

Numerical Computations of Quantum Phase Transitions in Cold Atoms

Bhanu Pratap Das

Indian Institute of Astrophysics
Bangalore

Co Workers:

Tapan Mishra (IIA, Bangalore)

Meetu Sethi (IIA, Bangalore)

Ramesh V. Pai (Univ. of Goa)

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SF-MI transition for bosons in a periodic lattice potential

Bose-Hubbard Model :

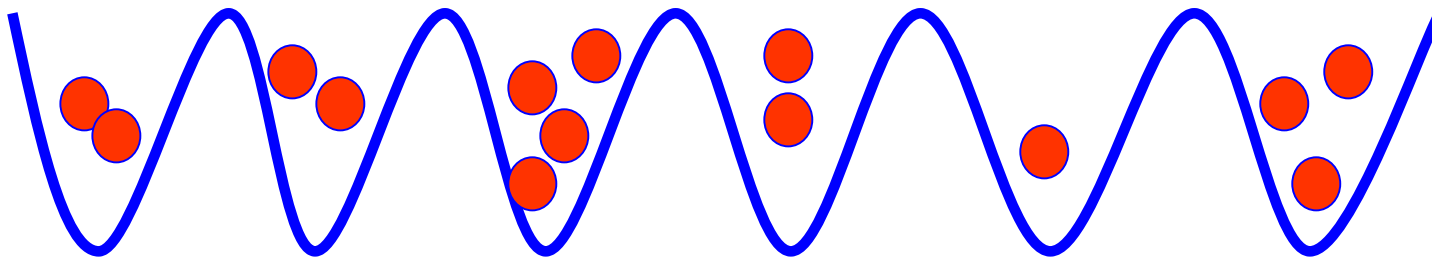
$$H = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + h.c) + \frac{U}{2} \sum_i n_i(n_i - 1)$$

