

Variational Study of hard-core Bosons in a 2-D Optical Lattice using Projected Entangled Pair States (PEPS)

V. Murg¹, F. Verstraete^{1,2} and J. I. Cirac¹

¹ Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Strasse 1, Garching D-85748, Germany
² Institute for Quantum Information, Caltech, Pasadena, US



Abstract

We study the system of **hard-core bosons on a 2-D optical lattice** using a variational algorithm based on **projected entangled-pair states (PEPS)**. We investigate the ground state properties of the system as well as the responses of the system to sudden changes in the parameters. We compare our results to mean field results based on a Gutzwiller ansatz.

Introduction

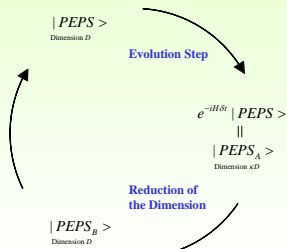
Main Idea

We study the ground state properties and the dynamics of **hard-core bosons in an optical lattice** by applying a variational algorithm based on PEPS.

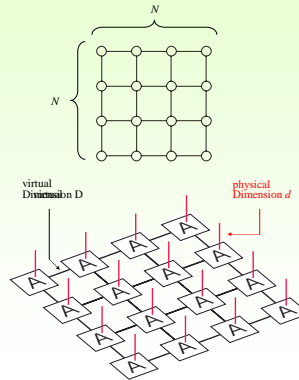
This algorithm simulates the time-evolution within the **subset of PEPS with a fixed virtual dimension D**.

It consists of two main elements:

- **Evolution Step**
The virtual dimension of the PEPS increases by a factor κ .
- **Reduction of the Dimension**
The state of the system is approximated by the „nearest“ PEPS with virtual dimension D .



Projected Entangled-Pair States (PEPS)



Definition:

$$|PEPS\rangle = \sum_{k_1, \dots, k_{N_1}=1}^d F(\{A_{\alpha\beta\gamma\delta}^k\}) |k_1, \dots, k_{N_1}\rangle$$

$$A_{\alpha\beta\gamma\delta}^k = \text{[Diagram of a tensor with four legs and an index k]}$$

PEP-states are favorable for variational calculations, because

- they are adequate for representing the **ground-state** of numerous **many-body systems** and
- they possess an **internal refinement parameter**, the **virtual dimension D**, that allows to control the precision of the calculation.

The Algorithm

Reduction of the Dimension

The aim is to optimize the coefficients of $|PEPS_A\rangle$ with virtual dimension κD , such that its distance to $|PEPS_B\rangle$ with virtual dimension D is minimal:

$$K = \|\langle PEPS_A | - | PEPS_B \rangle\|^2 \rightarrow \text{Min.}$$

This optimization is done site-by-site until convergence is reached.

Due to the special structure of PEPS, the distance K is **quadratic** with respect to the parameters B_i associated with one lattice site i . Because of this, the optimal parameters with respect to this site can simply be found by solving a **system of linear equations**.

$$|PEPS_A\rangle = e^{-iH\delta t} |PEPS\rangle \rightarrow |PEPS_B\rangle$$

$$K \propto \langle PEPS_B | PEPS_B \rangle - 2 \text{Re} \langle PEPS_A | PEPS_B \rangle$$

$$\uparrow \quad \quad \quad \uparrow$$

$$B_i^\dagger M B_i \quad \quad \quad \mathbf{w}^\dagger B_i$$

$$\frac{\partial K}{\partial B_i} = 0 \quad \Leftrightarrow \quad M B_i = \bar{\mathbf{w}}$$

Calculation of M and $\bar{\mathbf{w}}$

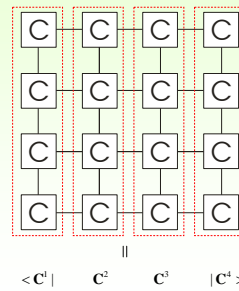
Calculation of M and $\bar{\mathbf{w}}$

The calculation of the **coefficient matrix M** and the **inhomogeneity $\bar{\mathbf{w}}$** of the system of linear equations is **intractable**. Because of this, an approximate method has to be used.

The approximate method consists in

- rewriting **M** and **w** in terms of products of **matrix product operators (MPO)** and a **matrix product state (MPS)** – which can be interpreted as a **time-evolution of a MPS**.

- This time-evolution can be performed **efficiently** by restricting the evolution to the subset of **MPS** with a fixed **virtual dimension**.



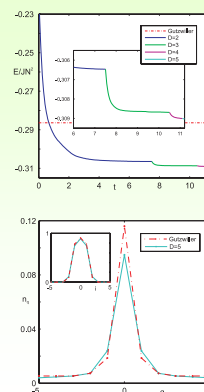
Ground State Properties

Imaginary Time Evolution

We calculate the **ground state** by means of an imaginary time evolution.

- **Upper Plot:**
The **imaginary time evolution** is performed with $D=2$ until convergence is reached; then evolutions with $D=3$, $D=4$ and $D=5$ follow. The energy of the final PEPS lies well below the Gutzwiller ansatz.

- **Lower Plot:**
There is a clear difference between the **momentum distribution** derived from the PEPS and the one derived from the Gutzwiller ansatz. In contrast, they both produce a similar **density distribution** (see inset).



System under Study

Hard-core bosons in a 11×11 optical lattice with a harmonic trap:

$$H = -J \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + \sum_i V_i \hat{n}_i$$

$$(a_i^\dagger)^2 = 0$$

$$\gamma = \frac{E_{\text{kin}}}{E_{\text{int}}} = \frac{U}{J} \rightarrow \infty$$

Dynamics of the System

Real Time Evolution

We investigate the responses of the system to sudden changes in the parameters.

- **Upper Plot:**
The plot shows the evolution of the condensed fraction of the condensate after a **sudden change of the trap frequency**. What can be observed is that the results obtained from using PEPS are qualitatively different from the results based on the Gutzwiller ansatz.

- **Lower Plot:**
The **overlap** between the PEPS with $D=2$ and $D=3$ is close to 1 – which indicates a fast convergence with increasing **virtual dimension D**.

