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Yann Magnin, K. Akabli, Hung The Diep, Isao Harada. Monte Carlo Study of the Spin Transport in Magnetic Materials. 2009. hal-00426291v1

**HAL Id: hal-00426291**

**<https://hal.science/hal-00426291v1>**

Preprint submitted on 24 Oct 2009 (v1), last revised 29 Dec 2010 (v3)

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# Monte Carlo Study of the Spin Transport in Magnetic Materials

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## Abstract

The resistivity in magnetic materials has been theoretically shown to depend on the spin-spin correlation function which in turn depends on the magnetic-field, the density of conduction electron, the magnetic ordering stability, etc. However, these theories involved a lot of approximations, so their validity remained to be confirmed. The purpose of this work is to show by extensive Monte Carlo (MC) simulation the resistivity of the spin current from low- $T$  ordered phase to high- $T$  paramagnetic phase in a ferromagnetic film. We take into account the interaction between the itinerant spins and the localized lattice spins as well as the interaction between itinerant spins themselves. We show that the resistivity undergoes an anomalous behavior at the magnetic phase transition in agreement with previous theories in spite of their numerous approximations. The origin of the resistivity peak near the phase transition in ferromagnets is interpreted here as stemming from the existence of magnetic domains in the critical region. This interpretation is shown to be in consistence with previous theoretical pictures. Resistivity in a simple cubic antiferromagnet is also shown. The absence of a peak in this case is explained.

*Key words:* spin transport, Monte Carlo simulation, magnetic resistivity, magnetic materials

*PACS:* 72.25.-b, 75.47.-m

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## 1. Introduction

The magnetic resistivity has been extensively studied by both theories and experiments in the last fifty years. Experiments have shown that the resistivity indeed depends on the itinerant spin orientation and the lattice spin ordering [1, 2, 3, 4, 5]. At low temperature ( $T$ ), the main magnetic scattering is due to spin-wave excitations [6, 7]. The resistivity is proportional to  $T^2$ . However at higher  $T$  the spin-wave theory is not valid, such a calculation of the resistivity is not possible, in particular in the critical region around the Curie temperature  $T_c$  in simple ferromagnets, let alone other complicated magnetic orderings. Experiments on various magnetic materials have found in particular an anomalous behavior of the resistivity at the critical temperature where the system undergoes the ferromagnetic-paramagnetic phase transition [2, 3, 4, 5]. de Gennes and Friedel's first explanation in 1958[8] for the resistivity behavior near  $T_c$  was based on the interaction between the spins of conduction electrons and the lattice spins. Therefore, the resistivity was expected to depend strongly on the spin ordering of the system. Theoretically, in this pioneer work, de Gennes and Friedel [8] have suggested that the magnetic resistivity is proportional to the spin-spin correlation. In other

words, the spin resistivity should behave as the magnetic susceptibility. This explained that the resistivity singularity is due to "long-range" fluctuations of the magnetization observed in the critical region. Craig et al [9] in 1967 and Fisher and Langer [10] in 1968 suggested that the shape of the singularity results mainly from "short-range" interaction at  $T \geq T_c$ . Fisher and Langer have shown in particular that the form of the resistivity cusp depends on the correlation range. A summary was given in 1975 by Alexander and coworkers [11] which highlighted the controversial issue. To see more details on the magnetic resistivity, we quote an interesting recent publication from Kataoka [12]. He calculated the spin-spin correlation function using the mean-field approximation and analyzed the effects of magnetic-field, density of conduction electron, the correlation range, etc. Recently, Zarand et al [14] have used the picture that the itinerant spin is mainly scattered by impurities which are characterized by a "localization length" in the sense of Anderson's localization. They found that the peak's height depends on this localization length. Note that since the so-called giant magnetoresistance (GMR) was discovered experimentally twenty years ago in magnetic multilayers [15, 16], intensive investigations, both experimentally and theoretically, have been carried out [17, 18]. The so-called "spintronics" was born with spectacular rapid developments in relation with industrial applications. For recent overviews, the reader is

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referred to Refs. [19] and [20].

