DMRG for Ultracold Bose Gases in Optical Lattices

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ECT* Workshop 2009
Linking Nuclei, Molecules, and Condensed Matter:
Computational Quantum Many-Body Approaches

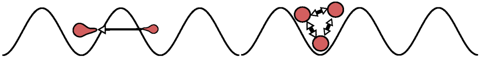
Overview

Hubbard Model (1963)

John Hubbard

Susono, November, 1980

periodic potential



- particles can tunnel to adjacent lattice sites and can interact on-site
- originally proposed as the simplest low temperature model for electrons in crystalline solids
- straight-forward generalization for bosons

Bose-Hubbard Hamiltonian

I lattice sites N particles $T = 0$

Occupation-Number Basis

$$|\,\psi\,\rangle = \sum_{\alpha} C_\alpha \,|\, \{n_1, n_2, \ldots, n_I\}_\alpha \,\rangle \qquad \sum_i n_i = N$$

Hamiltonian

$$\hat{\mathrm{H}} = \sum_{i=1}^{I} \Big\{ -J \left(\hat{\mathrm{a}}_{i+1}^\dagger \, \hat{\mathrm{a}}_i + \hat{\mathrm{a}}_i^\dagger \, \hat{\mathrm{a}}_{i+1} \right) + \frac{1}{2} U \left(\hat{\mathrm{n}}_i - 1 \right) \hat{\mathrm{n}}_i \Big\}$$

J tunneling matrix-element

U on-site interaction matrix-element

the only parameter is U/J

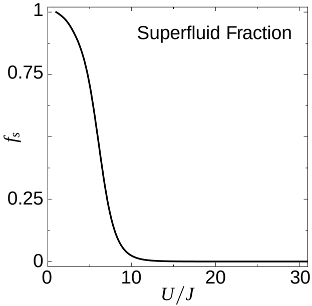
Quantum Phase-Transition

quantum phase-transition from

superfluid to
Mott-insulator

driven by interaction instead of temperature

Fisher et al., Phys. Rev. B 40, 546 (1989)

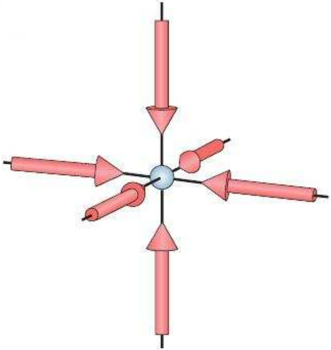


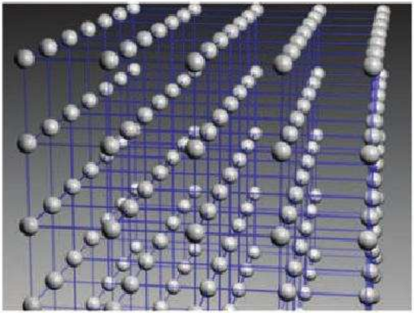
exact diagonalization for $I = N = 10$

where can this be observed?

Ultracold Atoms in Optical Lattices

Jaksch et al. (1998) proposed a setup to the observe SF-MI transition in ultracold atomic gases in optical lattices





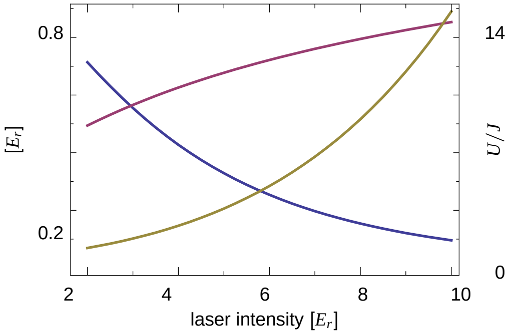
I. Bloch, Nature Physics 1, 23 (2005)

- standing laser-field
- perfect optical crystal
- 1D, 2D, 3D setups possible
- ultracold alkali gas, e.g. ^{87}Rb

U/J in the Experiment

laser intensity directly controls U/J

- blue: J $[E_r]$
- red: U $[E_r]$
- yellow: U/J



more details will follow...

