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SPIN RESISTIVITY IN THE FRUSTRATED $J_1 - J_2$ MODEL

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We study in this paper the resistivity encountered by Ising itinerant spins traveling in the so-called $J_1 - J_2$ frustrated simple cubic Ising lattice. For the lattice, we take into account the interactions between nearest-neighbors and next-nearest-neighbors, J_1 and J_2 respectively. Itinerant spins interact with lattice spins via a distance-dependent interaction. We also take into account an interaction between itinerant spins. The lattice is frustrated in a range of J_2 in which we show that it undergoes a very strong first-order transition. Using Monte Carlo simulation, we calculate the resistivity ρ of the itinerant spins and show that the first-order transition of the lattice causes a discontinuity of ρ.

Keywords: Spin transport; magnetism; Monte Carlo simulation.

1. Introduction

One of the most fascinating subjects in condensed matter physics is the study of the resistivity encountered by conduction electrons in crystals. Fifty years ago, the effect of the magnetic ordering of the crystal on the electron resistivity began to attract investigations. It has been shown that at very low temperature (T) the resistivity is dominated by spin-wave scattering, the spin resistivity ρ is then proportional to T^2 in ferromagnets.[1,2] In the region of the ferromagnetic phase transition, ρ shows a peak at the transition temperature T_C similar to the magnetic susceptibility. De Gennes and Friedel[3] have suggested that this behavior is due to the spin–spin correlation. Several approximations have been used to treat this correlation appearing in several formulations,[4,5] in particular in the Boltzmann's equation.[6,7] Recently, we have introduced a Monte Carlo (MC) simulation technique to deal with the spin resistivity. Our results for ferromagnets are in agreement with other theories, in particular the existence of the peak at T_C and its dependence on the strength of magnetic field and density of itinerant spins.[8,9] In unfrustrated antiferromagnets, there have been a few investigations. Some theories predicted the absence of a sharp peak at T_C.[6] We have shown by MC simulations that this is true, however the form of the rounded peak depends on the crystal structure and

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other interaction parameters.[10,11] Note that MC simulation has been used only recently to study spin transport. Among the works which are similar to ours one can mention the paper by Sen *et al.*[12] and the paper by Yuan *et al.*[13] The former has studied the transport in manganites by using a double-orbital model while the latter has investigated the case of doped manganese perovskites. Both have found a colossal magnetoresistance at the magnetic phase transition similar to our results obtained directly from the system Hamiltonian as seen in our previous works[8–11] and in this paper.

Experimentally, there has been a large number of works dealing with the spin resistivity in different magnetic compounds.[14–24] These experiments show the existence of an anomaly of ρ at the magnetic phase transition. The shape of this anomaly depends on the material. This observation stimulates us to consider various kinds of systems.

One class of interesting magnetic systems is called "frustrated systems" introduced in the 1970s in the context of spin glasses. The magnetic structure of these systems can be complex since degeneracy is expected to occur due to the competition between different kinds of interaction. However they are periodically defined (no disorder) and therefore subject to exact treatments. This is the case of several models in two dimensions,[25] but in three dimensions frustrated systems are far from being understood even on basic properties such as the order of the phase transition (first or second order, values of critical exponents, ...). Let us recall the definition of a frustrated system. When a spin cannot fully satisfy energetically all the interactions with its neighbors, it is "frustrated". This occurs when the interactions are in competition with each other or when the lattice geometry does not allow one to satisfy all interaction bonds simultaneously. A well-known example is the stacked triangular lattice with antiferromagnetic interaction between nearest-neighbors. The frustration in spin systems causes many unusual properties such as large ground state (GS) degeneracy, successive phase transitions with complicated nature, partially disordered phases, reentrance and disorder lines. Frustrated systems still constitute at present a challenge for investigation methods. For recent reviews, the reader is referred to Ref. 26.

