Almost Second Order Phase Transitions

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We investigate models which have more than one coupling constant and which have no (codimension one) fixed point in the renormalization group flow in an $\epsilon = 4 - d$ expansion. We show that the pseudocritical behavior of these systems is dominated by a minimum in the flow. By using the local potential approximation of the renormalization group, the properties of such minima are described. If a minimum is "good enough," it can fake a fixed point, but there are corrections to the relation between the exponents. Finally, we show that similar results hold in an ϵ expansion.

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In this Letter, we will study models that do not have a fixed point in the renormalization group (RG) flow in an $\epsilon = 4 - d$ expansion. The first class of models arises from the study of the long distance properties of frustrated antiferromagnets, or of the Stiefel nonlinear sigma model $V_{n,p} = O(n)/O(n-p)$ [1,2]. It can be viewed as a straightforward generalization of the Heisenberg model. The field φ is a real $n \times p$ matrix and the Hamiltonian is $O(n) \times O(p)$ invariant,

$$H = \int d^{d}x \operatorname{Tr} \nabla \varphi^{\dagger} \nabla \varphi + m \operatorname{Tr} \varphi^{\dagger} \varphi + \lambda_{1} \operatorname{Tr} (\varphi^{\dagger} \varphi)^{2} + \lambda_{2} (\operatorname{Tr} \varphi^{\dagger} \varphi)^{2}.$$
(1)

The main difference from the usual Heisenberg model is the appearance of a second quartic invariant (we assume $p \ge 2$). For p=2, the two columns of the matrix φ can be combined into a single complex *n*-component vector, and this model has been used to describe some superconductors, frustrated Josephson junction arrays, and superfluid helium 3. The second class of models arises from the study of phase transitions for superconductors, smectic liquid crystals, or electrodynamics. The fields are an *n*-component complex vector φ and a scalar gauge field A such that the Hamiltonian is globally U(*n*) invariant and locally U(1) invariant,

$$H = \int d^d x \left| (\nabla - ieA)\varphi \right|^2 + |dA|^2 + \mu |\varphi|^2 + \lambda |\varphi|^4.$$
 (2)

The important common feature with the model (1) is the presence of two coupling constants λ and e which have the same dimension $[\lambda] = [e] = 4 - d$.

Soon after the advent of the RG, the flow for these models was computed by using the $\epsilon = 4 - d$ expansion [see [1] for (1) and [3] for (2)]. Because there are two coupling constants, four fixed points can exist at one loop order. Two fixed points are always present. One is the trivial Gaussian fixed point (of codimension 3) and one describes a system with a different symmetry $[\lambda_1=0$ for (1) and e=0 for (2)] and is of codimension 2. Because we are interested in a phase transition, that is, in a fixed point of codimension one, we want to focus on the two other possible fixed points. The trouble is that they can or cannot be present depending on the value of *n*. If *n* is large enough $n > n_c$, with $n_c \approx 20p$ for (1) and $n_c \approx 183$ for (2), there is a pair of fixed points and one of them is the desired fixed point with codimension one. If n is smaller than n_c , these two solutions move into unphysical complex values. The introduction of higher order terms in the ϵ expansion will not change the situation for ϵ small, although it can for $\epsilon = 1$. For the experimental applications, we are interested precisely in this small n domain n = 1, 2, or 3. In this case, the flow runs away to infinity, and the usual conclusion is a "fluctuation induced first order" phase transition.

We feel uncomfortable with this conclusion for several reasons. First, it is based on a negative result (the absence of a fixed point in a perturbative expansion), but it does not show that, indeed, the system undergoes a first order phase transition below d=4 (however, see [3]). Second, we have the results of the Monte Carlo simulations in three dimensions. They indicate generically second order phase transitions (see [2] for the Stiefel model). Finally, on the experimental side, some of the systems which should fall in those universality classes exhibit first order transitions. Yet, there is also a whole body of experiments which exhibit continuous transitions.

