Critical behavior of compressible magnets*

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A model of a compressible n-component magnet which includes shearing forces is solved by the renormalization-group recursion relations to first order in $\epsilon = 4 - d$. Four fixed points are found and their relevance for critical behavior is discussed. The critical exponents of Heisenberg magnets have their rigid-lattice values. The leading correction to scaling has the exponent $\alpha\nu^{-1}$ with respect to inverse length. In Ising-like systems the transition is of the first order, but may appear as a second order.

I. INTRODUCTION

Consider an elastically isotropic n-component magnet which has a bulk modulus K_0 and a shear modulus μ_0. The surfaces are free. The question is can the system have a critical point, and if so, what are its critical exponents? The main tool in answering the question will be the renormalization-group equations.[1]

In the renormalization-group approach to critical phenomena[1,2] the first step is to set up a system of recursion relations for the thermodynamical fields[3] of the system. Then one looks for the fixed points of these equations. Each fixed point describes one type of critical behavior. Critical exponents can be determined by linearizing the recursion relations around the particular fixed point of interest. The fixed points differ by the degree of instability. The degree of instability is the number of thermodynamical fields which must be held at their critical values for the system to be at the critical point. Such fields are called thermodynamically relevant. A field which is irrelevant for some fixed point may be relevant for another. It may happen that the most stable fixed point does not control the behavior of the system. What is important to keep in mind is that each fixed point has a domain of attraction. If the values of the thermodynamical fields are outside the domain of the most stable fixed point the system will typically undergo a first-order transition, but in favorable cases it will be controlled by another, less stable, fixed point over a large range of experimentally controllable relevant fields (such as magnetic fields and temperature; sometimes there are relevant fields which are not experimentally controllable as we shall see below). The behavior just described is one we shall find for a compressible Ising model. The "critical" region is finite but may be large. The effective critical exponents are those of the rigid Ising model ($n=1$). The analysis by renormalization group thus confirms the results of Baker and Essam[4] and of Larkin and Pikin.[5]

Compressible Heisenberg systems ($n=3$), on the contrary, may have a genuine critical point, i.e., the fields can converge to a fixed point starting from physically admissible values. Critical exponents in this case are identical to those of the rigid Heisenberg model. The reason for the different effects that compressibility has on Ising and Heisenberg models, respectively, is the difference in the sign of the critical exponent α of the rigid systems. It is positive for the rigid Ising model and negative for the Heisenberg magnet in dimension $d=3$.

A fairly complete analysis of the problem is possible if the dimensionality of the system is close to 4 and the ϵ-expansion approximation to the renormalization-group equations can be used. To be able to make statements about real systems, one has to assume that the solution does not qualitatively change as the transition from $d=4-\epsilon$ to $d=3$ is made. (One has to be careful; for instance, in rigid lattices the critical exponent α changes its sign between $d=4-\epsilon$ and $d=3$ for the Heisenberg model with three components.)

II. RENORMALIZATION GROUP FOR COMPRESSIBLE MAGNETS

We shall start with the following Hamiltonian[5]:

$$-\mathcal{H}[S_i(\vec{x}), \vec{u}(\vec{x})] \equiv \frac{H}{T} = \int d^d x \left[\frac{1}{2} r \sum_i S_i^2(\vec{x}) + \frac{1}{2}\sum_{i,\beta}\left(\frac{\partial S_i}{\partial x_\beta}\right)^2 + u_0\left(\sum_i S_i^2(\vec{x})\right)^2 + \left(\tfrac{1}{2}K - \frac{1}{d}\mu\right)(\mathrm{div}\vec{u})^2 + \mu\sum_{\alpha,\beta}\left(\frac{\partial u_\alpha}{\partial x_\beta}\right)^2 + g\sum_i S_i^2(\vec{x})\,\mathrm{div}\vec{u}\right] . \qquad (1)$$

The first three terms represent the rigid n-component Heisenberg model in a form suitable for a study of the system by means of the renormalization group[1] in the ϵ-expansion approximation. $\vec{u}(\vec{x})$ is the displacement vector, K and μ are the bulk and shear moduli of the underlying lattice divided by the temperature, g is a spin-lattice coupling constant, and d is the dimensionality of the system. The spin and displacement variables are constrained by not having faster spatial variations than on the scale of the lattice constant.