Although many theoretical investigations have been carried out, there has been no Monte Carlo (MC) simulations performed regarding the temperature dependence of the dynamics of spins participating in the current. In our recent works [21, 22], we have investigated by MC simulations the effects of magnetic ordering on the spin current in magnetic multilayers. Our results are in qualitative agreement with measurements [23].

In this paper we improve our previous MC simulations to study the transport of itinerant electrons in ferromagnetic and antiferromagnetic crystals. We use the Ising model and take into account interactions between lattice spins and itinerant spins. We show that in ferromagnets the magnetic resistivity shows a huge peak at the transition temperature of the lattice spins while in simple cubic antiferromagnets, the resistivity does not show such a peak.

The paper is organized as follows. Section 2 is devoted to the description of our model and the rules that govern its dynamics. In section 3, we describe our MC method and discuss the results we obtained for ferromagnets. Results on antiferromagnets are shown in Section 4. Concluding remarks are given in Section 5.

## 2. Model

### 2.1. Interactions

We consider in this section a magnetic thin film. Periodic boundary conditions (PBC) are used in the  $xy$  planes. Spins localized at FCC lattice sites are called "lattice spins" hereafter. They interact with each other through the following Hamiltonian

$$\mathcal{H}_l = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)$$

where  $\mathbf{S}_i$  is the Ising spin at lattice site  $i$ ,  $\sum_{\langle i,j \rangle}$  indicates the sum over every nearest-neighbor (NN) spin pair  $(\mathbf{S}_i, \mathbf{S}_j)$ ,  $J$  being the NN interaction. We consider in this paper both  $J > 0$  (ferromagnets) and  $J < 0$  (antiferromagnets).

In order to study the spin transport in the above system, we consider a flow of itinerant spins interacting with each other and with the lattice spins. The interaction between itinerant spins is defined as follows,

$$\mathcal{H}_m = - \sum_{\langle i,j \rangle} K_{i,j} \mathbf{s}_i \cdot \mathbf{s}_j, \quad (2)$$

where  $\mathbf{s}_i$  is the itinerant Ising spin at position  $\vec{r}_i$ , and  $\sum_{\langle i,j \rangle}$  denotes a sum over every spin pair  $(\mathbf{s}_i, \mathbf{s}_j)$ . The interaction  $K_{i,j}$  depends on the distance between the two spins, i.e.  $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ . A specific form of  $K_{i,j}$  will be chosen below. The interaction between itinerant spins and lattice spins is given by

$$\mathcal{H}_r = - \sum_{\langle i,j \rangle} I_{i,j} \mathbf{s}_i \cdot \mathbf{S}_j, \quad (3)$$

where the interaction  $I_{i,j}$  depends on the distance between the itinerant spin  $\mathbf{s}_i$  and the lattice spin  $\mathbf{S}_i$ . For the sake of simplicity, we assume the same form for  $K_{i,j}$  and  $I_{i,j}$ , namely,

$$K_{i,j} = K_0 \exp(-r_{ij}) \quad (4)$$

$$I_{i,j} = I_0 \exp(-r_{ij}) \quad (5)$$

where  $K_0$  and  $I_0$  are constants.

### 2.2. Monte Carlo Method

The procedure used in our simulation is described as follows. First we study the thermodynamic properties of the film alone, i.e. without itinerant spins, using Eq. (1). We perform MC simulations to determine quantities as the internal energy, the specific heat, layer magnetizations, the susceptibility, ... as functions of temperature  $T$  [24]. From these physical quantities we determine the critical temperature  $T_c$  below which the system is in the ordered phase.

Once the lattice has been equilibrated at  $T$ , we inject  $N_0$  itinerant spins into the system. The itinerant spins move into the system at one end, travel in the  $x$  direction, escape the system at the other end to reenter again at the first end under the PBC. Note that the PBC are used to ensure that the average density of itinerant spins remains constant with evolving time (stationary regime).