The key observation of this work is the following: Even if the flow has no fixed point, it may have a minimum (i.e., a slow point), and if the minimum is "deep enough" it can mimic a fixed point for practical purposes. For example, the correlation length becomes very large, although not strictly diverging. The system behaves almost as if it had a second order phase transition.

In order to turn this idea into a quantitative theory, we need a norm for the flow and search for the points where this norm is minimum. A metric in the tangent space to the parameter space of the model should be introduced in order to define this norm. As a first step, we are working with the local potential approximation (LPA) of the RG. In this framework, the RG flow is given by a differential equation. From the differential equation, we inherit a natural mathematical structure, and in particular the necessary metric. We can then define a minimum in the flow and investigate the properties of the system in the neighborhood of the minimum. As a second step, we are carrying the structure built in the LPA into the perturba-

0031-9007/93/71(15)/2421(4)\$06.00 © 1993 The American Physical Society tive computation of the β functions in an ϵ expansion.

In the LPA, the RG is reduced to a semilinear partial differential equation, providing us with a natural mathematical structure. This approximation has been derived by several authors [4] and is discussed in [5]. It is similar to the hierarchical models in the sense that it involves only a potential $v(\varphi)$ and that $\eta \equiv 0$. For a model with *n* fields φ_i , $i = 1, \ldots, n$, $\partial_i = \partial/\partial \varphi_i$, the local potential approximation of the RG is given by

$$\mu(\varphi_i,t) = \partial_i^2 \mu - \frac{d-2}{2} \varphi_i \partial_i \mu + d\mu \ln \mu , \qquad (3)$$

with $\mu \ge 0$ and where $\mu(\varphi_i, t) = \exp[-v(\varphi_i, t)]$ is the density corresponding to the potential v, d is the space dimensionality, the "time" t corresponds to the cutoff $\Lambda = \Lambda_0 \exp(-t)$, and the time derivative is denoted by an overdot. We make no assumption about the symmetries of μ with respect to φ_i . Let us call Ω the space of μ ; then $\mu(\mu)$ is a mapping from Ω to the corresponding tangent space $T\Omega$. We define the operator L_{μ} , mapping $T\Omega$ to itself, by

$$L_{\mu} := \partial \dot{\mu} / \partial \mu = \partial_i^2 - \frac{d-2}{2} \varphi_i \partial_i + d(1 + \ln \mu).$$
 (4)

This operator is essentially self-adjoint on the space $L^{2}(\mathbb{R}^{n}, g(\varphi)d^{n}\varphi)$ with the measure given by $g(\varphi)$ $=\exp[-(d-2)/4\varphi^2]$. With respect to the scalar product in $T\Omega$ defined by $\langle \psi | \phi \rangle = \int d^n \varphi \psi(\varphi) g(\varphi) \phi(\varphi)$, L possesses real eigenvalues y_k and orthonormal eigenvectors ψ_k . A fixed point μ^* of the RG flow satisfies $\partial_t \mu^* = 0$, and the linearized flow around μ^* is given by L_{μ^*} . $\partial_t \delta \mu = L_{\mu^*} \delta \mu$. Therefore the eigenvalues of L_{μ^*} correspond to the critical exponents of the RG at the fixed point μ^* . The scalar product in $T\Omega$ induces the norm $\|\psi\| = \langle \psi | \psi \rangle^{1/2}$. As motivated above, we are interested in a more general condition where the density μ^* corresponds to a minimum of the flow, that is, when $\|\dot{\mu}\|$ is minimum. These densities are the solutions of the equation $\partial \|\mu\|^2 / \partial \mu(\varphi')|_{\mu=\mu^*} = 0$. By computing the derivative and inserting the definition of L, we get the equation for μ*****:

$$\frac{1}{2} \frac{\partial \|\dot{\mu}\|^2}{\partial \mu(\varphi')} \bigg|_{\mu^*} = \int d\varphi \,\dot{\mu}(\varphi) g(\varphi) L_{\mu}(\varphi,\varphi') \bigg|_{\mu^*} = 0.$$
 (5)