Motivated by their exotic behaviors, we have studied some frustrated systems and found that ρ depends drastically on the range of interaction, and that ρ shows a discontinuity at T_C reflecting the first-order character of the phase transition.[27]

This work aims at confirming the fact that in systems with first-order transitions, ρ should have a discontinuity at T_C. For that purpose, we consider in this paper the so-called $J_1 - J_2$ simple cubic lattice with Ising spins. This system is known to undergo a very strong first-order transition in the Heisenberg case.[28] The Ising case studied here shows also a very strong first-order transition as shown below.

In Sec. 2, we present our model and MC method. The results are shown in Sec. 3. Concluding remarks are given in Sec. 4.
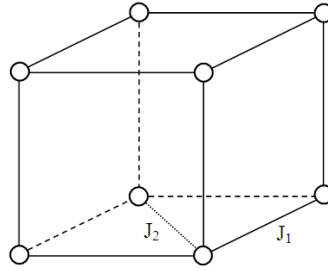
Fig. 1. Simple cubic lattice with nearest and next-nearest neighbor interactions, J_1 and J_2, indicated.

2. Model and Method

2.1. *Model*

We consider the simple cubic lattice shown in Fig. 1. The spins are the classical Ising model of magnitude $S = 1$. The Hamiltonian is given by

$$\mathcal{H} = -J_1 \sum_{(i,j)} \mathbf{S}_i \cdot \mathbf{S}_j - J_2 \sum_{(i,m)} \mathbf{S}_i \cdot \mathbf{S}_m \,, \tag{1}$$

where $\mathbf{S}_i$ is the Ising spin at the lattice site i, $\sum_{(i,j)}$ is made over the NN spin pairs $\mathbf{S}_i$ and $\mathbf{S}_j$ with interaction J_1, while $\sum_{(i,m)}$ is performed over the NNN pairs with interaction J_2. We are interested in the frustrated regime. Therefore, hereafter we suppose that $J_1 = -J$ ($J > 0$, antiferromagnetic interaction, and $J_2 = -\eta J$ where η is a positive parameter. The ground state (GS) of this system is easy to obtain, either by minimizing the energy, or by comparing the energies of different spin configurations, or just a numerical minimizing by a steepest descent method.[29] We obtain the antiferromagnetic (AF) configuration shown by the upper figure of Fig. 2 for $|J_2| < 0.25|J_1|$, or the configuration shown in the lower figure for $|J_2| > 0.25|J_1|$. Note that this latter configuration is three-fold degenerate by putting the parallel NN spins on x, y or z-axis. With the permutation of black and white spins, the total degeneracy is thus 6.

The phase transition of this model in the frustrated region ($|J_2| > 0.25|J_1|$) has been studied by Pinettes and Diep[28] in the case of the Heisenberg model. It has been found that the transition is strongly of first-order. The ordered phase is very unstable due to its degeneracy. As will be shown below, the case of the Ising case shows an even stronger first-order transition. It is therefore interesting to investigate the resistivity of itinerant spins traveling across such a system.

The model we use here to study the spin transport takes into account the following interactions:

- Interaction between lattice spins given by Eq. (1)
- Interaction between itinerant spins and lattice spins given by

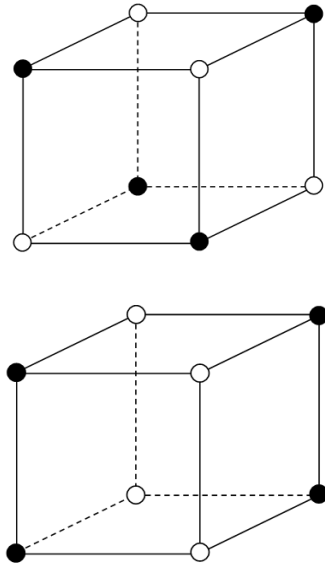$$\mathcal{H}_r = -\sum_{i,j} I_{i,j} \boldsymbol{\sigma}_i \cdot \mathbf{S}_j \,, \tag{2}$$

Fig. 2. Simple cubic lattice. Up-spins: white circles, down-spins: black circles. Upper: Ground state when $|J_2| < 0.25|J_1|$, lower: Ground state when $|J_2| > 0.25|J_1|$.

where σ_i is the Ising spin of itinerant electron and $I_{i,j}$ denotes the interaction that depends on the distance between an electron i and the spin $\mathbf{S}_j$ at the lattice site j. We use the following interaction expression:

$$I_{i,j} = I_0 e^{-\alpha r_{ij}} \quad with \quad r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|, \tag{3}$$

where I_0 and α are constants which will be chosen in Sec. 2.2. The interaction range is limited in a sphere of radius D_1.

