Influence of rare regions on magnetic quantum phase transitions

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(August 12, 2018)

The effects of quenched disorder on the critical properties of itinerant quantum magnets are considered. Particular attention is paid to locally ordered rare regions that are formed in the presence of quenched disorder even when the bulk system is still in the nonmagnetic phase. It is shown that these local moments or instantons destroy the previously found critical fixed point in the case of antiferromagnets. In the case of itinerant ferromagnets, the critical behavior is unaffected by the rare regions due to an effective long-range interaction between the order parameter fluctuations.

Rare regions and their influence on observables is an important, if intricate, aspect of systems with quenched disorder. An effect that has been known for a long time is the formation of a Griffiths region [1]. To explain this, let us consider a ferromagnet for definiteness. Disorder will decrease the critical temperature from its clean value, T_c^0, to a value $T_c < T_c^0$ in the disordered system. In the temperature region $T_c < T < T_c^0$ the system does not display global order, but one will find regions that are devoid of any impurities and hence show local magnetic order. The probability of finding such a 'rare region' in general decreases exponentially with its size. The resulting magnetization fluctuations have very slow dynamics. They are often called 'local moments' or 'instantons', and they lead to a nonanalytic free energy for all temperatures below T_c^0, even though no long-range order develops until the temperature reaches T_c. For generic classical systems this is a weak effect, the singularity being only an essential one. An important exception is the model studied by McCoy and Wu [2], which is a two-dimensional (2-d) Ising model with random bonds in one direction, but identical bonds in the second direction. The infinite correlation of the disorder in this model leads to much stronger effects, with the average magnetic susceptibility diverging in a finite-width temperature region above T_c. The transition at T_c is nevertheless sharp. The divergence of the average susceptibility for $T > T_c$ is caused by atypical fluctuations in the susceptibility distribution, and the averaged order parameter becomes nonzero only for $T < T_c$. The temperature region $T_c < T < T_c^0$ is known as a Griffiths region. Little is known about the influence of rare regions on the critical behavior at T_c, and in the conventional theory of the critical behavior of disordered magnets [3] the rare regions are neglected.

Recent work [4] on a random-T_c classical Ising model has suggested that the effects of the rare regions go beyond the formation of a Griffiths region, even in this simple model where the conventional theory [3] predicts standard power-law critical behavior. These authors showed that the conventional theory is unstable with respect to perturbations that break the replica symmetry. By approximately taking into account the rare regions, they found a new term in the action that actually induces such perturbations. In some systems replica symmetry breaking is believed to be associated with activated, i.e. non-power law, critical behavior. Although no final conclusion about the fate of the transition could be reached, Ref. [4] thus raised the possibility that the random-T_c classical Ising model shows activated critical behavior as a result of rare-region effects, as is believed to be the case for the random-field classical Ising model [5].

The problem of rare regions is even less well investigated for the case of quantum phase transitions, i.e. transitions that occur at $T = 0$ as a function of some non-thermal control parameter [6]. An important exception to this are certain 1-d systems. Fisher [7] has investigated quantum Ising spin chains in a transverse random field, which is closely related to the classical 2-d McCoy-Wu model (with time playing the role of the dimension along which the disorder is correlated). He found activated critical behavior due to rare regions, which has been confirmed by numerical simulations [8]. Recent simulations [9] suggest that this type of behavior may not be restricted to 1-d systems, raising the possibility that exotic critical behavior dominated by rare regions may be generic in quenched disordered quantum systems.

Apart from their relevance for disordered magnets and their critical properties, rare regions are believed to be a crucial ingredient for understanding other systems with quenched disorder. For instance, it has been proposed that a complete understanding of the properties of doped semiconductors, and of the metal-insulator transitions that are observed in such systems as a function of doping, requires the consideration of local moments [10–12].

