Onsager reaction field theory for 3d anisotropic xy model

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We discuss coupled XY spin chains in three dimensions and calculate the transition temperature and spin correlation lengths, as functions of the ratio of the interchain exchange coupling J' to the intrachain coupling J, for chain-like spatial anisotropy, $J' < J$. We use two different approaches of the Onsager Reaction Field (ORF) formalism. First we use the standard ORF theory, in which both the intrachain and interchain couplings are treated equally. Second, we treat one chain exactly and consider it in the effective field caused by the other chains, with the ORF formalism applied to the interchain interaction. The transition temperatures obtained are compared with results from Monte Carlo simulations.
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I. INTRODUCTION

Here we study a set of coupled XY chains in three-dimensions (3d) described by nearest neighbor exchange couplings J along the chains and J' between chains. We use the Onsager Reaction Field (ORF) approach,[1] and a modified version of it in order to treat the limit of *weakly* coupled chains ($J' \ll J$). This modified version – which we call CORF ("chain"-ORF) – was introduced in Ref. 2. We use a cluster Monte Carlo (MC) scheme to estimate the critical temperature as a function of anisotropy $\Delta \equiv J'/J$ to test the two theoretical calculations.

The ORF was first used in magnetism by Brout and Thomas[3] and has since been applied successfully to many problems.[4,5] ORF represents an improvement over the mean field approximation because it gives a more adequate treatment of the short-range order. The basic idea is that the spins surrounding any given spin are correlated to the motion of that spin and do not contribute to the mean field seen by that spin. This is incorporated into the theory by subtracting the reaction field from the mean field.

In the modified reaction field approach, CORF, the idea is to treat a linear chain exactly while its interaction with other chains is treated approximately using the reation field theory. Since individual chains are treated exactly, we expect this modified ORF approach to be more appropriate for weak interchain interactions ($\Delta \ll 1$). For strongly coupled chains ($\Delta \to 1$), we expect the standard ORF to work better. Obviously, both approaches are valid only for temperatures above the critical temperature T_c and outside a very small critical region around it.

II. THEORY

A. The standard ORF

The Hamiltonian for coupled XY chains is

$$\mathcal{H} = -\sum_{(\mathbf{n},\mathbf{m})} J_{\mathbf{n},\mathbf{m}} \ \vec{S}_{\mathbf{n}} \cdot \vec{S}_{\mathbf{m}} \tag{1}$$

where the sum is over nearest neighbor pairs $(\mathbf{n}, \mathbf{m})$ on a cubic lattice, and $J_{\mathbf{n},\mathbf{m}} = J$ for bonds along the chains (z-axis) and $J_{\mathbf{n},\mathbf{m}} = J' = \Delta J$ for bonds between neighboring chains (x and y axes). The Fourier transformed Hamiltonian has coupling in $\vec{q}$-space,

$$J(\vec{q}) = 2J\left[\cos q_z + \Delta(\cos q_x + \cos q_y)\right]. \tag{2}$$

In order to incorporate short-range order effects into the mean field approach we subtract from the molecular field acting on a given spin the part due to the polarization by that spin of its neighbors: this part is the reaction field. The procedure for obtaining the static susceptibility is analogous to the one used in the standard mean field approach and we subtract a self-consistent term $\lambda(T)$ from the molecular field $J(\vec{q})$, obtaining

$$\chi(\vec{q}) = \frac{\chi_0}{1 - \chi_0[J(\vec{q}) - \lambda(T)]} \tag{3}$$

where $\chi_0 = S^2/2T$ (henceforth, $S = 1$). The reaction field $\lambda(T)$ is determined self-consistently[2] and the critical temperature T_c is the highest temperature at which the susceptibility (3) diverges (See Ref. 5). T_c is given by

$$\frac{J}{T_c} = \frac{1}{\pi^2} \int_0^\pi \int_0^\pi \frac{dq_x dq_y}{\sqrt{[1 + \Delta(2 - \cos q_x - \cos q_y)]^2 - 1}} \tag{4}$$

The solid line in Fig. 1 shows T_c as a function of Δ. Notice that this procedure correctly predicts the absence of a phase transition for the 1d limit, $\Delta = 0$.