↪ hopping ↪ onsite interaction

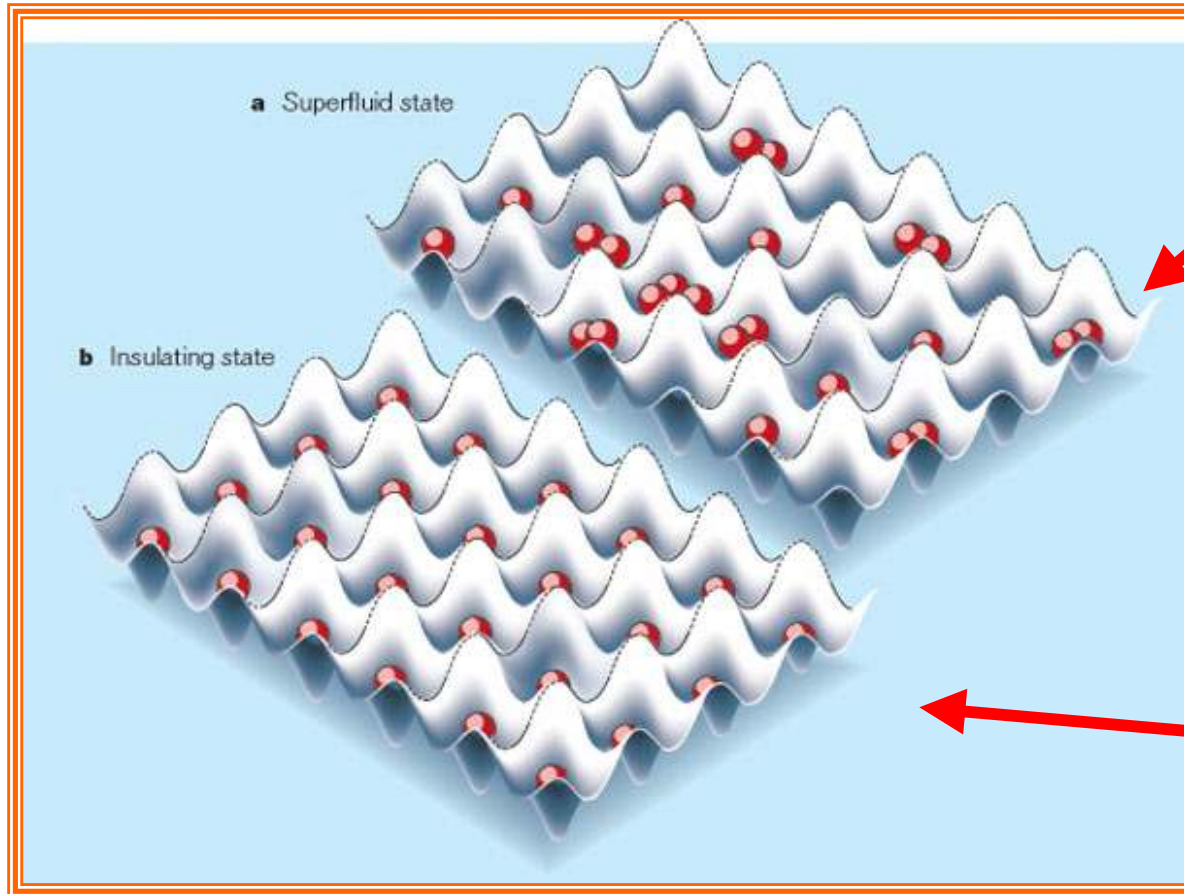
$U/t \ll 1$: Superfluid

Fisher et al, PRB(1989)

$U/t \gg 1$: Mott insulator



SF-MI Transition In Optical Lattice



- $U/t \ll 1$
- Random distribution of atoms
- superfluidity

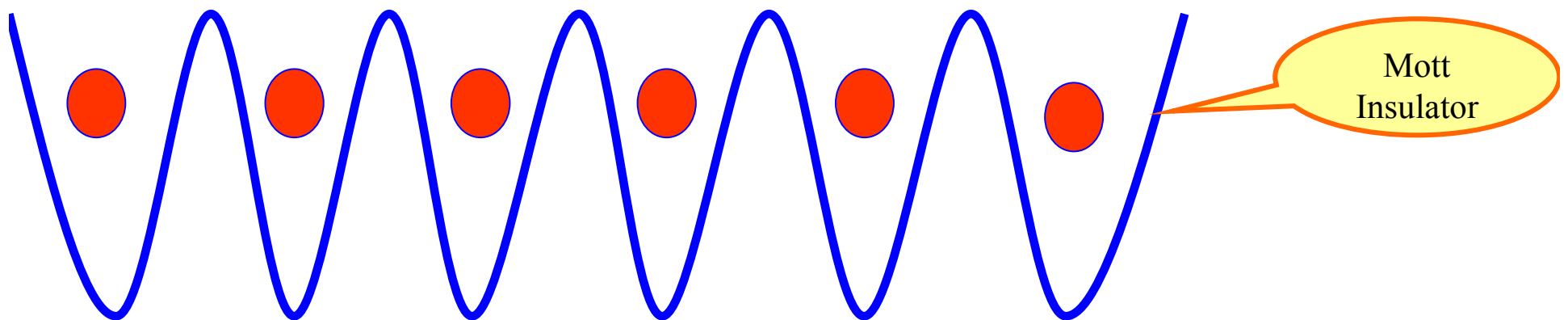
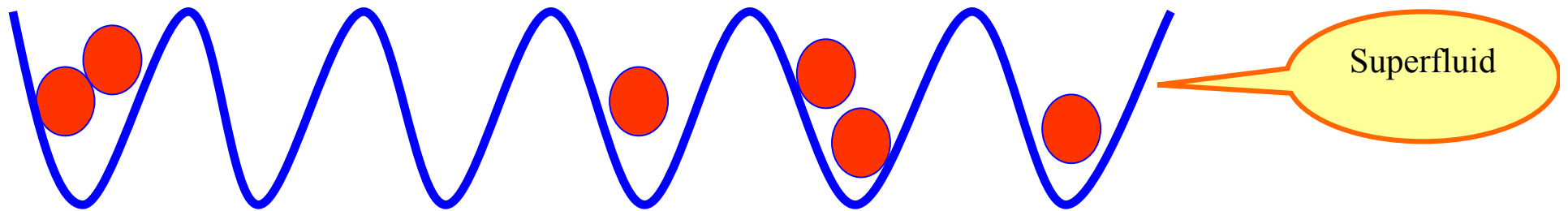
Uncertainty principle
 $\Delta x \Delta p \sim \hbar$

- $U/t \gg 1$
- Confined atoms
- Mott insulator

Greiner et al, Nature(2002) : 3D
Stoeflerle et al, PRL (2004) : 1D

Physics Noble prize(2001) for work on BEC

SF-MI transition in One component Boson with Filling factor = 1



Solve Schroedinger's equation, $H\psi = E\psi$

Necessary to know the ground state wavefunction ψ_0 and energy E_0 to determine the phase of the system.

$$\psi = \sum_i C_i \phi_i$$
$$\begin{pmatrix} H \end{pmatrix} \begin{pmatrix} C \end{pmatrix} = \begin{pmatrix} E \end{pmatrix} \begin{pmatrix} C \end{pmatrix}$$

Size of "H" increases with the increase in the system size as more lattice sites are included.

