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LETTER TO THE EDITOR

A Monte Carlo study of the critical behaviour of the longitudinal susceptibility for $S = \frac{1}{2}$ isotropic Heisenberg ferromagnetic films

I V Rojdestvensky† and I A Favorski‡§

† Department of Physics, University of Western Ontario, Canada N6A 3K7

‡ Faculty of Physics, Leningrad State University, Russia

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Abstract. The Handscomb Monte Carlo method is applied to investigate the critical behaviour of the $S = \frac{1}{2}$ isotropic Heisenberg ferromagnetic film on the simple cubic lattice with the number of monolayers $L \leqslant 3$. For the one-monolayer film we confirm the results of the renormalization group study of the two-dimensional model for a wide range of temperatures. For the two- and three-monolayer films for the temperature interval investigated we report a two-dimensional type of critical behaviour of the longitudinal susceptibility with renormalized exchange.

The critical properties of quasi-two-dimensional systems have been studied recently by a number of analytical and numerical methods [1–5]. Under discussion were the type of phase transition as well as the critical behaviour of the uniform longitudinal susceptibility and the correlation range in two dimensions. Now it is considered as established that the $S = \frac{1}{2}$ Heisenberg ferromagnet with nearest-neighbour interaction displays no phase transition in two dimensions [1–4] at finite temperatures. This is confirmed by the Mermin–Wagner theorem [5].

In [1, 2] the uniform longitudinal susceptibility and the correlation range for the model in two dimensions were investigated by means of the modified spin-wave theory. The susceptibility and the correlation range were reported to have the following dependences on the temperature:

$$\chi T = \frac{1}{6\pi JS} T \exp\left(\frac{8\pi JS^2}{T}\right)(1 + O(T)) \qquad \xi = \left(\frac{2JS}{T}\right)\exp\left(\frac{4\pi JS^2}{T}\right). \tag{1}$$

On the other hand, the reported renormalization group results [3] correspond to the expressions (1) only in one-loop order, giving an additional factor, proportional to T^2 in χT in the two-loop approximation:

$$\chi T = C_\chi \left[\frac{C_\xi}{2\pi}\right]^2 2^7 \left[\frac{T}{2J}\right]^3 \exp\left\{\frac{2\eta_\chi \pi J}{T}\right\} \tag{2a}$$

$$\xi \simeq (T/J)^{1/2} \exp\left\{\frac{2\eta_\chi \pi J}{T}\right\} \tag{2b}$$

§ Deceased.

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with $n_\chi = 1$ for $S = \frac{1}{2}$. The renormalization group results in [3] are confirmed by quantum Monte Carlo data for the two-dimensional system. We note here that the expressions (1) and (2) correspond to those in [2, 3] with the temperature being renormalized to $T/2$. This follows from the difference between the definitions of the Hamiltonian in the present paper and in the cited papers (see below).

In [4] the spin–spin static correlators $g(r)$ as well as the correlation range ξ are investigated by the Monte Carlo method in two dimensions. The temperature behaviour of the correlation range is compared to the results of HT expansion and the predictions of the spin-wave theories. The model discussed is also known to have a second-order phase transition in three dimensions (see e.g. [11] and references therein). It is interesting to find out how the crossover from two-dimensional to three-dimensional behaviour takes place in the case of a monocrystalline thin film.

The aim of this work is to investigate the critical properties of ultra-thin monocrystalline thin films with the $S = \frac{1}{2}$ isotropic Heisenberg ferromagnetic Hamiltonian on the simple cubic lattice with the number of monolayers $L \leqslant 3$.

Let us consider the thin film as a crystal having two equal surfaces in one direction and extending to infinity in the others. The Hamiltonian of the $S = \frac{1}{2}$ Heisenberg ferromagnet with nearest-neighbour interaction and of the described geometry can be written in the following general form:

$$H = -2\sum_{(ij)} j^{bb} S_i S_j = 2\sum_{(pq)} J^{sb} S_p S_q - 2\sum_{(lm)} J^{ss} S_l S_m \tag{3}$$

where the first sum is responsible for the interaction of the bulk spins, the second sum is a contribution of the bulk–surface interactions and the third one is the energy of surface spin interactions. In all the terms the sums are taken over the pairs of nearest neighbours. In the present work we have simplified this Hamiltonian by putting $J^{sb} \equiv J^{bb}$. This model has been used in numerical calculations of the longitudinal susceptibility in zero uniform field.

As the Monte Carlo method is appropriate only for finite crystals, we should explain the procedure used to approximate the real infinite crystal by the finite system. The usual method for bulk systems is to introduce periodic boundary conditions. In order to simulate the thin film we can also use periodic boundary conditions for those directions in which the crystal is infinite, keeping free boundary conditions for the surfaces of the film.

