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Corrections to leading singularities in systems at the upper critical dimension

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Abstract. Renormalisation group methods are used to calculate the behaviour of the order parameter on the coexistence curve and the critical isotherm of a one-component spin system at four dimensions, and the order parameter of a three-dimensional uniaxial dipolar ferromagnet. For the four-dimensional system, the amplitudes of the subleading corrections are obtained and found to be in disagreement with the results of a recent Monte Carlo study. We show how the discrepancy may be removed by fitting the Monte Carlo data to a crossover scaling function for the order parameter rather than to an asymptotic form. For the three-dimensional system the amplitude of the subleading correction is found to be in reasonable agreement with experimental results on the uniaxial dipolar ferromagnet $LiHoF_4$.

1. Introduction

Much work has recently been performed on the critical behaviour of systems at their upper critical or marginal dimension, the spatial dimension which separates classical mean-field theory from non-classical behaviour. At the upper critical dimension the Renormalisation Group (RG) equations can be solved exactly without recourse to ε-expansions and so independent experimental investigations provide important tests to the validity of RG predictions.

It is now well known that at the upper critical dimension RG theory predicts that the asymptotic critical behaviour is classical apart from logarithmic factors (Larkin and Khmel'nitskii 1969). RG theory, however, allows not only for the calculation of quantities which characterise the asymptotic critical behaviour, but also for additional quantities describing the approach to the critical regime. More specifically, it predicts that as we move away from the critical regime, the leading singularities will be modified by correction terms, some of whose amplitudes may also be calculated, at the marginal dimension, within the RG framework.

In a paper by Mouritsen and Knak Jensen (1979) a Monte Carlo study was made, to look at the subleading correction to the order parameter of a four-dimensional Ising ferromagnet. From their investigations they were able to quote a value for the critical amplitude of the subleading correction term assuming a form as predicted by the RG for the order parameter. In the course of this work we show that the RG prediction for this amplitude is in disagreement by an order of magnitude with that from the Monte Carlo study. We give a possible reason for the discrepancy and suggest that, rather than fitting the Monte Carlo data to an asymptotic function with a correction term, it should instead be fitted with a crossover scaling function as we move into a higher reduced temperature regime where crossover effects from Ising-to-Gaussian behaviour become important.

Therefore, in the first section of this paper we obtain a crossover scaling representation of the order parameter at four dimensions using the Gaussian–Ising crossover formalism following Bruce and Wallace (1976). We show that in the asymptotic limit $-t \equiv (T_c - T)/T_c \to 0$ this reduces to the asymptotic form used for fitting the Monte Carlo data but that the critical amplitude is in disagreement with the fit; we thus proceed to fit the full crossover scaling function to the data.

Following this we quote the result of a similar calculation for the critical isotherm and also compare with Monte Carlo investigations (Mouritsen and Knak Jensen, 1981 private communication).

In the final section of the paper we take a brief look at a different system, namely a uniaxial dipolar-coupled ferromagnet whose upper critical dimension is three. As for the short-range system we calculate the subleading correction to the leading singularity of the order parameter and compare it with recent experimental results on the three-dimensional uniaxial dipolar ferromagnet $LiHoF_4$ (Griffin *et al* 1980).

2. Two-loop crossover scaling function for the order parameter

2.1. Calculation

The problem we consider is based on the standard Ginzburg–Landau–Wilson effective Hamiltonian:

$$\mathscr{H} \equiv \int d^4x \left(\tfrac{1}{2}(\nabla\phi)^2 + \tfrac{1}{2}(m_{0c}^2 + t)\phi^2 + \tfrac{1}{2}\Lambda^{-2}(\nabla^2\phi)^2 + u\phi^4/4! - H\phi\right) \tag{2.1}$$

for a one-component field ϕ. The bare mass term m_0 enters in $m_0^2 = m_{0c}^2 + t$ where m_{0c} is the bare mass of the critical theory and t is a measure of the reduced temperature $(T - T_c)/T_c$. The fourth-order derivatives implement the large momentum cut-off and the quartic term is expressed in terms of the bare coupling u which is dimensionless at four dimensions. Finally we allow for the presence of an external field, H.

