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FINITE SIZE EFFECTS IN GRAPHITE-Cl₂Co INTERCALATION COMPOUNDS; A MONTE CARLO STUDY

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Abstract. - Magnetic susceptibility data of Cl₂Co - GIC have been compared with Monte Carlo simulations on finite size systems. The best fit is obtained for the XY model, free boundary conditions on a 50 x 50 spins lattice with $J_{\text{eff}} / k = 8.7$ K. The effect of small symmetry breaking fields is found to be negligible.

1. Introduction

The search for two dimensional, 2d, magnetic systems has centered a great deal of interest to compare the experimental data with the theoretical predictions [1]. Particularly, 2d systems with a Kosterlitz-Thouless (KT) phase transition are very scarce and, moreover, of difficult analysis since most of the theoretical predictions for KT transitions use simplifications like non interaction between spin waves and vortices excitations. (This is just the Villain approximation of the planar rotator (PR) model (spin dimensionality, $D = 2$) [2]. Even more, periodic boundary conditions (PBC) are needed to deal with bulk properties and to make use of the spin wave theory. However these assumptions are far from the real nature of graphite intercalated compounds (GIC). Specially Cl₂Co - GIC compounds behave as very good examples of magnetic 2d systems [3] but due to the synthesis procedure the Cl₂Co intercalant does not extend over the whole plane, and 2d clusters are formed. Therefore, finite size effects (FSE) may play a decissive role in their physical properties. To our knowledge only Szeto and Dresselhaus [4] have given an analytical treatment to FSE in KT transitions though their work has the limitations above exposed.

In previous studies [5] we have shown that the magnetic susceptibility is rather sensitive to FSE. Moreover, free boundary conditions (FBC) allow the appearance of single free vortices near boundaries and the pair vortex-antivortex excitations energy is lower than in the PBC case.

In this communication the PR ($D = 2$) and XY ($D = 3$) models, in the triangular lattice, namely

$$H_{\text{PR}} = -J_{\text{eff}} \sum_{(i,j)} \cos (\phi_i - \phi_j)$$

$$H_{\text{XY}} = -J_{\text{eff}} \sum_{(i,j)} \sin \theta_i \sin \theta_j \cos (\phi_i - \phi_j)$$

are dealt with, where $J_{\text{eff}} = JS^2$ and $\theta$ and $\phi$ are the polar and azimuthal spin direction angles, respectively. First a comparison of Cl₂Co - GIC $\chi$ data with the predictions obtained with High Temperature Series expansions (HTS) is performed. Second the data are compared with MC simulations. Finally the effects of the symmetry breaking fields (SBF) are analysed.

2. Analysis and comparisons

In previous analysis of Cl₂Co - GIC $\chi$ data [6, 7] were compared with theoretical estimations obtained by direct computations of the HTS for the PR model. Indeed, they were appropriated for high temperature but presented a very bad convergency in the region where they were used. In figure 1 the comparison of experimental data [4] with the HTS predictions for the PR model [8] is represented. This fit is similar to one done by Szeto et al. [6] and two features deserve attention: first, the $\chi$ data lie above HTS predictions for the infinite lattices whereas one would expect that, due to FSE, would lie below. The radius of HTS convergence may be enlarged using Padé approximants (PA). As
shown in figure 1, PA estimations deviate clearly from both HTS and experimental results. This difference invalidates the direct use of HTS and the agreement found by Szeto et al. [6] for the experimental data with the PR model is meaningless.

A more realistic model is the XY in which the HTS predictions have a behavior similar to the PR one. The best fit to $\chi$ gives a value $J_{\text{eff}} / k = 9.0$ K. Obviously, the experimental data separate from PA results and one of the cause may be the presence of FSE in the Cl$_2$Co clusters. However, from this comparison we deduce that it is better and more realistic to compare with XY model rather with PR one.

MC simulations enable us to modelize real systems in two ways. First, FSE are taken into account since clusters estimated size $(L \times L)$ is reasonably small $(L < 100)$. Second, different boundary conditions can be properly simulated. MC simulations have been performed using standard Metropolis algorithm. Spin lattices ranging from $30 \times 30$ to $60 \times 60$ for the XY model and with FBC and PBC have been considered. The average was done over $5 \times 10^5$ to $10 \times 10^5$ MC steps after discarding $3 \times 10^3$ steps for equilibration. The susceptibility is defined as $\tilde{\chi} = (1 / N) \langle S^2 \rangle$, where $S^2 = \left( \sum S_x^2 + \sum S_y^2 \right)$ and $N = L \times L$. This quantity has to be compared with the reduced experimental susceptibility $\chi_{\text{exp}} = \chi T / C$ $C$ being the Curie's constant obtained by fit at high enough temperatures. In figure 2 the fit of MC simulations with PBC to experimental data with $J_{\text{eff}} / k = 9$ K is shown. It is interesting to observe how MC simulations can discriminate different lattice sizes. In figure 3 the same fit is shown, but with FBC and $J_{\text{eff}} / k = 8.7$ K. In figure 3 a fair agreement between the experimental data and the theoretical calculations at the $50 \times 50$ spins lattice is found. This value is in agreement with one expect from experimental results (obviously an average on real clusters sizes) [9].

Other experimental characteristics in Cl$_2$Co – GIC is the existence of six-fold SBF [10]. This can be introduced in the XY Hamiltonian adding a term like

$$H_{\text{SBF}} = -h_5 \sum \sin \theta_i \cos (6\phi_i).$$

Experimentally it is found that $h_5$ has a value of $(10^{-3} - 10^{-4})$ J [10]. Simulations performed for the XY model with FBC and $h_5$ between $(10^{-4} - 1.0)$ J have not given appreciable corrections to $\chi$ in the temperature range of our interest. These results are in contradiction with the previously reported [4] in which SBF had a great influence on $\chi$ even at high temperatures. At $T / J \approx 0.4$ took place the predicted transition to an ordered phase [5] which is well below the temperature range considered here.

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