Many physical quantities, such as spin correlation functions, correlation lengths, specific heat, etc., can be obtained from the static susceptibility $\chi(\vec{q})$. The longitudinal (along z-axis) and transverse correlation lengths, ξ_z and ξ_{xy}, respectively, can be obtained from the relation

$$< \vec{S}_i . \vec{S}_j > = T \sum_{\vec{q}} \chi(\vec{q}) \exp[i\vec{q}.(\vec{R}_i - \vec{R}_j)] \tag{5}$$

by performing a small $\vec{q}$-expansion. This procedure yields

$$\xi_z(T) = \left[\frac{2T}{J} + \frac{\lambda}{J} - 2(1+2\Delta) \right]^{-1/2} \quad ,$$

$$\xi_{xy}(T) = \sqrt{\Delta} \;\; \xi_z(T) \quad . \tag{6}$$

In the isotropic limit $\Delta \to 1$, we correctly obtain $\xi_z = \xi_{xy}$ but, for $\Delta = 0$ and for low temperatures, Eq. (6) gives $\xi_z = J/T$ underestimating the exact asymptotic result[6] $\xi_z^{exact} = 2J/T$. However, considering the nature of the approximations we expect that the ORF procedure works better for the isotropic limit, when all spins surrounding a given one are almost equivalent. The procedure is more likely to fail in the 1d limit because the spins are much more strongly correlated to their neighbors along the chains than to those in adjacent chains.
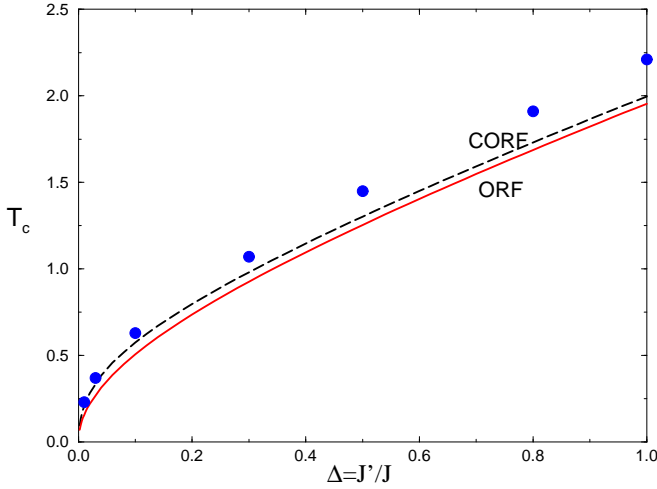

FIG. 1. T_c vs Δ, from ORF (continuous curve), CORF (dashed curve), and MC (points).

B. Chain-ORF: weakly coupled chains

In order to study quasi-one dimensional systems, $\Delta \approx 0$, we treat the linear *chain* exactly and consider the interchain interaction in the context of the Onsager reaction field. This kind of approach — but using mean field instead of ORF – was applied[7] to study coupled chains. Our proposal, first presented in Ref. 2, is that we consider each chain in the effective field of the neighboring chains. We refer to this procedure as CORF ("chain"-ORF). The steps that lead to the static susceptibility are analogous to those in a mean field approximation, but the "molecular" field is $J'(\vec{q}_\perp) = 2J\Delta(\cos q_x + \cos q_y)$. Here the temperature dependent Onsager correction term is designated by $\lambda^c(T)$. We find that the susceptibility is

$$\chi^c(\vec{q}) = \frac{\chi_{1d}(q_z)}{1 - \chi_{1d}(q_z)\left[J'(\vec{q}_\perp) - \lambda^c(T) \right]} \quad , \tag{7}$$

where superscripts c stand for *chain* approximation, and $\chi_{1d}(q_z)$ is the susceptibility of a single isolated chain, calculated exactly by Joyce[8]:

$$\chi_{1d}(q_z) = \frac{1}{2T} \frac{1 - u^2}{1 + u^2 - 2u \cos q_z} \quad , \tag{8}$$

where $u = I_1(J/T)/I_0(J/T)$, and $I_n(x)$ are the modified Bessel functions of order n.