The particular form of the renormalisation group we shall use is due to Zinn-Justin (1973). Such a formulation has been applied by Bruce and Wallace (1976) in a calculation of the crossover behaviour for the susceptibility in $d = 4 - \varepsilon$ dimensions and subsequently by Theumann (1980) for the specific heat.

In this paper we follow the approach of Bruce and Wallace but work directly in $d = 4$ dimensions. In the presence of an external field the order parameter obeys the renormalisation group equation (see e.g. Brézin *et al* 1976)

$$\left[\Lambda\frac{\partial}{\partial\Lambda} + \beta(u)\frac{\partial}{\partial u} - (\gamma_4(u) - \gamma_3(u))t\frac{\partial}{\partial t} + \tfrac{1}{2}\gamma_3(u)\left(1 + H\frac{\partial}{\partial H}\right)\right] M(u, t, H, \Lambda) = 0. \tag{2.2}$$

The coefficients $\beta(u)$, $\gamma_4(u)$ and $\gamma_3(u)$ have been obtained to two loops by Bruce and Wallace, so that at $d = 4$ for a one-component field:

$$\beta(u) = 3u^2 - \tfrac{17}{3}u^3 + O(u^4) \tag{2.3}$$

$$\gamma_4(u) = -u + u^2 + O(u^3) \tag{2.4}$$

$$\gamma_3(u) = \tfrac{1}{6}u^2 + O(u^3). \tag{2.5}$$

The RG equation (2.2) is integrated by the method of characteristics using the results for the coefficients (2.3)–(2.5). Hence we define $\tau = \ln \Lambda$ and introduce $u(\tau)$, $t(\tau)$ and $H(\tau)$ such that

$$du(\tau)/d\tau = \beta(u(\tau)) \tag{2.6}$$

$$dt(\tau)/d\tau = -(\gamma_4(u(\tau)) - \gamma_3(u(\tau)))t(\tau) \tag{2.7}$$

$$dH(\tau)/d\tau = \tfrac{1}{2}\gamma_3(u(\tau))H(\tau). \tag{2.8}$$

The initial conditions are $u(0) = u$, $t(0) = t$, $H(0) = H$ and correspond to the original physical system with coupling u, reduced temperature t, external field H and cut-off $\Lambda = e^0 = 1$. (2.2) then reduces to

$$M(u, t, H, 1) = \exp\left(\tfrac{1}{2}\int_u^{u(\tau)} \frac{\gamma_3(u(\tau))}{\beta(u(\tau))}\, du(\tau)\right) M(u(\tau), t(\tau), H(\tau), e^\tau). \tag{2.9}$$

By choosing τ so that $M(u(\tau), t(\tau), H(\tau), e^\tau)$ is the magnetisation of a system far from T_c, we can obtain $M(u, t, H, 1)$ for $t \ll 1$ and hence the critical behaviour of the system.

Further, since $M(u(\tau), t(\tau), H(\tau), e^\tau)$ is required outside the critical region, we can evaluate it using a Feynman graph expansion (see e.g. Wallace 1976).

$$M^2(u(\tau), t(\tau), 0, e^\tau) = -\frac{6t(\tau)}{u(\tau)}\{1 - u(\tau)[\ln(-2t(\tau)/e^{2\tau}) + 1] + O(u(\tau)^2)\} \tag{2.10}$$

where $H(\tau)$ has been set equal to zero since we wish to evaluate the spontaneous magnetisation in the absence of an external field.

A matching condition is now needed to fix the value of τ and a suitable choice is given by

$$t(\tau) = -e^{2\tau}. \tag{2.11}$$

Using (2.9), (2.10), (2.11) and integrating (2.6)–(2.8) we obtain a parametric representation of the crossover scaling function for the order parameter

$$M^2(t) = B(-t)u(\tau)^{-2/3}[1 + Cu(\tau) + O(u^2(\tau))] \tag{2.12}$$

with

$$-t = t_0 \exp(-2/3u(\tau))u(\tau)^{25/27}[1 + O(u(\tau))] \tag{2.13}$$

where B, t_0 and C are non-universal system-dependent factors.

