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LETTER TO THE EDITOR

Critical behaviour of the $S = 1/2$ isotropic Heisenberg ferromagnetic film with a diluted upper layer: a Monte Carlo study

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Abstract. We investigate the critical properties of an $S = \frac{1}{2}$ isotropic Heisenberg ferromagnetic film with a simple cubic structure, consisting of two monatomic layers with the upper layer being incomplete due to dilution. We demonstrate the effective two-dimensional character of the critical behaviour of the longitudinal susceptibility for this system and study the dependence of an effective in-plane exchange constant on the concentration of the spins in the upper layer. Within appropriate limits, we compare our results with the two-dimensional percolation theory.

In some recent publications [1, 2] we studied numerically the critical properties of ultrathin monocrystalline thin films described by an $S = \frac{1}{2}$ isotropic Heisenberg ferromagnetic Hamiltonian on a simple cubic lattice and with the number of monolayers $L \leqslant 3$. We found that, for the investigated range of temperatures, the critical behaviour of the longitudinal susceptibility χ and the correlation range ξ was effectively two-dimensional (2D) [1–3], i.e. for $T/J \gg 1$ they satisfy

$$\chi T = A\left(\frac{T}{J}\right)^3 \exp\left(\frac{2\eta_\chi \pi J}{T}\right) \qquad \xi = B(T/J)^{1/2} \exp\left(\frac{\eta_\chi \pi J}{T}\right) \tag{1}$$

with $\eta_\chi \simeq L$. We note that the analysis of our results cannot give us a proof that the behaviour of the system remains 2D to $T = 0$. This is because in our Monte Carlo calculations we use large but finite lattices and long but finite Markov chains. However, for the investigated temperature interval, the transverse (or interlayer) correlations were shown to be close to saturation [1, 2], not giving rise so far to any kind of finite-temperature phase transition, which is consistent with the two- and three-monolayer films being effectively 2D to $T = 0$. We suggested [2] that the anomalous value for the exchange constant deduced in [4] for the 2.5 monolayer thin ^{3}He film was due to in-plane exchange renormalization effects. There remains a possibility, however, that the third (incomplete) layer in the experiment of [4] could contribute to this renormalization.

Accordingly, the aim of the present paper is to study the effects of an incomplete layer. For simplicity, we consider a Heisenberg film consisting of two monatomic layers, of which one is complete, i.e. all the sites are occupied by spins, and the second is diluted or incomplete, having random distribution of vacant sites with a given concentration. We

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show that the critical behaviour of the susceptibility for such a system is effectively 2D within the explored range of temperatures with the index η_χ varying from 2 to 1 with the concentration. We discuss the concentration dependences of η_χ in relation to the percolation theory.

As in our previous paper [1, 2], the Handscomb Monte Carlo procedure had been utilized. We consider the thin film as a crystal having two equal surfaces in one direction and infinite in the others. The Hamiltonian of an $S = \frac{1}{2}$ Heisenberg ferromagnet with nearest-neighbour interactions and the described geometry can be written generally as

$$H = -2\sum_{(ij)} J^1_{ij} S^1_i \cdot S^1_j - 2\sum_{(pq)} J^2_{pq} S^2_p \cdot S^2_q - 2\sum_{l} J^{\rm T}_l S^1_l \cdot S^2_l \tag{2}$$

where the first and second sums are for the intra-layer interactions of the spins within the first and second layers, respectively, and the third sum is for the interlayer interactions of the spins. The superscripts 1 and 2 refer to the layer number whilst the subscripts label the positions of the sites in the film plane. Also, we assume the in-plane periodic boundary conditions [1] to be in effect.

