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Uniaxial systems with dipole–dipole interactions

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Abstract. Within the context of a model that allows for the exact calculation of the partition function, it is shown that a d-dimensional uniaxial system with dipolar interactions falls into the same universality class as a $(d + 1)$-dimensional, strictly short-range system.

An important feature which determines the critical behaviour of a phase transition is the range of the interactions between the microscopic degrees of freedom. In models where these interactions do not decay adequately fast with distance, the physics is substantially modified compared to models described by strictly short-range interactions. Long-range interactions are present in magnetic systems and particularly influence the behaviour of systems with relatively low critical temperatures (less than 300 K). Therefore, even though in most ferromagnets the dominant interaction for magnetic order is the short-range exchange interaction, the classical dipolar interactions cannot always be neglected. It is well known, for example, how the critical behaviour of a ferromagnet, is altered considerably when one considers the effect of the long-range interaction due to pairs of magnetic dipoles in addition to the short-range spin–spin interactions [1–8]. Specifically, in [2] renormalization group theory was applied to derive the critical exponents γ, ν and η, to order $\varepsilon = 4 - d$, for a d-dimensional ferromagnetic system with dipole–dipole interactions between its d-component spins. These results were extended in [3] where the Feynman-graph-expansion approach of Wilson [10] was used to calculate the exponent η to second order in ε, as well as to describe the behaviour of the 4-spin correlation function. In general, the behaviour of ferromagnets with this type of long-range interaction differs from that of ferromagnets with strictly short-range interactions, according to the number of components of the order parameter. For example, the pioneering work of Larkin and Khmel'nitskii [1], using Feynman-graph expansions for $d = 3$, showed that the critical behaviour of a uniaxial ferromagnet with both exchange and dipolar interactions has logarithmic corrections not expected classically. Aharony [7, 8] used exact renormalization group (RG) equations and the ε-expansion (where for this particular problem $\varepsilon = 3 - d$) to verify this, as well as to predict that the critical behaviour of a d-dimensional uniaxial Ising ferromagnet with dipole–dipole interactions belongs in the same universality class as a $(d + 1)$-dimensional, strictly short-range Ising ferromagnet [8]. In the present work, an alternative approach will be used to confirm and generalize this result. It will be shown that d-dimensional uniaxial systems with short-range ferromagnetic interactions as well as long-range dipole–dipole interactions have $d_c = 3$ as the upper marginal dimension above which mean-field behaviour fully sets in, and below (explicitly for $1 < d < 3$) which critical behaviour prevails. Unlike the ε-expansion where the validity of the results depends on the smallness of ε, the method used here derives the result for any d without any constraints. The study of such systems will be done by considering a model with reduced interactions of fluctuations, allowing for the exact calculation of the partition function. The model is a considerable improvement over mean-field theory, and has been previously successfully applied to a number of different systems [9, 11–17]. The results obtained by the model are in qualitative agreement with those obtained by RG theory, whenever there are results from both approaches for comparison. Furthermore, through the model, unlike in RG theory, fluctuation interactions can be controlled. Specifically, they can be easily suppressed, thus allowing one to see the crossover to mean-field behaviour.

The system of interest has the Ginzburg–Landau–Wilson functional with a scalar order parameter $S(\boldsymbol{x})$

$$F[S(\boldsymbol{x})] = \tfrac{1}{2}\int \mathrm{d}^d x \left[\tau S^2(\boldsymbol{x}) + c\,(\nabla S(\boldsymbol{x}))^2 + uS^4(\boldsymbol{x}) - hS(\boldsymbol{x}) - \int_{\boldsymbol{x}'\neq\boldsymbol{x}} \mathrm{d}^d x'\, gS(\boldsymbol{x})S(\boldsymbol{x}')\frac{\partial^2}{\partial z^2}(|\boldsymbol{x}-\boldsymbol{x}'|^{2-d})\right] \tag{1}$$

where $S(\boldsymbol{x})$ is a classical order parameter pointing in the direction of spatial anisotropy (the z-axis), located at site $\boldsymbol{x}$ of a d-dimensional lattice. Also, $\tau = (T - T_c)/T_c$, where T_c is a trial critical temperature for the order parameter, h is a constant external conjugate field, c and u are the usual constants of interactions and g is a measure of the strength of the dipole interaction.