These two equations provide a possible form with which one may attempt to fit the Monte Carlo data for $M(t)$ in the four-dimensional Ising model. In the asymptotic regime $t/t_0 \ll 1$, the expressions can be simplified. Clearly from (2.13), we see that $u(\tau)$ must then also be small, and we can solve systematically for $u(\tau)$:

$$u(\tau) = \frac{2}{3|\ln(-t/t_0)|}\left[1 + \frac{25}{27}\frac{\ln|\ln(-t/t_0)|}{|\ln(-t/t_0)|} + O\left(\frac{1}{|\ln(-t/t_0)|}\right)\right]. \tag{2.14}$$

Note that in this equation, the coefficient of the correction of order $1/|\ln(-t/t_0)|$ changes if we change the scale t_0. By a similar argument, when we substitute (2.14) into (2.12), we see that the term $Cu(\tau) \sim 2C/(3|\ln(-t/t_0)|)$ has the same character: *in the asymptotic regime*, the freedom of choice of both C and t_0 is illusory. Alternatively stated, in the asymptotic regime, C may be set to zero given the freedom of choice of t_0.

Hence, for $t \ll t_0$, an alternative parametric form for $M(t)$ is given by

$$M^2(t) = B(-t)u(\tau)^{-2/3}[1 + \mathrm{O}(u^2(\tau))]. \tag{2.15}$$

Yet another form may be obtained by effecting the above substitution:

$$M(t) = B\left(-\frac{t}{t_0}\right)^{1/2}\left|\ln\left(-\frac{t}{t_0}\right)\right|^{1/3}\left[1 - \frac{25}{81}\frac{\ln|\ln(-t/t_0)|}{|\ln(-t/t_0)|} + \mathrm{O}\left(\frac{1}{|\ln(-t/t_0)|}\right)\right] \tag{2.16}$$

where it should be understood that $\mathrm{O}(1/|\ln(-t/t_0)|)$ becomes $\mathrm{O}(1/|\ln(-t/t_0)|^2)$ with a suitable choice of t_0.

It is worth noting, however, that this discussion of the insignificance of $1/|\ln(-t/t_0)|$ corrections must be refined if we have two quantities at our disposal, e.g. the susceptibility $\chi(t)$ in addition to $M(t)$. The $1/|\ln(-t/t_0)|$ correction can, by an appropriate choice of t_0, be made to vanish for one or the other of these quantities but not in general for both. If this correction is set to zero in $M(t)$, the resulting correction in $\chi(t)$ is significant.

2.2. *Discussion*

Mouritsen and Knak Jensen (1979) have obtained a value for the coefficient of the subleading correction term by fitting an equation of the form

$$M(t) = B(-t)^{1/2}|\ln(-t)|^{1/3}[1 + Q(\ln|\ln(-t)|/|\ln(-t)|)] \tag{2.17}$$

to Monte Carlo data obtained on a four-dimensional spin-$\frac{1}{2}$ Ising ferromagnet in a simple hypercubic lattice over the reduced temperature range $0.01 < -t < 0.56$. The value they obtain for Q, namely

$$Q = -0.030 \pm 0.002, \tag{2.18}$$

is in disagreement, by an order of magnitude, with the RG result, (2.16).

A possible reason for this disagreement is that in extrapolating to relatively high values of $|t|$, ($|t| \simeq 1$), (2.17) is not a valid fitting function because of the slow variation of the logarithmic correction terms. As a result, the value of Q obtained by fitting (2.17) to the Monte Carlo data describes the effect of several subleading correction terms. In extending the range of reduced temperature out to $|t| \simeq 1$, it seems reasonable to describe the temperature variations of the order parameter not by an asymptotic series such as (2.17), but rather by a crossover scaling function, since we are presumably near the region where crossover from Ising-to-Gaussian behaviour is taking place. As a result we attempted to constrain a fit to the form of the crossover scaling representation of the order parameter. When two-parameter fits were made using the universal forms of the crossover scaling function, (2.15) (2.13) and (2.16), the overall quality of the fit was poor and strongly dependent on the temperature range over which the data was fitted. In a typical fit, we found t_0 to be of the order 1, so that $-t/t_0$ is not small if one attempts to fit out to $-t \simeq 1$. Since these universal forms have been shown, in the previous section, to be appropriate for use only in the asymptotic region where $-t/t_0 \ll 1$ or equivalently in the small-coupling regime, we assume that the poorness of fit is due to the bare coupling not being small in the model from which the Monte Carlo data was obtained. We thus proceeded to fit the data using the non-universal crossover scaling function, (2.12)–(2.13), which allows for a larger coupling by the inclusion of a term