Reduction of the system size by Density Matrix Renormalization Group(DMRG), which can be applied to 1D lattice systems.

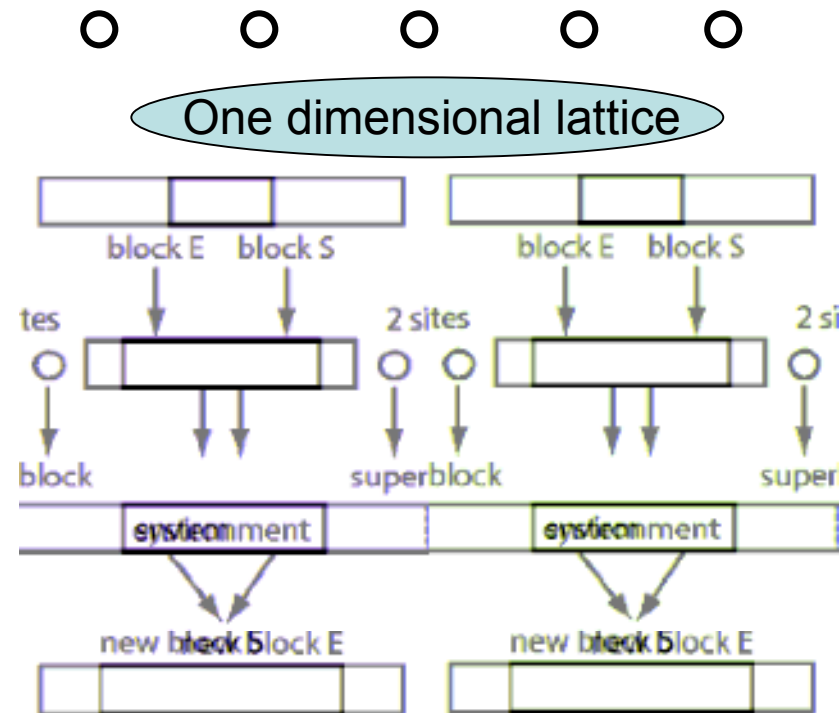
The most important states are the eigen states of the density matrix whose eigen values are above a particular threshold value.

DMRG method consists of two iterative diagonalizations:

- 1) Hamiltonian "H"
- 2) Density Matrix

The size of the above matrices is of the order of $10^5 \times 10^5$

Flow chart of the DMRG Method



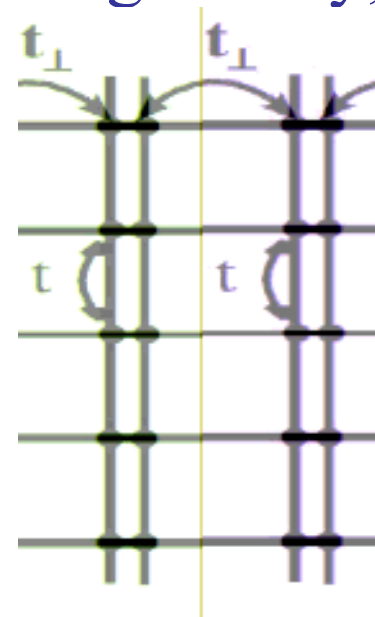
- Typical dimension of the Hamiltonian and density matrix is 400×400 at 4 sites level.
- That increases further by enlarging the system size
- Maximum dimensions of the Hamiltonian and the density matrix are both $10^6 \times 10^6$

- For our problem we deal with the ground state wave function $|\psi_0\rangle$ and the ground state energy E_0 .
- We need the above quantities for different values of hopping amplitude(t) and interatomic potential(U). This enables us to get the necessary phase diagram and find the critical points for the SF-MI transition.
- We therefore need to run multiple jobs for different values of “ t ” and “ U ”.