The critical temperature T_c^c can be obtained[2] by numerically solving the equation

$$\frac{2u_c}{1 - u_c^2} = \int_0^\pi \int_0^\pi \frac{dq_x dq_y/\pi^2}{\sqrt{[1 + B_c(2 - \cos q_x - \cos q_y)]^2 - 1}}, \tag{9}$$

where $B_c = \Delta(J/T_c^c)(1 - u_c^2)/2u_c$ is calculated at the transition temperature. The only differences of this equation compared with the ORF expression for T_c, Eq. (4) are the factors involving $2u_c/(1 - u_c^2)$. From this similarity, it can be seen that if the full ORF result $T_c(\Delta)$ over a range of Δ is known, then a mapping[9] to the corresponding CORF result can be obtained *without* a self-consistent solution of Eq. (9). In Figure 1, the dashed line shows T_c^c as a function of Δ.

Performing a small $\vec{q}$-expansion of Eq. (7), we obtain the longitudinal and transverse correlation lengths

$$\xi_z = \left\{ \frac{(1-u)}{u} \left[(1-u) - \frac{(4J' - \lambda^c)}{2T}(1+u) \right] \right\}^{-1/2} \quad ,$$

$$\xi_{xy} = \sqrt{\frac{J\Delta}{T} \frac{(1-u^2)}{2u}} \;\; \xi_z \tag{10}$$

In the 1d-limit we obtain $\xi_{xy} = 0$, and the correct low-temperature limit,[6] $\xi_z = 2J/T$, This shows that in the $\Delta \to 0$ limit, CORF is better than the standard ORF. In the other limit, $\Delta \to 1$, for temperatures where the Onsager Reaction Field approach is valid ($T > T_c$) the argument J/T of the Bessel functions appearing in u [Eq. (8)] is small. Then Eq. (10) gives $\xi_z \approx \sqrt{\Delta}\xi_z$ as in Eq. (6). This shows that for high temperature CORF and ORF are equivalent as $\Delta \to 1$.

III. MC CALCULATION OF T_C

A MC scheme based on the Wolff[10] single-cluster algorithm was used to estimate the critical temperatures, incorporating the spatially anisotropic exchange by building clusters as follows: First, a random seed site of a $L \times L \times L$ periodic lattice was chosen, and "flipped" by inversion of its component along a randomly chosen unit vector $\hat{\mathbf{r}}$ within the XY plane:

$$\vec{S}_{\mathbf{n}}{}' = \vec{S}_{\mathbf{n}} - 2(\vec{S}_{\mathbf{n}} \cdot \hat{\mathbf{r}})\hat{\mathbf{r}}. \tag{11}$$

Then each of the six neighboring sites $\mathbf{m}$ were tested to see if they should be included into the cluster according to a Metropolis-like decision, determined by the energy change $\Delta E_{\mathbf{n},\mathbf{m}} \equiv E^{\text{nobond}} - E^{\text{bond}}$ for *not* forming a bond from site $\mathbf{n}$ to site $\mathbf{m}$:
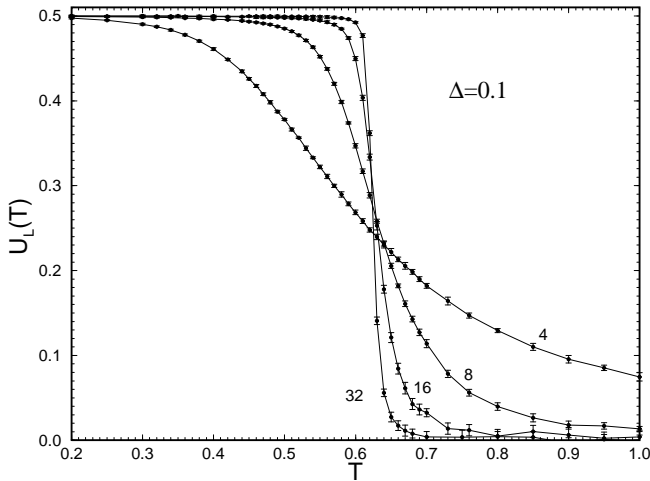
FIG. 2. Fourth order cumulant ratio [Eq. (14)] used to determine $T_c \approx 0.62J$ for $\Delta = 0.1$, for indicated system lengths L.

$$\Delta E_{\mathbf{n},\mathbf{m}} = -J_{\mathbf{n},\mathbf{m}} \vec{S}_{\mathbf{n}}{}' \cdot \left(\vec{S}_{\mathbf{m}} - \vec{S}_{\mathbf{m}}{}' \right). \tag{12}$$