This equation has the solution $\dot{\mu}^* = 0$, but we are interested here in the solution corresponding to $\dot{\mu}^* \neq 0$. The flow can be expanded on the base $\psi, \dot{\mu} = \sum_k \beta_k \psi_k$, and by hypothesis, some of the coefficients β_k are different from zero. By projecting Eq. (5) on ψ_j , we obtain $\frac{1}{2} \int d\varphi' \times \partial \|\dot{\mu}\|^2 / \partial \mu(\varphi') \psi_j(\varphi') = \beta_j y_j = 0$. Therefore, at a minimum of the flow, some of the eigenvalues of L_{μ} have to be zero. For the sake of simplicity, let us assume that the minimum behaves in a similar way to a fixed point corresponding to a second order phase transition; that is, it possesses only one relevant direction. In this case, the spectrum of L_{μ^*} has the structure

$$y_0 = d > y_1 = 1/v > y_2 = 0 > y_3 > \cdots$$
 (6)

with the corresponding density and flow

$$\mu^{*} = \alpha_{0}\psi_{0} + \alpha_{2}\psi_{2}, \qquad (7)$$

$$\mu^{*} = -d\alpha_{2}\psi_{2}, \quad \|\mu^{*}\| = d|\alpha_{2}|.$$

The first eigenvalue of L is equal to d since μ^* is positive. [The first eigenvector of an operator is of a given sign, let us say positive; by orthogonality, the next eigenvectors have no definite sign. In order to ensure $\mu^* \ge 0$, we must have $\alpha_0 > 0$. Because of Eq. (3) and because by hypothesis $y_1 > 0$, we obtain $y_0 = d$.] This first eigenvalue corresponds to a multiplication of μ by a constant, or to an additive constant on the potential. The corresponding eigenvalue is $y_0 = d$. This direction is therefore trivial because it does not enter into the thermodynamics of the system and it will be omitted below.

We can linearize the flow around the minimum μ^* by taking $\mu = \mu^* + \delta \mu$ with $\delta \mu = \sum_k \delta \alpha_k \psi_k$ and we obtain the flow for the coefficients:

$$k \neq 2, \quad \delta \alpha_k(t) = \delta \alpha_k(0) \exp(y_k t) ,$$

$$k = 2, \quad \delta \alpha_2(t) = -d\alpha_2 t + \delta \alpha_2(0) .$$
(8)

As usual, perturbations increase (decrease) exponentially along the relevant (irrelevant) directions corresponding to k=1 ($k \ge 3$). In the direction k=2, the flow has constant speed and the perturbations from the minimum are kept constant. The perturbations from the minimum are functions of the temperature T. As usual, we take the perturbation along the direction k=1 to be proportional to the reduced temperature $\delta \alpha_1(0) = C_\tau \tau$, $\tau = (T - T_c)/T_c$. In principle, $\delta \alpha_2(0)$ is also a function of T, but we assume that this dependence is regular enough and can be neglected.

Starting in the critical region, that is, close to the minimum, the "time" t needed to flow outside the critical domain measures the number of length scales that are integrated out and this is basically the correlation length. Neglecting the irrelevant directions, the time t necessary to flow at a distance c (c - 1) of the minimum μ^* is given by $c^2 = \|\mu(t) - \mu^*\|^2 = c_t^2 \tau^2 \exp(2y_1 t) + [d\alpha_2(0)t]^2$. The corresponding correlation length is given by $\Lambda_0 \xi = \exp(t)$. By eliminating t, we obtain the equation for the correlation length:

$$c_{\tau}^{2} \tau^{2} (\Lambda_{0} \xi)^{2/\nu} + \|\dot{\mu}\|^{2} \ln^{2} (\Lambda_{0} \xi) = c^{2}.$$
(9)

