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SPIN TRANSPORT IN MAGNETICALLY ORDERED SYSTEMS: EFFECT OF THE LATTICE RELAXATION TIME

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Spin resistivity R has been shown to result mainly from the scattering of itinerant spins with magnetic impurities and lattice spins. R is proportional to the spin–spin correlation so that its behavior is very complicated near and at the magnetic phase transition of the lattice spins. For the time being there are many new experimental data on the spin resistivity going from semiconductors to superconductors. Depending on materials, various behaviors have been observed. There is however no theory so far which gives a unified mechanism for the spin resistivity in magnetic materials. Recently, we have shown Monte Carlo results for different systems. We found that the spin resistivity is very different from one material to another. In this paper, we show for the first time how the dynamic relaxation time of the lattice spins affects the resistivity of itinerant spins observed in Monte Carlo simulation.

Keywords: Spin resistivity; spin transport in magnetic materials; Monte Carlo simulation.

1. Introduction

The resistivity is an important subject in condensed-matter physics. It has been studied experimentally and theoretically already with old classical physics. However, only from the fifties, with notions borrowed from microscopic modern physics that the resistivity has been viewed as a consequence of microscopic mechanisms which govern physical behaviors of materials through which conduction electrons travel. In this paper, we are interested in the resistivity caused by scattering of itinerant electronic spins by localized lattice spins in magnetic materials (ferromagnets and anfiferromagnets). The resulting resistivity is called hereafter "spin resistivity" which is to be distinguished from the resistivity due to spin-independent scattering, for example, by phonons and non-magnetic impurities.

The spin resistivity, R, was shown to depend on the spin–spin correlation in ferromagnetic crystals by de Gennes and Friedel,[1] Fisher and Langer[2] among

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others. At low temperatures (T), the spin-waves are shown to be responsible for the T^2 behavior of the spin resistivity in ferromagnets.[3,4] Note however that in these calculations the itinerant electrons have been considered as free electrons interacting with the lattice spins, but there is no interaction between them. We have shown[5,6] that when an interaction between itinerant electrons is introduced, the itinerant electrons can be crystallized at low T giving rise to an increase of R as $T \to 0$. Experimental data in various materials show this behavior,[7–11] but we would warn that there may be other mechanisms involved as well. At the magnetic phase transition temperature T_C, the spin–spin correlation diverges in magnetic materials with a second-order phase transition. The theory of de Gennes–Friedel predicts that R should show a divergent peak. However, experiments in various magnetic materials ranging from semiconductors to superconductors[7–17] show indeed an anomaly at the transition temperature T_C, but the peak is more or less rounded, not as sharp as expected from the divergence of the correlation length. It has been shown in fact that[2,18] the form of the peak depends on the length of the correlation included in the calculation of R. If only short-range correlations are taken into account, then the peak is very rounded. A justification for the use of only short-range correlations comes from the fact that the mean free path of itinerant spins is finite at T_C. When scattering is due to impurities, the peak has been shown to depend on the localization length.[19] In the case of antiferromagnets, Haas has shown the absence of a resistivity peak.[20] Our recent works using Monte Carlo (MC) simulations have shown that there is indeed an anomaly at T_C in various magnetic models from ferromagnets,[5,21,22] antiferromagnets[5,23] to frustrated spin systems.[6,24] The shape of the anomaly depends on many ingredients such as crystal structures, spin models, and interaction parameters.

In this paper, we will show new results obtained by MC simulation when we take into account the temperature dependence of the relaxation time of localized lattice spins in the simulation. We will show that this temperature dependence affects the shape of the peak in the phase transition region.

Section 2 is devoted to a description of the general model and the MC method. We introduce in this section the temperature dependence of the relaxation time. Results are shown and discussed in Sec. 3 for both ferro- and antiferromagnets in terms of critical slowing-down. Concluding remarks are given in Sec. 4.

2. Model and Method

The model we use in our MC simulation is very general. The itinerant spins move in a crystal whose lattice sites are occupied by localized spins. The itinerant spins are assumed to be of Ising type, but the method of simulation can be used for other spin models.[23] The localized spins may be of Ising, XY or Heisenberg models. Their interaction is usually limited to nearest-neighbors (NN) but this assumption is not necessary. It can be ferromagnetic or antiferromagnetic.