The Fourier transform of the dipolar term for small $\boldsymbol{q}$ is [2]

$$F_{dip} \equiv -\tfrac{1}{2}\int \mathrm{d}^d x \int_{\boldsymbol{x}'\neq\boldsymbol{x}} \mathrm{d}^d x'\, gS(\boldsymbol{x})S(\boldsymbol{x}')\frac{\partial^2}{\partial z^2}(|\boldsymbol{x}-\boldsymbol{x}'|^{2-d})$$

$$= -\tfrac{1}{2}\int_{\boldsymbol{q}\neq\boldsymbol{0}} \mathrm{d}^d q\; S^2(\boldsymbol{q})\left[-g_1\frac{q_z^2}{q^2} + g_2 q_z^2 + g_3 + g_4 q^2\right] \tag{2}$$

where constants resulting from integrations of d-dimensional Fourier transforms have been absorbed in the constants g_1, g_2, g_3 and g_4. In the Fourier transform terms of $\mathrm{O}(q^4 + q_z^4)$ have been dropped. Equation (2) will be used to express the partition function of the system in momentum space.

The exact model used here is one which uses the approximation of the quartic term in the functional (1) as follows:

$$\int \mathrm{d}^d x\; S^4(\boldsymbol{x}) \to \frac{1}{V}a^2[S(\boldsymbol{x})] \qquad a[S(\boldsymbol{x})] \equiv \int \mathrm{d}^d x\; S^2(\boldsymbol{x}) \tag{3}$$

where V is the volume of the system. Such an approximation, first proposed by Schneider *et al* [18] causes the model to consider the interaction of fluctuations with equal and antiparallel momenta. This can be seen if one rewrites equation (1) in the momentum representation. Then approximation (3) becomes equivalent to splitting the δ-function, which provides momentum conservation, into the product of two δ-functions:

$$\delta(\boldsymbol{q}_1 + \boldsymbol{q}_2 + \boldsymbol{q}_3 + \boldsymbol{q}_4) \to \delta(\boldsymbol{q}_1 + \boldsymbol{q}_2)\delta(\boldsymbol{q}_3 + \boldsymbol{q}_4).$$

Using a transformation analogous to that of Hubbard–Stratonovich,

$$\exp\left(-\frac{V}{2}K\left(\frac{a[S]}{V}\right)\right) = \int \mathrm{d}x\,\mathrm{d}y\,\exp\left(-\frac{V}{2}K\left(\frac{x}{V}\right) + \mathrm{i}(xy - ya)\right)$$

applied to an arbitrary function $K\,(a/V)$, where for functional (1), $K\,(a/V)$ is

$$K\left(\frac{a}{V}\right) = \frac{\tau a}{V} + \frac{ua^2}{V^2}$$

the Boltzmann factor in the partition function becomes bilinear with respect to $S(\boldsymbol{x})$. The consequence of this relative simplification is the introduction of two new variables, x and y. The free energy functional (1) then becomes

$$F[S(\boldsymbol{x})] = \frac{V}{2}K\left(\frac{a}{V}\right) + \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}^d x \left[c(\nabla S(\boldsymbol{x}))^2 - hS(\boldsymbol{x})\right] + F_{dip}$$

and after using equation (2), the partition function in momentum space takes the form

