Logarithmic Corrections for Dilute Uniaxial Ferromagnets at the Critical Dimension

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The leading logarithmic corrections to the critical behavior of a dilute uniaxial (Ising) ferromagnet in the disordered phase are derived using renormalization group methods. The values of the exponents in the logarithmic terms differ from those given by previous authors.

KEY WORDS: Dilute Ising; critical dimension; logarithmic corrections.

1. INTRODUCTION

While an understanding of the role of dilution (or nonmagnetic) impurities is important in the study of phase transitions in magnetic materials, its theoretical analysis remains extremely difficult.⁽¹⁾ A ferromagnet with short-range interactions has a critical dimension of $d_c = 4$ and consequently exhibits Gaussian critical behavior with logarithmic corrections when $d = 4.^{(2)}$ A determination of these logarithmic corrections by, for example, simulation of the model provides a direct test of the renormalization group description of critical phenomena. Aharony⁽³⁾ pointed out that the logarithmic corrections are modified in a dilute uniaxial (Ising) system (e.g., having a randomly distributed concentration of nonmagnetic impurities) and have an unusual form involving powers of the factor $\exp[-|(6/53)\ln(t)|^{1/2}]$, where t is the reduced temperature $t = (T - T_c)/T_c$ (see also ref. 4 and 5). These exponential factors are multiplied by powers of $|\ln(t)|$. Shalaev⁽⁶⁾ made the important observation that the correct powers of $|\ln(t)|$ are not obtained unless terms corresponding to graphs with up to three loops are included in the calculation of the β functions

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(only graphs with up to two loops has been included in the previous work⁽³⁻⁵⁾). Consequently, although the crossover from pure to dilute behavior is expected to be slow,^(1,3,5) the possibility of observing the dilute uniaxial behavior is of considerable interest, as it would provide a very direct test of our understanding of phase transitions in dilute systems.

In considering this problem we have derived the asymptotic critical behavior of the dilute system from the renormalization group equations for a massless ϕ^4 field theory. (As in the work of Shalaev,⁽⁶⁾ we consider only a short-range interaction model at its upper critical dimension.) Our results confirm Shalaev's conclusion that the three-loop graphs must be retained in the construction of the β functions in order to describe correctly the asymptotic behavior. However, our results differ from those of Shalaev both in the power of $\ln(p)$ which appears in the momentum dependence of the pair correlation function G(p) at $T = T_c$ and in the power of the ln(t) which appears in the singular part of the specific heat. Our results for the pair correlation function at $T = T_c$, G(p), the inverse susceptibility $\chi^{-1}(t)$, and the singular part of the specific heat $C_{sing}(t)$ may be summarized as follows:

$$G(p) \sim p^{-2} |\ln(p)|^{-\eta_2} \tag{1}$$

$$\chi^{-1}(t) \sim t \exp\{2\theta_1 [|\ln(t)|/2]^{1/2}\} |\ln(t)|^{\eta_2 + \theta_2}$$
(2)

$$C_{\rm sing}(t) \sim -\exp\{4\theta_1 [|\ln(t)|/2]^{1/2}\} |\ln(t)|^{1/2 + 2\theta_2}$$
(3)

$$\eta_2 = -1/212 \approx -0.00472 \tag{4}$$

$$\theta_1 = -(3/53)^{1/2} \approx -0.238 \tag{5}$$

$$\theta_2 = \frac{2375}{11236} + \frac{378}{2809} \zeta(3) \approx 0.373 \tag{6}$$

As the method used differs from that used by Shalaev,⁽⁶⁾ the derivation is briefly described below.

In order to generate the appropriate field theory in the replica representation of a disordered system, the *nm* model with reduced Hamiltonian

$$\mathscr{H} = \int_{\mathbf{k}} \frac{1}{2} (r+k^2) \sum_{i=1}^{n} \sum_{\alpha=1}^{m} \phi_i^{\alpha} \phi_i^{\alpha} + u \left(\sum_{i=1}^{n} \sum_{\alpha=1}^{m} \phi_i^{\alpha} \phi_i^{\alpha} \right)^2 + \Delta \sum_{i=1}^{n} \left(\sum_{\alpha=1}^{m} \phi_i^{\alpha} \phi_i^{\alpha} \right)^2$$
(7)