In the domain of temperatures where the term containing $\|\dot{\mu}\|$ is small, we obtain the correlation length as a function of the reduced temperature:

$$\Lambda_0 \xi = \left(\frac{c}{c_\tau |\tau|}\right)^{\nu} \left(1 - \frac{\nu}{2}\gamma^2 + \cdots\right), \quad \gamma \ll 1 , \qquad (10)$$

with $\gamma(\tau) = - \|\dot{\mu}\| v/c \ln(c_{\tau} |\tau|/c)$. This form is valid in the domain of reduced temperatures:

$$\exp[-c/(\|\dot{\mu}\|_{V})] \ll c_{\tau} |\tau|/c \ll 1.$$
(11)

Therefore, we see that the minimum of the flow will

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behave almost like a fixed point for a broad domain of reduced temperature around the transition. The quantity $\|\mu\|v/c$ measures the "quality" of the minimum. The smaller this number, the better the minimum will fake a true fixed point. It is only for reduced temperatures very close to zero, $c_{\tau} |\tau| / c \ll \exp(-c/||\dot{\mu}||v)$, corresponding to very large correlation lengths $\Lambda_0 \xi \gg \exp(c/\|\mu\|)$, that we will observe a significant deviation from the usual power law. In this case, since the flow is going neither to the high nor to the low temperature fixed point, the behavior of the system is given by the flow downstream of the minimum. We may ultimately reach another fixed point, or have a first order phase transition. Nevertheless, if the quality of the minimum is good enough, this domain may be out of reach, experimentally or by numerical computations. Therefore, although the system possesses no fixed point, it behaves practically as if it had one.

The constant c is fixed by the condition that, for the density μ , the corresponding correlation length is of order 1 and c may have different values in the low or high temperature phase. As the RG corresponds to a relative change of length scale, we have no information about absolute length and therefore we are not able to compute c. Besides, the metric g is defined up to an arbitrary multiplicative constant g_0 so that $c = \|\mu(t) - \mu^*\|$ will depend on the choice of g_0 . This constant also sets a scale for c_{τ} , but the quantities c_{τ}/c and $\|\mu\|/c$ are independent of the particular choice of g_0 .

The flow around a minimum shows, nevertheless, an important difference from the flow around a fixed point. For the sake of simplicity, let us neglect the irrelevant directions. Starting close to a fixed point, the flow leaves the critical region along the direction ψ_1 . In the case of a minimum, the flow exits the critical region in the plane span by ψ_1 and ψ_2 . This difference has consequences on the scaling relations. The minimum can be viewed as a very dispersive medium for the RG trajectories. Let us denote by θ the angle of exit from the critical region with $\sin\theta = c_{\tau} \tau (\Lambda_0 \xi)^{1/\nu} / c$ and we are interested in the region $\theta \simeq \pm \pi/2$. We obtain at lowest order $\theta(\tau) \simeq \pm [\pi/2]$ $-\gamma(\tau)$]. Let us consider now the free energy (per unit volume) f. It satisfies the scaling law $f(\mu)$ $=(\Lambda_0 L)^{-d} f(\mu')$ where μ' is computed at scale $L = \Lambda^{-1}$. Starting in the critical region $\mu = \mu^* + \delta \mu$, taking $L = \xi$, and taking τ such that $\theta \simeq \pi/2$, we obtain $f(\tau)$ = $(\Lambda_0 \xi)^{-d} \tilde{f}_{\pm}(\gamma)$ where \tilde{f}_{\pm} is a regular function of γ , the indices \pm referring to the high and low temperature phases. By expanding \tilde{f} into a power series around zero $\tilde{f}(\gamma) = \tilde{f}(0)[1 + f_1\gamma + O(\gamma^2)]$, at lowest order we obtain $f(\tau) \simeq (\Lambda_0 \xi)^{-d + f_1 \parallel \mu \parallel / c}$. The specific heat is given by the second derivative of f. When defining the exponent α by the usual scaling law $C_v \simeq \tau^{-\alpha}$, we obtain the relation between the exponents

$$\alpha = 2 - \nu (d - f_1 \| \mu \| / c) , \qquad (12)$$

where f_1 can differ whether in the high or low temperature phase. We can also introduce an external magnetic