Note that unlike in the previous works[21, 22] where the lattice spin configuration is frozen while calculating the resistivity, we use here several thousands of configurations in each of which the resistivity is averaged with many thousands passages. As will be shown below, this extensive configuration average improves the results with respect to those in previous works. The dynamics of itinerant spins is governed by the following interactions:

i) an electric field  $\mathbf{E}$  is applied in the  $x$  direction. Its energy is given by

$$\mathcal{H}_E = -e\mathbf{E} \cdot \mathbf{v}, \quad (6)$$

where  $\mathbf{v}$  is the velocity of the itinerant spin,  $e$  its charge;

ii) a chemical potential term which depends on the concentration of itinerant spins ("concentration gradient" effect). Its form is given by

$$\mathcal{H}_c = Dn(\mathbf{r}), \quad (7)$$

where  $n(\mathbf{r})$  is the concentration of itinerant spins in a sphere of radius  $D_2$  centered at  $\mathbf{r}$ .  $D$  is a constant taken equal to  $K_0$  for simplicity;

iii) interactions between a given itinerant spin and lattice spins inside a sphere of radius  $D_1$  (Eq. 3);

iv) interactions between a given itinerant spin and other itinerant spins inside a sphere of radius  $D_2$  (Eq. 2).

Let us consider the case without an applied magnetic field. The simulation is carried out as follows: at a given  $T$  we calculate the energy of an itinerant spin by taking into account all the interactions described above. Then we tentatively move the spin under consideration to a new position with a step of length  $v_0$  in an arbitrary direction. Note that this move is immediately rejected if the new position is inside a sphere of radius  $r_0$  centered at a lattice spin or an itinerant spin. This excluded space emulates the Pauli exclusion principle in the one hand, and the interaction with lattice phonons on the other hand. If the new position does not lie in a forbidden region of space, then the move is accepted with a probability given by the standard Metropolis algorithm.[24]

### 3. Results on Ferromagnetic Thin Films

We use here the Ising model and the face-centered cubic (FCC) lattice with size  $4N_x \times N_y \times N_z$ .

We show in Fig. 1 the lattice magnetization versus  $T$  for  $N_z = 8$ ,  $N_x = N_y = 20$ .

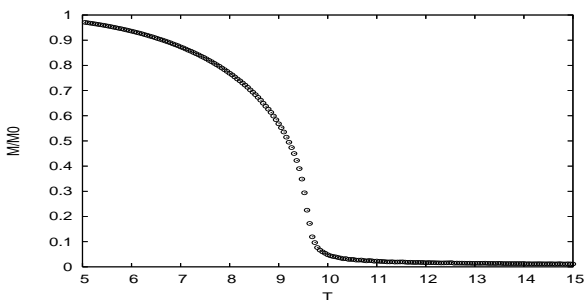


Figure 1: Lattice magnetization versus temperature  $T$  for  $N_z = 8$ .  $T_c$  is  $\simeq 9.58$  in unit of  $J = 1$ .

We let  $N_0$  itinerant spins travel through the system several thousands times until a steady state is reached. The parameters we use in most calculations, except otherwise stated are  $s = S = 1$  and  $N_x = N_y = 20$  and  $N_z = 8$ . Other parameters are  $D_1 = D_2 = 1$  (in unit of the FCC cell length),  $K_0 = I_0 = 2$ ,  $L_0 = 17$ ,  $N_0 = 8 \times 20^2$  (namely one itinerant spin per FCC unit cell),  $v_0 = 1$ ,  $k_F = \left(\frac{\pi}{a}\right)\left(\frac{n_0}{2}\right)^{1/3}$ ,  $r_0 = 0.05$ . At each  $T$  the equilibration time for the lattice spins lies around  $10^6$  MC steps per spin and we compute statistical averages over  $10^6$  MC steps per spin. Taking  $J = 1$ , we find that  $T_c \simeq 9.58$  for the critical temperature of the lattice spins (see Fig. 1).

We define the resistivity  $R$  as

$$R = \frac{1}{n}, \quad (8)$$

where  $n$  is the number of itinerant spins crossing a unit area perpendicular to the  $x$  direction per unit of time.