is considered in the limit $(m = 1, n \rightarrow 0)$.^(7,8) (As usual, the integration is over all momentum arguments of the ϕ 's and momentum conversation is applied to these arguments.) The isotropic coupling constant u of the *nm* model in the present application is negative and related to the mean square fluctuations of the random impurity potential. The coupling constant Δ is positive. The renormalized vertex functions of this model in the massless limit (r=0) satisfy the renormalization group equations

$$\left[\kappa\frac{\partial}{\partial\kappa} + \beta_{u}\frac{\partial}{\partial u} + \beta_{d}\frac{\partial}{\partial\Delta} - \frac{N}{2}\eta - \theta\left(L + t\frac{\partial}{\partial t}\right)\right]\Gamma^{(N,L)} = B^{(N,L)}$$
(8)

where N and L denote the number of ϕ fields and composite $\phi^2/2$ operators, respectively. In the cases of interest here

$$B^{(2,0)} = 0 \tag{9}$$

$$B^{(0,2)} = -nm/2 + O(u, \Delta)$$
(10)

The correlation function, inverse susceptibility, and specific heat of the dilute uniaxial magnetic system are given in terms of the vertex functions by

$$G^{-1}(p) \propto \Gamma^{(2,0)}(p;t=0)$$
 (11)

$$\chi^{-1}(t) \propto \Gamma^{(2,0)}(p=0;t)$$
(12)

$$C_{\rm sing}(t) \propto -\Gamma^{(0,2)}(p=0;t)/n$$
 (13)

(Note that $B^{(0,2)}$ is treated as a constant to leading order, as $\Gamma^{(0,2)}$ is to be divided by *n* before taking the limit $n \to 0$.)

As usual, the renormalization group equations may be solved by using the method of characteristics; the flow equations are:

$$-\frac{\partial\kappa(s)}{\partial s} = \kappa(s); \qquad \kappa(0) = \kappa \tag{14}$$

$$-\frac{\partial u(s)}{\partial s} = \beta_u(u(s), \Delta(s)); \qquad u(0) = u$$
(15)

$$-\frac{\partial \Delta(s)}{\partial s} = \beta_{\Delta}(u(s), \Delta(s)); \qquad \Delta(0) = \Delta$$
(16)

$$-\frac{\partial t(s)}{\partial s} = -\theta(u(s), \Delta(s)) t(s); \qquad t(0) = t$$
(17)

The (critical dimension) beta functions

$$\beta_{u}(u, \Delta) = u \{ 32u + 24\Delta + 2(-336u^{2} - 528u\Delta - 120\Delta^{2}) + [23680 + 16896\zeta(3)]u^{3} + [63264 + 36864\zeta(3)]u^{2}\Delta + [46224 + 13824\zeta(3)]u\Delta^{2} + 12096\Delta^{3} \}$$
(18)

$$\beta_{A}(u, \Delta) = \Delta \{ 48u + 36\Delta + 2(-656u^{2} - 1104u\Delta - 408\Delta^{2}) + [52544 + 43008\zeta(3)]u^{3} + [140400 + 110592\zeta(3)]u^{2}\Delta + [113184 + 82944\zeta(3)]u\Delta^{2} + [31320 + 20736\zeta(3)]\Delta^{3} \}$$
(19)

for the $(m = 1, n \rightarrow 0)$ case were obtained from the previously derived general expressions for the β functions of the *nm* models.⁽⁸⁾ Assuming solutions of the form

$$u(s) = \frac{u_1}{s^{1/2}} + \frac{u_2}{s} + \dots$$
 (20)

$$\Delta(s) = \frac{\Delta_1}{s^{1/2}} + \frac{\Delta_2}{s} + \dots$$
 (21)

for s large, we can obtain u_1 , u_2 , Δ_1 , and Δ_2 from the flow equations. On substituting these solutions into the Wilson functions

$$\theta = \frac{\theta_1}{s^{1/2}} + \frac{\theta_2}{s} \tag{22}$$

$$\eta = \frac{\eta_2}{s} \tag{23}$$

We obtain the values of the coefficients given in Eqs. (4)–(6). The MAPLE computer algebra system was used to perform the lengthy algebra required to solve the flow equations for u and Δ and to obtain the coefficients in the Wilson functions. At this point, the solutions for u(s) and $\Delta(s)$ are easily checked analytically to be consistent with Eqs. (15) and (16). Our β functions were also used to generate the known results in the ε expansion of θ and η for d < 4, ^(9,10) as an additional check.