field which scales with the exponent $d - d_{\varphi} = (d + 2)$ $-\eta$)/2. Proceeding along similar lines, we obtain the relations for the exponents β for the magnetization β $= v(d-2+\eta-2m_1 \|\dot{\mu}\|/c)/2$ and γ for the susceptibility $\gamma = v(2 - \eta + \chi_1 \| \dot{\mu} \| / c)$. The coefficients m_1 and χ_1 come from the Taylor expansion around $\theta = \pm \pi/2$ of the scaling function for the magnetization and susceptibility, respectively, and can differ whether in the high or low temperature phase. The coefficients f_1 , m_1 , ξ_1 , and $\|\mu\|$ are universal constants because they do not depend on the bare model but only on the critical point and its neighborhood. Therefore, the minimum manifests itself by universal corrections to the usual relation between the critical exponents. Let us add that these corrections may be difficult to observe experimentally because they are of the same order as the logarithmic scale of temperature where we can expect scaling.

The presence of a minimum also has consequences on the finite size scaling relation. Let us consider for example the free energy f with the above scaling law. Take the scale L as the finite size of the sample, and eliminate τ in the right-hand side for the (infinite volume) correlation length $\xi(\tau)$. We obtain the relation $f(\tau,L)$ $=L^{-d}\tilde{f}[L/\xi, (\|\mu\||/c)\ln(\Lambda_0 L)]$. Thus, the scaling function \tilde{f} does not depend only on L/ξ but still on $\ln L$ and, therefore, there is no finite size scaling.

The corrections to the relations between the exponents as well as the breakdown of the finite size scaling may be at the origin of the difficulties in the analysis of the numerical simulations for frustrated antiferromagnet systems [6,7], pyrochlore antiferromagnets [8], or the Stiefel models $V_{2,2}$, $V_{3,2}$, and $V_{3,3}$ [2]. In the latest, the poor finite size scaling of the system has already been observed, as well as a negative η exponent if the relation $\gamma = \nu(2 - \eta)$ is assumed valid. Besides, equation (3) can be solved numerically for model (1) with two n-component vectors [9]. In three dimensions, the models with n > 4.8 have a fixed point and a minimum for n < 4.8. This is in agreement with the Monte Carlo simulations of the system $V_{n,2}$ [2] and roughly in agreement with the $4-\epsilon$ expansion at second order [10]. The exponents v are v=0.69 (n=5), v=0.63 (n=4), and v=0.63(n = 3).

Let us now turn to the $\epsilon = 4 - d$ expansion. The usual description of the RG is a complex recipe involving loop expansion, Feynman diagrams, regularization, (minimal) subtraction of divergences, etc. In this recipe, we do not have the natural mathematical structure present in the LPA, and in particular we do not have a metric in the tangent space. Nevertheless, let us try to carry on the main idea of the LPA. Similarly to the preceding section, let us call Ω the space of parameters of the model, with dim $(\Omega) = N$, and μ a point in this space. For example, for the model $V_{n,p}$ let us take $\mu = \{\mu^1 = \lambda_1, \mu^2 = \lambda_2\}, N=2$. The beta functions define a vector field in $T\Omega: -\beta_{\mu} = \mu = \mu(\mu)$. Similarly, we define the operator L_{μ} as $L_{\mu}{}^{\alpha}{}_{\beta} = \partial \mu^{\alpha}/\partial \mu^{\beta}$, $\alpha, \beta = 1, \ldots, N$ with its eigenvalues and