In the partition function

$$Z = \mathrm{Tr}\exp\{\mathcal{H}[S_i(\vec{x}), \vec{u}(\vec{x})]\} \tag{2}$$

the integrals over the displacement variables will be done first. For that purpose the homogeneous deformation has to be separated from the phonon part of the displacement[5]:

$$\frac{\partial u_\alpha}{\partial x_\beta} = u_{\alpha\beta} + \frac{1}{\Omega}\sum_{\vec{k}} i k_\beta\, u_\alpha(\vec{k})\, e^{i\vec{k}\cdot\vec{x}} \; . \tag{3}$$

Ω is the volume of the system. The integrals over $u_{\alpha\beta}$ and $u_\alpha(\vec{k})$ are Gaussian. The result is

$$Z = Z_{el}\, \mathrm{tr}\, e^{\bar{\mathcal{H}}[S_i(\vec{k})]} \; , \tag{4}$$

where the trace is taken only over the spin variables and the equivalent spin Hamiltonian is

$$-\bar{\mathcal{H}}[S(\vec{k})] = \tfrac{1}{2}\int_{\vec{k}} (r + k^2)\sum_i S_i(k) S_i(-\vec{k}) + u\sum_{ij}\int_{\vec{k}_1}\int_{\vec{k}_2}\int_{\vec{k}_3} S_i(\vec{k}_1) S_i(\vec{k}_2) S_j(\vec{k}_3) \times S_j(-\vec{k}_1 - \vec{k}_2 - \vec{k}_3) + \frac{v}{\Omega}\left(\int_{\vec{k}}\sum_i S_i(\vec{k}) S_i(-\vec{k})\right)^2 \; . \tag{5}$$

The wave vectors are cut off from above by the inverse lattice constant. The parameters u and v are defined as follows:

$$u = u_0 - \frac{g^2}{4\{\frac{1}{2}K + [(d-1)/d]\mu\}} \; , \tag{6}$$

$$v = \tfrac{1}{4} g^2 - \left(\frac{1}{\frac{1}{2}K + [(d-1)/d]\mu} - \frac{2}{K}\right) \; . \tag{7}$$

The four-spin interaction u can be negative. Then one has to bring into the problem six-spin (or higher) interactions. The critical point as a function of g ends at a tricritical point, and for sufficiently large g the transition becomes of first order[6] (actually, it is a fourth-order point for Ising systems; see below).

If u is positive Eq. (5) represents a Heisenberg model with an infinite-range energy-density–energy-density coupling v. Formally this interaction vanishes, if the shear modulus goes to zero, but such a limiting process is illegal because Z_{el} in Eq. (4) diverges for $\mu = 0$ and special arrangements are necessary in this case.[7]

Now we apply the renormalization-group method[1] to the spin Hamiltonian (5). The recursion relations[8] for the fields r, u, v are shown in graphical form in Fig. 1. Analytically they read

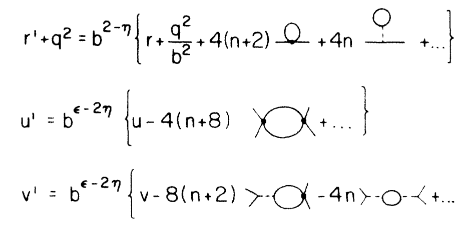

FIG. 1. Feynman diagrams when energy-energy coupling is present. The vertex u is denoted by a heavy dot and v is represented by dashed line. Only zero momentum can be carried by dashed lines. All diagrams having loops which contain a dashed line are negligible in the thermodynamic limit. All non-negligible diagrams have a tree structure with respect to dashed lines.

$$r' + q^2 = b^{2-\eta}\left(r + \frac{q^2}{b^2} + 4(n+2)u\int\frac{d^dq}{r+q^2} + 4nv\int\frac{d^dq}{r+q^2} + \cdots\right) , \tag{8}$$

$$u' = b^{\epsilon-2\eta}\left(u - 4(n+8)u^2\int\frac{d^dq}{(r+q^2)^2} + \cdots\right) , \tag{9}$$

$$v' = b^{\epsilon-2\eta}\left(v - 8(n+2)uv\int\frac{d^dq}{(r+q^2)^2} - 4nv^2\int\frac{d^dq}{(r+q^2)^2} + \cdots\right) . \tag{10}$$

All integrals are over the region $1 > |\vec{q}| > b^{-1}$, where $b > 1$ but otherwise arbitrary.

