

# Effects of Ferromagnetic Magnetic Ordering and Phase Transition on the Resistivity of Spin Current

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It has been shown experimentally a long time ago that the magnetic ordering causes an anomalous behavior of the electron resistivity in ferromagnetic crystals. Phenomenological explanations based on the interaction between itinerant electron spins and lattice spins have been suggested to explain these observations. We show by extensive Monte Carlo simulation that this behavior is also observed for the resistivity of the spin current calculated as a function of temperature ( $T$ ) from low- $T$  ordered phase to high- $T$  paramagnetic phase in a ferromagnet. We show in particular that across the critical region, the spin resistivity undergoes a huge peak. The origin of this peak is shown to stem from the formation of magnetic domains near the phase transition. The behavior of the resistivity obtained here is compared to experiments and theories. A good agreement is observed.

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## I. INTRODUCTION

The interplay between magnetic properties and transport behavior has been a subject of continuous experimental investigations.<sup>1,2,3</sup> It has been shown in these works that the resistivity has an anomalous peak in the magnetic transition temperature region. De Gennes and Friedel,<sup>4</sup> and later Fisher and Langer,<sup>5</sup> have suggested that the peak at the transition is due to the magnetic short-range interaction. Various analytical methods such as mean-field approximations<sup>6,7</sup> have been employed to explain experimental observations.

The problem of spin-dependent transport has been also extensively studied in magnetic

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thin films and multilayers. The so-called giant magnetoresistance (GMR) was discovered experimentally twenty years ago.<sup>8,9</sup> Since then, intensive investigations, both experimentally and theoretically, have been carried out.<sup>10,11</sup> Experimental observations show that when the spin of an itinerant electron is parallel to the spins of the environment it will go through easily while it will be stopped if it encounters an antiparallel spin medium. The resistance is stronger in the latter case resulting in a GMR. Although many theoretical investigations have been carried out, to date very few Monte Carlo (MC) simulations have been performed regarding the temperature dependence of the dynamics of spins participating in the current. In a recent work,<sup>12</sup> we have investigated by MC simulations the effects of magnetic ordering on the spin current in magnetic multilayers. Our results are in agreement with measurements.<sup>13</sup>

We study in this paper the transport of itinerant electrons traveling inside a bulk ferromagnetic crystal using extensive MC simulations. The electron spin is supposed to be the Ising model. Various interactions are taken into account, in particular interaction between itinerant spins and interaction between itinerant spins and lattice spins.

The paper is organized as follows. Section II is devoted to the description of our model and the rules that govern its dynamics. In section III, we describe our MC method and discuss the results we obtained. These results are in agreement with experiments and theories. Concluding remarks are given in Section IV.

## II. MODEL

We consider in this paper a bulk ferromagnetic crystal. We use the Ising model and the face-centered cubic (FCC) lattice with size  $4N_x \times N_y \times N_z$ . Periodic boundary conditions (PBC) are used in the three directions. 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  $(\mathbf{S}_i, \mathbf{S}_j)$ ,  $J(> 0)$  being the NN interaction.

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

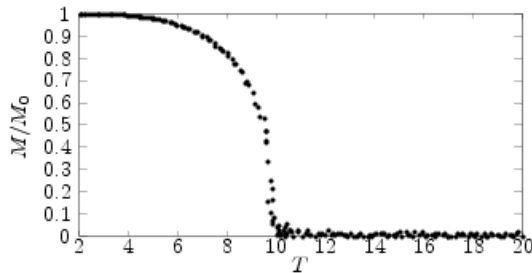


FIG. 1: Lattice magnetization versus temperature  $T$ .  $T_c$  is  $\simeq 9.75$  in unit of  $J = 1$ .

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 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.,  $r_{ij} = |\vec{r}_i - \vec{r}_j|$ . 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  $\mathbf{S}_j$ . For the sake of simplicity, we assume the same form for  $K_{i,j}$  and  $I_{i,j}$ , namely,  $K_{i,j} = K_0 \exp(-r_{ij})$  and  $I_{i,j} = I_0 \exp(-r_{ij})$ , where  $K_0$  and  $I_0$  are constants.

The procedure used in our simulation is described as follows. First we study the thermodynamic properties of the bulk system 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  $T$ .<sup>14</sup> From these physical quantities we determine the critical temperature  $T_c$  below which the system is in the ordered phase. We show in Fig. 1 the lattice magnetization versus  $T$ .