Primes indicate that the flipping operation (11) has been applied, using the same value of $\hat{\mathbf{r}}$ as for $\vec{S}_{\mathbf{n}}$. A bond (or link) from $\mathbf{n}$ to $\mathbf{m}$ is now placed with probability $(1 - p_{\mathbf{n},\mathbf{m}}^{\text{nobond}})$, where a Metropolis decision gives the probability for *not* putting a bond to be

$$p_{\mathbf{n},\mathbf{m}}^{\text{nobond}} = \min[1, e^{-\Delta E_{\mathbf{n},\mathbf{m}}/T}]. \tag{13}$$

When site $\mathbf{m}$ is added into the cluster, it is immediately flipped. The total energy E is then incremented by $\Delta E_{\mathbf{n},\mathbf{m}}$ and the total magnetization $\vec{M}$ is incremented by $(\vec{S}_{\mathbf{m}} - \vec{S}_{\mathbf{m}}{}')$, summing over all neighbors of the site $\mathbf{n}$ being considered, regardless of whether the neighbor $\mathbf{m}$ is included into the cluster or not. Any sites added to the cluster also have their neighbors tested for inclusion in the same way, until the cluster stops growing.

This process builds and flips one cluster. The cluster tends to be large at low temperature, leading to rapid changes in phase space. At high temperature, however, only small clusters are formed, leading to slower sampling of phase space. Therefore, we defined one MC cluster step to mean that we form and flip individual clusters until the total number of sites that were included into clusters is greater than $L^3/4$. Using similar numbers of steps at all temperatures we can get uniform error bars.

We made simulations with $L = 4, 8, 16, 32$, using 200,000 to 400,000 steps for averages, after a short relaxation of 2000 steps, since the Wolff scheme has an extremely short correlation time. We looked at the scaling of the results with system length, using the common crossing point of Binder's[11] fourth order cumulant ratio,

$$U_L(T) = 1 - \frac{\langle |M|^4 \rangle}{2 \langle |M|^2 \rangle^2}. \tag{14}$$

to estimate T_c for $0.01 \leq \Delta \leq 1.0$. A typical plot of $U_L(T)$, for $\Delta = 0.1$, is shown in Fig. 2. For $\Delta = 1.0$, we find $T_c \approx 2.20$, in agreement with Kohring *et al.*[12] on lattices with $L \leq 14$. For smaller anisotropies ($\Delta < 0.01$), however, it is difficult to get a single crossing point in the $U_L(T)$ plot for these values of L. For $\Delta = 0.01$ we found it necessary to go to $L = 64$ in order to get T_c accurately. There the finite size effects apparently are much stronger, as well as the MC becoming more difficult when $T \ll J$.

IV. DISCUSSION OF RESULTS

A. Critical Temperature and $\lambda(T)$

In Fig. 1 we compare T_c vs. Δ obtained from MC with the ORF and CORF results. The comparison to the MC values favors the CORF results in the whole Δ region, more so in the small Δ region ($\Delta < 0.1$). We could have anticipated this because the Onsager correction term (Fig. 3) is necessarily smaller in the CORF, leading to higher T_c, because it includes less spins than the ORF. At the other limit, $\Delta = 1$, ORF gives $T_c = 1.95J$, CORF gives $T_c^c = 2.00J$, both much more accurate than mean field theory, $T_c^{MF} = 3.0J$.

On intuitive grounds, we expect that the critical Onsager term, λ_c, shown in Fig. 3, should increase continuously with Δ in both treatments because the *interaction* with spins in neighboring chains becomes stronger as Δ increases. This is true in the CORF approach: a fit to the curve in Fig. 3 gives $\lambda_c^c = 1.45\Delta$, a result that can also be obtained analytically. The curve obtained for λ in the standard ORF shows a minimum around $\Delta \approx 0.1$: this unexpected result may show why the ORF treatment is not appropriate for $\Delta < 0.1$.
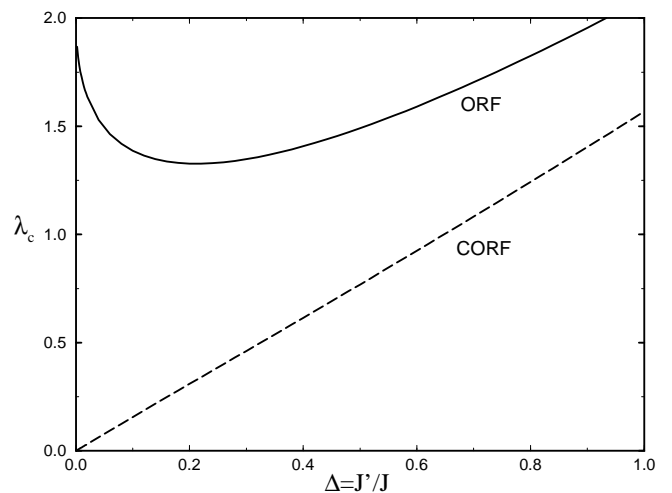

FIG. 3. λ_c vs Δ, from ORF (continuous curve) and CORF (dashed curve) calculations.