$$Z = \int DS_q\,\mathrm{d}x\,\mathrm{d}y \exp\Bigg[-\frac{V}{2}\Bigg(K(x) - xy - \frac{2hS_{q=0}}{\sqrt{V}} + \frac{yS^2_{q=0}}{V} + \sum_{\boldsymbol{q}\neq\boldsymbol{0}} \frac{S_q^2}{V}\left(y + cq^2 + g_1\frac{q_z^2}{q^2} - g_2 q_z^2\right)\Bigg)\Bigg] \qquad (4)$$

where the following substitutions, $x/V \to x, 2\mathrm{i}y \to y$, $g_4 - c \to c$, $g_3 - \tau \to \tau$, $S_q/\sqrt{V} \to S_q$, $h/(2V) \to h$ have been made. Furthermore, for materials with low critical temperatures (for which dipolar interactions are most effective) or large values of g_1 compared to τ, the term $g_2 q_z^2$ has an insignificant contribution and it is dropped for further consideration [8].

Consequently, all functional integrals in equation (4) may be calculated to give

$$Z = \int \mathrm{d}x\,\mathrm{d}y \exp -\frac{V}{2}\left[K(x) - xy + \frac{\ln|y|}{V} - \frac{h^2}{y} + \frac{1}{V}\sum_{\boldsymbol{q}\neq\boldsymbol{0}} \ln\left(y + cq^2 + g_1\frac{q_z^2}{q^2}\right)\right].$$

The summation over momentum must now be evaluated. To do so first note that

$$\sum_{\boldsymbol{q}\neq\boldsymbol{0}} \ln\left(y + cq^2 + g_1\frac{q_z^2}{q^2}\right) = \frac{V}{(2\pi)^d}\int_{\boldsymbol{q}\neq\boldsymbol{0}} \mathrm{d}^d q \ln\left(y + cq^2 + g_1\frac{q_z^2}{q^2}\right) \qquad (5)$$

and after writing the momentum integral in spherical coordinates in d-dimensional space and integrating all angles except the anisotropy angle θ, we derive

$$\int_{\boldsymbol{q}\neq\boldsymbol{0}} \mathrm{d}^d q \ln\left(y + cq^2 + g_1\frac{q_z^2}{q^2}\right) = \frac{2\pi^{(d-1)/2}}{\Gamma\left(\frac{1}{2}(d-1)\right)}\int_{\boldsymbol{q}\neq\boldsymbol{0}}^{\infty} \mathrm{d}^d q \int_{\boldsymbol{0}}^{\pi} \mathrm{d}\theta \left[q^{d-1}\sin^{d-2}\theta \ln\left(y + cq^2 + g_1\frac{q_z^2}{q^2}\right)\right] \qquad (6)$$

where $2\pi^{(d-1)/2}/\Gamma\left(\frac{1}{2}(d-1)\right)$ is the result of the angular integration. Since we consider large values of g_1 compared to g_2 then only integrals in q-space for small values of $q_z/q = \cos\theta$ will contribute. Thus, by combining equations (5) and (6), and defining $\mu \equiv g_1^{1/2}c^{-1/2}\cos\theta$ we obtain

$$\sum_{\boldsymbol{q}\neq\boldsymbol{0}} \ln\left(y + cq^2 + g_1\frac{q_z^2}{q^2}\right) = \frac{-Vg_1^{-1/2}c^{1/2}\Gamma\left(\frac{1}{2}d\right)}{(2\pi)^d\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{1}{2}(d-1)\right)}\int_{\boldsymbol{q}=\boldsymbol{0}}^{\infty} \mathrm{d}^d q \int_{\mu=\boldsymbol{0}}^{\infty} \mathrm{d}\mu \ln\left(y + cq^2 + c\mu^2\right).$$

