Many Body Physics Project Presentation

A Monte Carlo Study of Double Exchange Model

Presented by

Aritra Mukhopadhyay, Deependra Singh, Jabed Umar, Srijan Volety

School of Physical Sciences, NISER, Bhubaneswar

Supervisor :

Dr. Anamitra Mukherjee

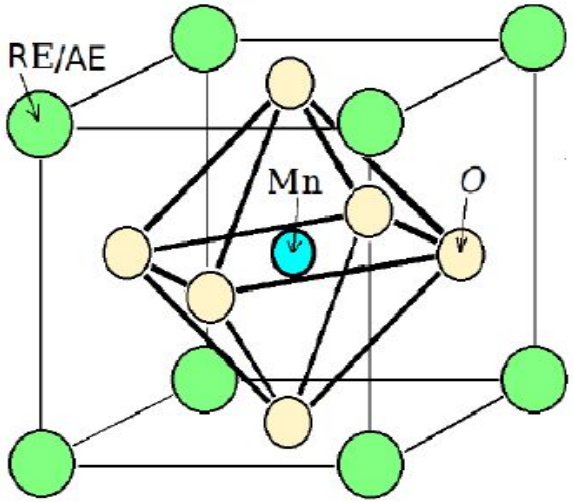
Contents

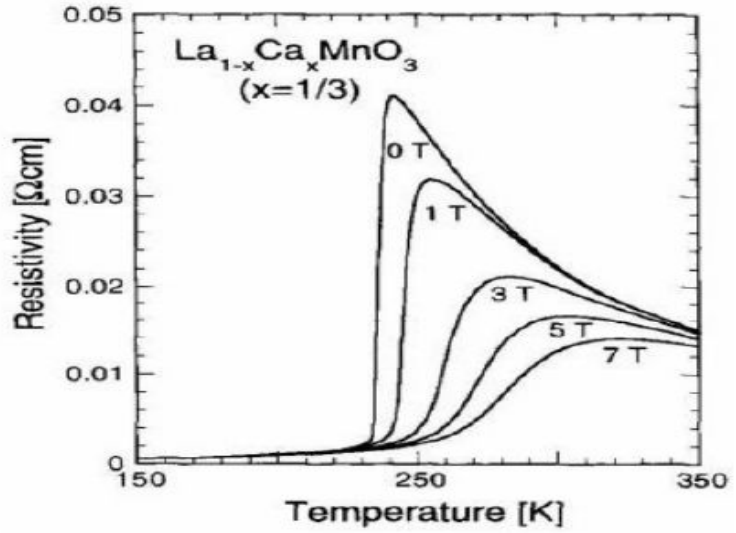
Introduction

- Manganites
- $A_{1-x}B_xMnO_3$

Mixed valency of Mn

Colossal magnetoresistance

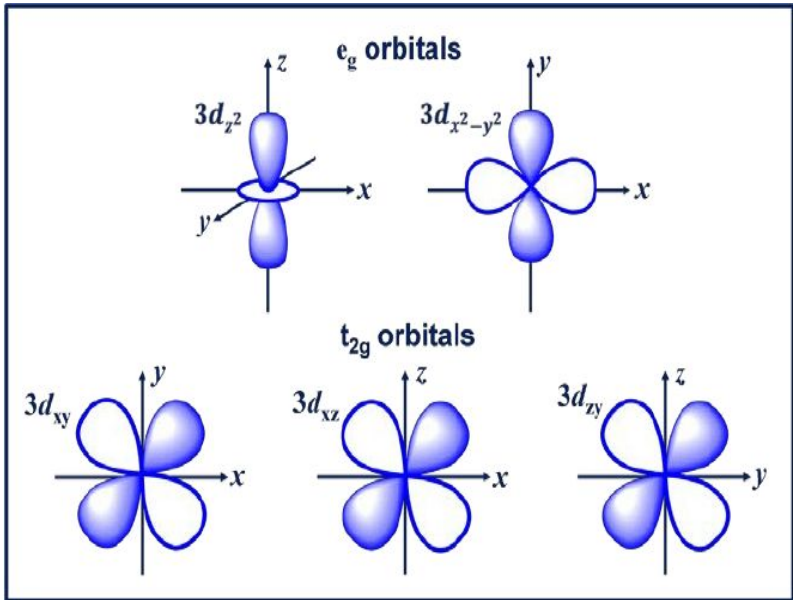


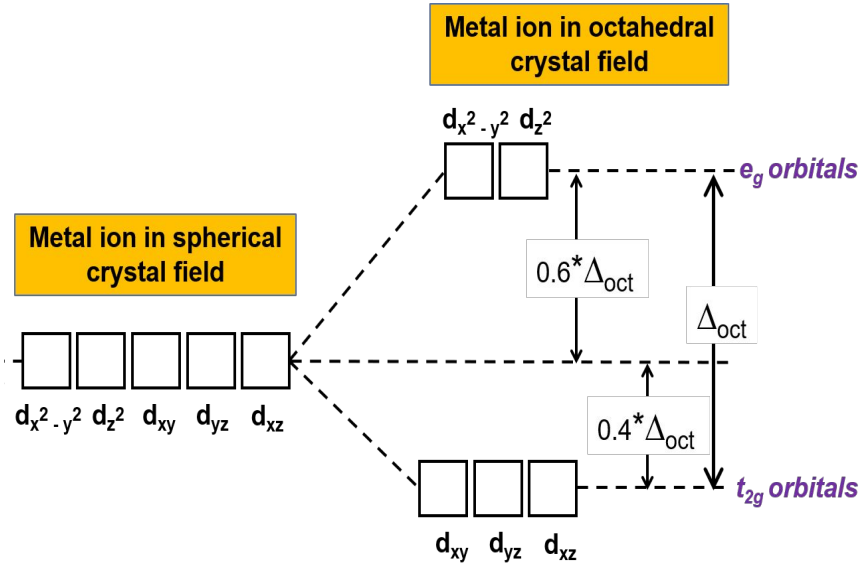


Anamitra Mukherjee, PhD thesis, HRI, 2009

Manganites and crystal field

- d orbitals are extended in space
- Interact with Crystal Field
- d orbital states becomes non degenerate (crystal field splitting)

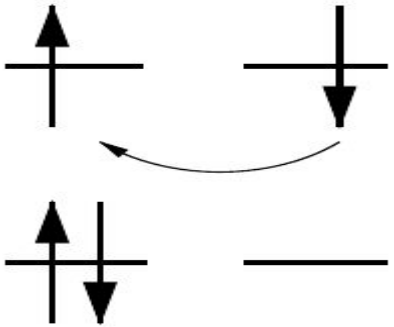




Direct Exchange and Superexchange

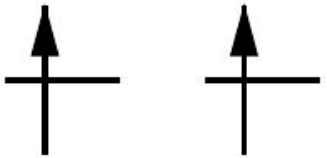
- Exchange mechanism is purely quantum effect → Pauli Principles