Superfluid to Mott-Insulator Transition – Experiment

time-of-flight image
(3D lattice)

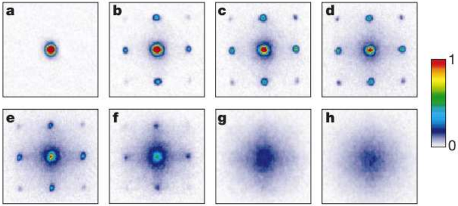
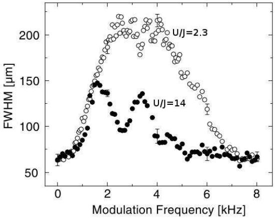


Figure 2 Absorption images of multiple matter wave interference patterns. These were obtained after suddenly releasing the atoms from an optical lattice potential with different potential depths V_0 after a time of flight of 15 ms. Values of V_0 were: **a**, 0 E_r; **b**, 3 E_r; **c**, 7 E_r; **d**, 10 E_r; **e**, 13 E_r; **f**, 14 E_r; **g**, 16 E_r; and **h**, 20 E_r.

Greiner et al., Nature Physics 415, 39 (2002)

absorption spectrum
(1D lattice)



Stöferle et al., Phys. Rev. Lett. 92, 130403 (2004)

perfect agreement between experiment and theory

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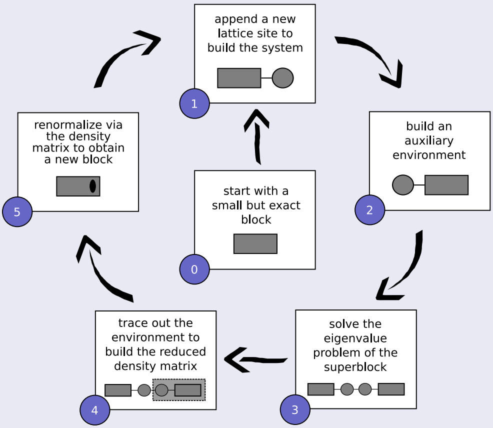
why are these systems of so much interest?

- simple model but rich physics
- perfect mapping of a Hamiltonian to an experiment
- perfect experimental control over the relevant parameters
- different quantum statistics: bosons, fermions, and mixtures
- genuine 1D and 2D systems can be realized
- optical lattices are a magnifying glass for solid state physics

Density-Matrix Renormalization Group (DMRG)

Schematic DMRG Cycle



1. $\mathcal{H}_{system(L)} = \mathcal{H}_{block(L-1)} \otimes \mathcal{H}_{site}$
2. $\mathcal{H}_{env(L)} = \tilde{\mathcal{H}}_{block(L-1)} \otimes \tilde{\mathcal{H}}_{site}$
3. $\mathcal{H}_{super(2L)} = \mathcal{H}_{system(L)} \otimes \mathcal{H}_{env(L)}$

   $\hat{\mathrm{H}}_{super(2L)} \mid \psi^{(0)} \rangle = E_0 \mid \psi^{(0)} \rangle$
4. $\hat{\rho}_{red} = \mathrm{Tr}_{env} \left(\mid \psi^{(0)} \rangle \langle \psi^{(0)} \mid \right)$
5. $\hat{\rho}_{red} \mid \omega_i \rangle = \omega_i \mid \omega_i \rangle$

   $\sum_i \omega_i = 1 \quad \omega_i \geq \omega_{i+1}$

   $\mathcal{O} = \left(\vec{w}_1, \cdots, \vec{w}_{D_b} \right)$

   $H_{block(L)} = \mathcal{O}^T \, H_{system(L)} \, \mathcal{O}$

DRMG Calculations

specifications

- block basis $D_b = 20 - 200 \longrightarrow$ superblock basis $D_s = 400 - 70000$
- usually $D_b = 60 \longrightarrow D_s = 5000$
- start with the infinite-size algorithm
- 3 sweeps in the finite-size algorithm

observables

- energy gap ΔE with and without targeting the excited state
- mean occupation number $\langle \hat{n}_i \rangle$
- particle fluctuation via $\langle \hat{n}_i^2 \rangle$
- one-body density-matrix via $\langle \hat{a}_i^\dagger \hat{a}_j \rangle$

