Monte Carlo study of Ising spin transport in Ferromagnets and antiferromagnets materials

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We study the spin current in different ferromagnetic and antiferromagnetic systems using Monte Carlo simulations. Many new experimental data on the spin resistivity have been shown, various behaviors have been observed, but there is however no theory which gives a unified mechanism for spin resistivity in magnetic materials. Spin resistivity ρ has been shown to depend on magnetic ordering stability. At low temperatures T, scattering of itinerants electrons is due to spin-waves. However at high temperatures, ρ is proportional to the spin-spin correlation so that its behavior is very complicated arround the magnetic phase transition of the lattice. Our purpose, is to show a new way to investigate spin transport mechanism.

Introduction : *Origin & genesis of resistivity*

**Resistance essentially depends on three mechanisms :
Phonons, static defects and magnons.**

$$\rho_{tot} = \rho_{phonon} + \rho_{magnetic} + \rho_{defects}$$

Our interest focuses on the magnetic contribution to the resistance.

- **1955-1956**: Turov and Kasuya show in a T^2 behavior and predict a constant resistivity after critical temperature T_c.
- **1958**: De Gennes and Friedel relate ρ to the correlation function. ρ shows a peak at T_c.
- **Recent works**: (Kataoka, Zarand, experimental data). Different kinds of behaviors of ρ at T_c depending on materials.

Aim & Interest

Magnetic resistivity attracted interest by "Giant Magneto Resistance".

Our motivation come from :

- Aboundance of experimental results.
- Many theorical studies with approximations.
- Abscence of Monte Carlo simulations.

Our aim is to :

- Develop a new Monte Carlo method to study spin transport.
- Study behavior of various kind of materilal near T_c.
- Include interaction between itinerant spins.
- Analyze effects of different physical parameters.

Model : *Hamiltonian & Algorithm*

$$\mathcal{H} = \underbrace{\sum_{i,j} J_{i,j}\vec{S}_i\vec{S}_j}_{\mathcal{A}} + \underbrace{\sum_{i,j} I_{i,j}\vec{\sigma}_i\vec{S}_j}_{\mathcal{B}} + \underbrace{\sum_{i,j} K_{i,j}\vec{\sigma}_i\vec{\sigma}_j}_{\mathcal{C}} - \underbrace{e\vec{\varepsilon}\vec{l}}_{\mathcal{D}} + \underbrace{D\vec{\nabla}_r n(\vec{r})}_{\mathcal{E}}$$

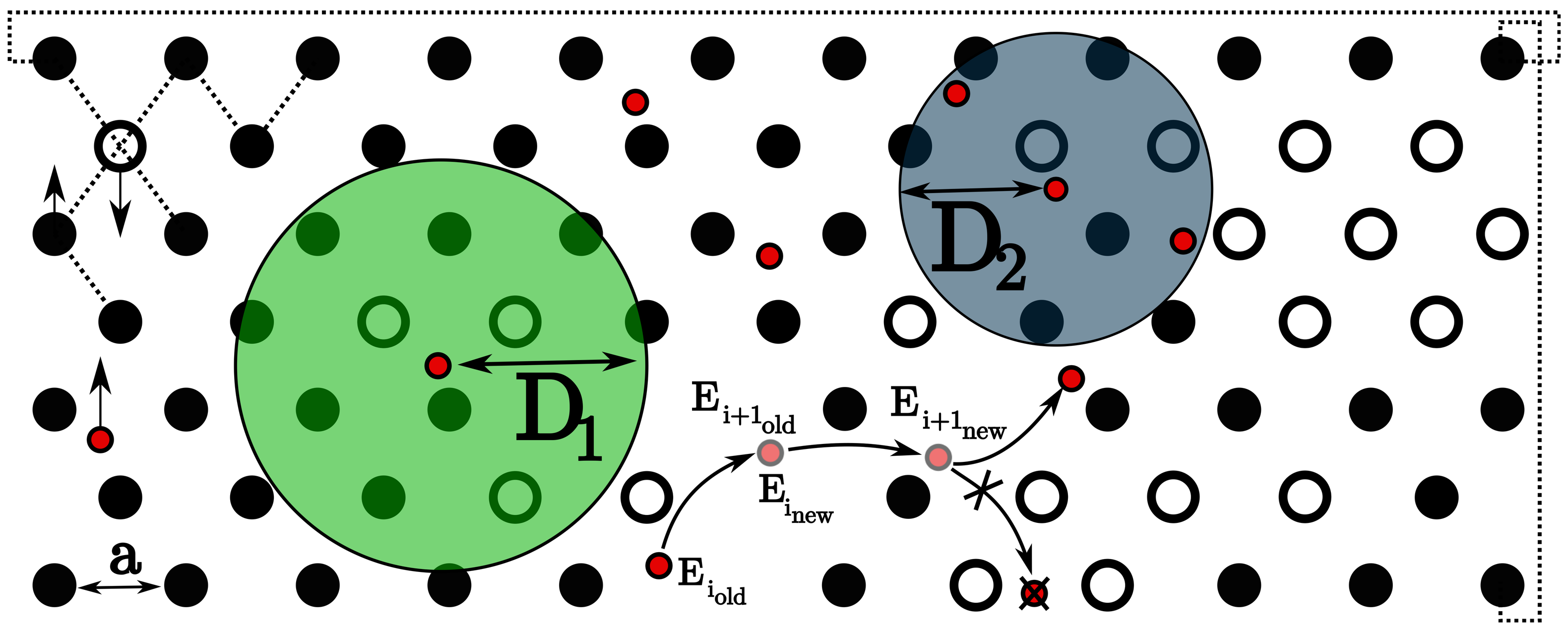
$\mathcal{A}$: Interaction between lattice spins limited on first neighbors with $J_{i,j} = J_0 e^{-r_{ij}}$ with $r_{ij} = |\vec{r}_i - \vec{r}_j|$.