We show in Fig. 2 the resistivity versus  $T$  without magnetic field.

Below the transition temperature, there exists a single large cluster of lattice spins with some isolated "defects"

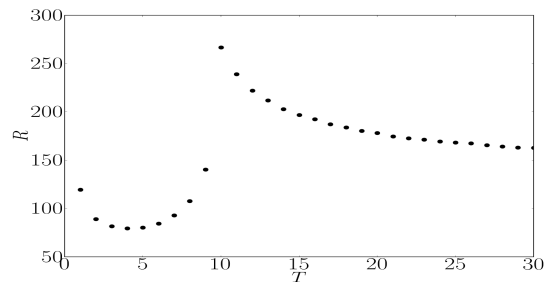


Figure 2: Resistivity  $R$  in arbitrary unit versus temperature  $T$  for  $N_x = N_y = 20$ ,  $N_z = 8$ ,  $E = 1$ ,  $I_0 = K_0 = 2$ .

(i. e. clusters of antiparallel spins), so that any itinerant spin having the parallel orientation goes through the lattice without hindrance. The resistance is thus very small but it increases as the number and the size of "defect" clusters increase with increasing temperature. The fact that it increases with decreasing  $T$  at very low  $T$  comes from the freezing of the itinerant spins due to their interaction with lattice spins and with themselves. This is very similar to the crystallization of interacting particles at low  $T$ . We have tested this interpretation by reducing the strength of the interactions. As a matter of fact,  $R$  reduces its augmentation with decreasing  $T$  as  $T \rightarrow 0$ .

At  $T_c$   $R$  exhibits a cusp at the transition temperature. We can explain this by the following argument: the cusp is due to the critical fluctuations in the phase transition region. We know from the theory of critical phenomena that there is a critical region around the transition temperature  $T_c$ . Fisher-Langer [10] and Kataoka [12] suggested that the form of peak is due mainly to short-range spin-spin correlation. These short-range fluctuations are known to exist in the critical region around the critical point. In a recent work, we found from our MC simulation [22] that the resistivity's peak is due to the formation of antiparallel-spin clusters of sizes of a few lattice cells which are known to exist when one enters the critical region. We have checked this interpretation by first creating an artificial structure of alternate clusters of opposite spins and then injecting itinerant spins into the system. We observed that itinerant spins do advance indeed more slowly than in the completely disordered phase (high- $T$  paramagnetic phase). We have also calculated directly the cluster-size distribution as a function of  $T$  using the Hoshen-Kopelman's algorithm [25]. The result confirms the effect of clusters on the spin conductivity. The reader is referred to our previous work [22] for those results.

In the paramagnetic phase,  $R$  is large and decreases with increasing  $T$ . As  $T$  increases, small clusters will be broken into single disordered spins, so that there is no more energy barrier between successive positions of itinerant spins on their trajectory. The resistance, though high, is decreasing with increasing  $T$  and saturated as  $T \rightarrow \infty$ .

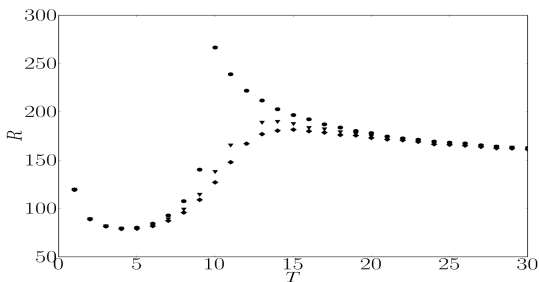


Figure 3: Resistivity  $R$  in arbitrary unit versus temperature  $T$ , for different magnetic fields  $B$ : 0 (circles), 0.5 (triangles), 0.75 (diamonds). Other parameters are the same as in Fig. 2.

### 3.1. Effect of magnetic field.

As it is well known, when a magnetic field is applied on a ferromagnet, the phase transition is suppressed because the magnetization will never tend to zero. Critical fluctuations are reduced, the number of clusters of antiparallel spins diminishes. As a consequence, we expect that the peak of the resistivity will be reduced and disappears at high fields. This is what we observed in simulations. We show results of  $R$  for several fields in Fig. 3.