Note that the purpose of this paper is to study the effect of the magnetic transition on the spin resistivity, in particular, the effect of the lattice relaxation time. This transition occurs at a high temperature where it is known that the quantum nature of itinerant electron spins does not make significant additional effects with respect to the classical spin model. In particular, in the context of spin transport, we have shown in previous works that the use of quantum spins through the Boltzmann's equation gives a good agreement with MC simulations using classical spin model[22,23] at the phase transition temperature. Therefore, to simplify the task, we consider here the classical Ising spin model.

2.1. *Interactions*

We consider a thin film of a given lattice structure where each lattice site is occupied by a spin. The interaction between the lattice spins is limited to NN with the following Hamiltonian:

$$\mathcal{H}_l = -\sum_{(i,j)} J_{i,j}\mathbf{S}_i \cdot \mathbf{S}_j \,, \tag{1}$$

where $\mathbf{S}_i$ is an Ising spin whose values are ± 1, $J_{i,j}$ the exchange integral between the NN spin pair $\mathbf{S}_i$ and $\mathbf{S}_j$. Hereafter, we take $J_{i,j} = J$ for all NN spin pairs, for simplicity. As a convention, ferromagnetic (antiferromagnetic) interaction has positive (negative) sign. The system size is $N_x \times N_y \times N_z$ where $N_i (i = x, y, z)$ is the number of lattice cells in the i direction. Periodic boundary conditions (PBC) are used in the x and y directions while the surfaces perpendicular to the z-axis are free. The film thickness is N_z.

We define the interaction between the itinerant spins and the localized lattice spins as follows

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

where σ_i is the Ising spin of the ith 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. For simplicity, we use the following interaction expression

$$I_{i,j} = I_0 e^{-\alpha r_{ij}} \,, \tag{3}$$

where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$, I_0 and α are constants. 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 $K_{i,j}$ being the interaction that depends on the distance between electrons i and j. The choice of the constants K_0 and β will be discussed below.

Note that we choose for the continuous distance-dependent interaction an exponential law, but this choice does not affect the general feature of our results presented in this paper because the short cut-off distance used here limits the interaction to a small number of neighbors (typically to second nearest neighbors) so the choice of another law such as a power law, or even discrete interaction values, for such a small cut-off will not make a qualitative difference in the results.

Dynamics of itinerant electrons is ensured by an electric field applied along the x-axis. Electrons travel in the x direction, and leave the system at the end. The PBC on the xy planes ensure that the electrons who leave the system at one end are to be reinserted at the other end. For the z direction, we use the mirror reflection at the two surfaces. These boundary conditions are used in order to conserve the average density of itinerant electrons. One has

$$\mathcal{H}_E = -e\boldsymbol{\epsilon} \cdot \boldsymbol{\ell}\,, \tag{6}$$

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

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

$$\mathcal{H}_c = D\boldsymbol{\nabla}_r n(\mathbf{r})\,, \tag{7}$$

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.

2.2. *Simulation method*

The procedure of our simulation can be split into two steps. The first step consists of equilibrating the lattice at a given temperature T without itinerant electrons. When equilibrium is reached, in the second step, we randomly add N_0 polarized itinerant spins into the lattice. Each itinerant electron interacts with lattice spins in a sphere of radius D_1 centered at its position, and with other itinerant electrons in a sphere of radius D_2.

The procedure of spin dynamics is described as follows. After injecting N_0 itinerant electrons in the equilibrated lattice, we equilibrate the itinerant spins using the following updating. We calculate the energy E_{old} of an itinerant electron taking into account all interactions described above. Then we perform a trial move of length ℓ taken in an arbitrary direction with random modulus in the interval $[R_1, R_2]$ where $R_1 = 0$ and $R_2 = a$ (NN distance), a being the lattice constant. Note that the move is rejected if the electron falls in a sphere of radius r_0 centered at a lattice spin or at another itinerant electron. This excluded space emulates the Pauli exclusion. We calculate the new energy E_{new} and use the Metropolis algorithm to accept or reject the electron displacement. We choose another itinerant electron

and begin again this procedure. When all itinerant electrons are considered, we say that we have made a MC sweeping, or one MC step/spin. We have to repeat a large number of MC steps/spin to reach a stationary transport regime. We then perform the averaging to determine physical properties such as magnetic resistivity, electron velocity, energy etc. as functions of temperature.