$\mathcal{B}$: Interaction of itinerant spins and lattice spins in a sphere radius D_1, $I_{i,j} = I_0 e^{-r_{ij}}$ with $r_{ij} = |\vec{r}_i - \vec{r}_j|$.

$\mathcal{C}$: Interaction between itinerant spins themselves in a sphere radius D_2, $K_{i,j} = K_0 e^{-r_{ij}}$ with $r_{ij} = |\vec{r}_i - \vec{r}_j|$.

$\mathcal{D}$: Motion of electrons driven by an applied electric field $\vec{\varepsilon_x}$ along x axis.

$\mathcal{E}$: Chemical potential allowing a diffusion by a gradient of electron concentration.



Discretization of motion does not affect final result if averaging is taken on a large number of micro states.

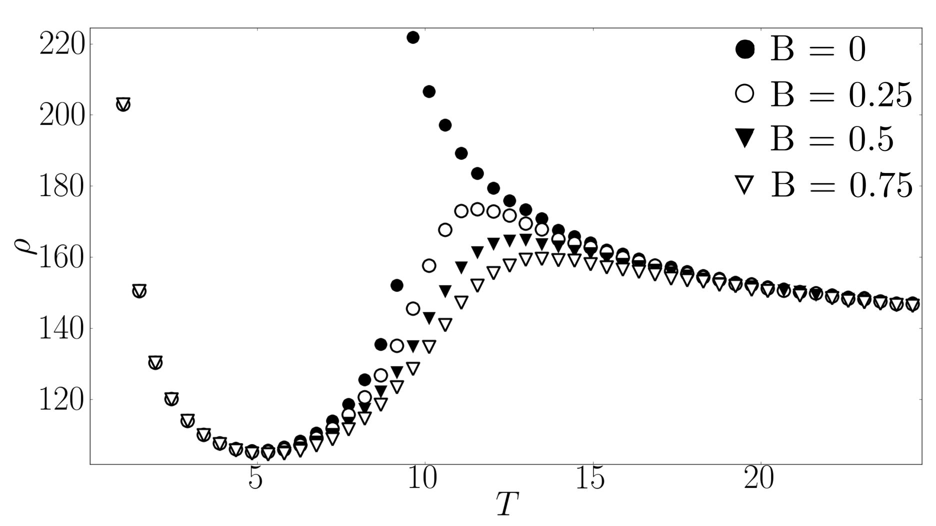
Algorithm

1. Perform a standard Monte Carlo thermalization at a given T for the lattice.
2. Inject N_0 polarized/non-polarized itinerant spins into the lattice.
3. Perform trial move of electrons to reach stationary regime.
4. Perform averaging and determine quantities like $R(T), \lambda(T), \sigma(T)$.
5. Rethermalize lattice and go to step (3) to improve statistical average.

