Spectral weight of bosonic excitations near Mott insulator-superfluid transition in 1D

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December 2, 2014

Outline

Density matrix renormalization group

DMRG is a numerical technique for finding approximate ground states and low lying excited states of low dimensional strongly correlated quantum models

- Roots in Wilson's RG
- Introduced by White in 1992
- Nowadays it is the most efficient method for treating 1D systems with applications in many fields

Real space renormalization group

Problem:

- Treating large quantum systems with limited memory

Solution:

- Break the system into blocks which can be diagonalized
- Choose the lowest lying eigenstates as an effective basis for the block
- Join two blocks
- Repeat

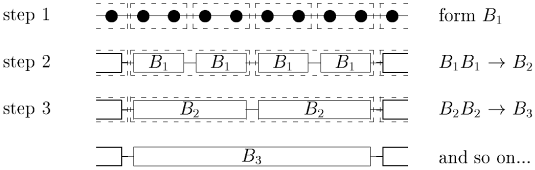

Figure: Formation of blocks in RSRG. [Till D Kühner. *Dynamics with the Density-Matrix Renormalization Group* (1990). PhD thesis]

Breakdown of RSRG:

- Lowest lying state of AA cannot be approximated properly using the lowest lying states of A
- This error is a consequence of the truncation procedure

Workaround: using different boundary conditions - only for non-interacting systems

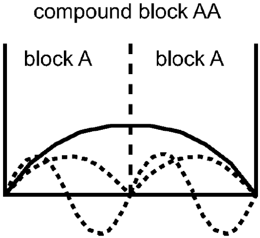

Figure: Block eigenstates for a tight binding model describing a single particle hopping on a chain. [Ulrich Schollwöck. *The density-matrix renormalization group*. Reviews of Modern Physics, 77(1):259, 2005.]

DMRG

In order to correct the errors of RSRG:

1. Embed the system in an environment
2. Change the way we choose the states we keep:

$$\| \, |\psi\rangle - |\tilde{\psi}\rangle \, \| \rightarrow \text{ min}$$

$\Rightarrow$ Satisfied when we truncate the states with the smallest density-matrix weight

Density matrix

$$\rho_{ii'} = \sum_j \psi^*_{ij} \psi_{i'j}$$

$|\psi\rangle = \sum_{ij} \psi_{ij} \, |i\rangle \, |j\rangle$ eigenstate of the block Hamiltonian

Infinite system DMRG

1. Start with block A
2. Add a site to form system block $A\bullet$
3. Reflect to obtain the environment block $\bullet A'$
4. Form the superblock $A \bullet \bullet A'$
5. Calculate the ground state $|\psi\rangle$ of the superblock
6. Form the density matrix $\rho = |\psi\rangle \langle\psi|$
7. Diagonalize the density matrix and keep the m eigenstates with the largest eigenvalues
8. $A \leftarrow A\bullet$ in the truncated basis, go to step 2

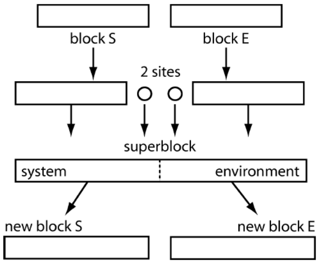

Figure: Infinite system DMRG blocks. [Ulrich Schollwöck. *The density-matrix renormalization group*. Reviews of Modern Physics, 77(1):259, 2005.]

Finite system DMRG

- By constantly increasing the size of the superblock, truncation is never made in terms of the correct target state
- Finite size DMRG changes the size of the system and the environment while keeping the superblock size constant

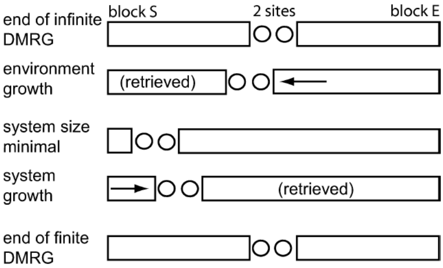

Figure: Finite system DMRG sweep. [Ulrich Schollwöck. *The density-matrix renormalization group.* Reviews of Modern Physics, 77(1):259, 2005.]