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 PBC. Note that PBC are used to ensure that the average density of itinerant spins remains constant during the time (stationary regime). 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  $\mathcal{H}_E = -\mathbf{E} \cdot \mathbf{v}$ , where  $\mathbf{v}$  is the velocity of the itinerant spin; ii) a chemical potential term which depends on the concentration of itinerant spins within a sphere of radius  $D_2$  ("concentration gradient" effect). Its form is given by  $\mathcal{H}_c = Dn(\mathbf{r})$ , 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.<sup>14</sup>

### III. MONTE CARLO RESULTS

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,  $s = S = 1$  and  $N_x = N_y = N_z = 20$ . Other parameters are  $D_1 = D_2 = 1$  (in unit of the FCC cell length),  $K_0 = I_0 = 2$ ,  $N_0 = 20^3$  (namely one itinerant spin per FCC unit cell),  $v_0 = 1$ ,  $r_0 = 0.05$ . 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 obtain  $T_c \simeq 9.75$  for the estimate of the critical temperature of the lattice spins (see Fig.1).

In Fig. 2 we sketch the characteristic traveling length  $\lambda$  computed after a fixed lapse of time as a function of temperature  $T$ . As can be seen,  $\lambda$  is very large for  $T < T_c$ . We note that there is a small depression in the transition region. We will show below that this has an important consequence on the spin current: the resistance undergoes a cusp.

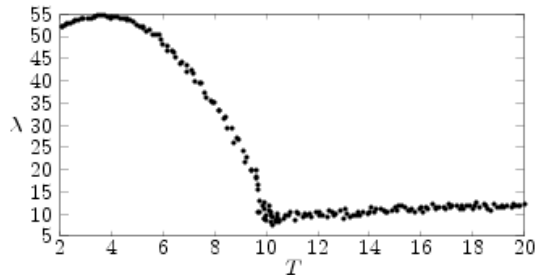


FIG. 2: Characteristic traveling length  $\lambda$  in unit of the FCC cell length versus temperature  $T$ , for 100 MC steps.

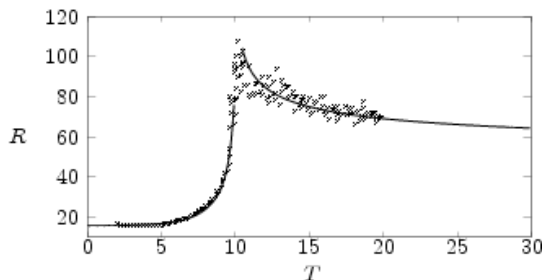


FIG. 3: Resistance  $R$  in arbitrary unit versus temperature  $T$ . Our result using the Boltzmann equation is shown by the continuous curve.

We define the resistance  $R$  as  $R = \frac{1}{n}$ , where  $n$  is the number of itinerant spins crossing a unit area perpendicular to the  $x$  direction per unit of time. In Fig. 3 we show the resistance  $R$  as a function of temperature.

There are several striking points observed here. First,  $R$  is very low in the ordered phase and large in the paramagnetic phase. Below the transition temperature, there exists a single large cluster with some isolated defects, so that any itinerant spin having the parallel orientation goes through the lattice without hindrance. The resistance is thus very small. Secondly,  $R$  exhibits a cusp at the transition temperature, the existence of which is due to the critical fluctuations in the phase transition region. De Gennes and Friedel<sup>4</sup> and later Fisher and Langer<sup>5</sup> and then Kataoka<sup>6</sup> among others have shown that the resistance is related to the spin correlation  $\langle S_i S_j \rangle$  which is nothing but the magnetic susceptibility. The latter diverges at the transition. This explains at least partially the cusp of  $R$  observed here. Another picture to explain the cusp is that when  $T_c$  is approached large clusters of up (resp. down) spins form 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 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, so that 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 overcome energy barriers. Note in addition that the cluster size is now comparable with the radius  $D_1$  of the interaction sphere, which in turns reduces the height of potential energy barriers. We have checked this interpretation by first creating an artificial structure of alternate clusters of opposite spins and then injecting itinerant spins into the structure. We observed that itinerant spins do advance indeed more slowly than in the completely disordered phase (high- $T$  paramagnetic phase). We have next calculated directly the cluster-size distribution as a function of  $T$  (not shown) using the Kopelman algorithm.<sup>15</sup> The result confirms the effect of clusters on the spin conductivity. The reader is referred to our previous work<sup>12</sup> for results of a multilayer case. Note that in Fig. 3 we also show the results from our theory using the Boltzmann equation in the relaxation-time approximation. The agreement is remarkable. We will show the details of this theory elsewhere.<sup>16</sup>

#### IV. CONCLUDING REMARKS

We have shown in this paper first results of MC simulations on the transport of itinerant spins interacting with localized lattice spins in a ferromagnetic FCC crystal. Various interactions have been taken into account. We found that the spin current is strongly dependent on the lattice spin ordering: at low  $T$  itinerant spins whose direction is parallel (antiparallel) to the lattice spins yield a strong (weak) current. At high temperatures, the lattice spins are disordered, the current of itinerant spins is very weak and does not depend on the input orientation of itinerant spins. As a consequence, the resistance is very high at high  $T$ . We found in the transition region between low- $T$  and high- $T$  phases a peak of the resistance which is due to the existence of domains of lattice spins. Experiments and theories support our finding.

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