Observables

Condensate Fraction (Onsager-Penrose Criterion)

- identify *natural orbitals* from the eigensystem of

$$\rho^{(1)}_{ij} = \langle\, \psi \,|\, \hat{a}^{\dagger}_{i} \hat{a}_{j} \,|\, \psi \,\rangle$$

- condensate fraction is defined via largest eigenvalue λ_{max} of $\rho^{(1)}$

$$f_c = \frac{\lambda_{max}}{N}$$

finite-size scaling: $\mathrm{Tr}\rho^{(1)} = N \quad \Longrightarrow \quad \lambda^{max} \geq N/I \quad \Longrightarrow \quad f_c \geq 1/I$

Observables

Interference Pattern and Visibility

- Fourier transformation of $\rho^{(1)}$ yields the interference pattern at δ

$$\mathcal{I}(\delta) = \frac{1}{I} \sum_{ij=1}^{I} e^{\mathbf{i}(i-j)\delta} \cdot \rho_{ij}^{(1)}$$

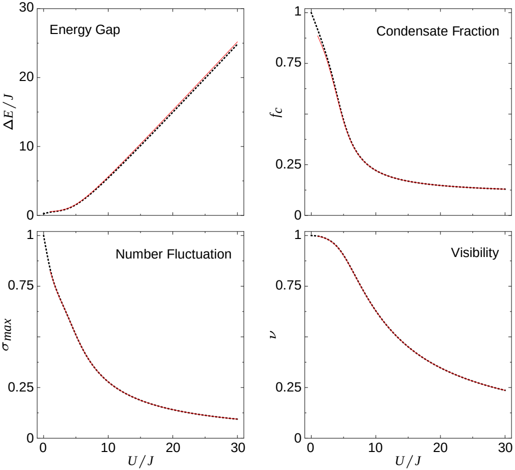
- visibility is defined as:

$$\nu = \frac{\max\{\mathcal{I}(\delta)\} - \min\{\mathcal{I}(\delta)\}}{\max\{\mathcal{I}(\delta)\} + \min\{\mathcal{I}(\delta)\}}$$

directly accessible to experiment via time-of-flight imaging

DMRG – Benchmark

- $I = N = 10$
- black: exact diagonalization
  ($D = 92\,378$)
- red: DMRG
  ($D_b = 21$, $D_s = 446$)
- perfect reproduction of all observables even in the SF phase

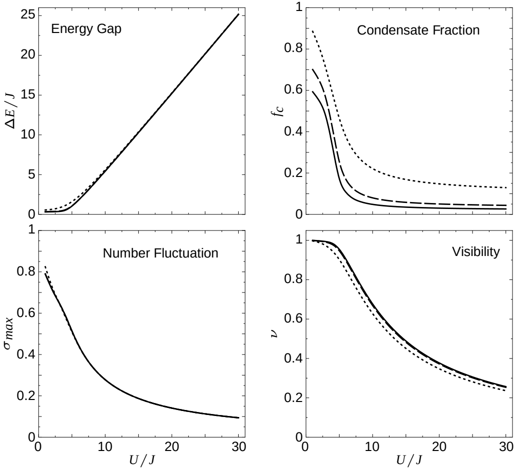


DMRG works fine

Observables – Finite-Size Effects

- dotted: $I = N = 10$
- dashed: $I = N = 30$
- solid: $I = N = 50$
- f_c shows expected finite-size effects