We emphasize here that in order to have sufficient statistical averages on microscopic states of both the lattice spins and the itinerant spins, we use the following procedure. After averaging the resistivity over N_1 steps for "each" lattice spin configuration, we thermalize again the lattice with N_2 steps in order to take another disconnected lattice configuration. Then we take back the averaging of the resistivity for N_1 steps for the new lattice configuration. We repeat this cycle for N_3 times, usually several hundreds of thousands times. The total MC steps for averaging is about 4×10^5 steps per spin in our simulations. This procedure reduces strongly thermal fluctuations observed in our previous work.[22]

Of course, the larger N_1 and N_3 are the better the statistics becomes. The question is what is the correct value of N_1 for averaging with each lattice spin configuration at a given T? This question is important because this is related to the relaxation time $\tau_L$of the lattice spins compared to that of the itinerant spins, τ_I. The two extreme cases are (i) $\tau_L \simeq \tau_I$, one should take $N_1 = 1$, namely the lattice spin configuration should change with each move of itinerant spins, and (ii) $\tau_L \gg \tau_I$, in this case, itinerant spins can travel in the same lattice configuration for many times during the averaging.

In order to choose a right value of N_1, we consider the following temperature dependence of τ_L in non-frustrated spin systems. The relaxation time is expressed in this case as[25]

$$\tau_L = \frac{A}{|1 - T/T_C|^{z\nu}} \tag{8}$$

where A is a constant, ν the correlation critical exponent, and z the dynamic exponent. From this expression, we see that as T tends to T_C, τ_L diverges. In the critical region around T_C the system encounters thus the so-called "critical slowing down": the spin relaxation is extremely long due to the divergence of the spin–spin correlation. In our previous papers,[5,6,21,22,24] we did not take into account the temperature dependence of τ_L. We propose to study here the spin resistivity using Eq. (8).

We define spin resistivity R as

$$R = \frac{1}{n_e}\,, \tag{9}$$

where n_e is the number of itinerant electron spins crossing a unit slice perpendicular to the x direction per unit of time.

2.3. *Choice of parameters and units*

The spin resistivity is dominated by the two interactions Eqs. (2) and (5). As said earlier, our model is very general. Several kinds of materials such as metals, semiconductors, insulating magnetic materials etc. can be studied with our model, provided an appropriate choice of the parameters. For example, non-magnetic metals correspond to $I_{i,j} = K_{i,j} = 0$ (free conduction electrons). The case of magnetic semiconductors corresponds to the choice of parameters K_0 and I_0 so as the energy of an itinerant electron due to the interaction $\mathcal{H}_r$ should be much lower than that due to $\mathcal{H}_m$, namely itinerant electrons are more tightly bound to localized atoms. Note that $\mathcal{H}_m$ depends on the concentration of itinerant spins. For example, the dilute case yields a small $\mathcal{H}_m$. We will show below results obtained for typical values of parameters which correspond more or less to semiconductors. 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 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 with that between lattice spins. To simplify, we take $\alpha = 1$. This case corresponds more or less to a semiconductor, as said earlier.
(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 (agglomeration) due to their attractive interaction [Eq. (5)].
(v) The electric field is chosen 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 much weaker than E_i, as said above in the case of semiconductors.

A variation of each parameter respecting the above requirements does not change qualitatively the results shown below. Only the variation of D_1 in some antiferromagnets does change the results (see Ref. 6).

The energy is measured in the unit of $|J|$. The temperature is expressed in the unit of $|J|/k_B$. The distance (D_1 and D_2) is in the unit of a.

3. Results and Discussion

In this section, we show for comparison the results obtained with and without temperature dependence of the lattice relaxation time for both ferromagnets and antiferromagnets. In each case, we use the same set of interaction parameters in order to outline the effect of the temperature-dependent relaxation time.

In this paper, we use the lattice size $N_x = N_y = 20$ and $N_z = 8$ and we consider the body-centered cubic (bcc) lattice for illustration. The lattice constant is a. The spin resistivity is calculated with $N_0 = (N_x \times N_y \times N_z)/2$ itinerant spins (one electron per two lattice cells). Except otherwise stated, we choose interactions $I_0 = 2$, $K_0 = 0.5$, $D_1 = a$, $D_2 = a$, $D = 0.5$, $\epsilon = 1$, $N_0 = 1600$, and $r_0 = 0.05a$. A discussion on the effect of a variation of each of these parameters is given above.