In this Letter we study this important problem analytically for quantum phase transitions in $d > 1$. We concentrate on magnetic transitions, and contrast the cases of itinerant ferromagnets (FMs) and antiferromagnets (AFMs), respectively. We find that for the latter, the rare regions destroy the critical fixed point (FP) found in a previous study [13], and thus have a profound effect on the critical behavior. In contrast, for itinerant FMs we find that, for certain realizations of the disorder, the previously found critical behavior [14] is stable with respect to rare regions, due to an effective long-range interaction between the spin fluctuations. In addition, we find that the ultimate effects of the rare regions depend on how the disorder is realized in a particular system. Therefore, no generally valid conclusions are possible, and the effects of rare regions must be studied carefully and separately for each system under consideration.

Let us first consider the case of itinerant quantum antiferromagnets. Our starting point is the same as in Ref. [13], namely Hertz's action, which is a ϕ^4-theory for a p-component order parameter field $\boldsymbol{\phi}$ whose expectation value is proportional to the staggered magnetization. The action reads

$$S = \int dx\, dy\ \boldsymbol{\phi}(x)\, \Gamma(x,y)\, \boldsymbol{\phi}(y) + u \int dx\ \left(\boldsymbol{\phi}(x)\cdot\boldsymbol{\phi}(x)\right)^2\ . \tag{1a}$$

Here $x \equiv (\mathbf{x},\tau)$ comprises position $\mathbf{x}$ and imaginary time τ, and $\int dx \equiv \int d\mathbf{x} \int_0^{1/T} d\tau$. We use units such that $\hbar = k_{\rm B} = 1$. $\Gamma(x,y)$ is the bare two-point vertex function, whose Fourier transform is

$$\Gamma(\mathbf{q},\omega_n) = (t + \mathbf{q}^2 + |\omega_n|)/2 \quad . \tag{1b}$$

Here t denotes the distance from the critical point, $\mathbf{q}$ is the wavevector, ω_n is a bosonic Matsubara frequency, and we measure both $\mathbf{q}$ and ω_n in suitable units.

Disorder is introduced by making t a random function of position, $t = t_0 + \delta t(\mathbf{x})$, where $\delta t(\mathbf{x})$ obeys a Gaussian distribution with zero mean and variance Δ. The standard procedure is to integrate out the 'random mass' $\delta t(\mathbf{x})$ by means of the replica trick [3], which produces a term of order $\boldsymbol{\phi}^4$ with coupling constant Δ, in addition to the ordinary quantum fluctuation term in Eq. (1a) with coupling constant u. The resulting theory does not easily allow for saddle-point solutions that are inhomogeneous in space, and to incorporate rare regions into it would be very difficult. We therefore follow a different procedure. In analogy to Ref. [4], we consider inhomogeneous saddle-point solutions of the theory for a *fixed* realization of the disorder. The inhomogeneity comes about since $\delta t(\mathbf{x})$ has 'troughs' that make $t < 0$ in some region in space, even though $t_0 > 0$. Troughs that are sufficiently deep and wide support locally nonzero saddle-point solutions. These regions we will refer to as 'islands'. Outside of the islands, the solution is exponentially small. This means that for a system with N islands, and in the case of an Ising model ($p = 1$), there will be 2^N almost degenerate saddle-point solutions that can be constructed by considering all possible distributions of the sign of the order parameter on the islands. For $p > 1$ there is a whole manifold of almost degenerate saddle points.

Let $\boldsymbol{\Phi}(\mathbf{x})$ be one of these saddle-point solutions, and let us consider fluctuations about it, $\boldsymbol{\phi}(x) = \boldsymbol{\Phi}(\mathbf{x}) + \boldsymbol{\varphi}(x)$ [15]. The different saddle points are far apart in configuration space and separated by large energy barriers. If we restrict ourselves to small fluctuations about each saddle point, we can therefore write the partition function approximately as the sum of all contributions obtained from the vicinity of each saddle point,

$$Z \approx \int D[\boldsymbol{\Phi}(\mathbf{x})]\, P[\boldsymbol{\Phi}(\mathbf{x})] \int_< D[\boldsymbol{\varphi}(x)]\, e^{-S[\boldsymbol{\Phi}(\mathbf{x})+\boldsymbol{\varphi}(x)]}, \tag{2}$$

where $P[\boldsymbol{\Phi}(\mathbf{x})]$ denotes the distribution of saddle points, and $\int_<$ indicates an integration over small fluctuations only. It is clear that this approximation takes into account effects that one would call 'non-perturbative' in a standard treatment of quenched disorder. Also, consistent with our approximations, it can be shown that the inhomogeneous saddle-point solutions lead to a lower free energy than the homogeneous saddle point $\boldsymbol{\phi}(x) \equiv 0$.