### 3.2. Discussion

De Gennes and Friedel [8] have shown that the resistivity  $R$  is related to the spin correlation  $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ . They have suggested therefore that  $R$  behaves as the magnetic susceptibility  $\chi$ . However, unlike the susceptibility which diverges at the transition, the resistivity observed in many experiments goes through a finite maximum, i. e. a cusp, without divergence. To explain this, Fisher and Langer [10] and then Kataoka [12] have shown that the cusp is due to short-range correlation. This explanation is in agreement with many experimental data but not all (see Ref. [11] for review on early experiments).

Let us recall that  $\langle E \rangle \propto \sum_{i,j} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$  where the sum is taken over NN (or short-range) spin pairs while  $T\chi \propto \langle (\sum_i \mathbf{S}_i)^2 \rangle = \sum_{i,j} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$  where the sum is performed over *all* spin pairs. This is the reason why short-range correlation yields internal energy and long-range correlation yields susceptibility.

Roughly speaking, if  $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$  is short-ranged, then  $R$  behaves as  $\langle E \rangle$  so that the temperature derivative of the resistivity, namely  $dR/dT$ , should behave as the specific heat with varying  $T$ . Recent experiments have found this behavior (see for example Ref. [4]).

Now, if  $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$  is long-ranged, then  $R$  behaves as the magnetic susceptibility as suggested by de Gennes and Friedel [8]. In this case,  $R$  undergoes a divergence at  $T_c$  as  $\chi$ . One should have therefore  $dR/dT > 0$  at  $T < T_c$  and  $dR/dT < 0$  at  $T > T_c$ . In some experiments, this has been found for example in magnetic semiconductors (Ga,Mn)As [5] (see also Ref. [11] for review on older experiments). We think that all systems are not the same because of

the difference in interactions, so one should not discard a priori one of these two scenarios.

Here, we suggest another picture to explain the cusp: when  $T_c$  is approached, large clusters of up (resp. down) spins are formed in the critical region above  $T_c$ . As a result, the resistance is much larger than in the ordered phase: itinerant electrons have to steer around large clusters of opposite spins in order to go through the entire lattice. Thermal fluctuations are not large enough to allow the itinerant spin to overcome the energy barrier created by the opposite orientation of the clusters in this temperature region. Of course, far above  $T_c$ , most clusters have a small size, the resistivity is still quite large with respect to the low- $T$  phase. However,  $R$  decreases as  $T$  is increased because thermal fluctuations are more and more stronger to help the itinerant spin to overcome energy barriers.

In ferromagnets, what we have found here is a peak of  $R$ , not a peak of  $dR/dT$ . So, our resistivity behaves as the susceptibility although the peak observed here is not sharp and no divergence is observed.

## 4. Results on Antiferromagnetic Thin Films

In the case of antiferromagnets, we use a film with simple cubic (SC) lattice structure. This is because the FCC lattice used in the ferromagnetic case shown above becomes fully frustrated if we use an antiferromagnetic interaction. The frustrated case is very particular [26], it cannot be treated on the same footing as the non frustrated case.

We show first in Fig. 4 the sublattice magnetization versus  $T$  in a simple cubic antiferromagnet with Ising spins. Note that the Neel transition temperature is  $T_N \simeq 4.51$  in the bulk.

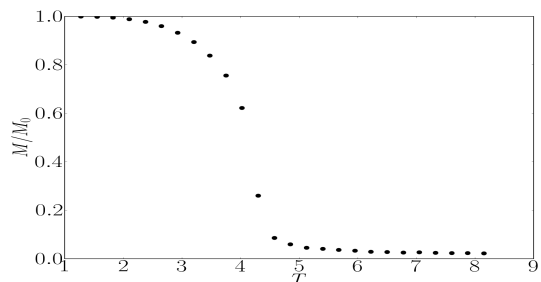


Figure 4: Sublattice magnetization versus temperature  $T$  for  $N_x = N_y = 20$ ,  $N_z = 8$ .  $T_c$  is  $\simeq 4.2$  in unit of  $|J| = 1$ .