finite-size effects are under control

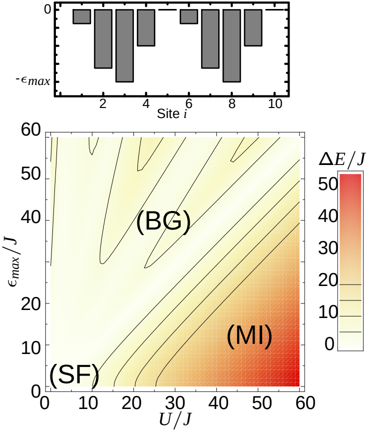


Phase Diagram – Two-Color Superlattice

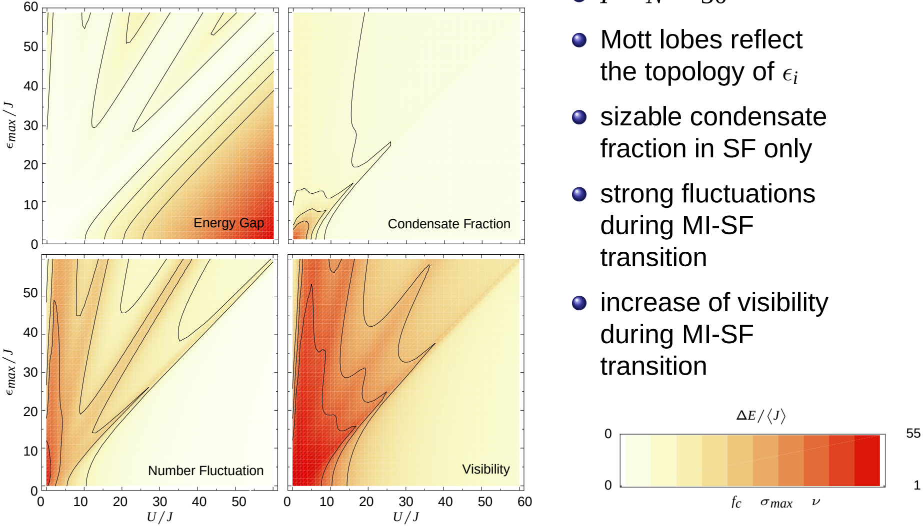
Hamiltonian

$$\hat{\text{H}} = \sum_{i=1}^{I} \left\{ -J \left(\hat{a}^\dagger_{i+1}\, \hat{a}_i + \hat{a}^\dagger_i\, \hat{a}_{i+1} \right) + \frac{1}{2} U \left(\hat{n}_i - 1 \right) \hat{n}_i + \epsilon_i\, \hat{n}_i \right\}$$

- on-site potential energy introduces irregularities
- subtle interplay of the different energy scales
- rich phase diagram:
  - superfluid (SF)
  - Mott-insulating (MI)
  - quasi Bose-glass (BG)



Observables – Generic Parameters

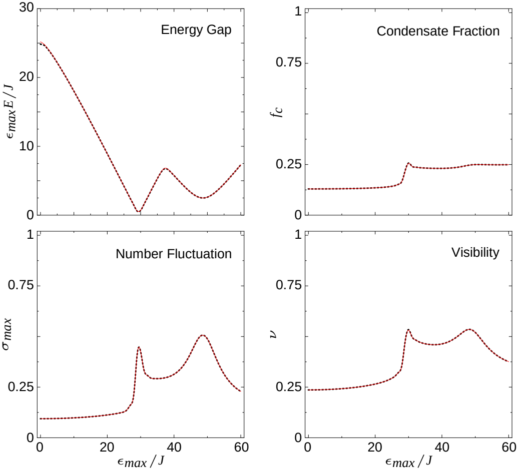


- $I = N = 30$
- Mott lobes reflect the topology of ϵ_i
- sizable condensate fraction in SF only
- strong fluctuations during MI-SF transition
- increase of visibility during MI-SF transition

DMRG – Benchmark

- $I = N = 10$
- $U/J = 30$
- black: exact diagonalization
  ($D = 92\,378$)
- red: DMRG
  ($D_b = 21$, $D_s = 446$)

DMRG does a good job in superlattices too

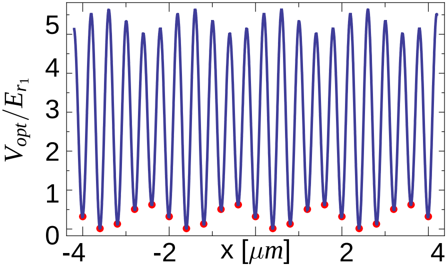


From Experiment to Hubbard Model

- two standing-wave laser-fields with wavelengths $\lambda_1,\ \lambda_2$
- natural energy scale is the *recoil energy* $E_{r_i} = \frac{h^2}{2m\lambda_i^2}$
- experimental knobs are the intensities $s_i = \frac{V_i}{E_{r_i}}$