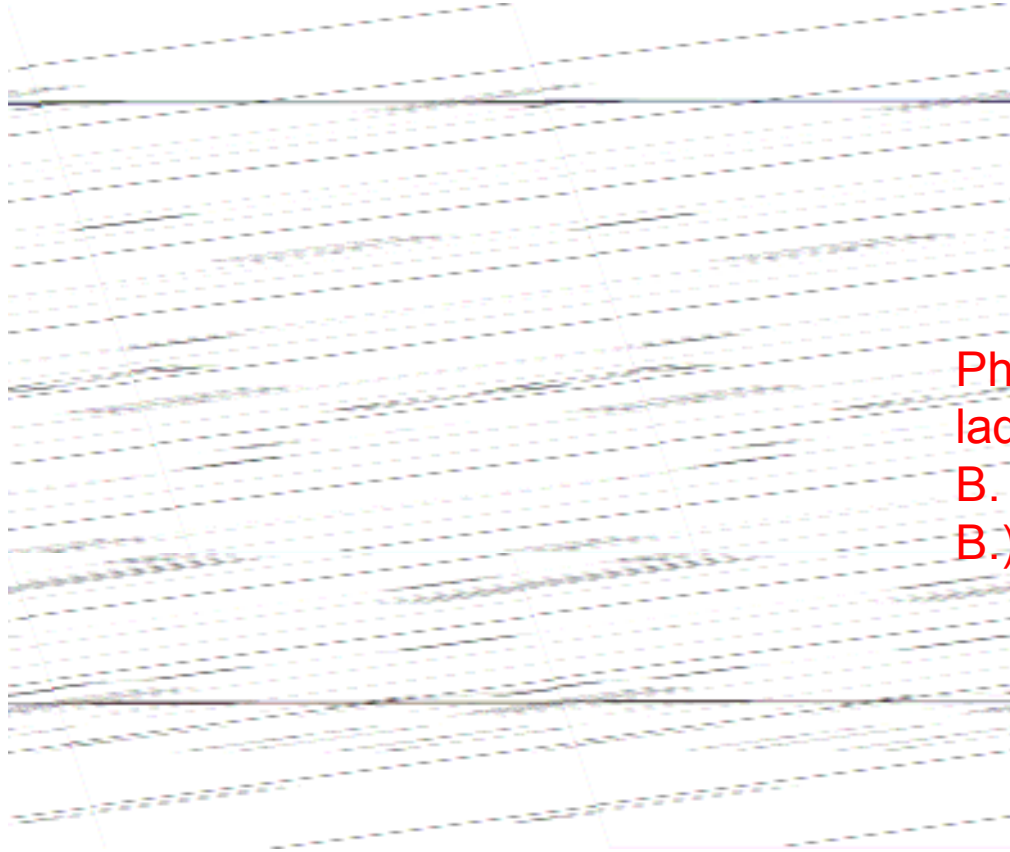
Results using GARUDA

- We have studied the SF-MI transition in a two leg bosonic ladder.
- The model Hamiltonian in this case is given by,

$$\begin{aligned}
 & \sum_{i,a} a_{i,a}^\dagger \left(t_{1,\alpha} a_{i+1,\alpha} + t_{2,\alpha} a_{i+2,\alpha} \right) + h.c. \sum_{i,a} \left(a_{i,a}^\dagger a_{i+1,\alpha} + t_{2,\alpha} a_{i+2,\alpha} \right) + h.c. \sum_{i,a} \left(a_{i,a}^\dagger a_{i+1,\alpha} + t_{2,\alpha} a_{i+2,\alpha} \right) \\
 & + n_{i,a} (n_{i,a} - 1) \frac{U}{2} \sum_{i,a} n_{i,a} (n_{i,a} - 1) \frac{U}{2} \sum_{i,a} \\
 & + (a_{i,1}^\dagger a_{i,2} + h.c.)_{\perp} \sum_i (a_{i,1}^\dagger a_{i,2} + h.c.)_{\perp} \sum_i
 \end{aligned}$$



Phase Diagram



Phase diagram of two leg Bose ladder, M. Sethi, T. Mishra, R. V. Pai, B. P. Das (Submitted to Phys. Rev. B.)

For a fixed value of t_{\perp} we used various clusters available in GARUDA to calculate the energies and the wavefunctions for a series of values of t_{\perp} and U and got above phase diagram .

Clusters used in the work are from : (a) IGIB, Delhi (b) RRI , Bangalore (c) Chennai (d) Hyderabad

Future Plans

- Parallelization of the Davidson method for the diagonalization of the Hamiltonian.
- Parallelization of the diagonalization of the density matrix
- Parallelization of the calculation of various correlation functions
- Automatic generation of the Hamiltonian matrix elements using artificial intelligence methods.

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