We use the Monte Carlo method developed by Handscomb [6, 7]. It is unnecessary to reproduce the details of the original method here because it is discussed well in the literature [6–11]. Here we represent only the expression for the estimator of the susceptibility χT [7]:

$$\Omega_{\chi T} = \frac{1}{2n}\sum_i a_i^2 \tag{4}$$

where $n = N \times N \times L$ = the total number of spins in the system.

We calculated the susceptibility for systems with number of sites $N \times N$, where $N = 10$, 15, 20, 30, 40, 60, 80 and 120 within the temperature interval $0.4 \leqslant T/J \leqslant 1.3$. Markov chains were in the range from 200 MC steps/spin for $T/J \geqslant 1.0$ to 500 MC steps/spin for $0.4 \leqslant T/J \leqslant 1.0$. The averaging was made over the second half of the Markov chain, the first half being left for the relaxation. For the purpose of extrapolation of our susceptibility results to the infinite lattice, we plotted $\ln(\chi T/J)$ versus $\ln(N)$ (figure 1). Using this plot we can make a reliable extrapolation to the infinite lattice for the temperatures down to as low as $T/J \simeq 0.5$, which corresponds to $T/J = 0.25$ with the Hamiltonian taken as in

[3]. To check the validity of (2) we plotted $\ln(\chi J/T^2)$ versus inverse temperature J/T (see figure 2). It can be seen that the data presented fit a straight line with slope 5.99 throughout the temperature interval investigated, the given theoretical slope being equal to 2π for $S^2 = \frac{1}{4}$. We note that our fit is better than the value of 5.92 obtained in [3]. The insignificant difference in the vertical intercept is due to the difference between the normalization of the susceptibility in the present paper and that in [3]. We conclude that our results confirm the validity of (2) for a wider range of temperatures.

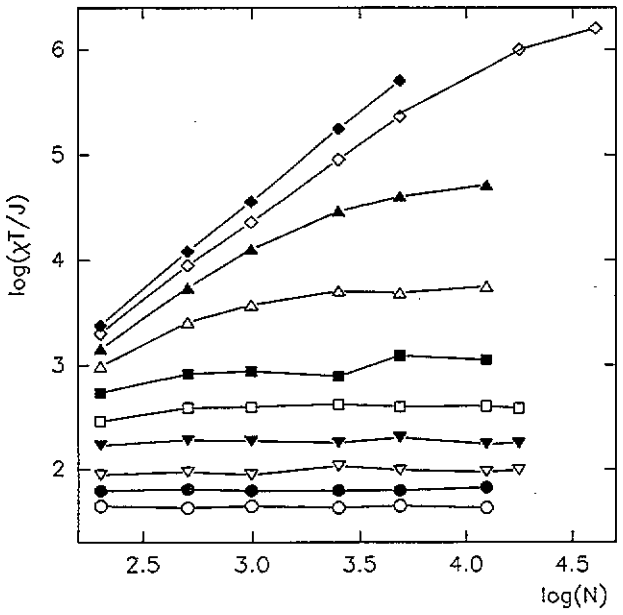

Figure 1. The finite scaling analysis of the susceptibility for the one-layer film, for T/J = ○, 1.3; ●, 1.2; ▽, 1.1; ▼, 1.0; □, 0.9; ■, 0.8; △, 0.7; ▲, 0.6; ◇, 0.5; ◆, 0.4.

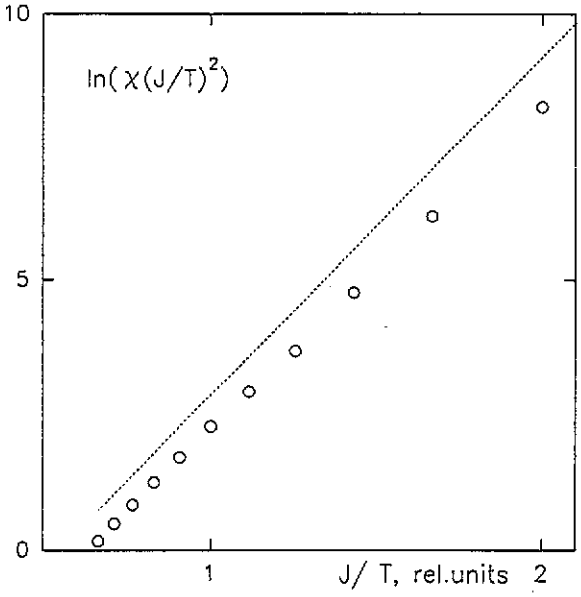

Figure 2. The temperature dependence of the susceptibility for the one-layer film. ○—MC data, fit $5.99J/T - 3.77$; ----—fit from [3], $5.92J/T - 3.51$.