1D Optical Two-Color Superlattice

$$V_{opt}(x) = s_1 E_{r_1} \sin^2\left(\frac{2\pi}{\lambda_1}x + \phi\right) + s_2 E_{r_2} \sin^2\left(\frac{2\pi}{\lambda_2}x\right)$$

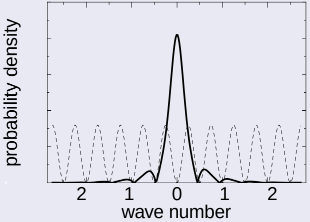


- commensurate lattice
- $\lambda_2 = 800\,nm$
  $s_2 = 5$
- $\lambda_1 = 1000\,nm$
  $s_1 = 1$
- $\phi = \pi/4$

Single-Particle Band-Structure Calculation (1D)

1. experimental parameters
   - laser wavelengths: λ_1, λ_2
   - laser intensities: s_1, s_2
   - scattering length: a_s
   - transverse trapping frequency: $\omega_\perp$
2. obtain localized Wannier function $w_i(x)$ from 1D bandstructure calculation
3. calculate Hubbard parameters for each site

Wannier function $w_i(x)$



$$-J_{i,i+1} = \int dx\, w_i^*(x) \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_{opt}(x) \right) w_{i+1}(x)$$

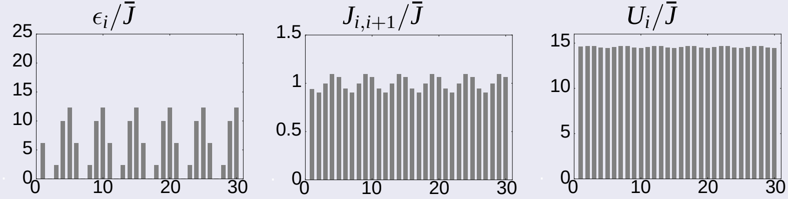
$$\epsilon_i = \int dx\, w_i^*(x) \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_{opt}(x) \right) w_i(x)$$

$$U_i = 2\, \omega_\perp \hbar\, a_s \int dx\, |w_i(x)|^4$$

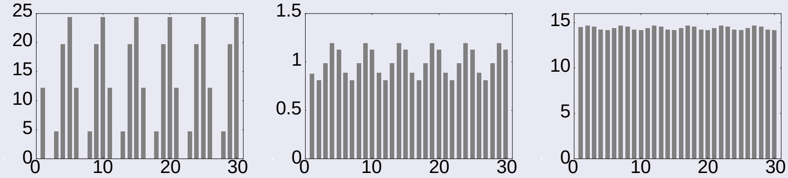
Site-Dependent Hubbard Parameters

$\lambda_2 = 800\,nm$, $\lambda_1 = 1000\,nm$, $\phi = \pi/4$, $\omega_\perp = 30 E_{r_1}$, ^{87}Rb

$s_2 = 10$, $s_1 = 0.5$

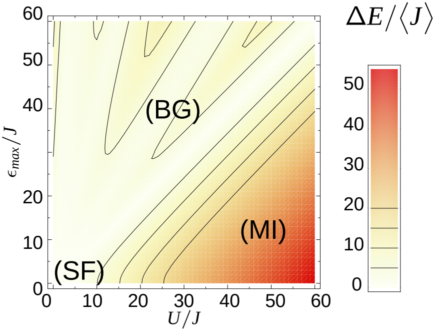


$s_2 = 10$, $s_1 = 1$

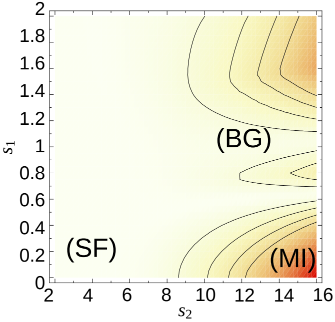


Phase Diagram – Commensurate Lattice

Hubbard parameters[1]