- Interaction between itinerant spins. In the same way, interaction between itinerant electrons is defined by

$$\mathcal{H}_m = -\sum_{i,j} K_{i,j} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, \tag{4}$$

$$K_{i,j} = K_0 e^{-\beta r_{ij}}, \tag{5}$$

with σ_i the spin of itinerant electron and $K_{i,j}$ the interaction that depends on the distance between electrons i and j. The choice of the constants K_0 and β is discussed in Sec. 2.2. The interaction range is limited in a sphere of radius D_2.

- Chemical potential term: Since the interaction between itinerant electron spins is attractive, we need to add a chemical potential in order to avoid a possible collapse of electrons into some points in the crystal and to ensure a homogeneous distribution of electrons during the simulation. The chemical potential term is given by

$$\mathcal{H}_c = D\boldsymbol{\nabla}_r n(\mathbf{r}), \tag{6}$$

where $n(\mathbf{r})$ is the concentration of itinerant spins in the sphere of D_2 radius, centered at $\mathbf{r}$. D is a constant parameter appropriately chosen.

- Electric field term:

$$\mathcal{H}_E = -e\boldsymbol{\epsilon} \cdot \boldsymbol{\ell} \tag{7}$$

where e is the charge of electron, $\boldsymbol{\epsilon}$ the applied electric field and $\boldsymbol{\ell}$ the displacement vector of an electron.

Note that in Eq. (6) the chemical potential proportional to density, as it is for perfect gases, leads to a density gradient term in the Boltzmann's equation. This electrochemical potential contains a term proportional to electron density times the electric potential as written in Eq. (7) in the case of a uniform electric field. Of course the difference between Eqs. (6) and (7) is due to the fact that the electric field in Eq. (6) is due to internal charges while in Eq. (7) it is due to an external potential.

2.2. *Choice of parameters and units*

Note that the effect of the crystal magnetic ordering on the resistivity is dominated by the first two interactions. We will show below the results obtained for typical values of parameters. The choice of the parameters has been made after numerous test runs. We describe the principal requirements which guide the choice:

 (i) We choose the NN interaction between lattice spins as unity, i.e. $|J| = 1$.
 (ii) We choose interaction between an itinerant and its surrounding lattice spins so as its energy E_i in the low T region is the same order of magnitude as that between lattice spins. To simplify, we take $\alpha = 1$.
(iii) Interaction between itinerant spins is chosen so that this contribution to the itinerant spin energy is smaller than E_i in order to highlight the effect of the lattice ordering on the spin current. To simplify, we take $\beta = 1$.
(iv) The choice of D is made in such a way to avoid the formation of clusters of itinerant spins (collapse) due to their attractive interaction [Eq. (5)].
 (v) The electric field is chosen to be not so strong in order to avoid its dominant effect that would mask the effects of thermal fluctuations and of the magnetic ordering.
(vi) The density of the itinerant spins is chosen in a way that the contribution of interactions between themselves is neither so weak nor so strong with respect to E_i.

Within these requirements, a variation of each parameter does not change qualitatively the results shown below. As will be seen, only the variation of D_1 changes the results drastically. That is the reason why we will study in detail the effect of this parameter. For larger densities of itinerant spins, the resistivity is larger as expected because of additional scattering process between itinerant spins.