Note that, due to the form of the interaction given by Eq. (5), the itinerant spins have a tendency to form compact clusters to gain energy. This tendency is neutralized by the concentration gradient term, i.e. a chemical potential, given by Eq. (7). The value of D has to be chosen so as to avoid an agglomeration of itinerant spins. This choice depends of course on the values of D_1 and D_2. Examples have been shown elsewhere.[6,24] For the temperature dependence of the lattice relaxation time τ_L, we take $\nu = 0.638$ (3D Ising universality) and $z = 2.02$.[26] By choosing $A = 1$, we fix $\tau_L = 1$ at $T = 2T_C$ deep inside the paramagnetic phase far above T_C. This value is what we expect for thermal fluctuations in the disordered phase.

Figure 1 shows the spin resistivity R in bcc ferromagnetic and antiferromagnetic thin films. Note that the transition temperature for this thin film of size

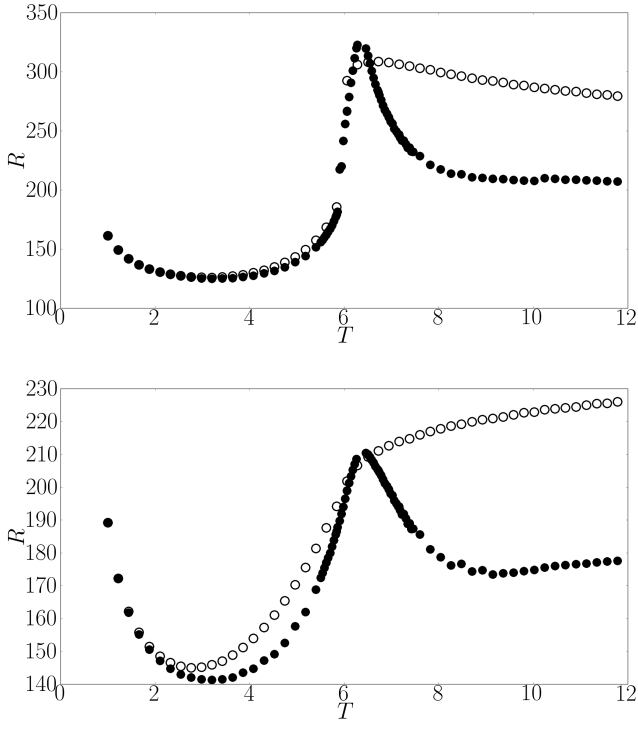

Fig. 1. Resistivity R calculated with temperature-independent relaxation (white circles) and temperature-dependent relaxation (black circles) in arbitrary unit versus temperature T, in zero magnetic field, with electric field $\epsilon = 1$, $I_0 = 2$, $K_0 = 0.5$. Upper: bcc ferromagnetic thin film, lower: bcc antiferromagnetic thin film.

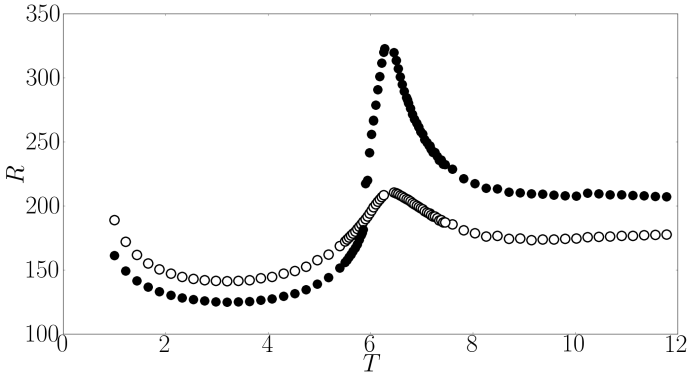

Fig. 2. The bcc ferromagnetic and antiferromagnetic films. Resistivity R with temperature-dependent relaxation for ferro- (black circles) and antiferromagnet (white circles) in arbitrary unit versus temperature T, in zero magnetic field, with electric field $\epsilon = 1$, $I_0 = 2$, $K_0 = 0.5$.

$20 \times 20 \times 8$ with Ising spins interacting via the NN coupling is $T_C \simeq 6.35$. For the ferromagnetic case, several remarks are in order:

(i) The results obtained with and without temperature-dependent relaxation time for $T < T_C$ coincide with each other.
(ii) At T_C, for the set of parameters used here, the results using the temperature-independent relaxation shows a broad maximum above T_C while those using the temperature-dependent relaxation strongly decreases at T_C giving rise to a sharp peak.

