Numerical study of the Bose-Hubbard model

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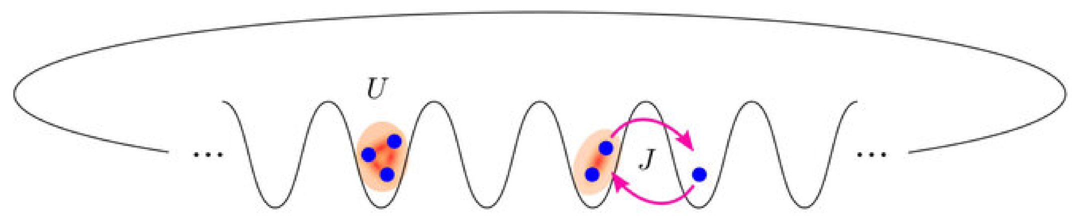
Abstract

The **Bose-Hubbard model** describes interacting bosons on a lattice and is central to the study of the **superfluid–Mott insulator transition**. We compare two methods to obtain its ground state energy, **one-body** and **two-body** reduced density matrices: **exact diagonalization** and a **semidefinite programming (SDP) approach**. This formulation reduces the complexity and enables the study of larger systems.
For a ring configuration of M sites we write the Hamiltonian as follow:

$$\hat{H} = -J\sum_{j=1}^{M}\left(\hat{a}^\dagger_{j+1}\hat{a}_j + \hat{a}^\dagger_j\hat{a}_{j+1}\right) + U\sum_{j=1}^{M}\frac{\hat{n}_j(\hat{n}_j-1)}{2}$$



J is the **tunneling amplitude** between neighboring sites, and U is the **on-site repulsive interaction** strength.

Exact diagonalisation in the Fock basis

The **Fock basis** describes quantum states by **occupation numbers** at each site. For N bosons on M lattice sites, a Fock state is written as:

$$|n_1, n_2, \ldots, n_M\rangle, \quad \text{with} \sum_{j=1}^{M} n_j = N,$$

where n_j is the number of particles on site j.
The number of Fock states $\mathcal{N}_N^M$ grows exponentially with N and M:

$$\mathcal{N}_N^M = \binom{N+M-1}{M-1}$$

To efficiently construct the Bose-Hubbard Hamiltonian, each Fock state is assigned a **unique integer label**, using the *Ponomarev ordering* [1]. This reversible mapping between labels and occupation vectors allows us to quickly locate any state in the Hamiltonian matrix and reduce the naive complexity of $\left(\mathcal{N}_N^M\right)^2$ matrix entries to $\mathcal{N}_N^M(M+1)$.

Some usefull tools of many-body physics

One-body reduced density matrix (1RDM):

$$\rho^{(1)}_{ij} = \langle\phi|\hat{a}^\dagger_i\hat{a}_j|\phi\rangle$$

→ particle probabilities (diag.) + coherences (off-diag.)

Two-body reduced density matrix (2RDM):

$$\rho^{(2)}_{ij,kl} = \langle\phi|\hat{a}^\dagger_i\hat{a}^\dagger_j\hat{a}_l\hat{a}_k|\phi\rangle$$

→ pair probabilities + pair coherences

Condensed fraction:

$$f_{\text{cond}} = \frac{\lambda_{\max}}{\text{Tr}\,\rho^{(1)}} \qquad \lambda_{\max} \text{ is the largest eigenvalue of the 1RDM}$$

→ occupation of the most populated single-particle state

SDP approach

Key idea. Variational principle
For any normalized state $|\phi\rangle$ in the Hilbert space:

$$E_{\text{gs}} \le \langle\phi|\hat{H}|\phi\rangle,$$

with equality when $|\phi\rangle = |\psi_{\text{gs}}\rangle$ is the ground state.

Key equality.

$$\langle\phi|\hat{H}|\phi\rangle = \text{Tr}(H^{(1)}\rho^{(1)}) + \text{Tr}(H^{(2)}\rho^{(2)}),$$

with

$$H^{(1)}_{ij} = -J\,\delta_{|i-j|,1}, \quad H^{(2)}_{ij,kl} = \frac{U}{2}\,\delta_{ijkl}.$$

We replace the many-body wavefunction $|\phi\rangle$ by the 1RDM and 2RDM, reducing the number of variables from $\mathcal{N}_N^M$ to $M^2 + M^4$.

