Computational Studies On Ultra-Cold Atoms: Recent Results from Garuda

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Outline of systems with Ultra-cold Atoms: Bosons in a periodic potential

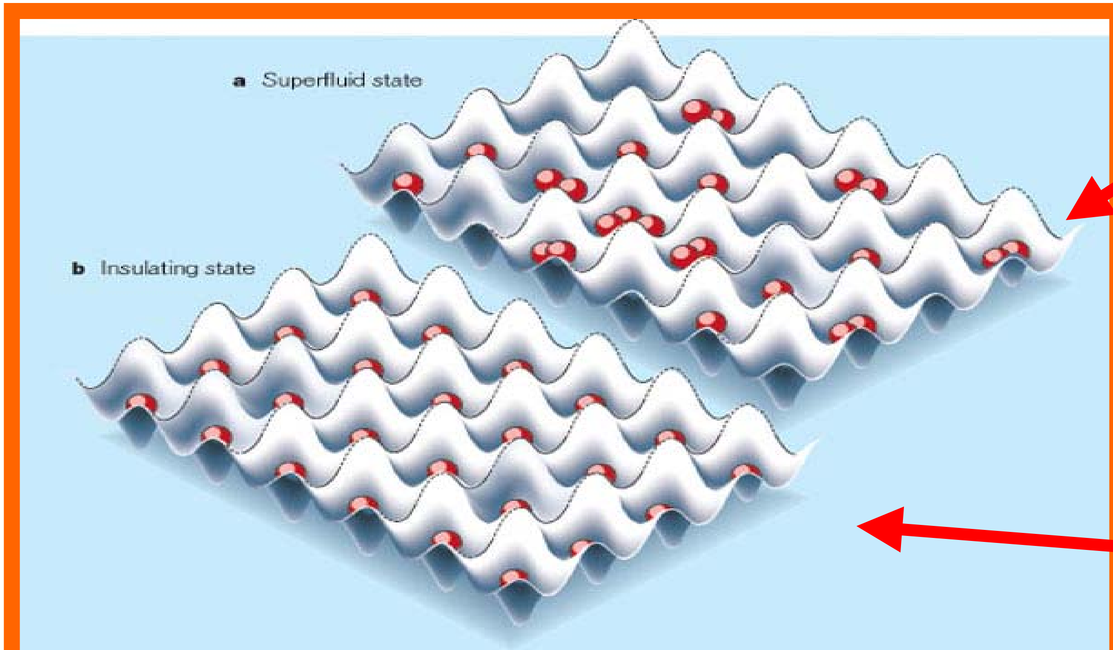
Bose-Hubbard Model :

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

hopping

onsite interaction

- U/t << 1
- Random distribution
- of atoms -Superfluid

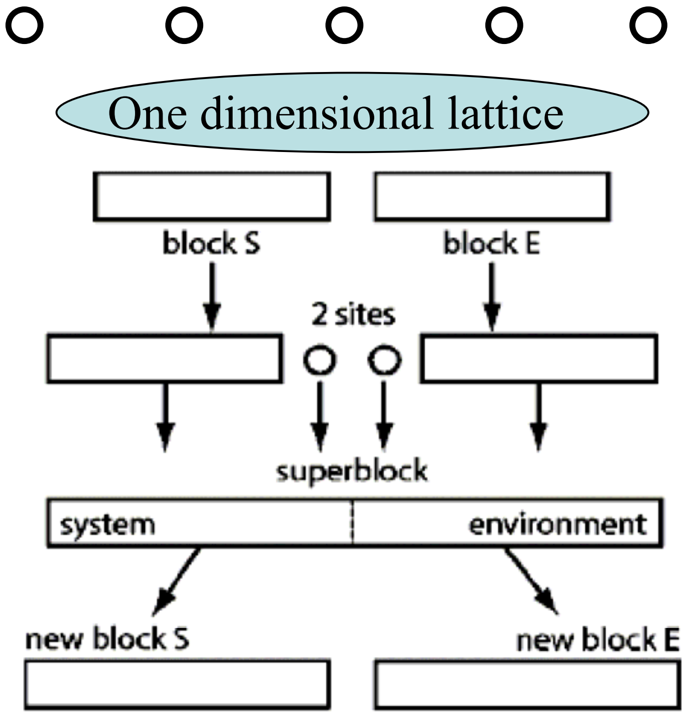


Integer density =>
SF-MI transition
Quantum Phase Transition!

