Onsager reaction field theory of the one-dimensional ferromagnet with long-range interactions

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We have studied the one-dimensional ferromagnets with $1/r^p$ exchange, using the Onsager reaction field theory. We have shown the existence of a phase transition at finite temperatures for $1 \le p \le 2$ and estimated its critical temperature.

The Onsager reaction field (ORF) theory, proposed by Onsager¹ in 1936, has recently seen a resurgence in the literature. Logan, Szechech, and Tusch² used it to study the two-dimensional Heisenberg model. The theory predicted correctly the absence of long-range order for any T>0, produced an exponentially divergent correlation length as $T\rightarrow 0$, and gave good quantitative agreement over a wide temperature range with both Monte Carlo and high-temperature series expansion. Also ORF ideas have been extended successfully to spin glasses³ and itinerant electron systems.⁴ The ORF theory is extremely simple, physically transparent, and captures many of the essential features inferred from highly sophisticated approaches.²

The theory provides a self-consistent modification of the mean-field approximation (MFA) to account for the crucial effects of local correlations. In magnetic systems the MFA approach does not give a self-consistent correlation function between spins located in different sites: $\langle S_0^{\alpha} S_r^{\alpha} \rangle$ (with $\alpha = x, y, z$) is replaced by $S_0^{\alpha} \langle S_r^{\alpha} \rangle$ for $T > T_c$, whereas this same correlation function obtained from the susceptibility $\chi(\vec{q})$

$$\langle S_0^{\alpha} S_r^{\alpha} \rangle = T \sum_q \chi(\vec{q}) e^{i\vec{q}\cdot\vec{r}}$$
(1)

does not vanish.

The central idea in the ORF is that the part of the local field, acting on a given spin, which arises from the surrounding polarization due to the instantaneous orientation of the spin in question, should not be included in the effective orienting field. That polarization simply follows the motion of the spin in question and thus does not favor one orientation over another. This is a short-range order effect which the MFA does not take into account. Generally this short range is included only for temperatures T above the critical temperature T_c ; the problem for $T < T_c$ is considerably more difficult, and the reaction field, in this case is only a small correction to the mean field associated with the spontaneous magnetization, except for T very close to T_c . In this report we apply the ORF formalism to study the one-dimensional ferromagnet with long-range interactions.

It is well known that long-range attractive interactions can induce critical behavior in low-dimensional spin systems,⁵ and over the last years, the study of spin systems associated with a low-dimensional lattice, and interacting via longrange potentials has attracted a significant amount of theoretical work.^{6–11} For the *d*-dimensional Heisenberg and *XY* model with ferromagnetic interactions decaying as r^{-p} , it has been shown that^{6,12} an ordering transition, at finite temperature, to a ferromagnetically ordered phase exists when $d and that the system becomes disordered at all finite temperatures when⁷ <math>p \ge 2d$. The condition p > d is needed in order to avoid a ground state with an infinite energy per spin.

The Hamiltonian for the one-dimensional Heisenberg and *XY* model with long-range ferromagnetic interaction is

$$H = -\sum_{n,m} J_{nm} \vec{S}_n \cdot \vec{S}_m , \qquad (2)$$

with

$$J_{nm} = J | n - m |^{-p}, (3)$$

where S has three components for the Heisenberg model and two for the XY model.

We start with a brief summary of the basic ORF theory.^{2,13} The usual procedure is to subtract $\lambda(T)$, the self-consistent determined Onsager reaction field, from the simple molecular field J(q), where

$$J(q) = \sum_{n,m} J_{nm} e^{iq(n-m)},$$
(4)

and we have taken the lattice constant a=1. This leads to a wave-vector-dependent spin susceptibility

$$\chi(q) = \frac{\chi_0}{1 - \chi_0 [J(q) - \lambda]},\tag{5}$$

with $\chi_0 = S(S+1)/nT$, where n=2 for the planar rotator, n=3 for the Heisenberg model, and we have taken $K_B=1$. We renormalize *T* as T/S(S+1). This has the advantage that our calculations can be directly compared with Monte Carlo simulations for the classical models. Now to calculate λ in a self-consistent way we start with the relation