SDP formulation:

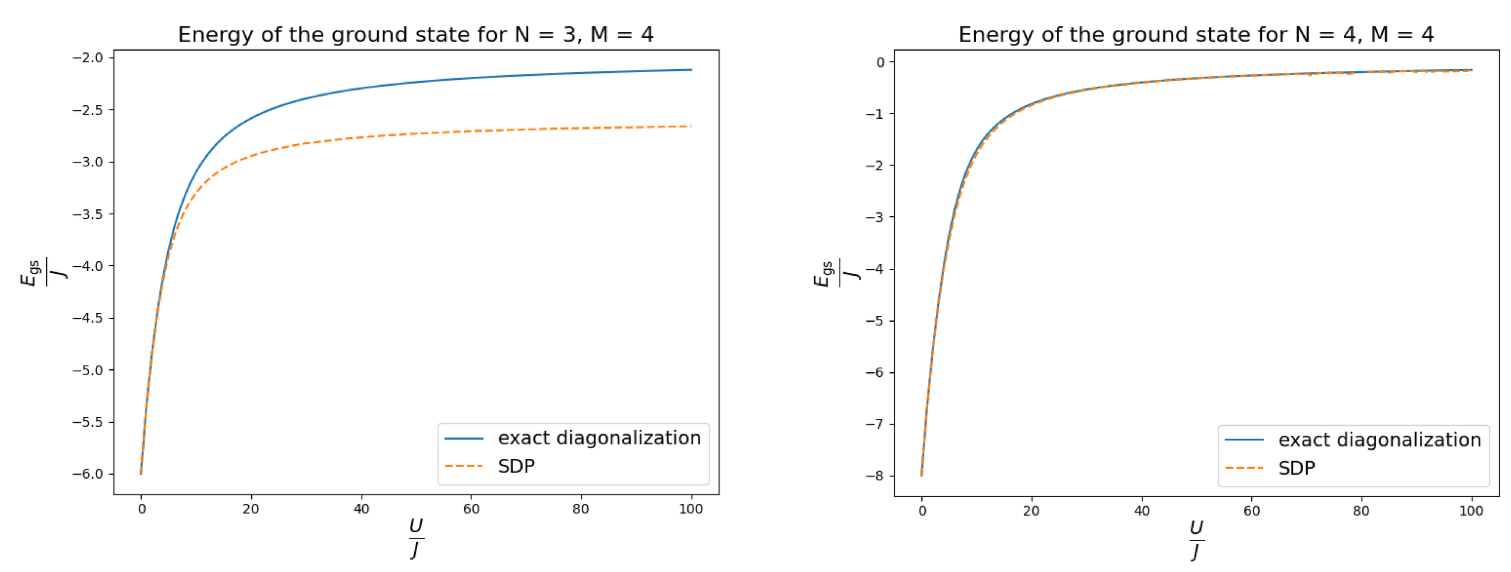
$$\begin{aligned}&\text{minimize } \text{Tr}(H^{(1)}\rho^{(1)}) + \text{Tr}(H^{(2)}\rho^{(2)})\\ &\text{subject to } \rho^{(1)}, \rho^{(2)} \succeq 0, \text{ plus many others necessary constraints! [2]}\end{aligned}$$

N-representability

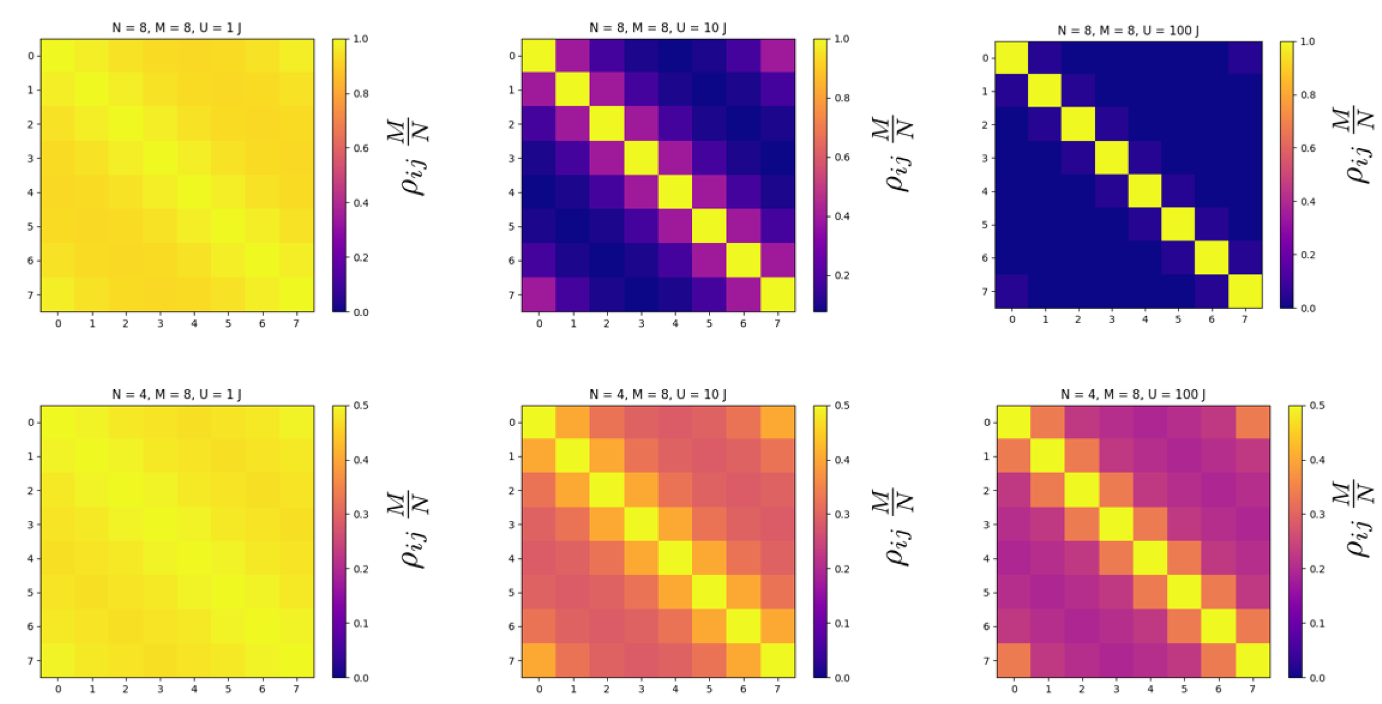
Determining whether a given set of 1RDM and 2RDM comes from a true N-particle quantum state is **intractable** (QMA-hard). The constraints we use are **necessary but not sufficient**, and the SDP solution provides **a lower bound** to the ground-state energy.