1. Kinetic exchange



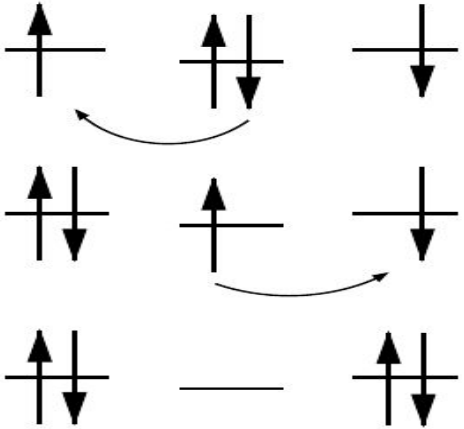
Antiferromagnetism

2. Potential exchange



Ferromagnetism

3. Superexchange

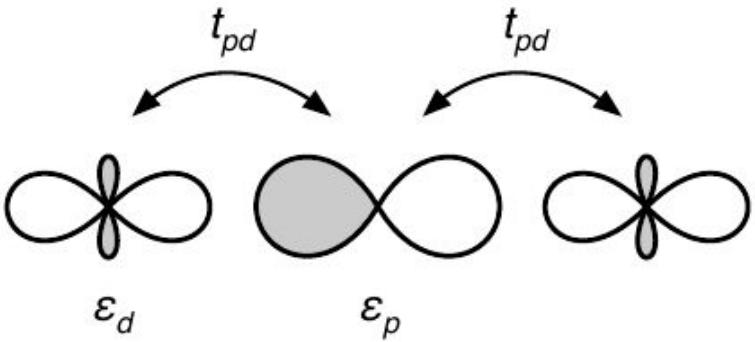


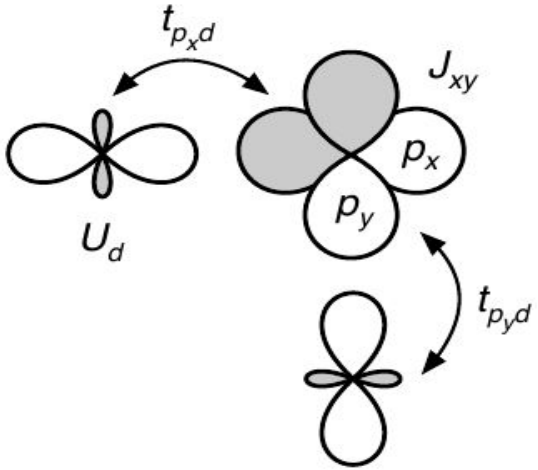
Antiferromagnetism

Erik Koch, Exchange Mechanisms, 2012

Double exchange

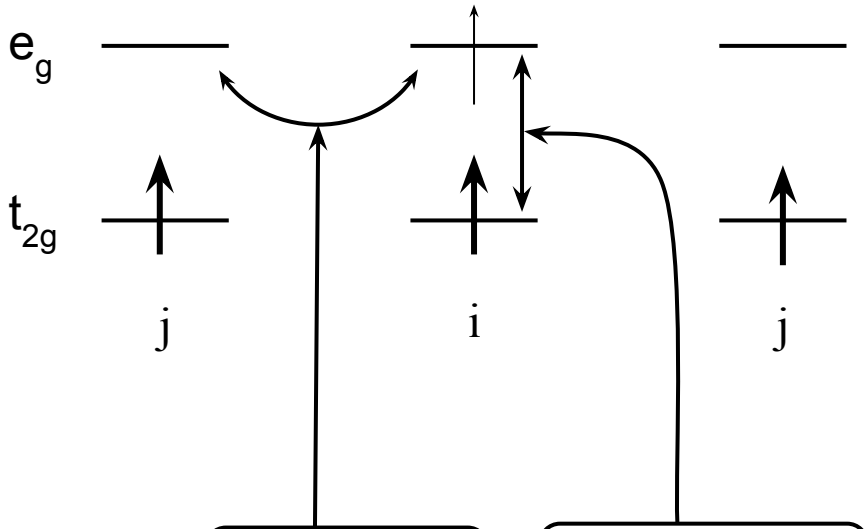
- Interaction mediated via intermediate oxygen atom





- Exchange interaction of e_g electrons which couples to t_{2g} spins → double exchange

The Hamiltonian



$$H = \sum_{\langle i,j\rangle,s} -t_{ij} a^{\dagger}_{i,s} a_{j,s} - J_H \sum_i \mathbf{S}_i \cdot \mathbf{s}_i$$