Finite size DMRG

1. Use infinite system DMRG algorithm to build up the system
2. Use finite system DMRG sweeps to tune it

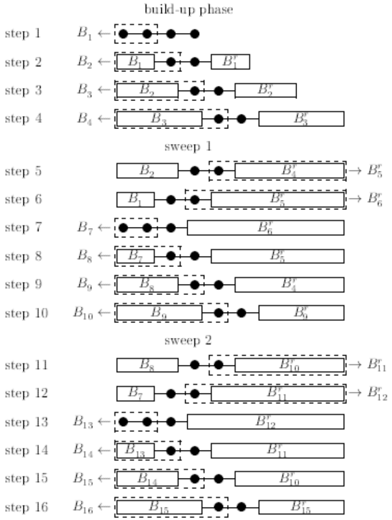

Figure: Finite size DMRG. [Till D Kühner. *Dynamics with the Density-Matrix Renormalization Group* (1990). PhD thesis]

Bose-Hubbard model

System of bosons on a lattice chain having repulsive on-site interaction, and lowering energy by hopping to neighburing sites on the lattice

Bose-Hubbard Hamiltonian in 1D

$$H = \underbrace{-t\sum_i (b_i^\dagger b_{i+1} + b_i b_{i+1}^\dagger)}_{\text{hopping term}} + \underbrace{\frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1)}_{\text{interaction term}} - \mu \sum_i \hat{n}_i$$

$b_i^\dagger / b_i$ - bosonic creation/annihilaton operators on site i
$n_i = b_i^\dagger b_i$ - number of particles on site i
t - hopping matrix element
U - on-site Coulomb repulsion
μ - chemical potential

Phases of the Bose-Hubbard model

Competition between

- **the hopping term**, which tries to delocalize the system
- **the on-site interaction term**, which tries to localize the particles and reduce the fluctuations

gives rise to two distinct phases:

Superfluid phase: single-particle wavefunctions spread out over the entire lattice, non-integer filling

Mott insulator phase: localized wavefunctions with a fixed number of atoms per site, integer filling

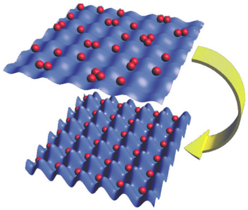

Figure: Superfluid-Mott insulator transition

[greiner.physics.harvard.edu]

Phase diagram of the 1D Bose-Hubbard model

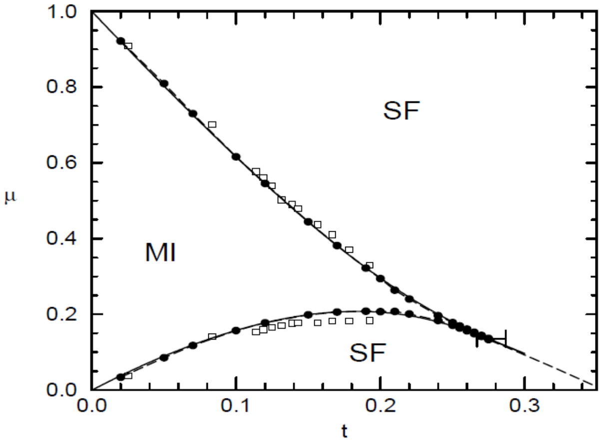

Figure: Phase diagram of the Bose-Hubbard model. [Till D Kühner and H Monien. *Phases of the one-dimensional Bose-Hubbard model*. Physical Review B, 58(22):R14741, 1998.]

Treating the Bose-Hubbard model with DMRG

- Cut-off number of particles per site introduced
- Ground state particle number is equal to the number of sites
- Both infinite and finite size algorithms are used
- Increased accuracy by targeting multiple states

$$\rho = \sum_{i=1}^{n} \omega_i \rho_i$$

- Address operator representation

Representation of operators

Make use of the fact that the particle number is conserved
$\Rightarrow$ Operators can be broken into sectors

$$H = \begin{pmatrix} \boxed{H_1} & & & & \\ & \boxed{H_2} & & & \\ & & \boxed{H_3} & & \\ & & & \boxed{H_4} & \\ & & & & \boxed{H_5} \end{pmatrix}$$