We fix $J_1 = -J = -1$ (AF interaction) for NN coupling of lattice spins as said above. The energy is thus measured in the unit of J. The temperature is expressed in the unit of J/k_B. The distance (D_1, D_2) is in the unit of a, the lattice constant. The resistivity is in atomic units and the magnetization is dimensionless.

2.3. *Simulation Method*

We consider a film with a thickness of N_z cubic cells in the z-direction. Each of the xy planes contains $N_x \times N_y$ cells. The periodic boundary conditions are used on the xy planes to ensure that the itinerant electrons who leave the system at the second end are to be reinserted at the first end. For the z-direction, we use the mirror reflection at the two surfaces. These boundary conditions conserve thus the average density of itinerant electrons. Dynamics of itinerant electrons is created by an electric field applied along the x-axis.

Simulations are carried out in the following manner. The lattice spins are equilibrated at a temperature T. Itinerant spins are then injected into the system. Before calculating thermal averages of transport properties, we equilibrate itinerant spins during a large number of MC steps. The multi-step averaging procedure has been used to get good statistics:[11] Averaging is made between re-equilibrating periods of lattice and itinerant spins to explore a maximum number of microscopic spin configurations.

3. Results

We show first the result of the lattice alone, namely without itinerant spins. The lattice in the frustrated region, i.e. $|J_2/J_1| > 0.25$, shows a strong first-order transition as seen in Fig. 3. The sublattice magnetization and the energy per spin as functions of T for $J_2 = -0.26|J_1|$ for the lattice size $N_x = N_y = 20$, $N_z = 6$ show a discontinuity at the transition temperature. To check further the first-order nature of the transition, we have calculated the energy histogram at the transition temperature T_C. This is shown in Fig. 4. The double-peak structure indicates the coexistence of the ordered and disordered phases at T_C. The distance between two peaks represents the latent heat.

Now we consider the lattice with the presence of itinerant spins. As far as the interaction between itinerant spins is attractive, we need a chemical potential to avoid the collapse of the system. The strength of the chemical potential D depends on K_0. We show in Fig. 5 the collapse phase diagram which allows to choose for a given K_0, an appropriate value of D.

We show now the main result on the spin resistivity versus T for $|J_2| = 0.26|J_1|$ for several values of D_1. Other parameters are the same as in Fig. 3. As said in Sec. 2.2, within the physical constraints, the variation of most of the parameters does not change qualitatively the physical effects observed in simulations, except for the parameter D_1. Due to the AF ordering, increasing D_1 means that we include successively neighboring down and up spins surrounding a given itinerant spin. As
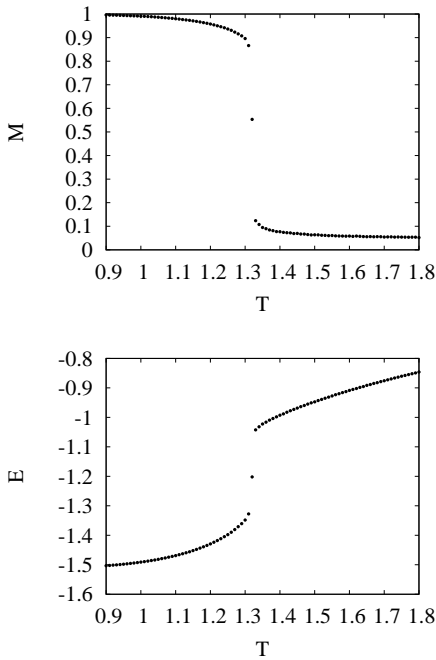
Fig. 3.   Upper: Sublattice magnetization M versus T, Lower: Energy versus T, for $|J_2| = 0.26|J_1|$, $N_x = N_y = 20,\ N_z = 6$.
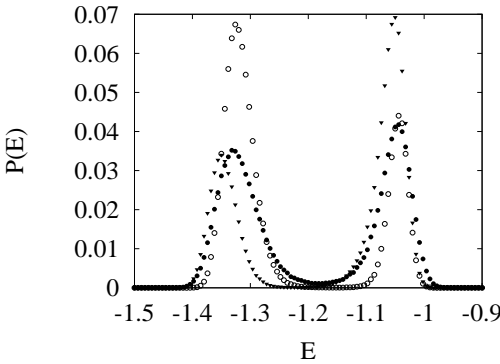