$$\mathbf{s}_i \cdot \sigma = \begin{pmatrix} S_i^z & S_i^- \\ S_i^+ & -S_i^z \end{pmatrix}$$

$$s_i = \frac{1}{2} \sum_{s,s'} a^{\dagger}_{i,s} \sigma_{s,s'} a_{i,s'}$$

The Simplified Hamiltonian ($J_H >> 1$)

$$H_t = -\sum_{\langle i,j \rangle} \tilde{t}_{ij} c_i^\dagger c_j$$

$$\tilde{t}_{ij} = t_{ij} \sqrt{\frac{1}{2}\left(1 + \frac{\mathbf{S}_i \cdot \mathbf{S}_j}{S^2}\right)}$$

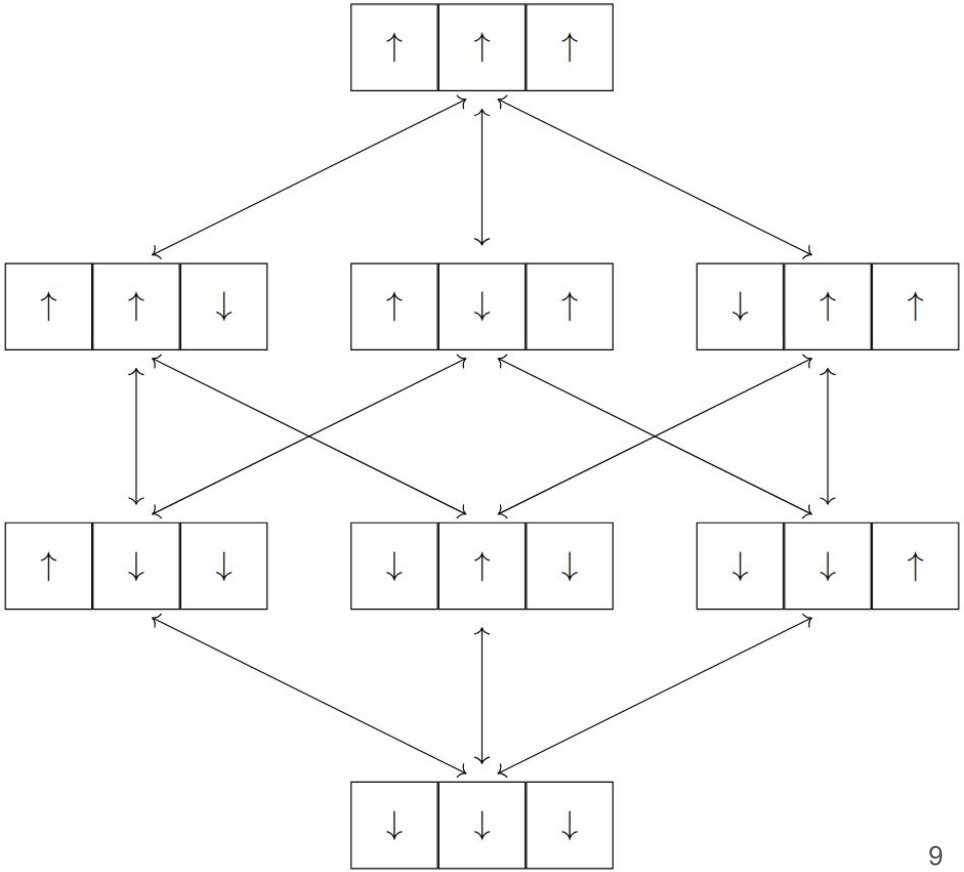
$$c_i^\dagger = d_{i\uparrow}^\dagger = \cos\frac{\theta_i}{2} a_{i\uparrow}^\dagger + \sin\frac{\theta_i}{2} e^{i\varphi_i} a_{i\downarrow}^\dagger$$