Representation of operators in the wavevector space

$$A_q = \frac{1}{N} \sum_n A_n \cos(q x_n) f(x_n)$$

$f(x_n)$ is the filtering function
$N = \sum_{n=1}^{L} f(x_n)$

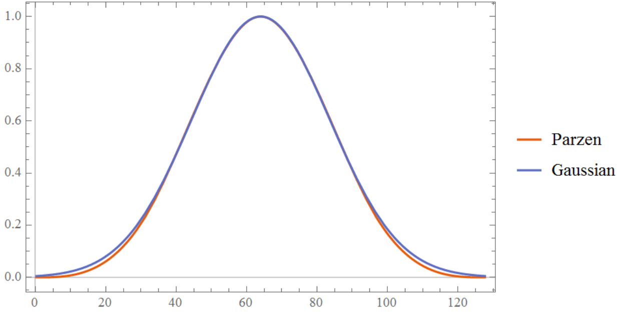

Figure: Parzen filter

Phase diagram of the 1D Bose-Hubbard model

Obtaining the phase diagram:

- Three states are targeted: ground state g and ground state with an added particle p or hole h

$$\mu_p = E_p - E_g$$

$$\mu_h = E_g - E_h$$

- Critical point expected around $t_c/U = 0.27$

Parameters used:

- $L = 128$
- $n_{max} = 4$
- $n_{states} = 16$
- $n_{sweeps} = 2$

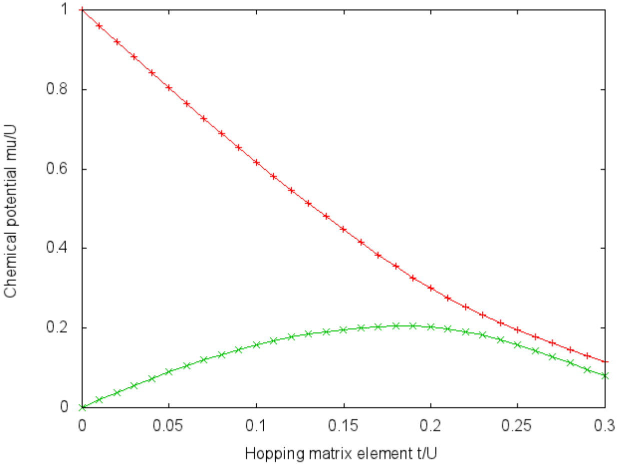

Figure: Phase diagram of the Bose-Hubbard model

Spectral weight of the bosonic excitations

Calculated value:

$$Z(q) = |\langle 1|b_q^\dagger|0\rangle|^2$$

Expected result:

- High values in the Mott and superfluid phase
- Drop around the critical point

Parameters:

- $L = 128$
- $n_{max} = 3$
- $n_{states} = 8$
- $n_{sweeps} = 2$

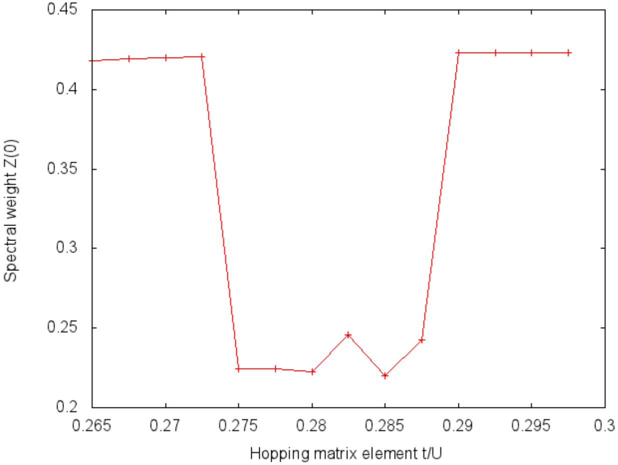

Figure: Spectral weight of the bosonic excitations

Summary and outlook

- DMRG - an effective method for treating low dimensional strongly correlated systems
- Bose Hubbard model - a simple bosonic model, realized in experiments with ultracold atoms
- Applying DMRG to the system, we are able to see the superfluid-Mott insulator transition
- Improve the code to obtain better accuracy and resolution of the results

Thank you for your attention