Ultracold Gases in 1D Optical Lattices
Exact Diagonalisation and more

Q 24 Quantengase (Bosonische Gitter II)

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Overview

1. Working Environment
   - Hubbard model in Wannier and Bloch bases
2. Solutions
   - exact diagonalisation
   - runcated diagonalisation
   - perturbative calculation
3. Summary

The Hubbard Model

- 1D optical lattice with I sites and N bosonic particles
- T=0K, nearest neighbour hopping and on-site interaction

Hamiltonian in Wannier Basis Representation

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

interaction term is diagonal in this basis

Hamiltonian in Bloch Basis Representation [1]

$$\hat{\mathrm{H}} = -J \sum_{k=0}^{I-1} 2\cos\left(\frac{2\pi}{I}k\right) \hat{\mathrm{n}}_k + \frac{V}{2I} \sum_{k,k',l}^{I-1} \hat{\mathrm{c}}_k^{\dagger}\, \hat{\mathrm{c}}_l^{\dagger}\, \hat{\mathrm{c}}_{k'}\, \hat{\mathrm{c}}_{k-k'+l}$$

tunnelling term is diagonal in this basis

J: hopping matrix element V: on-site interaction energy

[1] **Q 64.29** (Thursday 16:30, Poster C)

Many–Particle Eigenstates

Occupation Number Representation

$$|\,\nu\,\rangle = \sum_{\alpha=1}^{D} C_\alpha^{(\nu)}\;|\,\{\mathrm{n}_1,\mathrm{n}_2\ldots,\mathrm{n}_\mathrm{I}\}_\alpha\,\rangle$$ Wannier basis

Eigenvalue Problem

$$\sum_{\alpha=1}^{D}\langle\,\{\mathrm{n}_1,\mathrm{n}_2\ldots,\mathrm{n}_\mathrm{I}\}_\beta\,|\;\hat{\mathrm{H}}\;|\,\{\mathrm{n}_1,\mathrm{n}_2\ldots,\mathrm{n}_\mathrm{I}\}_\alpha\,\rangle\,C_\alpha^{(\nu)} = E_\nu C_\beta^{(\nu)}$$

D: dimension of the Hilbert space

- problem is the factorial growth of the Hilbert space
- worse for mixtures due to direct product of Hilbert spaces
- solvable on an ordinary PC up to $I = N = 12$ ($D \approx 10^6$) via Lanczos algorithms

Truncate the Hilbert Space

1. use an appropriate reference state
   - strongly correlated regime $V > J$: one particle per lattice site — Wannier basis $| \{1, 1, ..., 1\} \rangle$
   - superfluid regime $V \leq J$: all particles in quasimomentum zero state — Bloch basis $| \{N, 0, ..., 0\} \rangle$

2. successive particle-hole excitations
   - full np-nh space up to a given order
     similar to **C**onfiguration**I**nteraction
   - importance truncated space
     only number-states that satisfy the inequality:

$$\langle \{n_1, ...n_I\}_\alpha \mid \hat{H} \mid \{n_1, ...n_I\}_\alpha \rangle \leq \mathcal{E}_T$$ [1]

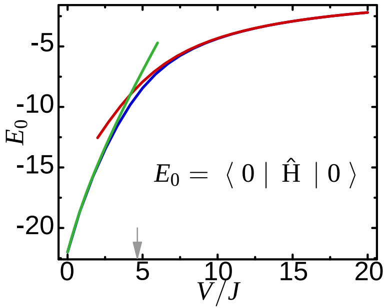
$\mathcal{E}_T$: truncation energy

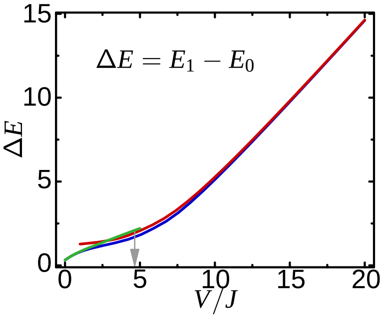
[1] F. Schmitt et. al. J.Phys.B: **40** 371-385 (2007)

Results I

$I = 11$ Particles on $N = 11$ Lattice Sites

blue	exact	$D_{complete} = 352\,716$
green	truncation in Bloch basis (6p6h)	$D/D_{complete} < 4\%$
red	truncation in Wannier basis (3p3h)	$D/D_{complete} < 3\%$





- Bloch basis: good agreement in the superfluid regime
- Wannier basis: good agreement in the strongly correlated regime

Results II

$I = 11$ Particles on $N = 11$ Lattice Sites

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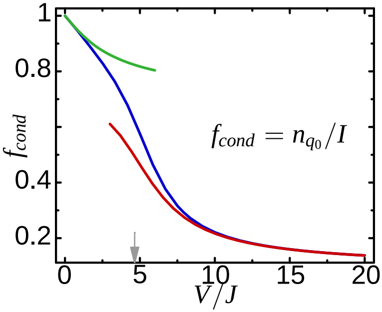
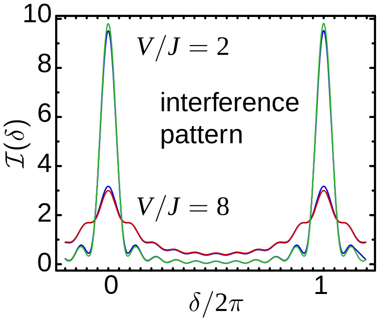