- U/t >> 1
- Confined atoms
- Mott insulator

Physics Noble prize(2001) for work on BEC

Flow chart of the DMRG Method



DMRG - An iterative method
starting with a 4-site problem-100 sites
Each time adding two sites.

- Solve Schrodinger'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.

$$\psi = \Sigma_i C_i \Phi_i$$

$$\begin{pmatrix} & & \\ & H & \\ & & \end{pmatrix} \begin{bmatrix} \\ C \\ \\ \end{bmatrix} = \begin{pmatrix} & & \\ & E & \\ & & \end{pmatrix} \begin{bmatrix} \\ C \\ \\ \end{bmatrix}$$

- 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 Method ,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.These are the most probable states of the block in the ground state of the Superblock
- Only a certain no. of states of the Density Matrix (decided by the cut-off) with highest eigen-values kept.
- These are the eigen-states of the block in the next iteration.
- DMRG method consists of two iterative diagonalizations done using Davidson's algorithm::
- Hamiltonian “H”
- Density Matrix
- Density Matrix is block-diagonalised based on the occupation number.
- Size of the Hamiltonian matrix increases in each iteration.

➢Typical dimensions of the Hamiltonian matrix at four site level with density =1 and maximum occupancy of each site restricted to three bosons:

- Single species bosons – 31x31
- Bosonic Ladder – 3800x3800.

➢That increases further by enlarging the system size.

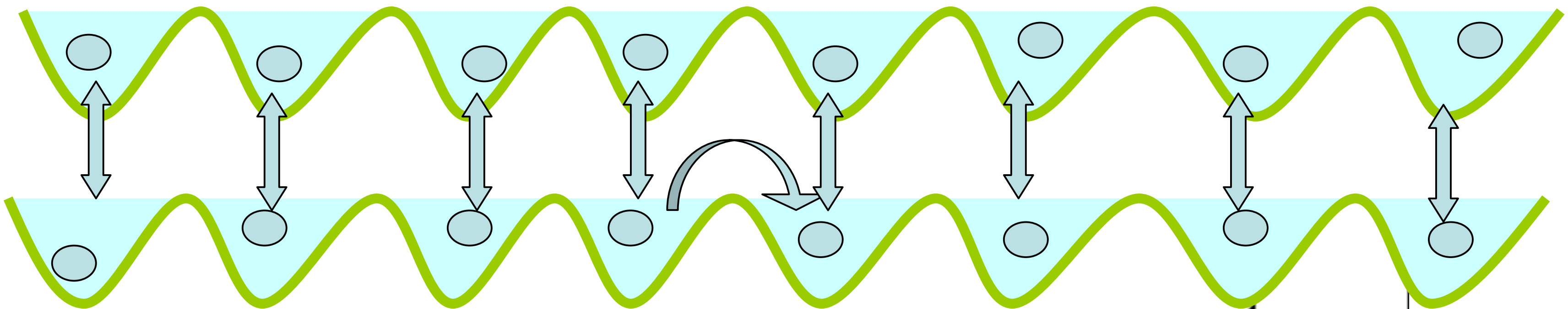
➢Dimensions of the Hamiltonian matrix for various systems for 100 sites:

- Single species - 25,000 x 25,000
- Ladder case - 4,00,000 x 4,00,000

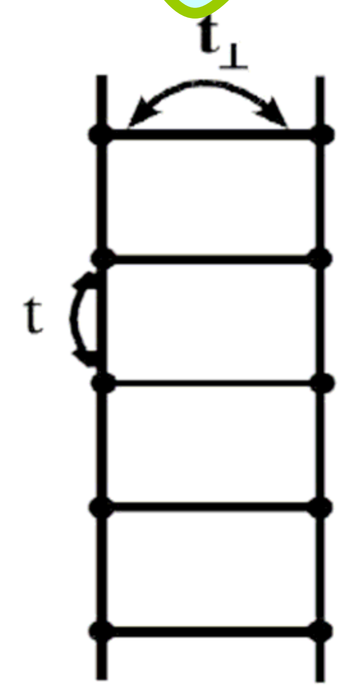
- For our problem we deal with the ground state wave function $|\psi_0>$ and the ground state energy E_0
- We need the above quantities for different values of hopping amplitude(t) and interatomic potential(U). This enables us to get the necessary phase diagram and find the critical points for the SF-MI transition.
- We therefore need to run multiple jobs for different values of "t" and "U".
- Depending on the system, we can have more variable parameters,like the trap potential, nearest neighbour interaction and so on.