Before showing the results on a SC antiferromagnet, let us emphasize the following point. The picture of defect clusters of down spins embedded in a up-spin sea that we used above to explain the behavior of the resistivity in ferromagnets should be modified in the case of antiferromagnets: in antiferromagnets defects are domain walls, clusters on the two sides of a wall both have antiferromagnetic ordering with opposite parity. An itinerant spin crossing a domain wall does not have the same scattering

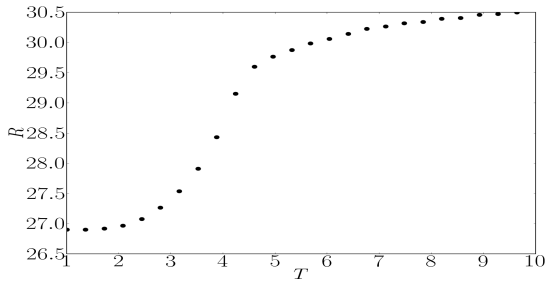


Figure 5: SC AF case. Resistivity  $R$  in arbitrary unit versus temperature  $T$ , in zero magnetic field, with electric field  $E = 1$ ,  $I_0 = K_0 = 0.5$ .

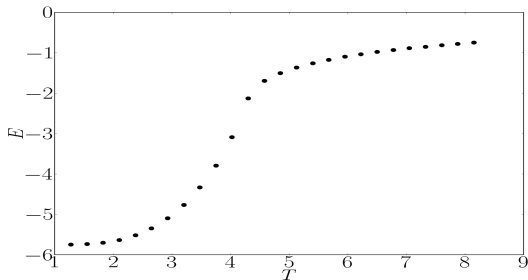


Figure 6: SC AF case. Internal energy  $\mathcal{E}$  in unit  $|J| = 1$  versus temperature  $T$ , in zero magnetic field, with electric field  $E = 1$ ,  $I_0 = K_0 = 0.5$ .

as in a ferromagnet. Its scattering depends on the numbers of up spins and down spins in the sphere of radius  $D_1$ . In other words, the scattering depends on the energy landscape in the crystal: the itinerant spin will stay a longer time where its energy is low, and a shorter time where its energy is high.

The resistivity versus  $T$  in zero magnetic field is shown in Fig. 7 with  $D_1 = D_2 = 1$ . Several remarks are in order: i) the absence of a peak of  $R$ ; ii) the variation of  $R$  with  $T$  has the same shape as the internal energy versus  $T$  shown in Fig. 6, therefore  $dR/dT$  shows a peak similar to the specific heat. This is the second scenario described in section 3.2 above. The peak of  $dR/dT$  has been experimentally observed in many materials, in particular in MnSi [3, 4] among others [2].

The absence of a peak at  $T_N$  observed here is certainly comes from the fact that the motion of an itinerant electron is not sharply slowed down at  $T_N$  by numerous clusters of opposite spins. Let us say it again in another manner: the absence of a peak at the transition is due to the fact that the motion of an itinerant spin depends on its immediate environment: in ferromagnets, the variation of its energy  $\Delta E$  going from a "parallel" cluster to a nearby "defect" (or antiparallel) cluster is much larger than the energy variation going from a cluster of antiferromagnetic ordering to a cluster which is a defect but a defect with an antiferromagnetic structure in the SC antiferromagnetic case. The smaller  $\Delta E$  gives rise to a larger spin mobility i. e. a smaller  $R$ .

