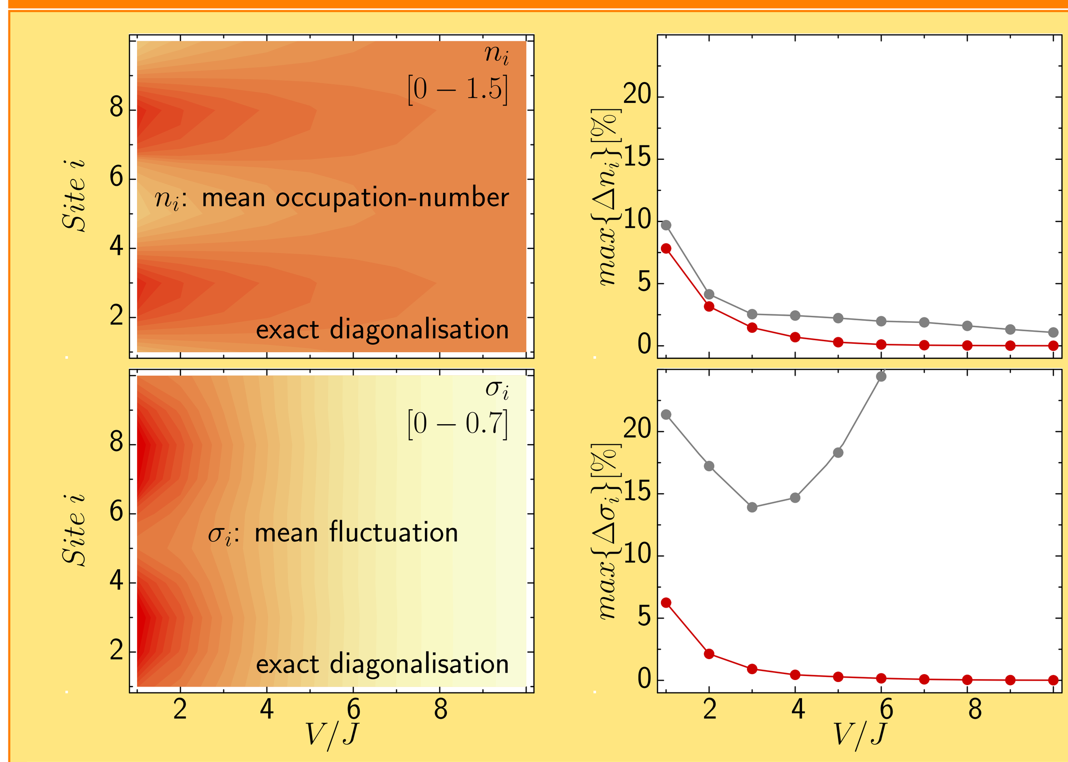
- $max\{|C_\alpha^{(0)}|^2\}$ reflects the composition of the ground state
- commensurate systems exhibit a rich phase-diagram [3,4]
- subtle interplay between the different energy scales (J, V and Δ)
- test DMRG calculations in the transition regimes of the phase diagram

DMRG Algorithm



1. $\mathcal{H}_{system} = \mathcal{H}_{block}\otimes\mathcal{H}_{site}$
2. $\mathcal{H}_{env} = \tilde{\mathcal{H}}_{Block}\otimes\tilde{\mathcal{H}}_{Site}$
3. $\mathcal{H}_{super} = \mathcal{H}_{system}\otimes\mathcal{H}_{env}$
   $\hat{H}_{super}\,|\,\psi^{(0)}\,\rangle = E_0\,|\,\psi^{(0)}\,\rangle$
4. $\hat{\rho}_{red} = \text{Tr}_{env}\left(|\,\psi^{(0)}\,\rangle\langle\,\psi^{(0)}\,|\right)$
5. $\hat{\rho}_{red}\,|\,\omega_i\,\rangle = \omega_i\,|\,\omega_i\,\rangle$
   $\sum_i\omega_i = 1 \quad \omega_i \geq \omega_{i+1}$
   $\mathcal{O} = \left(\vec{w}_1,\cdots,\vec{w}_{D_b}\right)$
   $H_{block(L)} = \mathcal{O}^T\,H_{system(L)}\,\mathcal{O}$