Performing the integration over the $\boldsymbol{\Phi}$ in Eq. (2) explicitly is very difficult, and the result will in general depend on the properties of the distribution function P, which in turn depend on the details of the miscroscopic disorder. However, a very basic observation simplifies our task: The $\boldsymbol{\Phi}(\mathbf{x})$ represent static randomness, and the average over this randomness is performed for the partition function. That is, we are dealing with static, annealed disorder. This is physically sensible, as the local moments are a self-generated part of the system and therefore in equilibrium with the rest of the degrees of freedom [15]. In addition, of course, there is quenched disorder due to the underlying random mass term. This we handle by means of the replica trick. If we assume that the distribution of the $\boldsymbol{\Phi}$ is short-range correlated (which will be the case for certain classes of realizations of the disorder, but not for others), we can immediately write down the effective action up to and including terms of $O(\boldsymbol{\varphi}^4)$:

$$\begin{aligned} S_{\rm eff} = \sum_\alpha &\int dx\, dy\ \boldsymbol{\varphi}^\alpha(x)\, \Gamma_0(x,y)\, \boldsymbol{\varphi}^\alpha(y) \\ &+ u \sum_\alpha \int dx\ \left(\boldsymbol{\varphi}^\alpha(x)\cdot\boldsymbol{\varphi}^\alpha(x)\right)^2 \\ &- \sum_{\alpha,\beta} (\Delta + w\,\delta_{\alpha\beta}) \int dx\, dy\, \delta(\mathbf{x}-\mathbf{y})\ \left(\boldsymbol{\varphi}^\alpha(x)\right)^2 \\ &\qquad\qquad \times \left(\boldsymbol{\varphi}^\beta(y)\right)^2 + O(\boldsymbol{\varphi}^6) \quad . \end{aligned} \tag{3}$$

Here Γ_0 is the Gaussian vertex, Eq. (1b), with $t = t_0$, Δ is the variance of the Gaussian random mass distribution, and α and β are replica indices. w is the coupling constant of the annealed disorder term. We have also derived Eq. (3) by means of a detailed technical procedure which will be reported elsewhere [16]. The technical derivation shows that w has the form $w = u^2\, v$, with v characteristic of the distribution P, and it also yields terms of $O(\boldsymbol{\varphi}^6)$ and higher. These turn out to be less relevant for the critical behavior than the quartic terms shown in Eq. (3). Notice that the annealed disorder contribution becomes indistinguishable from the usual $\boldsymbol{\varphi}^4$ or u-term in the case of a classical transition. This is the reason why the authors of Ref. [4], who studied classical magnets, considered replica symmetry breaking in order to describe nontrivial effects of the rare regions. In the quantum case we get a nontrivial effect even at the level of a replica symmetric theory, which means that the influence of rare regions on quantum transitions is stronger.

To discuss the properties of the effective action, Eq. (3), we proceed as in Ref. [13]. We consider $d = 4 - \epsilon$ space dimensions and ϵ_τ time dimensions, and control perturbation theory by means of a double expansion in ϵ and ϵ_τ [17]. Defining $\bar{w} = w\,T^{-\epsilon_\tau}$, and putting $T = 0$, we obtain the following renormalization group (RG) flow equations to one-loop order,

$$\frac{du}{dl} = (\epsilon - 2\epsilon_\tau)u - 4(p+8)u^2 + 48u\Delta \quad , \qquad \text{(4a)}$$

$$\frac{d\Delta}{dl} = \epsilon\Delta + 32\Delta^2 - 8(p+2)u\Delta + 8p\Delta\bar{w} \quad , \qquad \text{(4b)}$$

$$\frac{d\bar{w}}{dl} = (\epsilon - 2\epsilon_\tau)\bar{w} + 4p\bar{w}^2 - 8(p+2)u\bar{w} + 48\Delta\bar{w} \quad . \qquad \text{(4c)}$$