Results : *on FCC ferromagnets BCC antiferromagnets and FCC frustrated antiferromagnets*

FCC ferromagnets versus T for different values of magnetic field

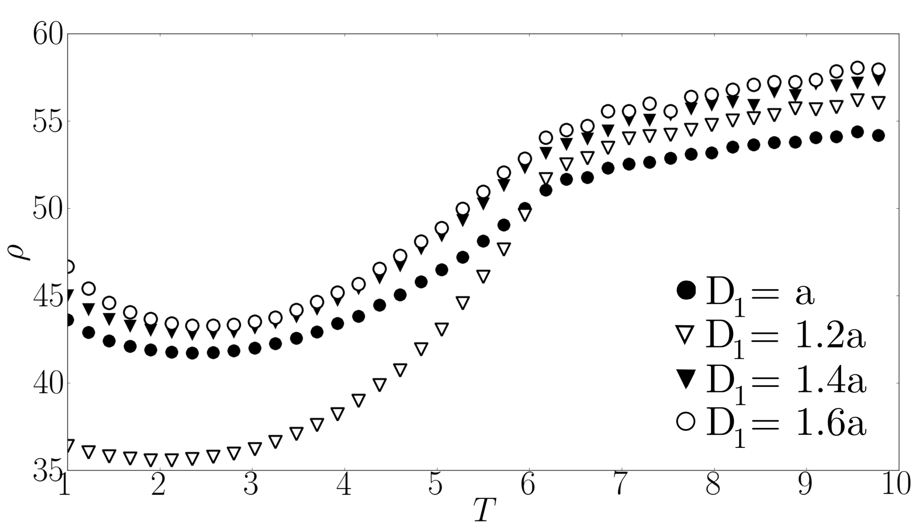
At T_c ρ shows a peak, whose origin can be interpreted by the scattering of itinerant spins with defect lattice spin cluster. Peak height depends on magnetic field...



ρ versus T in function of magnetic field $\vec{B}$. Parameters are $J = 1$, $I_0 = 1$, $K_0 = 0.5$, $D_1 = D_2 = a$. Electron density $n = 0.5$ one electron per cell, lattice size of $N_x = N_y = 20a$ and $N_z = 8a$.

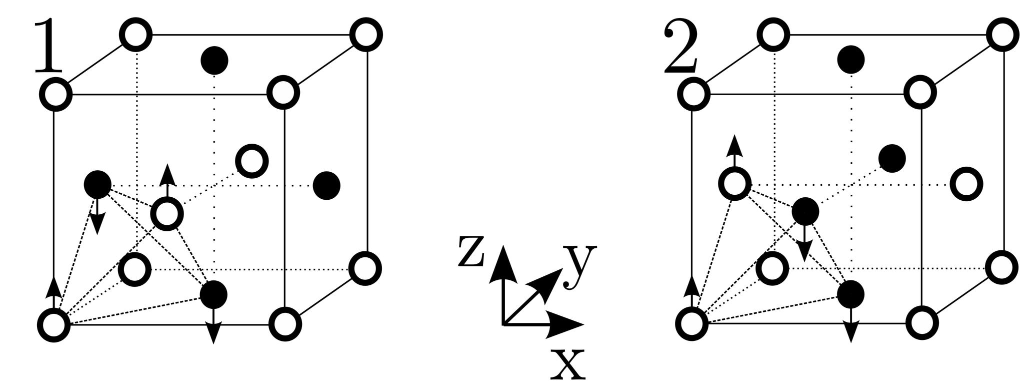
BCC antiferromagnet versus T

In BCC antiferromagnets ρ does not show a peak due to antiferromagnetic ordering.



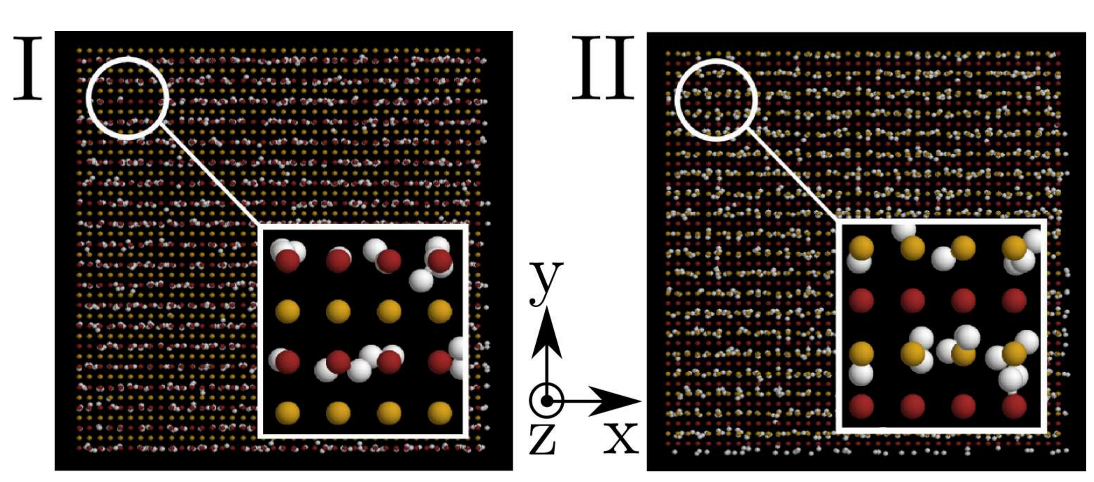
ρ versus T for different values D_1. Parameter are $J = 1$, $I_0 = K_0 = -1$, $D_2 = a$, $n = 0.5$ one electron per cell.