To first order in $\epsilon = 4 - d$ recursion relations (9) and (10) have four fixed points:

$$u^* = 0 \; , \qquad v^* = 0 \; ; \tag{11}$$

$$u^* = \frac{2\pi^2}{n+8}\epsilon \; , \qquad v^* = 0 \; ; \tag{12}$$

$$u^* = 0 \; , \qquad v^* = \frac{2\pi^2}{n}\epsilon \; ; \tag{13}$$

$$u^* = \frac{2\pi^2}{n+8}\epsilon \; , \qquad v^* = \frac{2\pi^2(4-n)}{n(n+8)}\epsilon \; . \tag{14}$$

Linearizing the recursion relations in the neighborhoods of the fixed points we obtain the critical exponents ϕ_u, ϕ_v, and ν^{-1} of the fields u, v, and r, respectively. The results are shown in Table I. Instead of ν^{-1} we give the result for $\alpha = 2 - d\nu$. The exponent η is determined from the q-dependent part of Eq. (8) and is zero to first order in ϵ.

Three statements can be made about the exponents which are valid to all orders in ϵ. First, the exponent η (and also δ and ϕ_u) are unaffected by the presence of the field v. This follows from the diagrammatic expansion of the spin-spin correlation function $\langle S_i(\vec{k}) S_i(-\vec{k})\rangle$ and the fact that dashed lines cannot carry nonzero momentum and cannot be edges of closed loops. The only way the interaction v can be present in a diagram is in the

TABLE I. Fixed points and exponents to first order in ϵ.

Fixed point	ϕ_u	$\phi_v=\alpha/\nu$	α	η
Eq. (11)	ϵ	ϵ	$\frac{1}{2}\epsilon$	0
Eq. (12)	$-\epsilon+O(\epsilon^2)$	$\frac{4-n}{n+8}\epsilon+O(\epsilon^2)$	$\frac{4-n}{2(n+8)}\epsilon+O(\epsilon^2)$	$0+O(\epsilon^2)$
Eq. (13)	ϵ	$-\epsilon+O(\epsilon^2)$	$-\frac{\epsilon}{2}+O(\epsilon^2)$	0
Eq. (14)	$-\epsilon+O(\epsilon^2)$	$\frac{n-4}{n+8}\epsilon+O(\epsilon^2)$	$\frac{n-4}{2(n+8)}\epsilon+O(\epsilon^2)$	$0+O(\epsilon^2)$

form of a branch of a tree growing on spin lines. Such decorations of diagrams cause a shift of the critical temperature but do not change the momentum dependence of the correlation function.

The second comment is about a relation between the values of the exponent $2-\alpha$ (and also ν and γ) at fixed points (12) and (14). Let α_H and α be the values of α at these fixed points, respectively. The calculation to the first order in ϵ is consistent with the relation

$$2-\alpha=(2-\alpha_H)/(1-\alpha_H) \ . \tag{15}$$

This is reminiscent of, but different from, the renormalization of exponents by hidden variables studied by Fisher.[9] In Fisher's theory the renormalization is a consequence of a constraint imposed on the system, while Eq. (15) describes the relation between two sets of exponents of an unconstrained system. Now we give an argument for the validity of Eq. (15) in general. The last term in the Hamiltonian (5) is a coupling between energy densities of infinite range and thus can be treated by a mean-field-theory assumption. Put another way, the theory has no graphs with loops containing dashed lines. A theory which has only trees is a mean-field theory. These considerations suggest that we substitute for the last term in (5) the expression

$$v\epsilon(r,u,v)\sum_i \int S_i^2(x)\,d^dx \ , \tag{16}$$

where $\epsilon(r,u,v)$ is the average energy density. The Hamiltonian is now formally identical to one of a rigid Heisenberg model:

$$\int d^dx\left[\tfrac{1}{2}\tilde{r}\sum_i S_i^2(\vec{x})+\frac{1}{2}\sum_{i,\mu}\left(\frac{\partial S_i}{\partial x_\mu}\right)^2+u\left(\sum_i S_i^2\right)^2\right] ,$$

where

$$\tilde{r}=r+2v\epsilon(r,u,v) \ .$$

Let $r_c(u,v)$ and $\tilde{r}_c(u,v)$ denote the critical-point values of r and $\tilde{r}$. By a generalization of Wilson's theorem[10] it is possible to choose values u_0 and v_0 of the fields u and v such that the perturbation expansions for the renormalized coupling constant u_R and for the variable $\tilde{r}-\tilde{r}_c$ exponentiate to the expected scaling behavior:

$$u_R\approx \text{const}\,(r-r_c)^{\gamma(\epsilon-2\eta)/(2-\eta)} \ , \tag{17}$$

$$\tilde{r}-\tilde{r}_c\approx \text{const}\,(r-r_c)^{1-\alpha} \ . \tag{18}$$

The singular part of the free energy F_{sing} scales with the variable $\tilde{r}-\tilde{r}_c$ with the rigid Heisenberg exponent $2-\alpha_H$: $F_{\text{sing}}\sim(\tilde{r}-\tilde{r}_c)^{2-\alpha_H}\sim(r-r_c)^{(1-\alpha)(2-\alpha_H)}\sim(r-r_c)^{2-\alpha}$. Thus we have $2-\alpha=(1-\alpha)(2-\alpha_H)$, which implies (15).