Results using GARUDA

1. We have studied the SF-MI transition in a two leg bosonic ladder.



$$\mathcal{H} = -t\sum_{i,\alpha}(a^{\dagger}_{i,\alpha}a_{i+1,\alpha} + h.c) + \frac{U}{2}\sum_{i,\alpha} n_{i,\alpha}(n_{i,\alpha} - 1) - t_{\perp}\sum_{i}(a^{\dagger}_{i,1}a_{i,2} + h.c).$$

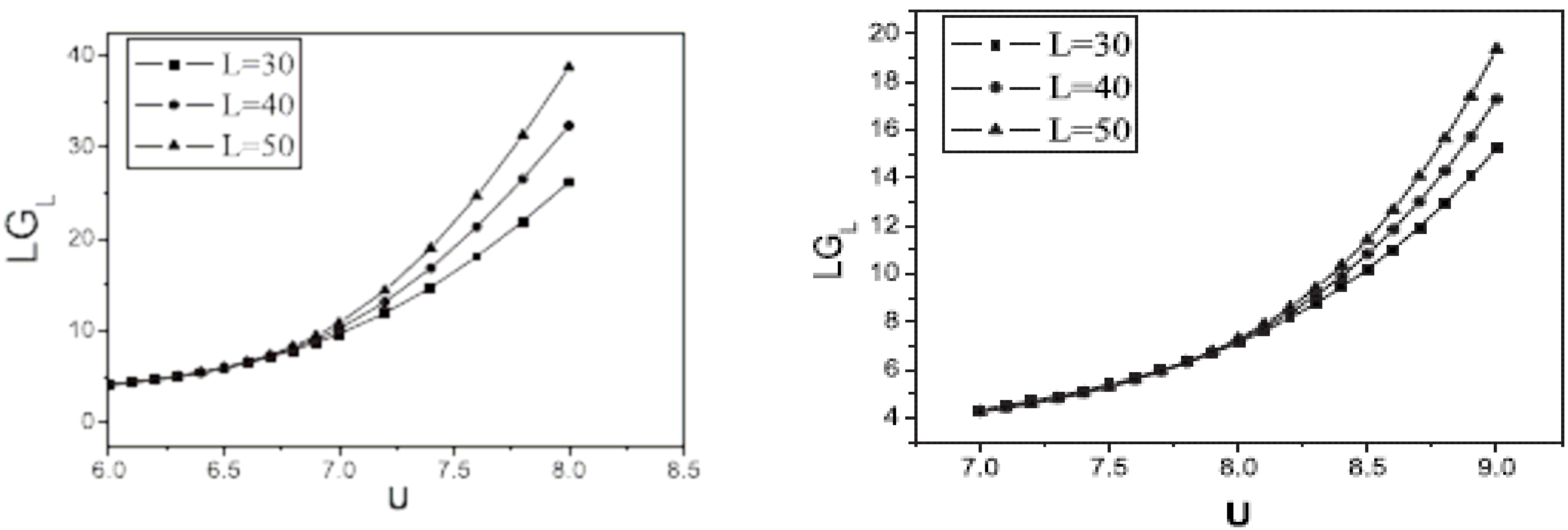


We calculate the single particle excitation gap for different sets of the system parameter;