FCC fully frustrated antiferromagnet versus T



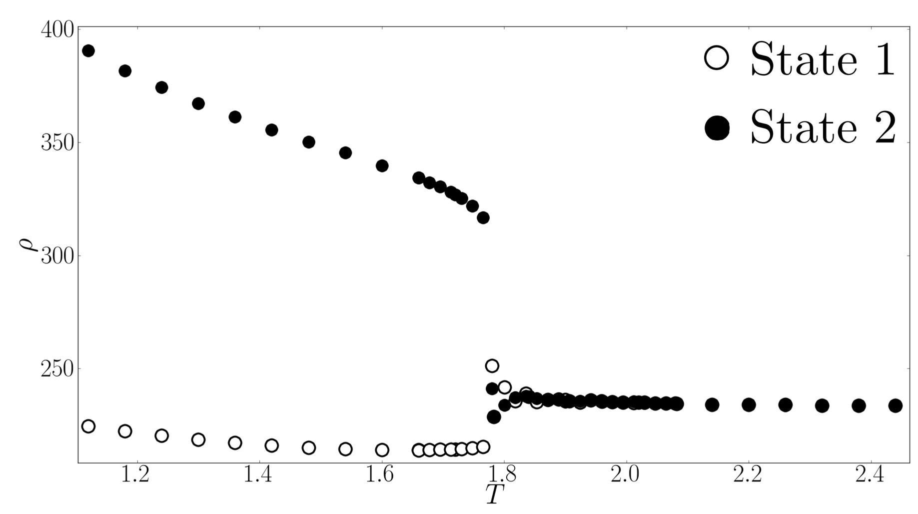
Degenerate ground state spin configurations of the FCC cell.

D_1 drasticly modifies energy landscape felt by electrons. Electrons traveling path depends on the number of $S_\uparrow$, $S_\downarrow$, lattice spins in the D_1 sphere.

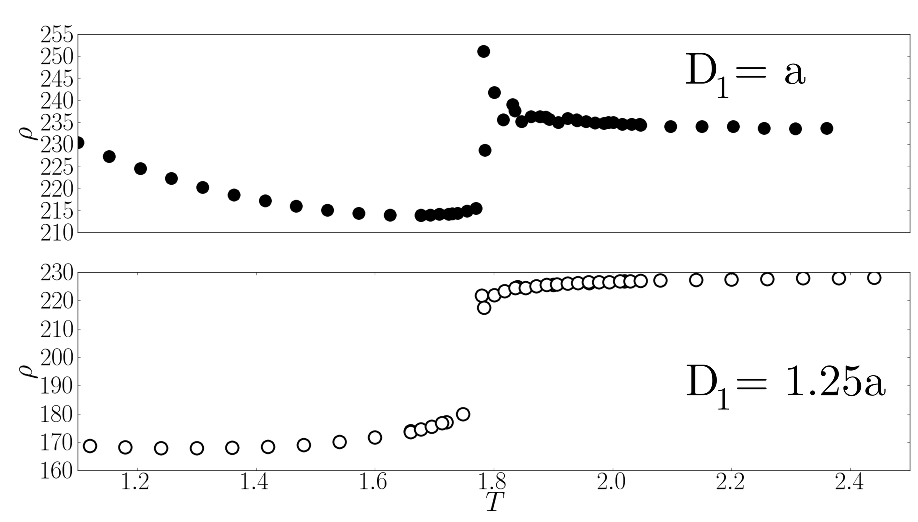


3D antiferromagnetic lattice at $T = 1$, with $S_\downarrow$ in red, $S_\uparrow$ in yellow and itinerant spins $\sigma_\uparrow$ in white. (I) $D_1 = a$. (II) $D_1 = 1.4a$

At transition ρ exhibits an upward jump or downward fall depending on degenerate state and D_1.



ρ versus T for $D_1 = a$ with $N_z = 8$, $n = 1/4$, $J_s = J = -1.0$, $I_0 = K_0 = 0.5$, $D = 0.35$.



ρ versus T in state 1 for $D_1 = a$ (upper) and $D_1 = 1.25a$ (lower). With $N_z = 8$, $n = 1/4$, $J_s = J = -1.0$, $I_0 = K_0 = 0.5$, $D = 0.35$.

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