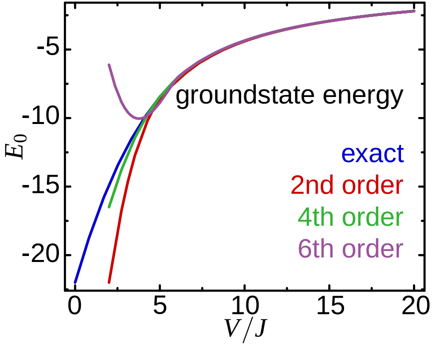
Perturbative Approach

Perturbation Series for $\hat{\mathrm{H}} = \hat{\mathrm{H}}_0 + \lambda\hat{\mathrm{H}}_1$

$$C_{n\nu}^{(k)} = \sum_{\mu\neq n} C_{n\mu}^{(k-1)} \frac{\langle\, \nu \mid \hat{\mathrm{H}}_1 \mid \mu \,\rangle}{E_n^{(0)} - E_\nu^{(0)}} - \sum_{i=1}^{k-i} C_{n\nu}^{(k-i)} \frac{E_n^{(i)}}{E_n^{(0)} - E_\nu^{(0)}}$$

$$E_n^{(k+1)} = \sum_{\mu\neq n} C_{n\mu}^{(k)} \langle\, \mathrm{n} \mid \hat{\mathrm{H}}_1 \mid \mu \,\rangle\,, \quad E_\nu^{(0)} = \langle\, \nu \mid \hat{\mathrm{H}}_0 \mid \nu \,\rangle$$

- Wannier basis
  - $\hat{\mathrm{H}}_0 = \hat{\mathrm{V}}\,,\ \hat{\mathrm{H}}_1 = \hat{\mathrm{J}}$
  - converges for $V/J > 5$
  - size consistent
  - numerical expensive
- Bloch basis
  - $\hat{\mathrm{H}}_0 = \hat{\mathrm{J}}\,,\ \hat{\mathrm{H}}_1 = \hat{\mathrm{V}}$
  - breakdown due to quasi-degenerate energy denominator



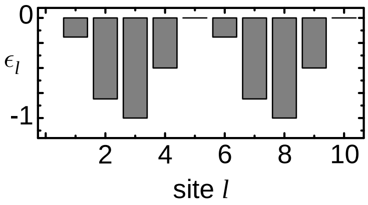
Application: Bose-Fermi Mixtures

Bose-Fermi Hubbard Hamiltonian with Superlattice Potential [1]

$$\hat{\mathrm{H}} = \hat{\mathrm{J}}_a + \hat{\mathrm{J}}_c + \hat{\mathrm{V}}_{aa} + \hat{\mathrm{V}}_{ac} + \Delta \sum_{l=1}^{I} \epsilon_l \left(\hat{\mathrm{n}}_l^{(a)} + \hat{\mathrm{n}}_l^{(c)} \right)$$

$\hat{\mathrm{J}}_a, \hat{\mathrm{J}}_c$	boson, fermion hopping operator ($J_a = J_c = J$)
$\hat{\mathrm{V}}_{aa}, \hat{\mathrm{V}}_{ac}$	boson-boson, boson-fermion interaction operator
Δ, ϵ_l	superlattice amplitude, superlattice topology

- two-colour superlattice
- Mott-insulator to quasi Bose-glass transition in pure bosonic systems [2]



[1] F. Schmitt et. al. J.Phys.B: **40** 371-385 (2007)

[2] R. Roth et. al. Phys. Rev. A **68**, 023604 (2003)

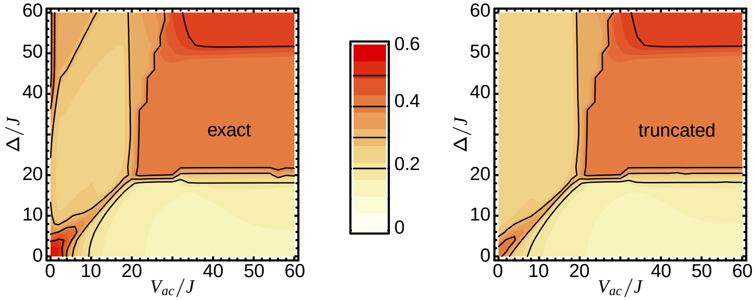
Application: Bose-Fermi Mixtures

$N_a = 5$ Bosonic, $N_c = 5$ Fermionic Particles on $I = 10$ Lattice Sites

exact	$D_{complete} = 504\,504$
truncated in Wannier basis	$D/D_{complete} < 15\%$

$V_{aa}/J = 20$ fixed   truncated basis optimised for $V_{aa} = V_{ac} = \Delta$

condensate fraction f_c of the bosonic species



- truncation scheme also works with mixtures

Summary

- looking for methods to solve the Bose-Hubbard model
- developed a truncation scheme to reduce the dimensionality of the Hilbert spaces
- access the phase diagram from both sides using Bloch- or Wannier-functions as single particle basis
- applied a straight forward perturbative calculation
- performed calculations for Bose-Fermi mixtures in two-colour superlattices