The asymptotic critical behavior of the vertex functions may be obtained from the general solution of the renormalization group equations. For example, the equation for $\Gamma^{(0,2)}$ has a general solution

$$\Gamma^{(0,2)}(0; u, \Delta, \kappa, t) = \Gamma^{(0,2)}_{\text{hom}} + \Gamma^{(0,2)}_{\text{inhom}}$$
(24)
$$\Gamma^{(0,2)}_{\text{hom}} = A_1 \Gamma^{(0,2)}(0; u(s), \Delta(s), \kappa(s), t(s))$$
$$\times \exp\left[\int_{s_0}^s -2\theta(s') \, ds'\right]$$
(25)

$$\Gamma_{\text{inhom}}^{(0,2)} = A_2 \int_{s_0}^{s} B(s') \exp\left[2 \int_{s_0}^{s'} \theta(s'') \, ds''\right] ds' + A_3 \qquad (26)$$

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The constants A_1, A_2 , and A_3 arise from the lower limit placed on the integrals. This limit is necessary, as the solutions of the flow equations given above are valid only in the large-*s* regime. In the large-*s* regime the dominant behavior of $\Gamma^{(0,2)}$ is determined by the second term, i.e., Eq. (26). After performing the integral in the exponential the remaining integral can be done by parts. To leading order the result is proportional to

$$-\exp(4\theta_1 s^{1/2}) s^{(1+4\theta_2)/2}$$
(27)

In order that B(s) and $\Gamma^{(0,2)}$ on the right-hand side of Eq. (24) can be evaluated in the perturbative regime, s is chosen to be

$$s = -\ln[t(s)/\kappa^2]/2$$
 (28)

Substituting this into Eq. (24), we obtain the result stated in Eq. (3). Similar manipulations of the general solution for $\Gamma^{(0,2)}$ give Eqs. (1) and (2).

The discrepencies between our results and those of Shalaev can be traced to two sources. In the case of the correlation function at $T = T_c$ the discrepency arises from Shalaev's Lie equation [ref. 6, Eq. (17)], which is inconsistent with expressions for η given later. The reason is that Shalaev's running variable is associated with the scaling of the square of a momentum, whereas the Lie equation which is consistent with Shalaev's equation (32) uses a variable *s* associated with the scaling of the momentum linearly. As a result, explicit use of Shalaev's equation (17) introduces an erroneous factor of two in the exponent η . In the case of the singular part of the specific heat, the discrepancy appears to arise from Shalaev's equation (43), which contains approximations familiar from parquet graph arguments. In this case, the approximations are not sufficiently accurate to obtain all subleading logarithmic factors.

Even if the asymptotic regime of the dilute system can be probed by experiment for a given material or Monte Carlo simulation, it seems unlikely that the powers of the multiplying factors of $|\ln(t)|$ could be convincingly resolved in the presence of the exponential factors. It is therefore natural to consider combinations of the observable properties in which the exponential factors are eliminated. From Eqs. (2) and (3) it can be seen that

$$t^{2}C_{\text{sing}}\chi^{2} \sim |\ln(t)|^{1/2 - 2\eta_{2}}$$
(29)

is such a combination. (Shalaev's results give the exponent as 1/2 rather than $1/2 - 2\eta_2$.) In the pure case the corresponding result is

$$t^2 C_{\rm sing} \chi^2 \sim |\ln(t)| \tag{30}$$

Therefore, as the critical temperature is approached, the effective exponent of this logarithmic factor would exhibit crossover from the pure value to the dilute value.

Lastly we note that dipolar uniaxial ferromagnets (and ferroelectrics) have a critical dimension of $d_c = 3$.^(2,11) Therefore, these materials may provide an opportunity to study the effects of dilution at the critical dimension experimentally (although the precise nature of the logarithmic corrections might be expected to differ from that discussed above). Indeed, it was the possibility of dilution effects in Gd, which previous studies indicated has asymptotic critical behavior determined by dipolar interactions,⁽¹²⁻¹⁴⁾ which motivated this work. Logarithmic corrections in the case of pure dipolar systems have been observed experimentally.^(15,16) Recently the dilute dipolar magnetic systems LiTb_{0.3}Y_{0.7}F₄ and LiHo_{0.3}Y_{0.7}F₄ were studied by neutron scattering techniques.⁽¹⁷⁾ However, the data analysis did not give detailed information about the form of the logarithmic corrections.

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