Formulate Problem in terms of Markov Chains

Let us imagine a graph data structure consisting of Nodes and Edges.

- **Nodes:** All d^N configurations
- **Edges:** Nodes at single spin flip distance (N for each node)

In this Figure the whole graph for N = 3 has been shown for example.



The Detailed Balance Condition

Markov Chains at equilibrium need to follow the *'detailed balance'* condition:

$$P_y \pi_{yx} = P_x \pi_{xy}$$

From Boltzmann distribution, we know that the probability of being in some state x is:

$$P_x = \frac{e^{-\beta E_x}}{Z}$$

Putting this in the detailed balance condition, we get:

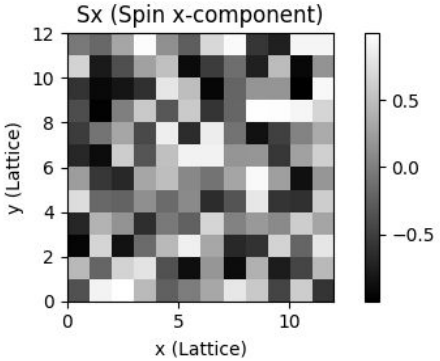
$$\begin{aligned} \pi_{xy} &= \pi_{yx} e^{-\beta(E_y - E_x)} \\ &= \pi_{yx} e^{-\beta \Delta E} \end{aligned}$$

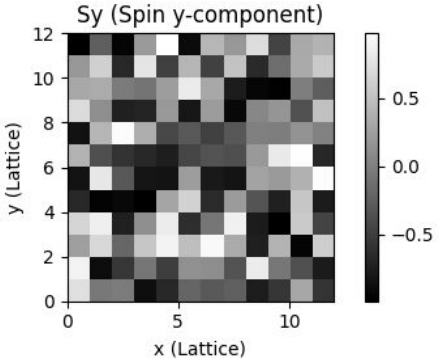
The Metropolis Algorithm

Start with a random configuration (equivalent to picking a random node in the graph). Decide on the hamiltonian ($\mathcal{H}$), temperature (β) and the number of steps (n) to run the simulation for. Then call the following function to evolve the state:

```
1: function METROPOLIS(state, n, β, ℋ)
2:     for i = 1 to n do
3:         Pick a site S_i on the state uniformly at random for flipping
4:         ΔE ← energy change if site S_i is flipped using ℋ
5:         if ΔE < 0 or with probability e^{−βΔE} then
6:             Flip S_i in the state    # make the transition
7:         end if
8:     end for
9:     return state
```