The above looks like a $D \equiv (d+1)$-dimensional integral with μ the extra $(d+1)$st component of the momentum vector. This is, in fact, the reason for the new behaviour of the uniaxial dipolar-interaction system as will be seen in detail below. The final result of the original sum will then be

$$\sum_{\boldsymbol{q}\neq\boldsymbol{0}} \ln\left(y + cq^2 + g_1\frac{q_z^2}{q^2}\right) \equiv V\left(f_d(y) + y\Theta_d(\Lambda)\right)$$

for which

$$f_d(y) = \begin{cases} \dfrac{-g_1^{-1/2} c^{(1-D)/2} 2^{(1-d)} \pi^{(2-d)/2} (-1)^{(D-1)} \Gamma\left(\frac{1}{2}d\right)}{D\Gamma\left(\frac{1}{2}(d+1)\right)\Gamma\left(\frac{1}{2}(d-1)\right)} y^{D/2} \\ \equiv \kappa_1(c) y^{D/2} \qquad D \neq \text{even} \\ \dfrac{-g_1^{-1/2} c^{(1-D)/2} 2^{(1-d)} \pi^{-d/2} (-1)^{D/2} \Gamma\left(\frac{1}{2}d\right)}{D\Gamma\left(\frac{1}{2}(d+1)\right)\Gamma\left(\frac{1}{2}(d-1)\right)} y^{D/2} \ln|y| \\ \equiv \kappa_2(c)\, y^{D/2} \ln|y| \qquad D = \text{even} \end{cases}$$

$$\Theta_d(\Lambda) = \begin{cases} \dfrac{-g_1^{-1/2} c^{-1/2} 2^{(1-d)} \pi^{-d/2} \Gamma\left(\frac{1}{2}d\right)}{(D-2)\Gamma\left(\frac{1}{2}(d+1)\right)\Gamma\left(\frac{1}{2}(d-1)\right)} \Lambda^{D-2} & D \neq 2 \\ \dfrac{-g_1^{-1/2} c^{-1/2} 2^{(1-d)} \pi^{-d/2} \Gamma\left(\frac{1}{2}d\right)}{2\Gamma\left(\frac{1}{2}(d+1)\right)\Gamma\left(\frac{1}{2}(d-1)\right)} \ln\left(c\Lambda^2\right) & D = 2 \end{cases}$$

where Λ is a momentum cut-off.

The function $\Theta_d(\Lambda)$ diverges when $\Lambda \to \infty$ and $D \geqslant 2$. However, critical asymptotics do not depend on a particular momentum cut-off and such a divergence is absorbed by renormalizing x and τ. This is done by defining $x + \Theta_d(\Lambda) \equiv x$ and $\tau x + 2u\Theta_d(\Lambda)x \equiv tx$. The partition function may now be written as

$$Z = \int \mathrm{d}x\, \mathrm{d}y \exp\left(-\tfrac{1}{2} V F(x, y, h)\right)$$

with

$$F(x, y, h) = tx + ux^2 - yx - \frac{h^2}{y} + \begin{cases} \kappa_1(c) y^{D/2} & D \neq \text{even} \\ \kappa_2(c)\, y^{D/2} \ln|y| & D = \text{even.} \end{cases} \tag{7}$$

In the thermodynamic limit $V \to \infty$, the calculation of the partition function becomes exact and can be performed using the method of steepest descent. The equilibrium free energy can be calculated by solving for x and y in the saddle-point equations $\partial F/\partial x = 0$ and $\partial F/\partial y = 0$. An expression for the equilibrium order parameter S is given by

$$S = \left[\frac{-\partial F(x, y, h)}{\partial h}\right]_{y=y(h)} = \frac{2h}{y(h)} \to \frac{h}{y(h)}. \tag{8}$$