For the antiferromagnetic case, note that the transition temperature is the same as that of the ferromagnetic counterpart shown above. We observe that R in the case of temperature-dependent relaxation is lower than that in the case of temperature-independent one in the whole temperature range. Note that the value of the peak is much smaller here than in the ferromagnetic case.

We show in Fig. 2 the two curves of ferromagnet and antiferromagnet with T-dependent relaxation time. We observe here that below T_C, the resistivity of antiferromagnet is higher than that of ferromagnet, while for $T > T_C$ the reverse is true.

It is interesting to calculate the relaxation time τ_I of the itinerant spins. We define τ_I in the simulations as the MC time (in unit of one MC step/spin) between two "MC collisions", namely the lapse of time between two "rejections" of a spin to advance. Of course this quantity is averaged over all itinerant spins and over the simulation time. Figure 3 shows τ_I^{-1} obtained by simulation using τ_L. As for R seen above, the temperature dependence and independence are markedly different only for $T > T_C$ for both cases of ferromagnet and antiferromagnet shown in Fig. 3.

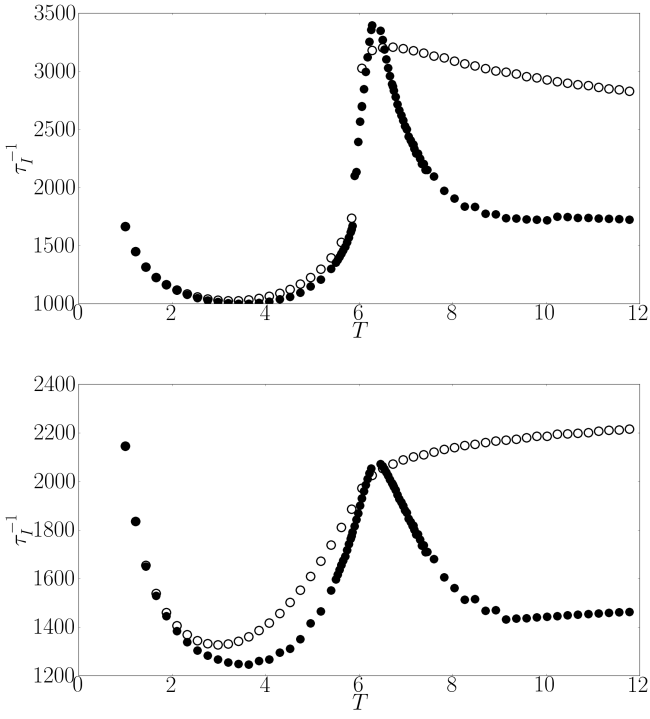

Fig. 3. Inverse of relaxation time of itinerant spins τ_I^{-1} calculated with temperature-independent (white circles) and temperature-dependent (black circles) of the lattice spins versus temperature T, in zero magnetic field, with electric field $\epsilon = 1$, $I_0 = 2$, $K_0 = 0.5$. Upper: bcc ferromagnetic film, lower: bcc antiferromagnetic film.

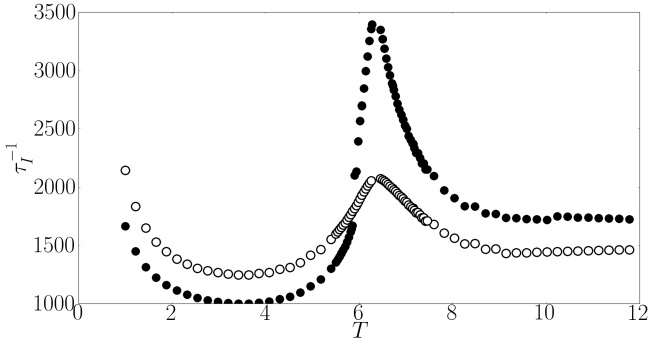

Fig. 4. The bcc ferromagnet and antiferromagnet cases. Inverse of relaxation time of itinerant spins τ_I^{-1} calculated with temperature-dependent relaxation time of the lattice spins for ferromagnet (black circles) and antiferromagnet (white circles) versus temperature T, in zero magnetic field, with electric field $\epsilon = 1$, $I_0 = 2$, $K_0 = 0.5$.

Figure 4 shows τ_I^{-1} for both ferro- and antiferromagnetic cases, for comparison. The antiferromagnet has τ_I^{-1} larger at $T < T_C$. Note that the resistivity is proportional to τ_I^{-1}.