Results


Sx (Spin x-component)
y (Lattice)
x (Lattice)
0
2
4
6
8
10
12
0
5
10
0.5
0.0
−0.5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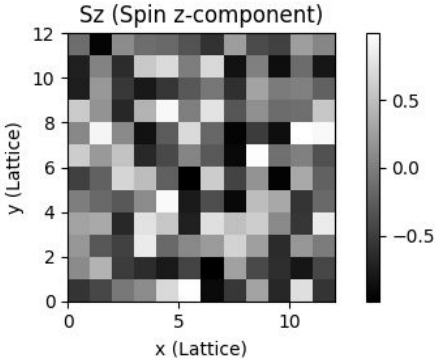
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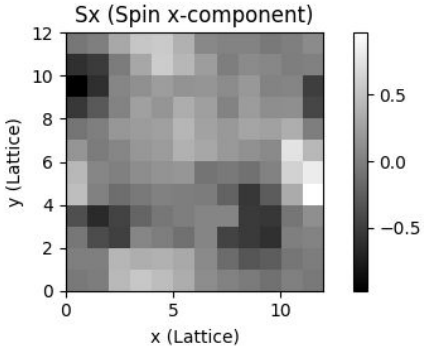
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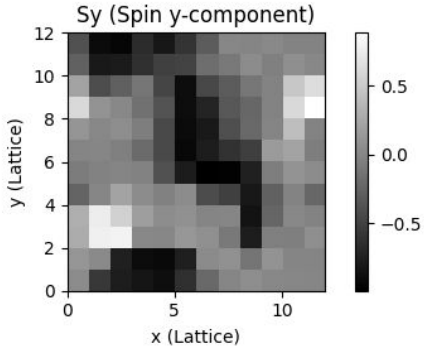
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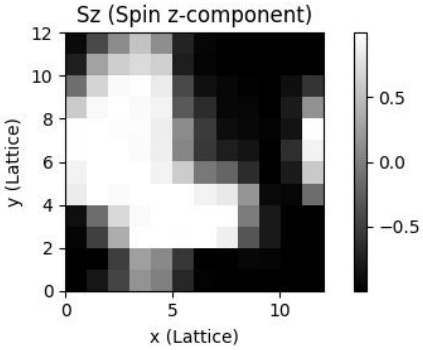
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y (Lattice)
x (Lattice)
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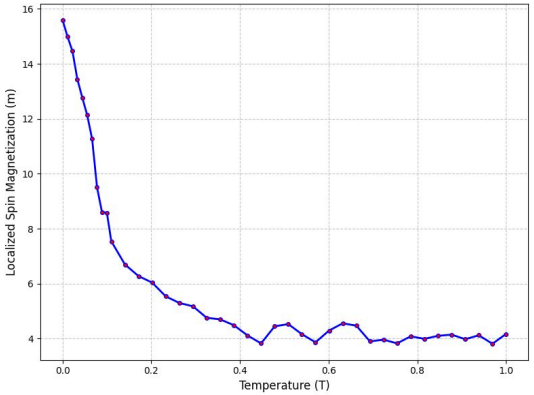
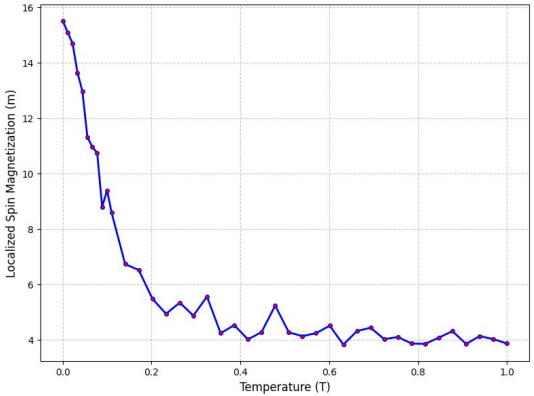
4
6
8
10
12
0
5
10
0.5
0.0
−0.5

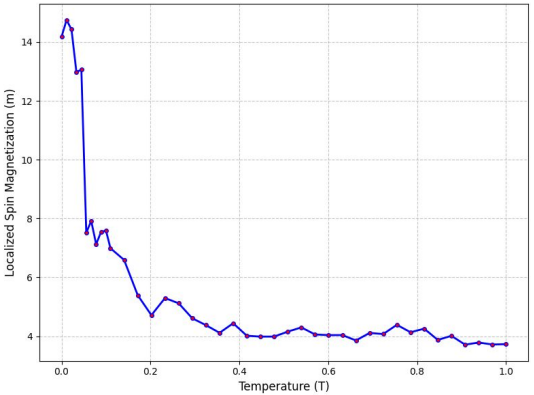
Localized Spin Magnetization vs Temperature