Using $\partial F(h)/\partial x = 0$, $\partial F/\partial y = 0$ and the expression for S (equation (8)), an equation for the order parameter is derived. This parameter depends, among other things, on the constant conjugate field h, the dimensionality d of space, and the scale of microscopic interactions of fluctuations c. One can write these expressions for S for all possible values of D (and consequently of d), including non-integers, as shown below,

$$S^2 + \frac{t}{2u} - \frac{h}{2uS} + \frac{D}{2}\kappa_1(c)\left(\frac{h}{S}\right)^{\left(\frac{1}{2}(D-2)\right)} = 0 \qquad D = \text{non-even}$$

$$S^2 + \frac{t}{2u} - \frac{h}{2uS} + \frac{D}{2}\kappa_2(c)\left(\frac{h}{S}\right)^{\left(\frac{1}{2}(D-2)\right)} \ln\left|\frac{h}{S}\right| + \kappa_2(c)\left(\frac{h}{S}\right)^{\left(\frac{1}{2}(D-2)\right)} = 0 \qquad D = \text{even.} \tag{9}$$

As $h \to 0$, whether S has a solution and whether the behaviour of the system will be critical or mean-field, depends on the values of the space dimensionality D as well as the scale of microscopic interactions c. In the absence of the external field h, a real solution for S exists only for $D > 2$ and $t < 0$ and is given by $S = \sqrt{-t/2u}$. This shows that $D = 2 \Rightarrow d = 1$ is the lower marginal dimension for the uniaxial dipolar system. The critical exponent $\beta = \frac{1}{2}$. The model finds more interesting results when the critical exponent δ is calculated. At $t = 0$ and as $h \to 0$ the solutions of equations (9) are

$$\begin{aligned} S &= \left(-\tfrac{1}{2}D\kappa_1(c)\right)^{2/(D+2)} h^{(D-2)/(D+2)} && 2 < D < 4 \\ S &= \left(-\frac{4}{3}\kappa_2(c)h\ln\left|\frac{\sqrt{3}}{2\sqrt{\kappa_2(c)}}h\right|\right)^{1/3} && D = 4 \\ S &= \left(\frac{h}{2u}\right)^{1/3} && D > 4. \end{aligned} \tag{10}$$

It follows from the above result that $D = 4 \Rightarrow d = 3$ is the upper marginal dimension. Explicitly, the critical exponent δ has the value $\delta = (D+2)/(D-2) \Rightarrow \delta = (d+3)/(d-1)$ which is true for the range $2 < D < 4 \Rightarrow 1 < d < 3$. If, however, $D > 4 \Rightarrow d > 3$ then $\delta = 3$ which is the usual mean-field value. Finally, at $D = 4 \Rightarrow d = 3$ the value of δ has logarithmic corrections. As can be seen from this discussion, within the context of the exactly solvable model, the consequences of the dipolar interactions is to increase by one the effective space dimension of the uniaxial system. This is also in agreement with the result obtained within the framework of renormalization group theory [7, 8]. Thus a three-dimensional uniaxial system with dipole–dipole interactions falls into the universality class of a four-dimensional strictly short-range system whose behaviour is mean-field with subtle logarithmic corrections which reflect the non-mean-field behaviour that sets in fully below four space dimensions. In the absence of the dipole–dipole interactions, which are eliminated by taking $g = 0$ in equation (1), the exactly solvable model finds critical behaviour for $2 < d < 4$ with subtle logarithmic corrections at $d = 4$ and a classical mean-field behaviour for $d > 4$ [9]. This is in accordance with RG analysis [19–22]. It is not contradictory that within the context of the exactly solvable model a system with a one-component order parameter, has a lower critical dimension $d_c = 2$. Indeed, the functional (1) with $g = 0$ corresponds to the classical Ising model which has $d_c = 1$. However, after the approximation (3) the model belongs to the spherical model universality class and, therefore, has symmetry $O(N = \infty)$ [23]. On the one hand, this makes the model less realistic. However, on the other hand, knowing the effect various perturbation terms have on non-physical models, such as the spherical one, could be used as a qualitative basis for understanding the behaviour the same perturbation may have on more realistic models.

Since c is the scale of microscopic interactions of fluctuations and is also related to the width of the fluctuation region, suppressing the fluctuations can be done in the limit $c \to \infty$. Then it is seen that all results reduce to strictly mean-field ones as expected regardless of dipolar interactions.

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