Let us discuss the reason why the temperature dependence of the lattice relaxation time affects so strongly the shape of the spin resistivity for $T \geq T_C$. First, we emphasize on two "empirical" rules that we observed and verified in a number of cases:

(a) Itinerant spins move easily when they are energetically unstable. The electric field then drives them easily forward. On the other hand, when they are "at ease" with surrounding spins, namely their energy is low, they will not move easily. We have checked this rule by calculating their velocity as a function of their energy.[6]
(b) In the case where the energy of an itinerant spin is low, the move of itinerant spins depends on the energy difference between its initial and final positions. Consider the ordered phase of the lattice: the energy at any point is very low and the energy difference between any two points is close to zero (ordered state). Hence, by the MC updating criterion, the electric field dominates again the move of itinerant spins. This explains the very small resistivity at low T with respect to that at high T (except when $T \to 0$ where other mechanisms come to play).

For the effect of τ_L, several important points are in order:

(i) For $T < T_C$ the lattice is ordered, therefore itinerant spins do not see the difference when the lattice changes its microstates more frequently or less frequently. This explains the same values obtained for R with and without temperature dependence of τ_L in ferromagnets. In antiferromagnets, one observes a small difference due to the presence of lattice down spins which act differently on up-polarized itinerant spins.
(ii) For $T > T_C$, the lattice is disordered: the lattice spins are frequently flipped. Itinerant spins have to move constantly to accommodate themselves to the fluctuating environment. Thus, τ_I is long by definition because there are very few rejections to move. Consequently, R is small in the paramagnetic phase.
(iii) Finally, it is striking to observe a strong correlation between τ_L and τ_I: Since τ_L is very large in the transition region where the lattice is in the regime of critical slowing down, itinerant spins have time to find themselves in energetically favorable positions. Then they refuse to move (first rule mentioned above). As a consequence, τ_I is very small (for example, $\tau_I = 1$, if they refuse to move at every update trial). R is thus very high. We have showed the inverse of τ_I in Figs. 3 and 4 because R is inversely proportional to τ_I. The correlation between τ_L and τ_I is thus "high τ_L corresponds to low τ_I" and vice-versa.

Now, let us show the effect of the choice of A of Eq. (8) in Fig. 5. The higher A (i.e. higher τ_L) induces an increase of R near T_C but gives the same value as T is far away from the critical point. Thus, the width of R at the transition temperature can serve as a measure of the relaxation time of the lattice spins.

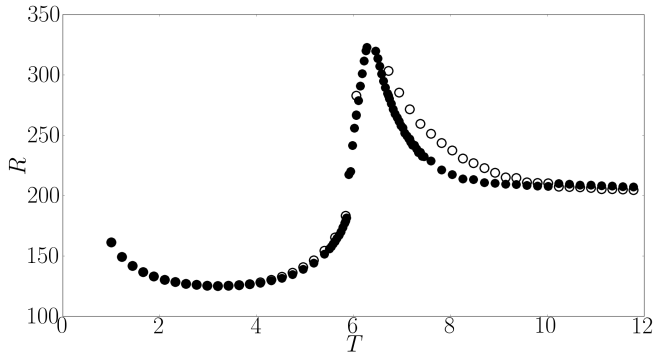

Fig. 5. The bcc ferromagnet. Effect of the choice of the constant A: (i) $A = 1$ (black circles), (ii) $A = 2$ (white circles) versus temperature T, in zero magnetic field, with electric field $\epsilon = 1$, $I_0 = 2$, $K_0 = 0.5$. See text for comments.

4. Conclusion

In this paper, we have shown the effect of the temperature dependence of the relaxation time on the spin resistivity for both ferromagnetic and antiferromagnetic films with bcc lattice structure.

In the ferromagnetic case, the long relaxation time in the critical region compared to that of the paramagnetic phase gives rise to a sharp peak of the spin resistivity at T_C. The resistivity in the low-T region is insensitive to the relaxation time while in high-T region, the resistivity is much smaller than that obtained with the temperature-independent relaxation time. The same tendency is observed for the antiferromagnetic case: while the spin resistivity in the case of temperature-independent relaxation time does not show a peak at T_C, the extremely long relaxation in the critical region with respect to that of the paramagnetic phase gives rise to a pronounced rounded peak at T_C. It is very interesting to study other systems such as spin glasses where the relaxation time is extremely long even at temperatures far below T_C.

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