eigenvectors $L_{\mu}\psi_k = y_k\psi_k$. We want to introduce a metric in $T\Omega$, with $\langle \varphi | \psi \rangle = \varphi^a g_{a\beta} \psi^\beta$ for $\varphi, \psi \in T\Omega$, such that we can define the norm of $\dot{\mu}$. What are the natural constraints on g? We want the eigenvectors ψ_k of L_{μ} to form an orthogonal basis. This is equivalent to the condition $(gL_{\mu})^{\dagger} = gL_{\mu}$ and this gives N(N-1)/2 equations fixing basically the off-diagonal terms of g. In order to satisfy these equations, g has to depend on μ (this is not the case in the LPA). Because the eigenvectors are defined up to multiplicative constants, there are no normality constraints; i.e., the equations $\langle \psi_k | \psi_k \rangle = 1$ are meaningless. Another natural set of conditions for g is $\mu^{\alpha} \partial_{\gamma} g_{\alpha\beta} \mu^{\beta} = 0$ for $\gamma = 1, ..., N$ and this gives N more equations, so that g is completely specified (up to a multiplicative constant). Because g depends on μ , this leads to partial differential equations for the diagonal elements of g. This approach is therefore more complicated than with the LPA. Having such a metric, we can now search for a minimum μ^* in the flow $\frac{1}{2} \partial_{\alpha} \langle \dot{\mu} | \dot{\mu} \rangle = g_{\alpha\beta} L^{\beta} {}_{\gamma} \dot{\mu}^{\gamma} = 0.$ By assuming that such a metric exists, we can take a short cut in order to define the minima. As for the LPA, we can expand the vectors μ and $\dot{\mu}$ in the base ψ_k . At a minimum μ^* (with one relevant direction), we have

$$y_2 = 0$$
, (13)

 $\dot{\mu}$ is parallel to ψ_2 or $L_{\mu^*}\dot{\mu} = 0$,

and we take these two equations as a definition of μ^* . These equations do not contain the metric and are therefore much simpler. We can add the remark that we can weaken the second condition on g by requiring it to be true only at μ^* and not everywhere in Ω . At this point, we have the necessary mathematical structure and we can parallel the computations of the preceding section. The same general behavior of a minimum will hold. Moreover, in an $\epsilon = 4 - d$ expansion, a minimum will be of order ϵ , and therefore $\|\mu\| \sim \epsilon$. We now see how a system can continuously change its behavior from mean field. There is a region of temperature of order $\tau - \exp(-1/\epsilon)$ which is not controlled by the minima and in which the thermodynamic singularity differs.

Let us add some general remarks, not necessarily related to the particular scheme used for the RG. The presence of a minimum in the flow can be viewed as the consequence of the two complex solutions for the zero of the flow. Even if these complex solutions are unphysical, they will dominate the behavior of the system through the minimum. These fixed points and the corresponding minimum are bifurcating from the trivial solution at d=4. Therefore, in principle we can compute the properties of the minimum in a systematic ϵ expansion (or in a λ expansion at fixed dimensions). Eventually for finite ϵ , the two complex zero and the minimum will meet and produce a pair of real fixed points. But there is no need to do a simultaneous analytic continuation in the *n* space [10] to follow the real fixed point; we can work with a fixed model. The LPA indicates that the three-dimensional Stiefel models with p=2 and n=3 or n=4 are indeed governed by a minimum [9], and this seems in agreement with Monte Carlo simulations [2]. On the other hand, if a system has a pair of fixed points close to collapsing, the second eigenvalue of the tangent operator should be close to zero. This means that important corrections to the leading scaling are to be expected, a behavior close to that of a minimum. Besides, there is the possibility of several fixed points and/or minima, with their respective basins of attraction.

The properties of a minimum may appear similar to a crossover phenomena. In this case, the system behavior crosses over from a codimension two fixed point toward a codimension one fixed point. But a minimum is similar to a codimension one fixed point in the sense that only one parameter should be adjusted in order to be a pseudocriticality. The analogy holds in the sense that in one direction, the minimum leaks toward a fixed point. But the rate of the flow is very different, exponential for a crossover whereas linear for a minimum. Therefore the analogy is to be taken only in the very broad sense that different domains of temperatures are governed by two different domains of the RG flow.

To conclude, we have shown that systems which have no fixed points in the RG flow may have an almost second order transition. The system will "mimic" a transition with well-defined critical exponents. Experimentally, such a behavior manifests itself by corrections to the relation between the exponents, and, if accessible, by crossoverlike phenomena. In Monte Carlo simulations, besides the previous effects, finite size scaling does not hold.

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