B. Correlation Lengths

Typical correlation lengths for $\Delta = 0.1$, $\Delta = 1.0$, are displayed in Fig. 4. The overall behavior does not differ appreciably from one treatment to the other, and in both cases the longitudinal and transverse correlation lengths behave as $\xi \approx t^\eta$ with the exponent η being independent of the interchain coupling J' (typically, η is in the range $0.80 - 0.90$). However, based on the behavior obtained for the correlation lengths in the $\Delta = 0$ limit and for the transition temperatures in the $\Delta \leq 0.1$ region, we can believe that $\Delta = 0.1$ is better described by the CORF results. We note that at $\Delta = 1$ the CORF and ORF procedures give completely equivalent results for high temperatures $T \gg T_c$, with $\xi_z = \xi_{xy}$ as they should (see discussion after Eq. (10)). This is an interesting result. For $\Delta = 1$ all neighbors of a given spin, whether in the same or neighboring chains, are completely equivalent. This is represented correctly in the ORF where all neighbors are included equivalently in the reaction field. In the CORF procedure, on the other hand, only the spins in the neighboring chains are included in the reaction field; those along the chain are treated exactly.
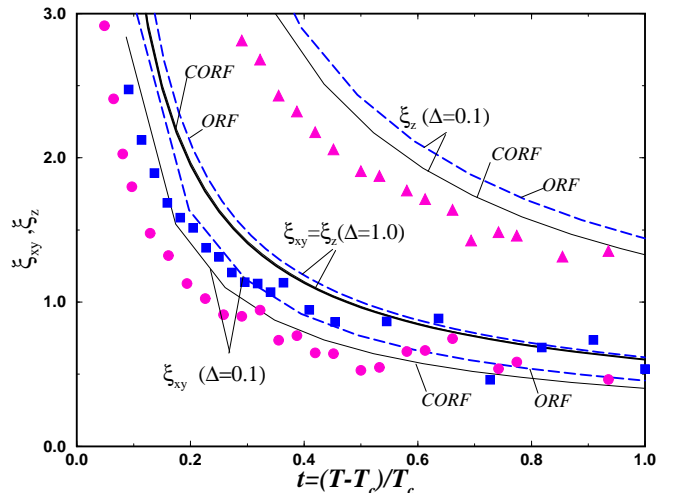

FIG. 4. Longitudinal and transverse spin correlation lengths compared with MC data for $L = 32$, for $\Delta = 0.1$ (triangles and circles, respectively), and $\Delta = 1.0$ (squares).

V. CONCLUSIONS

We have discussed two ways of implementing the Onsager Reaction Field formalism to study three-dimensional systems built from weakly coupled magnetic chains. In the standard ORF, exchange interactions in different directions were treated equivalently, although the exchange couplings are different. In the CORF, we considered each magnetic *chain* in the modified mean field due to the neighboring chains, integrating the spatial anisotropy into the calculational approach. It seems reasonable to expect that the CORF approach gives a better description of the system when $J' \ll J$ while for $J' \approx J$ the standard ORF treatment should work better because in this limit, all neighbors to a given spin are approximately equivalent, independent of being along the chain or not. In fact, in the $\Delta \to 1$ limit, the two procedures give almost indistinguishable results, except for small differences in T_c. Both CORF and ORF estimate values for T_c in good agreement with our MC data, however, the entire range $0 \leq \Delta \leq 1$ is better described by CORF. This was anticipated from the spin correlation lengths obtained in each treatment: for $\Delta = 0$ and low temperatures, CORF gives the exact result for ξ_z while the ORF underestimates it by a factor of 2. Thus we suggest that the CORF approach can be a useful improvement over the mean-field and ORF theories for other models with strongly anisotropic couplings.

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