optical lattice parameters[2]



all phases accessible via s_1 and s_2

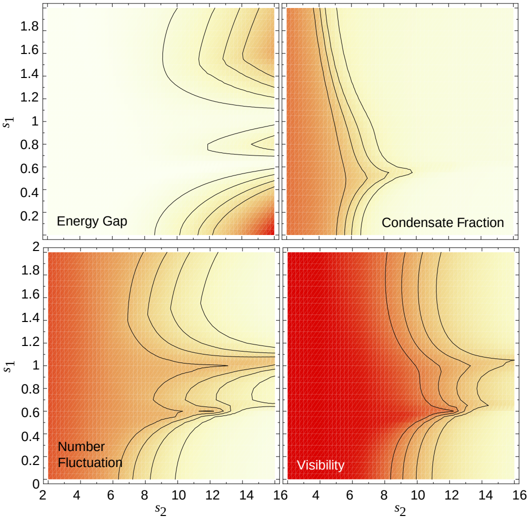
- superfluid phase (SF)
- quasi Bose-glass phase (BG)
- homogeneous Mott insulator (MI)

$$I = N = 30$$
$$\lambda_2 = 800\,nm,\ \lambda_1 = 1000\,nm$$
$$a_s = 109\,r_{Bohr},\ m = 85.5\,u$$
$$\omega_\perp = 30\,E_{r_1}/\hbar$$

[1] Roth et al. *Phys. Rev. A* **68**, 023604 (2003), Rapsch et al. *Europhys. Lett.* **46**, 559 (1999)

[2] Schmitt et al. *arXiv:0904.4397v1*

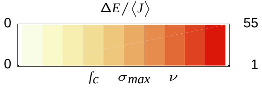
Observables – Commensurate Lattice



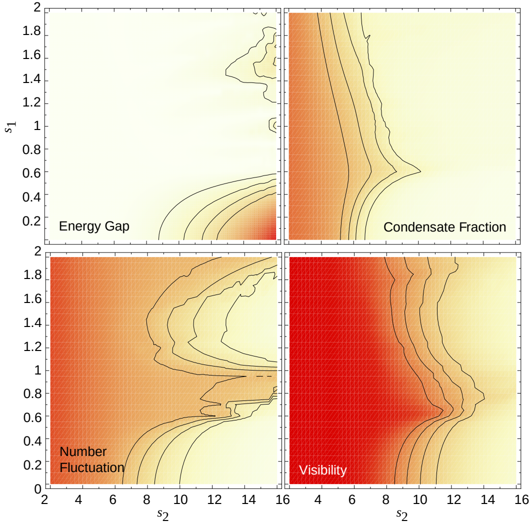
- commensurate lattice
- $\lambda_2 = 800\,nm$
- $\lambda_2 = 1000\,nm$

Transition to quasi Bose-glass

go to MI
$s_2 > 10$
and increase
$s_1 = 0 \rightarrow 2$

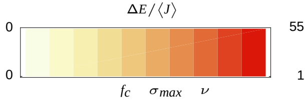


Observables – Incommensurate Lattice



- incommensurate lattice
- $\lambda_2 = 830\, nm$
- $\lambda_2 = 1076\, nm$

energy gaps in the BG are reduced



Summary

- Hubbard model & cold atoms in optical lattices
- observables in experiment & theory
- DMRG & benchmarks
- experimental parameters to Hubbard parameters
- phase diagrams expressed only by experimental parameters

Credits

Related Publications

- F. Schmitt, M. Hild, R. Roth: arXiv: 0904.4397
- M. Hild, F. Schmitt, I. Türschmann, R. Roth: Phys. Rev. A 76, 053614 (2007)
- F. Schmitt, M. Hild, R. Roth: J. Phys. B: At. Mol. Opt. Phys. 40, 371 (2007)
- M. Hild, F. Schmitt, R. Roth: J. Phys. B: At. Mol. Opt. Phys. 39, 4547 (2006)
- R. Roth, K. Burnett: Phys. Rev. A 68, 023604 (2003)

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