Summary & Motivation

- ultracold, dilute atomic gases in optical lattices are well described by the single-band Bose-Hubbard Hamiltonian\[2\]
- these are perfect laboratories to investigate the rich physics of strongly correlated quantum systems [1,5,6,7]
- the Bose-Hubbard Hamiltonian is transformed from the Wannier to the Bloch representation
- the ground state is obtained by an exact diagonalisation of the corresponding Hamilton matrix using Lanczos algorithms
- for reasons of symmetry only a small fraction of the coefficients of the ground state is non-zero
- with this reduced amount of number-states the static observables are accessible with the same precision as with the full basis [3,4]

Bose-Hubbard Model

- 1D optical lattice with \( I \) lattice sites and \( N \) bosonic particles
- nearest neighbour hopping, and on-site two-particle interactions

\[
H = -J \sum_{l=1}^{I} \left( \hat{a}_l^\dagger \hat{a}_{l+1} + h.c. \right) \text{ tunneling term} + U \sum_{l=1}^{I} \hat{n}_l (\hat{n}_l - 1) \text{ interaction term}
\]

\( \hat{a}_l^\dagger, \hat{a}_l \) creation, annihilation, occupation-number operators

\( U \) two particle interaction energy

Transformation to Bloch Basis

- operators transformed into Bloch basis \( q_j = \frac{2\pi j}{I} \)

\[
\hat{c}_j^\dagger = \frac{1}{\sqrt{I}} \sum_{l=1}^{I} e^{-iq_j l/a} \hat{a}_l, \quad \hat{c}_j = \frac{1}{\sqrt{I}} \sum_{l=1}^{I} e^{iq_j l/a} \hat{a}_l
\]

\( \Rightarrow \) Bose-Hubbard Hamiltonian in Bloch basis

\[
H = -J \sum_{j=0}^{I-1} \sum_{m=0}^{I-1} \cos(q_j - q_m) \hat{n}_j + U \sum_{j=0}^{I-1} \sum_{k=0}^{I-1} \sum_{m=0}^{I-1} \sum_{n=0}^{I-1} \hat{c}_j^\dagger \hat{c}_k^\dagger \hat{c}_m \hat{c}_n
\]

- states are represented in a quasimomentum occupation number basis with dimension \( D \)

\[
| \psi^{(0)} \rangle = \sum_{\alpha} C^{(0)}_{\alpha} | \{ n_0, \ldots, n_{I-1} \} \alpha \rangle
\]

Reduced Basis

- in many cases only the ground state observables are of interest
- to calculate those we only have to take into account the Fock-states with quasimomentum equal zero
- thus we can reduce the size of the Hilbert space without any loss of information

\[
\langle \psi^{(0)}_{\text{reduced}} | \psi^{(0)}_{\text{full}} \rangle = 1
\]

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<th>Reduced Dimension</th>
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</table>

Energy Spectrum

- energy-bands of eight particles and different interaction strengths

Some Observables

- mean occupation number \( \bar{n} \) and fluctuation of the mean occupation number \( \sigma \), for 10 particles with varying interaction strength \( U/J \)
- the mean occupation number at \( q_j = 0 \) is equal to total particle number for \( U/J = 0 \)
  \( \Rightarrow \) a perfect condensate
- for larger \( U/J \) the condensate is depleted

- the maximum coefficient \( C_{\text{max}} \) decreases with increasing \( U/J \)
- \( C_{\text{max}} \) is strongly correlated to the mean occupation number of the quasimomentum zero state
- for strongly correlated systems the interference pattern forms a broad bump, whereas for small \( U/J \) on \( q_j = 0 \) there is a sharp peak