To introduce incompleteness into the second layer, we assume the following structure of the exchange interaction matrices J^1_{ij}, J^2_{pq} and $J^{\rm T}_l$: (i) $J^1_{ij} \equiv J$ for all the pairs of nearest neighbours, i and j; (ii) to construct the matrices J^2_{pq} and $J^{\rm T}_l$ we at first introduce the fractional concentration x of the occupied sites, where $0 < x < 1$ and $x = 1$ represents the complete second layer. Then, using this concentration as the probability for the single site to be occupied, we construct the vacancy distribution within the second layer. After that, we put $J^2_{pq} = 0$ if either of the sites p and q are vacant, otherwise we put $J^2_{pq} = J$ if both are occupied. Similarly, we put $J^{\rm T}_l = 0$ if in the second layer the site l is vacant, otherwise $J^{\rm T}_l = J$. We note that in our simple model we do not account for the possibility of the interlayer exchange being different from the in-plane exchange.

For our calculations we chose the same temperature interval as before [1, 2], i.e. $0.7 < T/J < 1.3$. Since we had already made a simple finite-scaling analysis for this interval for the one- and two-monolayer films [1, 2], we can assume that a square with the linear size equal to 70 sites represents the infinite system fairly well. We note, however, that the finite-size effects are expected to be more important for diluted systems than for systems without structural disorder [5]. However, in our case, having made several test calculations, we did not observe these effects to be significant in the chosen temperature interval. All the other details of the computer simulation, including the lengths of the Monte Carlo runs, are similar to before [1, 2].

The analysis of the numerical results for the temperature dependences of the longitudinal susceptibility included making fits to an expression of the form (1) and defining the exchange renormalization index η_χ. We should note here that, according to the expression (1), the exact value of the exponential power is $2\pi\eta_\chi J/T \simeq 6.28\eta_\chi J/T$. However, both we [1, 2] and others [3] obtained this power for the one-monolayer system as $\sim 6\eta_\chi J/T$. The difference might be due either to systematic numerical error or to an inaccuracy in the derivation of (1). Therefore, for calculation of η_χ, we used our value of 6 instead of 6.28 from (1).

In figure 1 we present the results of this fitting procedure for several values of the concentration x. Analysing the presented data, we may conclude that the investigated system displays effectively 2D behaviour with the values of η_χ lying in between those for the two-monolayer and one-monolayer systems. When x is small, the value of η_χ appears to depend strongly on x, dropping rapidly from $\eta_\chi \simeq 1.5$ for $x = 0.8$ to $\eta_\chi \simeq 1.2$ for $x = 0.6$.

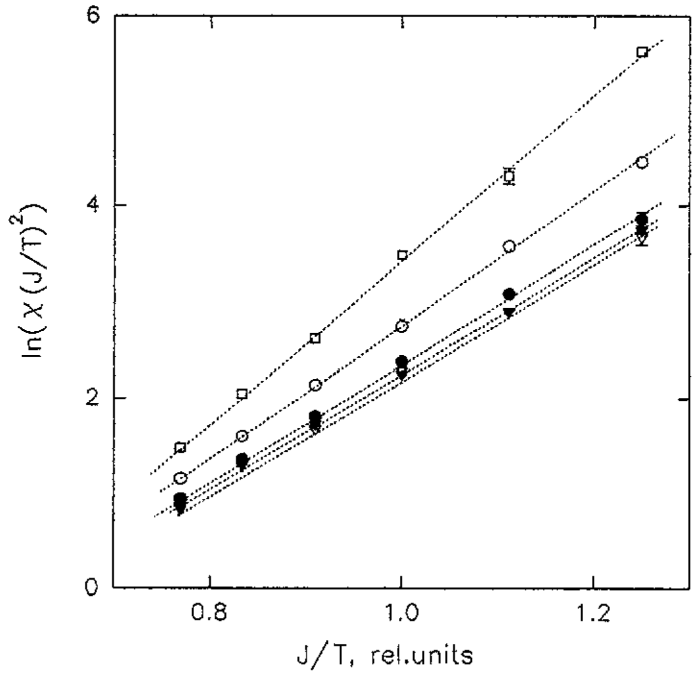

Figure 1. The temperature behaviour of the susceptibility for the film with two layers, one of them diluted with an occupancy concentration x. Broken curves: fits to the function $AJ/T - B$. Key: □: $x = 0.8$, $A = 8.6$, $B = 5.1$; ○: $x = 0.6$, $A = 7.0$, $B = 4.2$; ●: $x = 0.4$, $A = 6.3$, $B = 3.9$; ▽: $x = 0.2$, $A = 6.0$, $B = 3.9$; ▼: $x = 0.02$, $A = 6.0$, $B = 3.8$.