Results

Ground state energy:

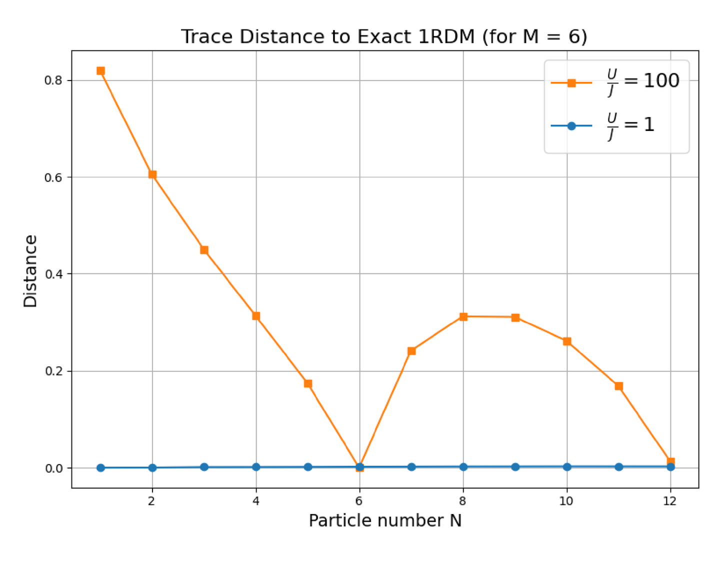


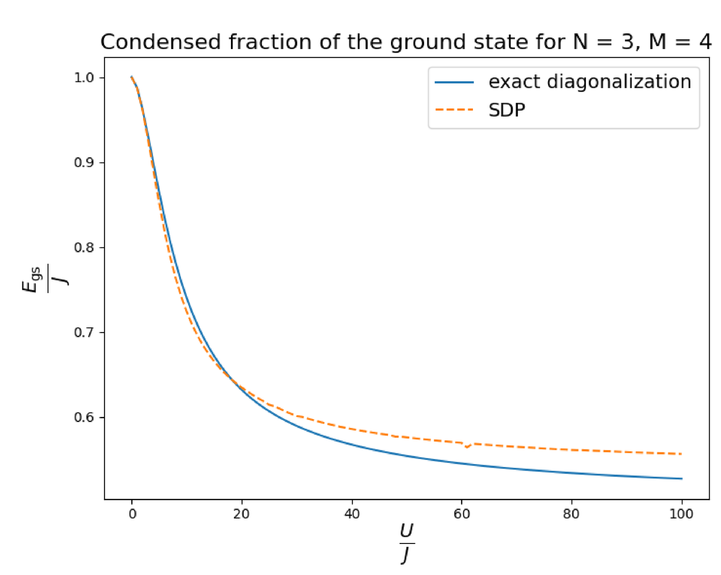
1RDM (exact diagonalization):



1RDM for filling factor 1 and $\frac{1}{2}$; $\frac{U}{J}$=1, 10 and 100.

Accuracy of SDP





References

[1] David Raventós i Ribera. *Exact diagonalization studies of quantum simulators.* Phd thesis, Institute of Photonic Sciences (ICFO), 2019.

[2] Mitchell J. Knight, Harry M. Quiney, and Andy M. Martin. *Reduced density matrix approach to one-dimensional ultracold bosonic systems.* School of Physics, University of Melbourne, March 2025.