$$G_L = E_L(N+1) - E_L(N) - [E_L(N) - E_L(N-1)]$$

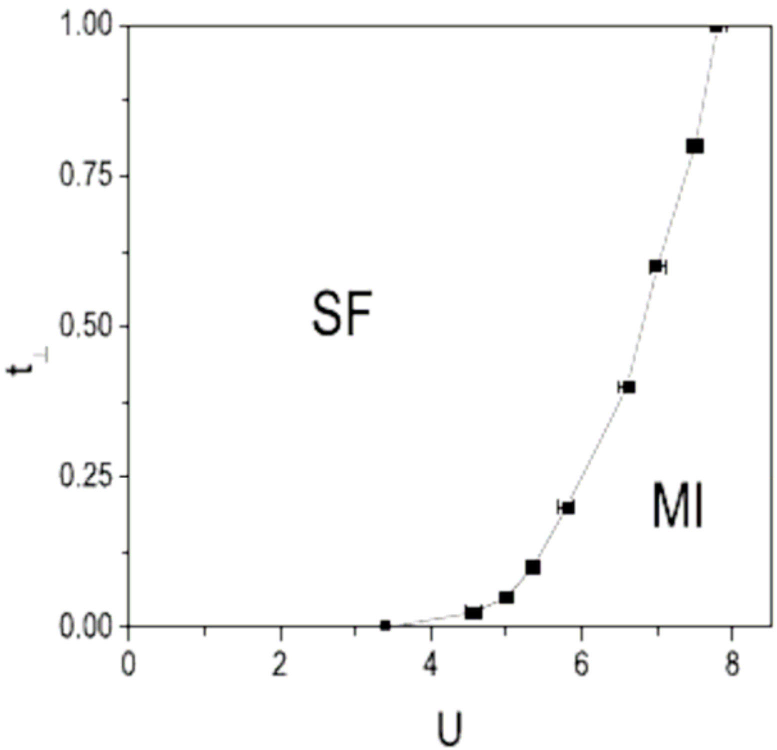
By doing the finite size scaling we get the critical point of the SF-MI transition.

When $t_\perp = 0$ then $U_c = 3.4$. U_c increases when $t_\perp$ increases.