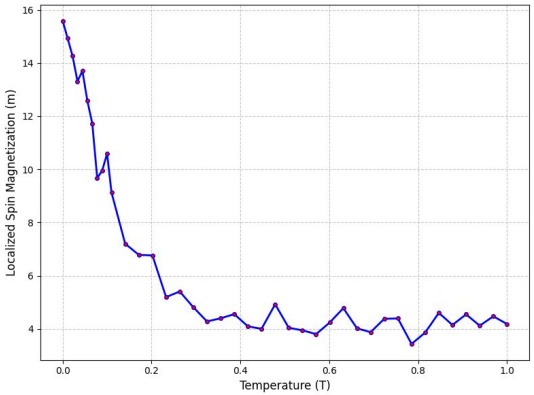
n = 0.25



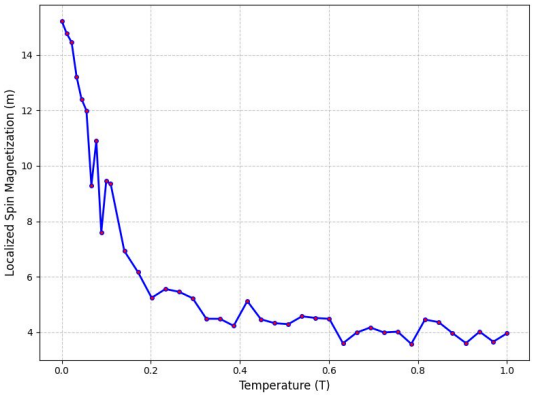
n = 0.38



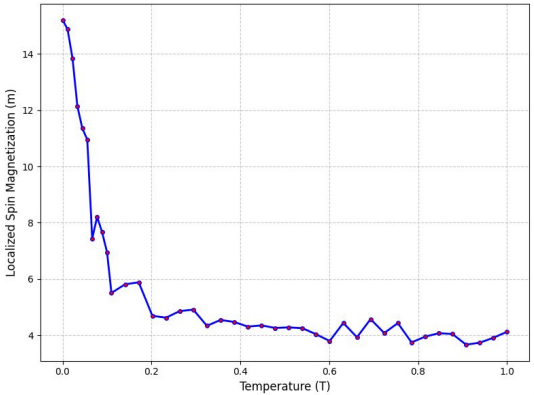
n = 0.50



n = 0.63

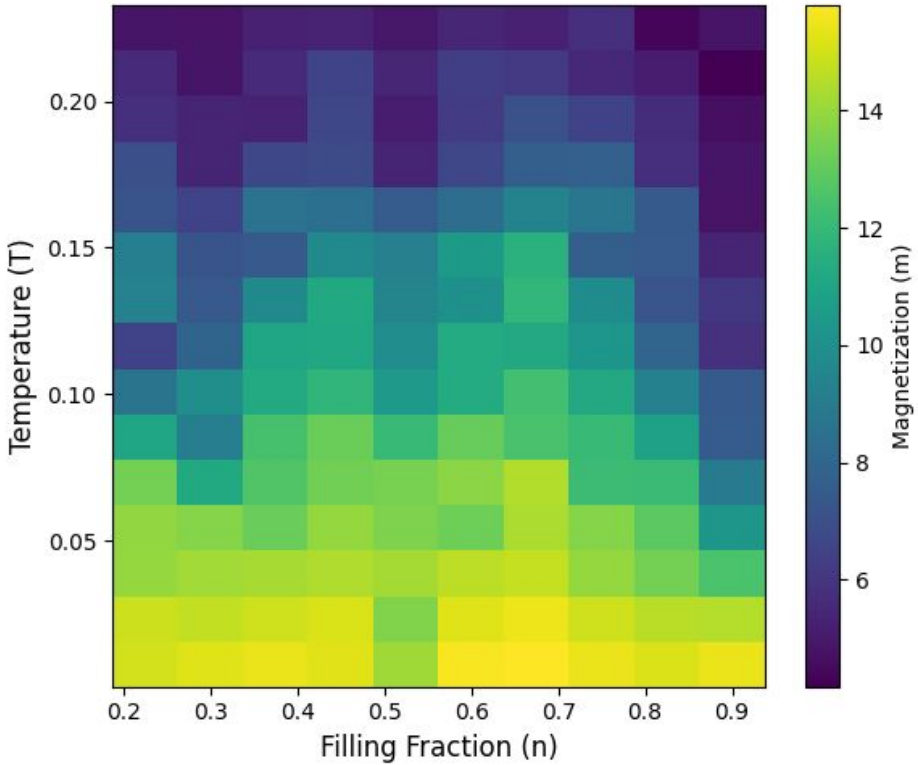


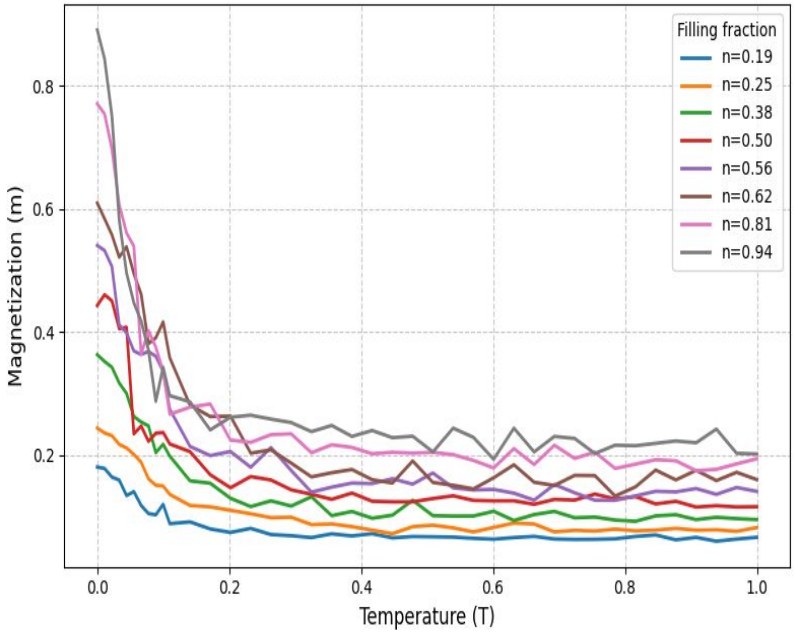
n = 0.81



n = 0.94