$$\chi(q) = T^{-1} \langle S_a^{\alpha} S_{-a}^{\alpha} \rangle, \qquad (6)$$

and sum over q obtaining

$$N^{-1}\sum_{q} \chi(q) = T^{-1} \langle (S_{n}^{\alpha})^{2} \rangle = (nT)^{-1}, \qquad (7)$$

which leads to the self-consistent equation

$$\frac{1}{N}\sum_{q} \frac{1}{1-\chi_0[J(q)-\lambda]} = 1.$$
(8)

The MFA limit is, trivially, $\lambda = 0$, leading to the critical temperature $T_c^{\text{mf}} = J(0)/n$. The critical temperature T_c at which $\chi(0)$ diverges occurs when

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which leads to the following expression for T_c :

$$\frac{nT_c}{2J} = \left[\frac{1}{N} \sum_{q} \left(\frac{1}{\eta(q)}\right)\right]^{-1},\tag{10}$$

where

$$\eta(q) = \sum_{n=1}^{\infty} n^{-p} (1 - \cos nq).$$
(11)

For small q and $1 \le p \le 3$ the dispersion $\eta(q)$ is given by⁸

$$\eta(q) = \omega(p)q^{p-1/2}, \qquad (12)$$

where $\omega(p)$ is defined by

$$\omega(p) = \pi \{ \Gamma(p) \sin[\pi(p-1)/2] \}^{-1}, \quad (13)$$

and $\Gamma(p)$ is the Gamma function.

Approximating the sum in Eq. (10) by an integral and using expression (12) we find for the critical temperature

$$\frac{nT_c}{2J} = \frac{(2-p)\pi^p}{2\Gamma(p)\sin[\pi(p-1)/2]}.$$
 (14)

We see that, in marked contrast to the MFA limit, the ORF theory correctly predicts the existence of an ordering transition when 1 . [Using the low-*q* $expression for <math>\eta(q)$ in two dimensions given in Ref. 9 we can show that the ORF correctly predicts the condition 2 for the existence of a phase transition in two dimensions].

The critical temperature near $p \sim 1$ can be estimated as

$$nT_c/2J \approx [(1-b\varepsilon)\varepsilon]^{-1}, \qquad (15)$$

where b = 0.577 and $\varepsilon = p - 1$.

In Fig. 1 we show T_c/J for the classical XY model as a function of p. (The reason for us to present the data for the XY model is that this model has been studied in the literature using Monte Carlo simulations.) For p=3/2 we have from Eq. (14) $T_c/J=2.22$. [We obtain this same value using Eq. (10) and performing the sum numerically.] This result is in very good agreement with the Monte Carlo estimate¹⁰ $T_c/J=2.16$.

For T above T_c , λ can be calculated from Eq. (8) rewritten as



FIG. 1. The critical temperature of the classical XY model as a function of p.

$$\frac{1}{\pi} \int_{0}^{\pi} \frac{dq}{z + 2J\eta(q)} = \frac{1}{nT},$$
(16)

where $z = (\lambda - \lambda_c) + 2(T - T_c)$ and we have used the relation $\lambda_c = J(0) - nT_c$. In the limit $T \rightarrow \infty$ we have $\lambda \rightarrow 0$. For the *XY* model and p = 3/2 inserting Eq. (12) into (16) we find, for *T* near T_c , the following expression:

$$(z/4T_c)\ln(z/4T_c) = (T_c - T)/T.$$
 (17)

Of course the ORF theory predicts a phase transition only when we have an ordered phase, and it is not suitable to study topological phase transitions, such as the Kosterlitz-Thouless transition. Kosterlitz-Thouless-like transitions occur⁹ in one dimension for p=2, and in two dimensions, for the classical XY model $p \ge 4$.

We have thus shown that the ORF treatment appears consistent not only with the fact that a transition to the ordered phase exists when d , but also that the system is of necessity disordered when <math>p > 2d.

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