For the two-layer film we introduce different constants of the exchange interactions within the surfaces and inside the film. Under consideration were systems with linear size N = 10, 20, 30, 40, 60 and 80 spins.

The results of our investigation of the temperature dependence of the susceptibility in the case when $J^{ss} = J^{bb}$ are presented in figures 3 and 4. In figure 3 we show our finite scaling analysis, making conclusions about the possibility of extrapolating our data to the infinite-lattice case for temperatures $T/J \geqslant 0.9$.

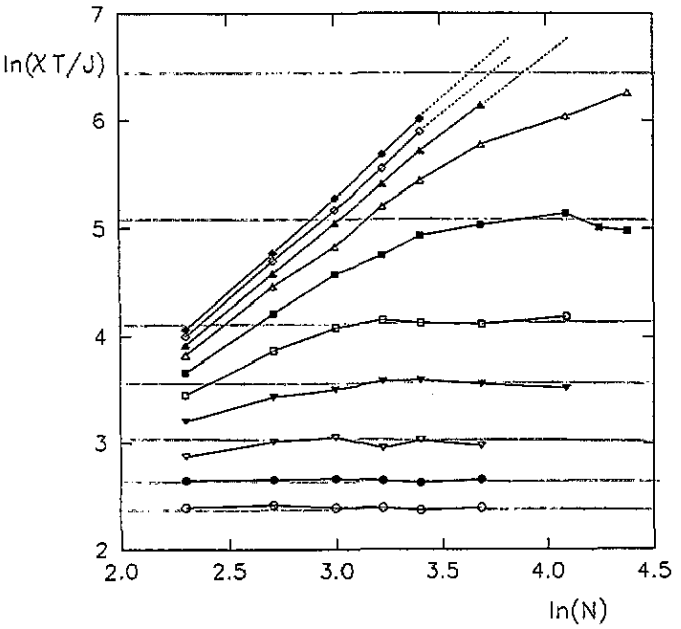

Figure 3. The finite scaling analysis of the susceptibility for the two-layer film, where $J^{ss} = J^{bb}$. T/J = ○, 1.5; ●, 1.4; ▽, 1.3; ▼, 1.2; □, 1.1; ■, 1.0; △, 0.9; ▲, 0.8; ◇, 0.7; ◆, 0.6.

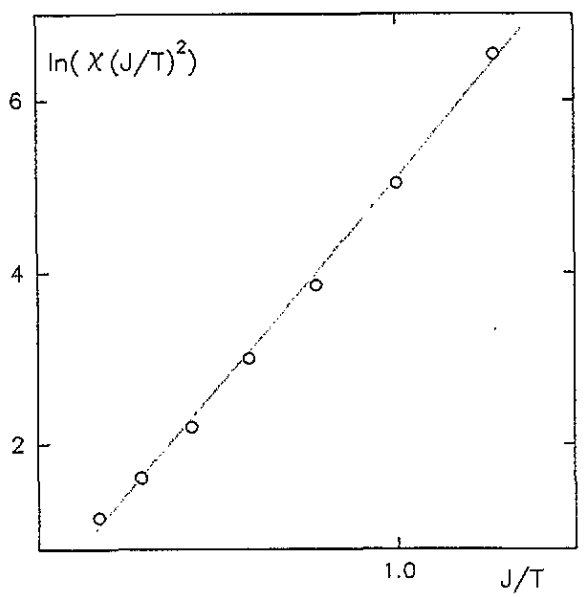

Figure 4. The temperature dependence of the susceptibility for the two-layer film, where $J^{ss} = J^{bb}$. ○—MC data, extrapolated to the infinite lattice; ·····—fit $12.1J/T - 7.0$.

We interpret figure 4 as evidence that in the given case the susceptibility displays two-dimensional behaviour of the same type as in (2a), but with the power in the exponential equal to 12.1, i.e. close to 4π.

We have calculated the surface–surface correlation function, by considering the two spins belonging to the opposite surfaces of the film. The temperature dependence of this quantity is presented in figure 5. We should notice here that within the temperature interval investigated this correlation function is rather close to the saturation value 0.25, which means that the surface spins are well correlated.