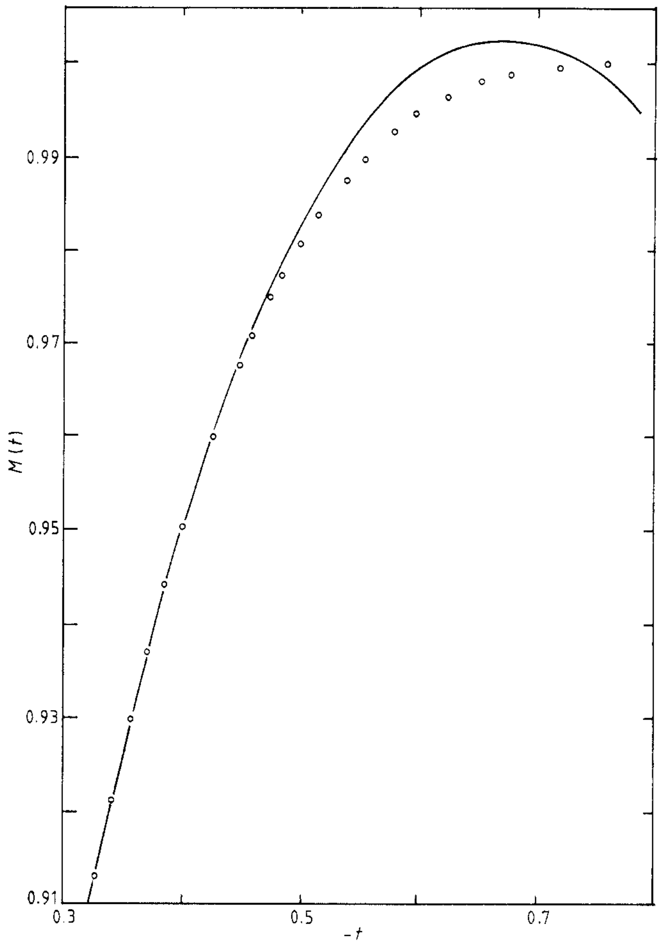

Figure 1. Temperature variation of the order parameter at four dimensions: open circles, Monte Carlo data; full curve, two-loop crossover, equations (2.12)–(2.13) with $B = 1.530$, $C = -2.832$, $t_0 = 30.00$.

proportional to $u(\tau)$ in the square brackets of equation (2.12). The result of this three-parameter fit is displayed in figure 1.

In the range of reduced temperatures over which the Monte Carlo data was fitted by the asymptotic form (2.17), namely $0.01 < -t < 0.56$, we obtained a fit, using this crossover scaling function, of comparable quality to that using the asymptotic function (2.17). The improvement, however, is that this crossover scaling form reduces to the theoretically correct asymptotic function (2.17) as shown in the previous section and thus there is no real discrepancy between data and theory. Nevertheless, it is also clear that the fit is still in disagreement with the data as one proceeds to higher reduced temperatures. Again this is only to be expected; for example, we have taken $t \equiv (T - T_c)/T_c$ as our scaling field and we have therefore assumed that we are working in a temperature regime where t is small enough so that we can use a scaling field that is linear in t. As we proceed into the crossover region it is no longer clear that this linearity hypothesis remains valid (Riedel and Wegner 1974).