Phase Diagram for 4 × 4 Lattice

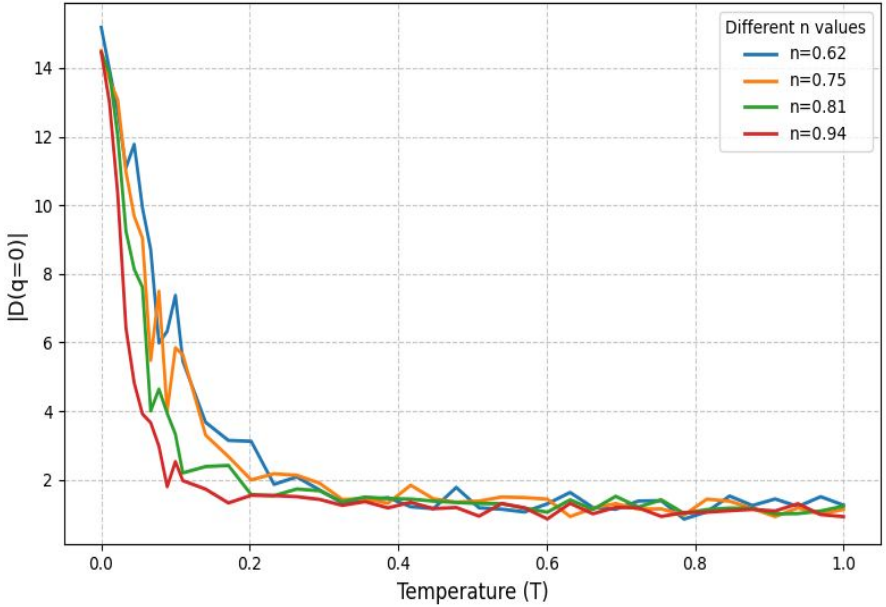




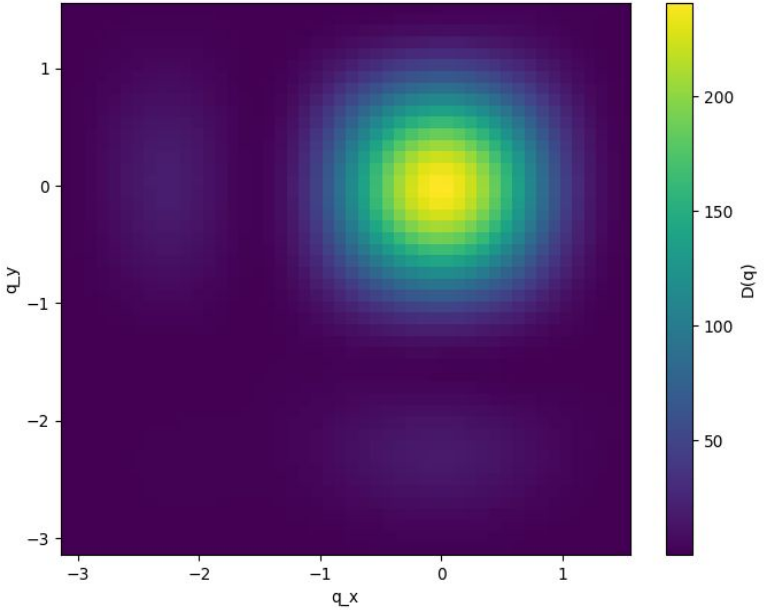
eg M vs T (at different n)

Spin-Spin Correlation vs Temperature

$$D_{\vec{q}} = \frac{1}{N^2} \sum_{ij} S_i \cdot S_j e^{\vec{q} \cdot (\vec{r}_i - \vec{r}_j)}$$