Plot showing the SF-MI transition for $t_\perp = 0.4$ and 1

Phase Diagram

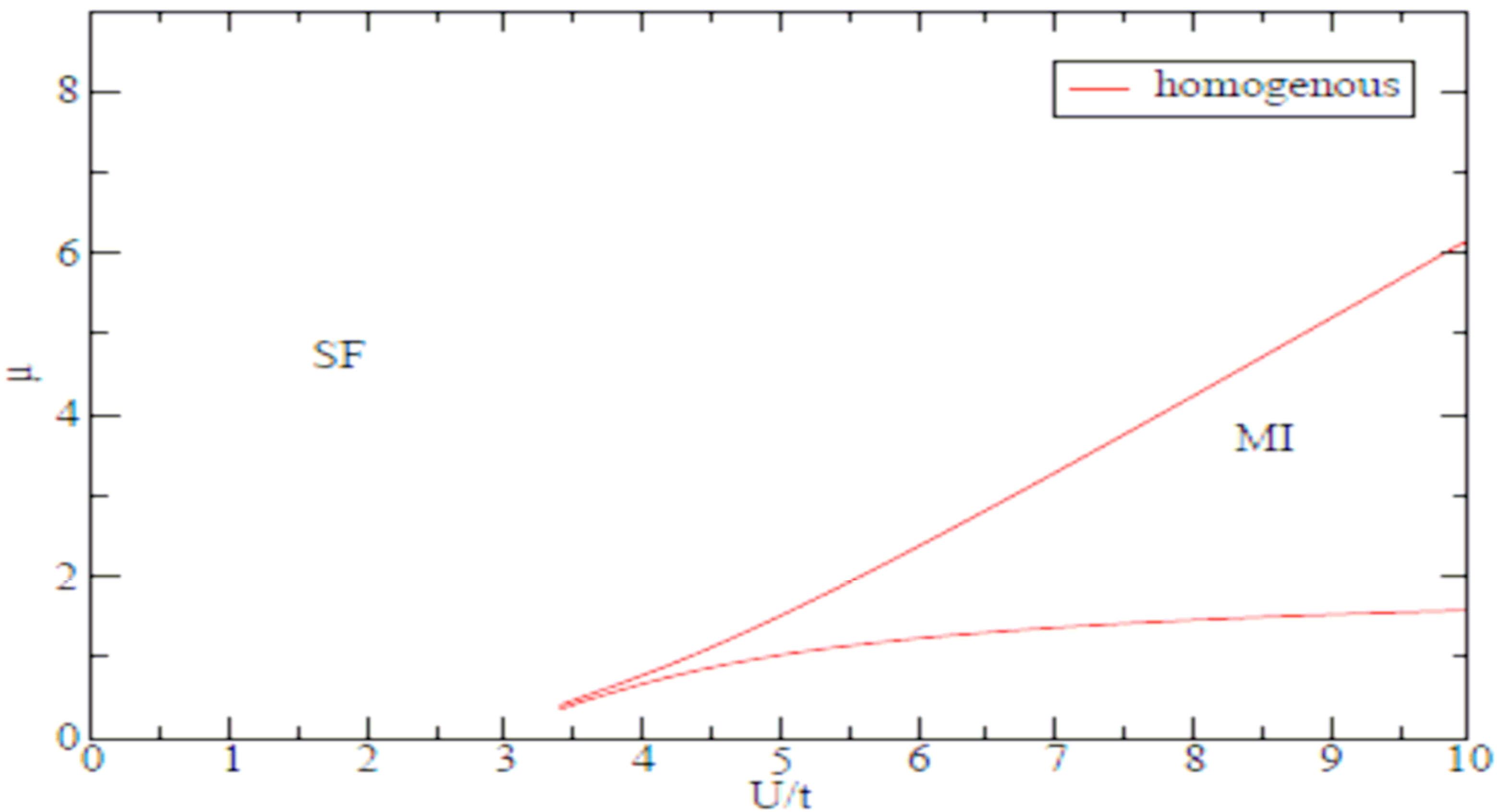


Phase diagram of two leg Bose ladder, M. Sethi, T. Mishra, R. V. Pai, B. P. Das, Phys. Rev. B **78**, 165104 (2008)

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) IITG,(b) IGIB, Delhi (c) RRI , Bangalore.

2. We have obtained the phase diagram of a single species homogenous system as well as a system confined by a trap.



This shows that there is a QPT at Uc=3.4. The system completely goes to MI phase from SF phase at n=1

QPT in the presence of Trap

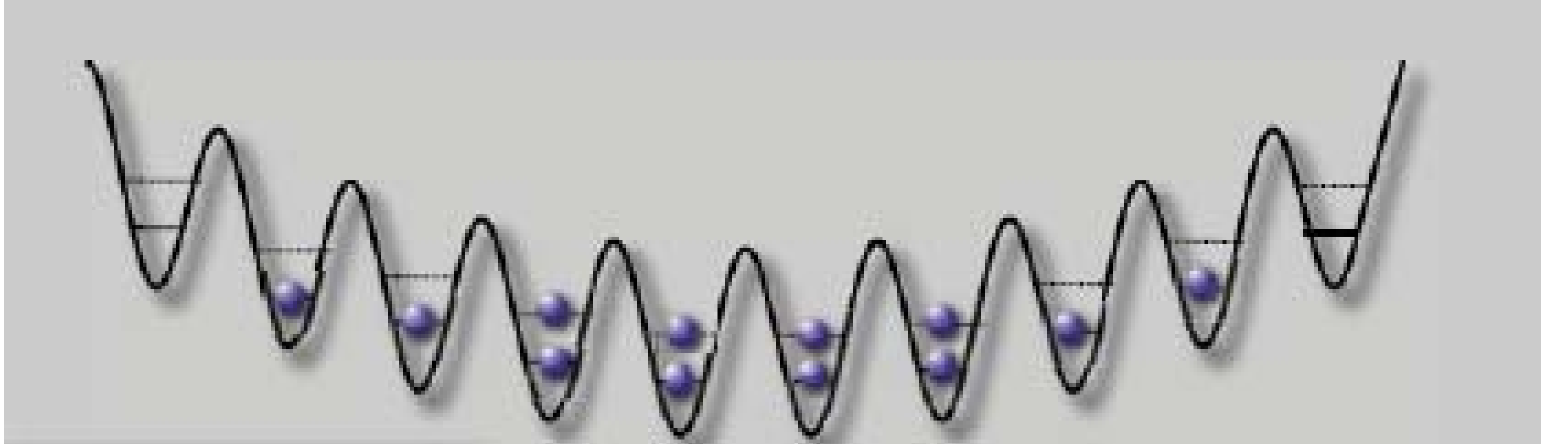
In the presence of the trap the Bose-Hubbard Hamiltonian takes the following form:

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

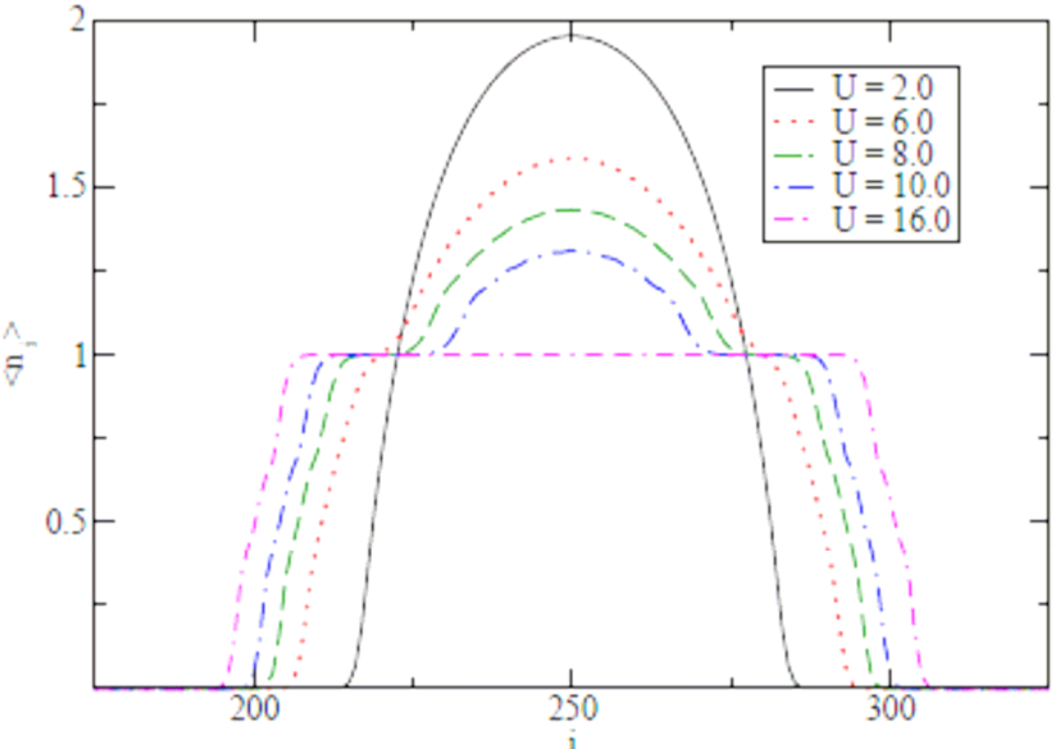
Contribution from harmonic confinement

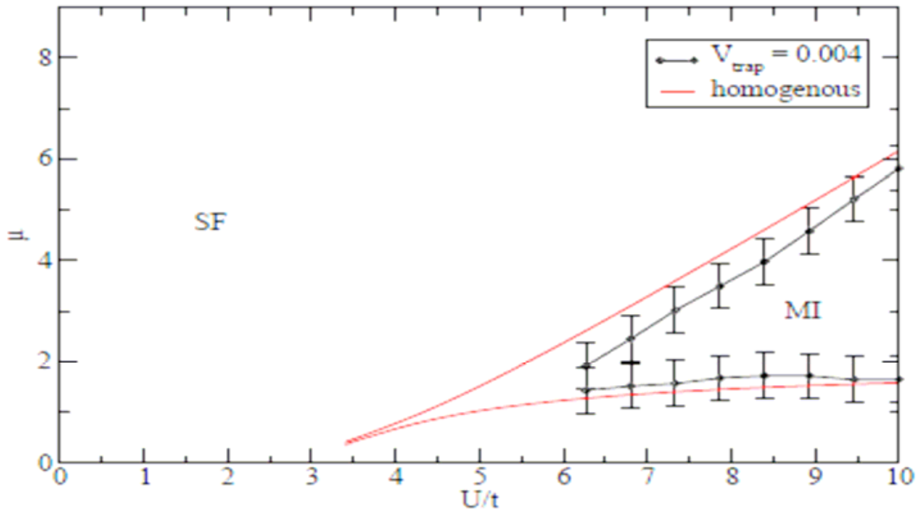
- We can have simultaneous occurrence of SF and MI phase

Density distribution in 1D



Density distribution in 1D





Phase Diagram in the presence of Trap

- For most of the above results, we have run our computationally intensive DMRG codes on Garuda clusters.
- Simultaneously run multiple values of the parameters, to obtain faster output.
- Due to Availability of a no. of nodes on IITG cluster, obtained quick results

Future Plans

- Parallelization of the diagonalization of the density matrix
- Parallelization of the Davidson method for the diagonalization of the Hamiltonian.
- Parallelization of the calculation of various correlation functions
- Using Novel features of Grid computing as and when we learn them!!
- Collaboration between users and Grid support team – Essential!!

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