Similar remarks can be made for other quantities of interest. In particular, for the critical isotherm we find, by a similar calculation to that performed above

$$M(H) \propto H^{1/3}|\ln H|^{1/3}\left[1-\frac{25}{54}\frac{\ln|\ln H|}{|\ln H|}+\mathrm{O}\left(\frac{1}{|\ln H|}\right)\right]. \tag{2.19}$$

Once again the value of the correction amplitude has been obtained by performing a fit to Monte Carlo data with the trial function (Mouritsen and Knak Jensen, private communication)

$$M = BH^{1/3}|\ln H|^{1/3}\left(1+Q\frac{\ln|\ln H|}{|\ln H|}+\frac{P}{|\ln H|}\right) \tag{2.20}$$

and a preliminary analysis is consistent with $Q \simeq -0.3$, in slightly better agreement with the theoretical prediction than for the coexistence curve result.

3. Three-dimensional uniaxial dipolar ferromagnet

Although the discussion so far has been restricted to a four-dimensional system, it is also relevant when considering other systems at their upper critical dimension. In particular, theory predicts that there is a correspondence, at leading order, between the four-dimensional short-range Ising system and the three-dimensional uniaxial ferromagnet with long-range dipolar coupling (Larkin and Khmel'nitskii 1969, Brézin and Zinn-Justin 1976). Recently the critical behaviour of the spontaneous magnetisation in the uniaxial dipolar-coupled ferromagnet $LiHoF_4$ has been measured using a light scattering technique (Griffin *et al* 1980) and the results fitted to an equation of the form

$$\frac{M(T)}{M(0)} = B(-t)^{1/2}|\ln(-t)|^{1/3}\left(1+C_1\frac{\ln|\ln(-t)|}{|\ln(-t)|}+\frac{C_2}{|\ln(-t)|}\right). \tag{3.1}$$

The values obtained for the amplitudes are $C_1 = 0.07 \pm 0.30$ and $C_2 = 0.29 \pm 0.07$ in the reduced temperature range $1.3\times10^{-3} < -t < 1.3\times10^{-1}$.

We have performed a calculation following Brézin and Zinn-Justin (1976) for the magnetisation below T_c and find

$$M(t) \propto (-t)^{1/2}|\ln(-t)|^{1/3}\left[1-\tfrac{1}{243}(108\ln\tfrac{4}{3}+41)\frac{\ln|\ln(-t)|}{|\ln(-t)|}+\mathrm{O}\left(\frac{1}{|\ln(-t)|}\right)\right]. \tag{3.2}$$

Thus RG predicts that $C_1 \simeq -0.30$.

One should note that although there is an additional $1/|\ln(-t)|$ correction term in (3.1), its coefficient C_2 is again non-universal in the sense discussed in § 2.

4. Concluding remarks

To summarise, we have calculated using field-theoretical methods the renormalisation group values for the amplitudes of the subleading corrections to the order parameter and critical isotherm of a four-dimensional Ising ferromagnet and to the order parameter of a three-dimensional unaxial dipolar-coupled ferromagnet. For the four-dimensional short-range system it is found that the theoretical predictions are not in good agreement with the values obtained by fitting an asymptotic form with a subleading correction to Monte Carlo data. For the three-dimensional long-range system, there is better agreement, although the subleading correction amplitude is, as yet, poorly determined experimentally.

A likely reason for these differences seems to be that in extending into a regime where crossover phenomena become important, it may no longer be valid to use asymptotic functions, with the slowly varying logarithmic corrections that are characteristic of systems at their upper critical dimensions, as fitting equations. It is suggested that, in these cases, more suitable fitting functions are the full crossover scaling functions. We have found that, for the order parameter of the four-dimensional short-range system, the crossover scaling form provides as good a fit to the data as does the asymptotic form, but by employing the crossover fitting form we remove the discrepancy between theory and data since the crossover scaling function reduces, in the limit $-t \to 0$, to the theoretically correct asymptotic form. However, there still remains some disagreement between data and theory, even when a crossover scaling function is used, and we suggest that this is due to the use of linear scaling fields in a region where the linearity hypothesis is no longer justifiable.

In conclusion, the moral seems to be the need to exercise extreme caution when fitting slowly varying asymptotic forms away from the critical region even when correction terms are included.

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