Fig. 4.   Energy histogram taken at the transition temperature T_C for $J_2 = -0.26|J_1|$: black circles are for $N_x = N_y = 20, N_z = 6, T_C = 1.320$, void circles for $N_x = N_y = 30, N_z = 6, T_C = 1.320$ and black triangles for $N_x = N_y = 20, N_z = 10, T_C = 1.305$. Other parameters are $I_0 = K_0 = 0.5$, $D_1 = 0.8a,\ D_2 = a,\ D = 1,\ \epsilon = 1$.

a consequence, the energy of the itinerant spin oscillates with varying D_1, giving rise to the change of behavior of ρ: ρ can make a down fall or an upward jump at T_C depending on the value of D_1 as shown in Fig. 6. Note the discontinuity of ρ at T_C. This behavior has been observed and analyzed in terms of the averaged magnetization in the sphere of radius D_1 in the frustrated FCC antiferromagnet.[27]
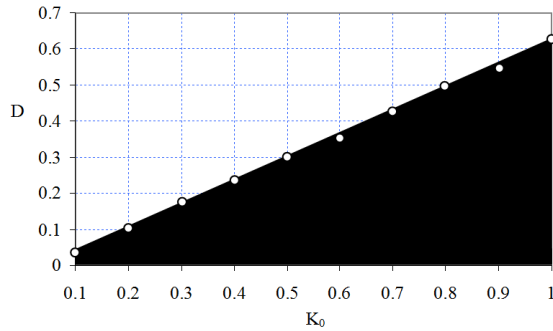
Fig. 5.   Phase diagram in the plane (K_0, D). The collapse region is in black, for $|J_2| = 0.26|J_1|$. Other parameters are $D_1 = D_2 = a$, $I_0 = 0.5$, $\epsilon = 1$.
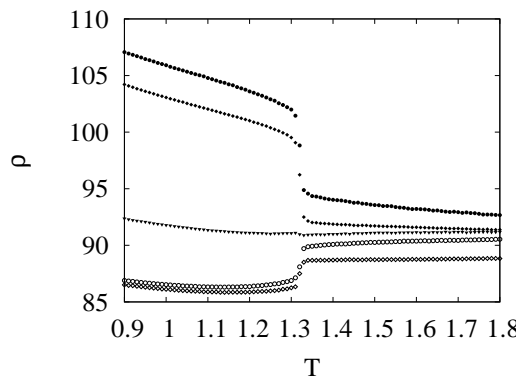

Fig. 6.   Spin resistivity versus T for $|J_2| = 0.26|J_1|$ for several values of D_1: from up to down $D_1 = 0.7a$, $0.8a$, $0.94a$, a, $1.2a$. Other parameters are $N_x = N_y = 20$, $N_z = 6$, $I_0 = K_0 = 0.5$, $D_2 = a$, $D = 1$, $\epsilon = 1$.

4. Concluding Remarks

From the results shown above for the strongly frustrated $J_1 - J_2$ model, we conclude that the spin resistivity reflects the nature of the first-order transition: it undergoes a discontinuity at the transition temperature. The fact that as $T \to 0$, ρ increases slowly stems from the freezing of itinerant spins with decreasing T. This has been experimentally observed in ferromagnets and antiferromagnets as seen in Fig. 11 of the paper by Chandra *et al.* on CdMnTe,[16] Fig. 2 of the paper by Du *et al.* for MnFeGe,[22] Fig. 6(a) of the paper by McGuire *et al.* on AF superconductors LaFeAsO,[24] Fig. 2 of the paper by Lu *et al.* on AF LaCaMnO,[21] and Fig. 7 of the paper by Santos *et al.* on AF LaSrMnO.[19]

We hope that these MC results will stimulate further theoretical calculations and experiments.

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