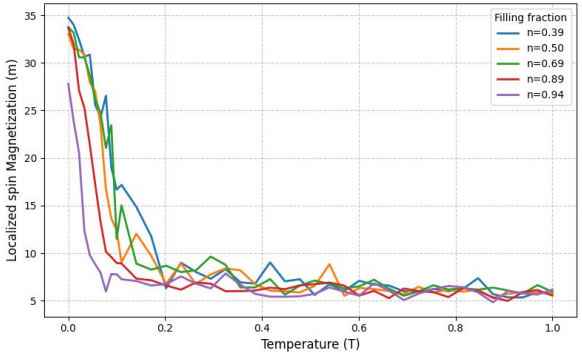


Spin-Spin correlation vs Temperature

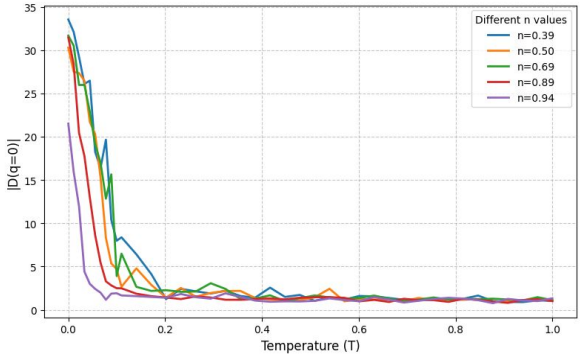


|D(q)| vs $\vec{q}$

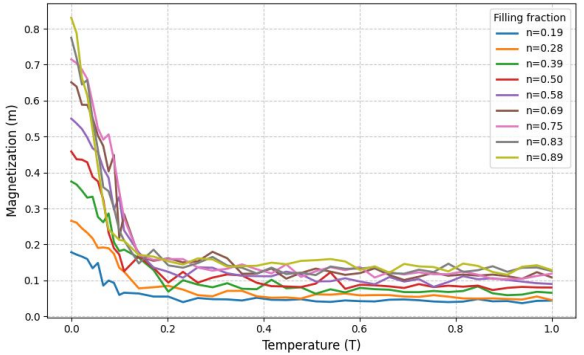
Plots for 6 × 6 lattice



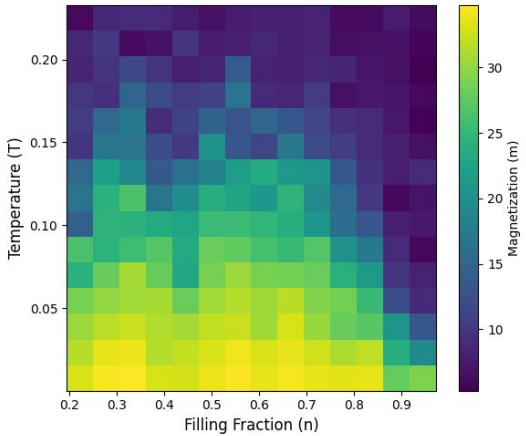
Localized spin M vs T

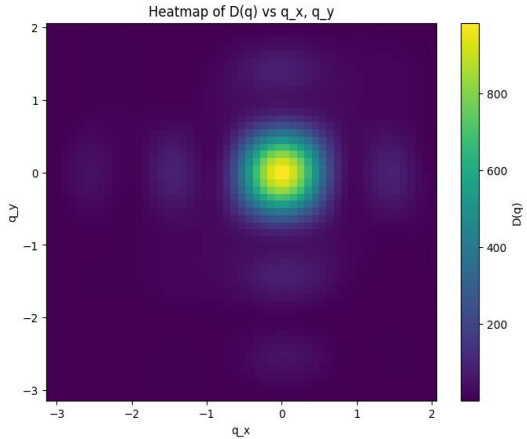


Spin-spin correlation vs Temperature



eg M vs T (at different n)





Conclusion

1. Discuss briefly about Manganites
2. Derive the effective models for Double exchange Model.
3. Simulate the Model using Monte Carlo simulation.
4. Compute Magnetization and Spin - Spin correlation as a function of Temperature and filling fraction.

Thank You

Plot Analysis-II

- **Why is eg magnetization higher for higher n?**
  Higher filling fractions involve more electrons contributing to magnetization, resulting in larger residual alignment even at higher temperatures.

- **Why does the phase diagram shows maxima around 0.5-0.6?**
  At a filling fraction close to 0.5-0.6, double exchange is maximized because electrons can hop most efficiently between neighboring sites, stabilizing spin alignment even at higher temperatures. At lower filling fractions, the number of electrons available for hopping is small, limiting conduction. At higher filling fractions, electrons face competition and blocking due to Pauli exclusion, reducing effective hopping.

Plot Analysis-I

- **Why does magnetization decrease with temperature?**
  Thermal energy disrupts the alignment of localized spins as temperature increases. Increased random motion reduces the net Magnetization.

- **Why does M not reach zero at high temperatures, with a maximum around 16 and a minimum around 4?**
  In a finite 4×4 lattice, finite-size effects constrains the system's ability to achieve perfect disorder.

- **Why are there bumps/spikes on the plot?**
  The spikes arise from statistical fluctuations in the Monte Carlo simulation. Small lattice sizes cause abrupt changes in magnetization due to discrete spin configurations.