Finally, it can be shown that $\phi_v=\alpha\nu^{-1}$. This follows from counting dimensions in the last term in (5), using the dimension of energy density $(1-\alpha)\nu^{-1}$ (with respect to inverse length) and the scaling law $d\nu=2-\alpha$. The naive counting of dimensions is permitted here because the theory has a structure of a mean-field theory with respect to the field v and the operator $[\int S_i^2(x)\,d^dx]^2$ does not have an anomalous dimension of its own.

III. CRITICAL BEHAVIOR OF COMPRESSIBLE ISING AND HEISENBERG MAGNETS

At this stage we want to determine which of the fixed points (11)–(14) gives the correct description of the critical behavior of a compressible magnet. The cases $n=1$ (Ising model) and $n=2$ or 3 (XY or Heisenberg model) will be discussed separately.

Consider $n=1$ first. The degree of instability of a fixed point is given by the number of fields which have positive exponents. All the fixed points are unstable to magnetic field and deviations from the critical temperature $r-r_c$. Table I tells us that fixed point (11) is also unstable to u and v. Fixed points (12) and (13) have only one additional degree of instability with respect to v and u, respectively. The remaining fixed point is the most stable one. However, this fixed point cannot be approached starting from physically admissible values of the fields. Namely, v must be negative [see Eq. (7)]. To approach fixed point (14) v would have to pass through zero, but that cannot happen. To see this, write Eq. (10) in the differential form ($b-1$ is infinitesimally small):

$$\frac{dv}{db}=v\left(\epsilon-\frac{n+2}{\pi^2}u-\frac{n}{2\pi^2}v\right) \ . \tag{19}$$

The rate of change of v goes to zero as v approaches zero. The physical reason for such behavior is that the shear modulus cannot be negative. For the same reason we discard fixed point (13) and are left with only two possibilities, (11) and (12), which are just the two fixed points of an incompressible Ising model. The degrees of instability are higher by one so that we have a fourth-order and a tricritical point. The relevant field v has the critical value equal to zero for any choice of u (and higher spin interactions) but it cannot be manipulated to this value, since μ cannot be zero and, strictly speaking, the compressible Ising system does not have a critical point.

Some systems, such as β-brass[11] or FeF_2,[12] behave as if the critical point existed. The reason for this is well known. The exponent of v is small, $-\alpha$, with respect to temperature, so that if the value of v is small it will remain small over a wide range of temperatures (stiff lattice and weak spin-lattice coupling are favorable) and the first-order transition takes place so close to T_c of the rigid system that it is unobservable. Baker and Essam[4] discuss β-brass in great detail.

Things are different for an isotropic magnet ($n=3$). It is known that α is negative for the Heisenberg model.[13] In ϵ expansion the first order predicts positive α, but the sign switches in the second and third orders for $\epsilon = 1$.[10,14] The most stable fixed point is (12) and it is accessible. Thus the isotropic compressible magnet has the same exponents as the rigid one. However, there is a difference in the corrections to scaling[2] because v is less irrelevant than u, which provides the leading correction for the rigid model. For example, the magnetic susceptibility is given by an expansion of the form

$$\chi = A t^{-\gamma}(1 + B t^{-\alpha} + \cdots) , \qquad (20)$$

where $t = \text{const}\,(r - r_c)$ is the reduced temperature, A and B are constants, and the dots stand for terms which vanish faster than $t^{-\alpha}$ as $t \to 0$.

The above conclusions extend also to the case $n=2$ (XY model) since it appears that α is negative in this case also.[13]

A word of caution must be added. Magnets with strictly spherical symmetry do not exist and the question arises about the stability of the fixed points with respect to crystal-field perturbations.[15,16] This is a difficult problem to solve by ϵ expansion because the answer fluctuates with increasing amplitude with the order of ϵ. The Heisenberg fixed point for $n=3$ and $\epsilon = 1$ is stable to first and third orders but is unstable in the second order.

Note added in manuscript. After this paper was completed the author learned about the work of F. Wegner on the same subject (to be published in J. Phys. C). The two papers used different lines of reasoning but the final results coincide. Dr. Wegner pointed out that Eq. (3) does not represent the most general deformation of a body with free surfaces. Indeed, the first term of expression (3) describes only such displacements which leave the surfaces planar. "Warping" deformations are not included. However, it is shown in Wegner's paper that these additional degrees of freedom do not change the critical behavior.

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