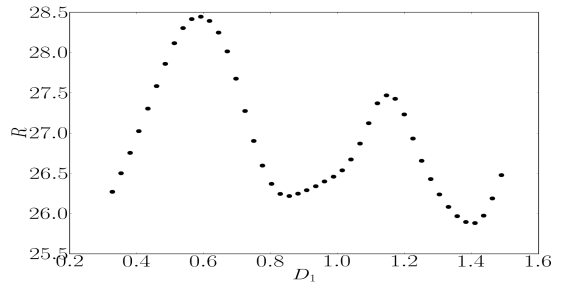


Figure 7: SC AF case. Resistivity  $R$  in arbitrary unit versus  $D_1$  at  $T = 1$ , in zero magnetic field, with electric field  $E = 1$ ,  $I_0 = K_0 = 0.5$ .

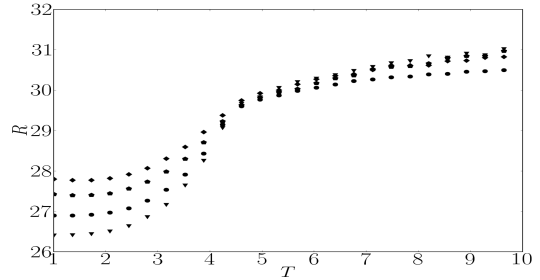


Figure 8: SC AF case. Resistivity  $R$  versus  $T$  for several values of  $D_1$ : 1 (circles), 1.2 (diamonds), 1.4 (triangles), 1.6 (pentagons),  $E = 1$ ,  $B = 0$ ,  $I_0 = K_0 = 0.5$ .

We show now in Fig. 7 the effect of  $D_1$  on the resistivity at a given temperature. We observe here an oscillatory behavior of  $R$ . By analyzing the ratio of numbers of up spins and down spins in the sphere of radius  $D_1$ , we found that this ratio oscillates with varying  $D_1$ : the maxima (minima) of  $R$  correspond to the largest (smallest) numbers of spins antiparallel (parallel) to the itinerant spin. This finding is coherent with what we said before, namely  $R$  is large when the energy of itinerant spin is low (i. e. large number of parallel spins).

We show in Fig. 7 the resistivity versus  $T$  for several  $D_1$ .

## 5. Conclusion

In this work, we have improved our MC simulations by averaging the resistivity over a large number of lattice spin configurations. The results shown above are much better than those in our previous works [21, 22]. Though the physics in the ferromagnetic case are not qualitatively altered but the precision on the peak position of  $R$  is excellent and the statistical fluctuations in the paramagnetic phase are reduced. The spin current is strongly dependent on the lattice spin ordering: in ferromagnets, at low  $T$  itinerant spins whose direction is parallel to the lattice spins yield a strong current, namely a small resistivity. At the ferromagnetic transition, the resistivity undergoes a huge peak. At higher temperatures, the lattice spins are disordered, the resistivity is still large but it decreases with

increasing  $T$ . The existence of the peak in ferromagnets is in agreement with theories, in particular those of Zaránd et al [14] and Haas [13] where interaction between itinerant spins and lattice spins is dominant.

We note that early theories have related the origin of the peak to the spin-spin correlation, while our interpretation here is based on the existence of defect clusters formed in the critical region. This interpretation has been verified by calculating the number and the size of clusters as a function of  $T$  by the use of Hoshen-Kopelman's algorithm. We have formulated a theory based on the Boltzmann's equation which has been shown elsewhere [22]. We solved this equation using numerical data obtained for the number and the size of average cluster at each  $T$ . The results on the resistivity in ferromagnets are in a good agreement with MC results [22].

We have also shown here some results of the SC anti-ferromagnetic case. The absence of a peak of  $R$  confirmed the prediction of Haas [13]. Note that the peak in  $dR/dT$  is similar to that of the specific heat as experimentally observed in MnSi [3, 4]. As a last remark, let us emphasize that our results on FCC AF [26] and on BCC AF [27] show that the shape of the resistivity in antiferromagnets depends on the lattice structure. This is not a surprise when we examine closely the channels by which the itinerant spins flow in the crystals. The extension of the Boltzmann's theory to the case of antiferromagnets is under way [27].

KA acknowledges a financial support from the JSPS for his stay at Okayama University. IH is grateful to the University of Cergy-Pontoise for an invitation during the course of the present work.

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