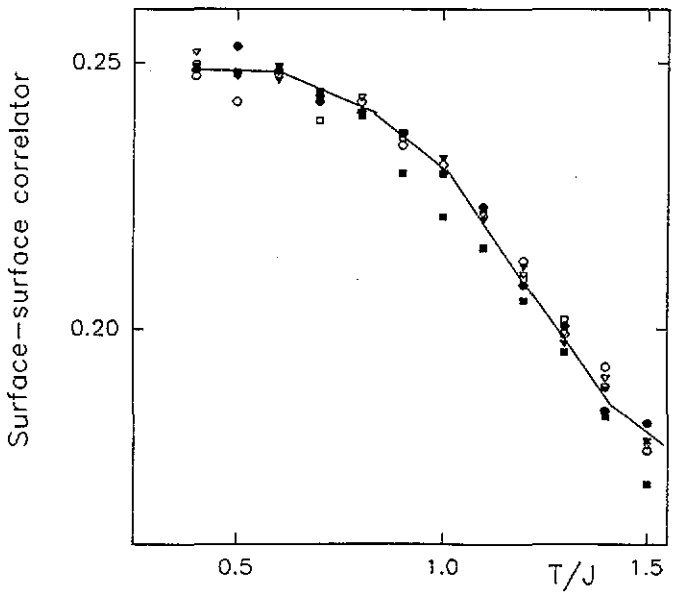

Figure 5. The temperature dependence of the surface–surface correlator for the two-layer film, where $J^{ss} = J^{bb}$. N = ○, 10; ●, 20; ▽, 30; ▼, 40; □, 60; ■, 80.

We simulated three-layer films with linear sizes N = 10, 20, 30, 40 and 60 spins and $J^{ss} = J^{bb}$. Our susceptibility results are presented in figure 6. As with previous cases, when trying to fit our results to the two-dimensional dependence (2a) we get the exponential power equal to 18, i.e. close to 6π.

We treat our results as evidence that in a certain temperature interval and for $J^{bb} = J^{ss}$, the temperature dependences of the susceptibility and the correlation range obey the two-dimensional law (2) with J replaced by LJ, L being the number of monolayers in the film. We present here simple arguments that suggest this to be true for the two-layer film. Having used a well-known transformation from spin operators to the transposition operators for the $S = \frac{1}{2}$ case (see e.g. [7]), we can re-write the Hamiltonian (3) as follows:

$$H = -\sum_{m=1}^{2}\sum_{(ij)} J^{ss} E_{ij}^{m} - \sum_{(pq)} J^{bb} E_{pq} + \text{constant} \tag{5}$$

where the operators E_{ij}^{m} and E_{pq} are, respectively, the transposition operators for the sites i and j within the mth layer and the sites p and q, belonging to neighbouring layers, respectively. The first sum corresponds to the energy of the exchange interaction within the layers, and the second sum is the exchange interaction energy between the layers. When the surface–surface correlations are strong, the most significant contribution to the

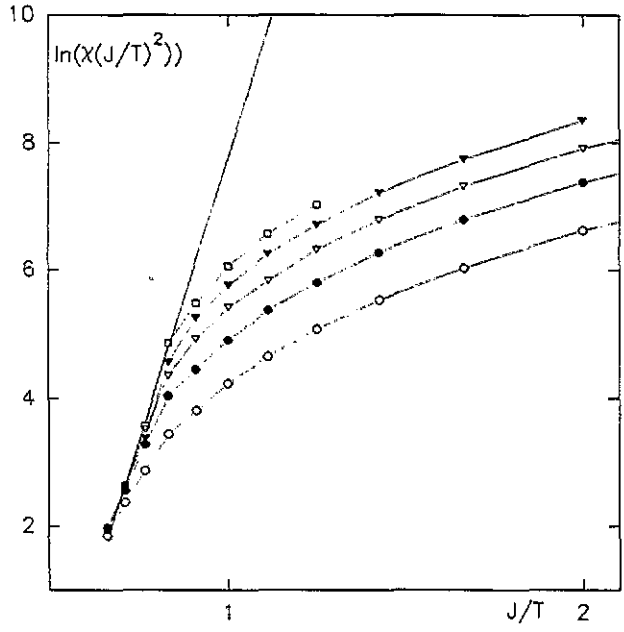

Figure 6. The temperature dependence of the susceptibility for the three-layer film where $J^{ss} = J^{bb}$. N = ○, 10; ●, 20; ▽, 30; ▼, 40; □, 60; ·····—fit $18J/T - 10$.

thermodynamic properties is given by the spin configurations in which the z-projection values of the spin operators along the direction perpendicular to the film surface are the same throughout the film thickness. For these configurations the transposition operators in the latter sum are equal to the identity operator, the latter sum then being effectively constant. The first sum for the same configurations can effectively be rewritten as

$$\sum_{(ij)} 2J^{ss}E_{ij}$$

which corresponds to the Hamiltonian of the two-dimensional model with the exchange renormalized to the value $2J^{ss}$. Of course, this simple explanation lacks rigour and cannot be treated as final and satisfactory.

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