For better analysis of these dependences, we plotted the values of η_χ versus concentration x in figure 2. This shows that for $x > 0.7$, η_χ decreases with the decreasing of x in such a way that the tangent line to this dependence is pointing to the limit of purely 2D behaviour ($\eta_\chi = 1$), close to the 2D percolation limit $x = 0.6$ (see, e.g. [5]). However, when x becomes less than 0.7, substantial deviations from this tangent line occur, making the crossover interval from two-layer to one-layer behaviour as wide as $0.3 < x < 0.7$. Finally, for $x < 0.3$ the curve flattens to an almost horizontal line.

The simple arguments for the interpretation of these results can be provided by the percolation theory. The magnetic long-range order in the incomplete layer, being taken separately, depends on the existence of exchange paths connecting the spins in the plane. If the number of the bonds is insufficient to form the mentioned paths, then the long-range order vanishes. However, in the presence of the second (complete) layer, the spins in the upper layer can be connected by the paths that avoid the broken bonds in the upper layer and partially go through the lower layer.

When the occupancy concentration x is sufficiently high, the main ordering in the upper layer occurs due to the paths lying within this layer. This situation can be adequately described by the 2D percolation theory, that results in the tangent line pointing straight to the percolation limit. However, in the vicinity of the percolation threshold, the paths involving both of the layers play a significant role, thus flattening the curve in the range of intermediate values of x. Finally, for small values of x, the total number of spins in the upper layer becomes so small that they do not contribute significantly to the susceptibility

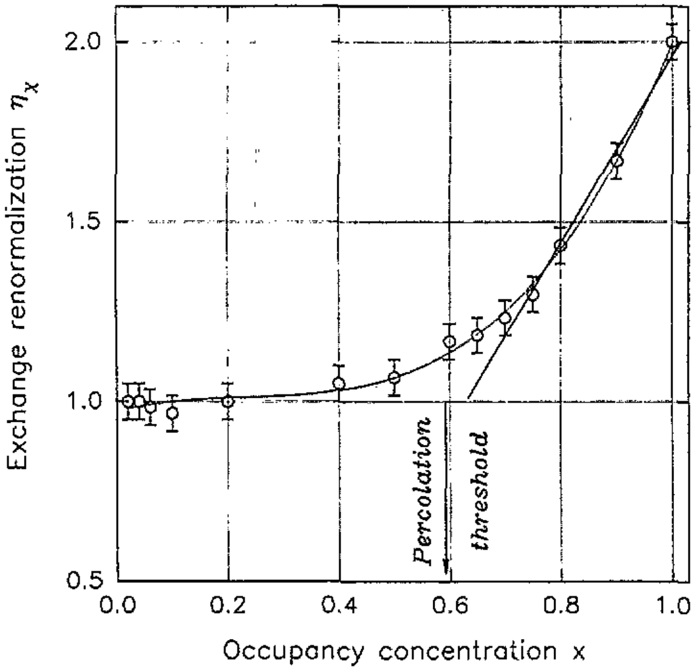

Figure 2. Exchange renormalization index η_x versus the occupancy concentration x.

of the whole system. Moreover, the paths connecting the remaining spins in the upper layer then lie mostly in the lower layer, contributing to the lower layer susceptibility.

The results depicted in figure 2 might be useful in the context of a rough interpretation of the data from [4], where the system in question had 2.5 layers of ^3He. This means that the occupancy concentration of the upper layer then is 0.5. As this is lower than the percolation limit, we can conclude that the upper layer should not contribute much to the susceptibility of the system. However, as the total number of layers in this system is 3, the curve analogous to figure 2 might be flatter than ours, as the bonds through the lower layers can be of more importance, thus increasing the upper layer contribution to the total susceptibility.

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