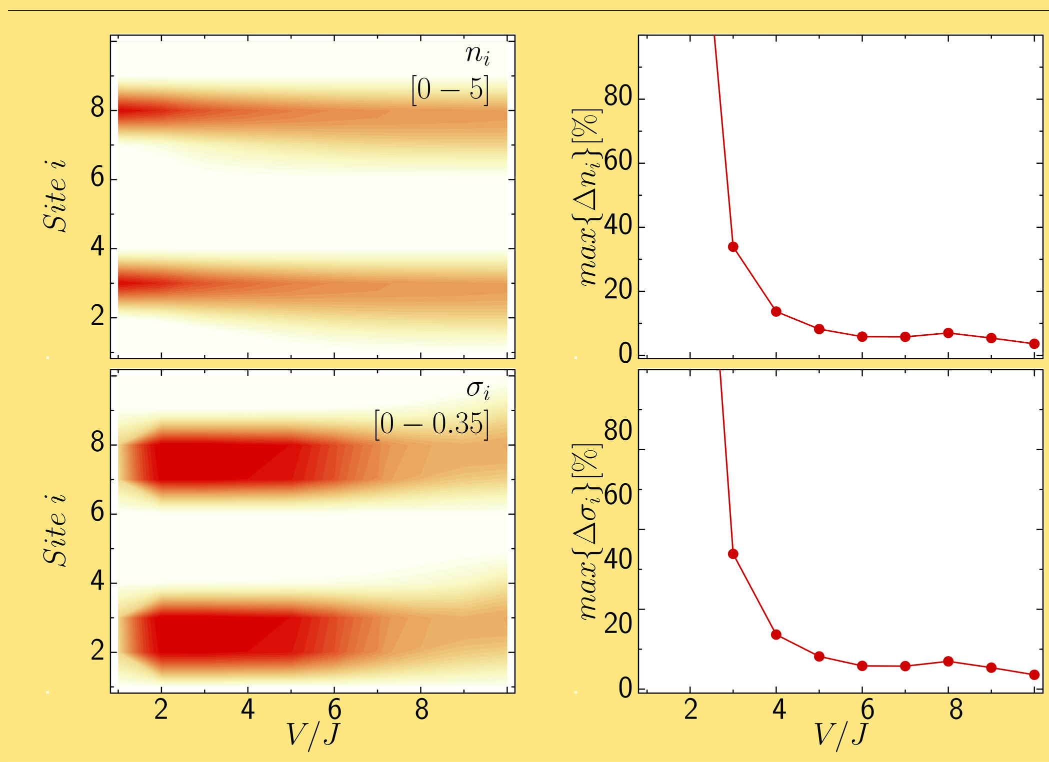
Results



- 2D plots show the maximum relative error of the DMRG calculations
- gray: DMRG without sweep
- red: DMRG with one sweep

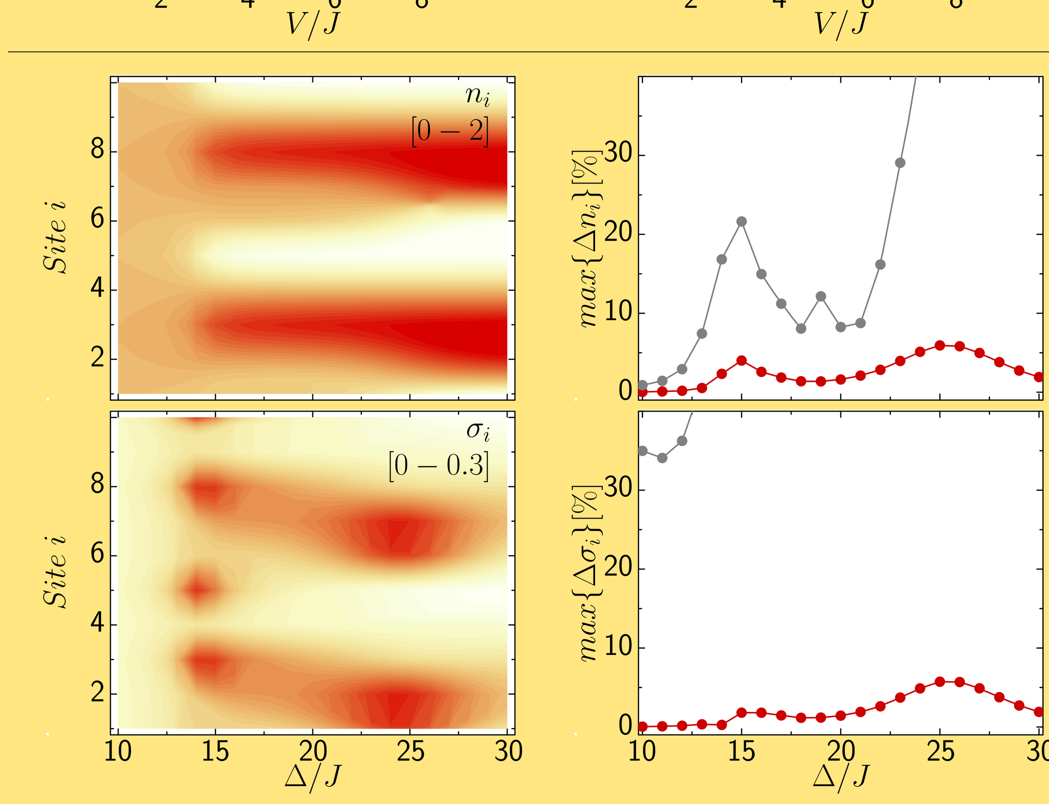
Superfluid to Mott-Insulator $(\Delta/J=1)$

- lattice sites are almost equal, ground state is nearly homogenous
- good results even without sweeping



Localized to Bose-Glass $(\Delta/J=50)$

- ground state is strongly inhomogeneous
- DMRG needs at least the average number of particles per unit-cell to reproduce the localized phase
- sweeping leads to good results as soon as delocalization of particles occurs



Mott-Insulator to Bose-Glass $(V/J=15)$

- intermediate inhomogeneity
- redistribution of particles is well reproduced by DMRG calculations with sweeps

- exact calculations involve a $D\approx10^5$ eigenvalue problem
- DMRG calculations involve a $D\approx400$ eigenvalue problem

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[2] Immanuel Bloch, Physics World (2004)
[3] R. Roth and K. Burnett, Phys. Rev. A 67 031692(R) (2003)
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[6] S.R. White, Phys. Rev. B 48 10345 (1993)
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[8] M. Greiner et al., Nature (London) 415, 39 (2002)