An analysis of Eqs. (4) shows that they possess eight FPs. Four of them have a vanishing FP value of $\bar{w}$, $\bar{w}^* = 0$, and have been discussed before in Ref. [13]. Of particular interest is the nontrivial critical FP $u^* = (\epsilon + \epsilon_\tau)/16(p-1)$, $\Delta^* = [(4-p)\epsilon + 4(p+2)\epsilon_\tau]/64(p-1)$, $\bar{w}^* = 0$, which on the $\bar{w} = 0$ hypersurface is stable for p smaller than some p_c. To one-loop order, and for $\epsilon = \epsilon_\tau$, $p_c = 16$. A linear stability analysis reveals that the third eigenvalue, $\lambda_{\bar{w}} = (4-p)(\epsilon + 4\epsilon_\tau)/4(p-1)$, is positive for $p < 4$. In the most interesting case $p = 3$, $\bar{w}$ is thus a relevant operator with respect to this FP, which means that the rare regions destroy the FP. It is, however, interesting to note that for $p > 4$ the FP is stable and describes power-law critical behavior. There also are four FPs with $\bar{w}^* \neq 0$. They are all unstable except for one with $\bar{w}^* = (p-4)(\epsilon + 4\epsilon_\tau)/8p(10-p)$, which is negative for $p < 4$. Since the bare value of $\bar{w}$ is positive, and the structure of the flow equations does not allow for $\bar{w}$ to change sign, this FP is unphysical. There is thus no new FP for $p < 4$, and a numerical solution of the flow equations reveals runaway flow in all of physical parameter space.

We conclude that for $p < 4$ the AFM long-range order found in Ref. [13] is unstable against effects induced by rare regions, a result that is consistent with the previous suggestion that AFM long-range order is strongly suppressed by quenched disorder [10]. However, other possibilities exist. For instance, there could be a transition to a long-range ordered state, but with activated critical behavior which manifests itself as runaway flow in a perturbative RG calculation. The viability of this latter suggestion is underscored by the fact that a calculation of the local moment contribution to the order parameter susceptibility yields $\chi_{\rm LM}(T) \sim 1/T$ [16]. This is similar to Fisher's 1-d result $\chi(T) \sim 1/T^\gamma$ with $\gamma < 1$ [7]. (Our exponent value of unity is a result of our saddle-point approximation for the local moments.) This shows that we are really describing a Griffiths region, which was shown in Ref. [7] to lead to a transition with activated critical behavior in $d = 1$. A third possibility is that a conventional critical FP exists, but cannot be described with perturbative RG methods. This possibility is consistent with the stability of conventional critical behavior against $\bar{w}$ for $p > 4$, as discussed above.

We now turn to the case of itinerant ferromagnets, which constitute an interesting contrast to the AFM case. In Ref. [14] it was shown that a description of itinerant FMs that neglects rare regions leads to an action that has the same form as Eq. (3) with $w = 0$, except that the bare two-point vertex function reads

$$\Gamma_0^{\rm FM}(\mathbf{q}, \omega_n) = \left(t_0 + |\mathbf{q}|^{d-2} + \mathbf{q}^2 + |\omega_n|/\mathbf{q}^2\right)/2 \quad , \qquad (5)$$

and that the field $\boldsymbol{\varphi}(x)$ now describes ferromagnetic fluctuations. There are two crucial, and related, differences between Eq. (5) and its AFM counterpart. The first one is the structure of the frequency dependence, which enters as $|\omega_n|/\mathbf{q}^2$ [18] and reflects the diffusive nature of the spins in a disordered environment. In Ref. [14] it was shown that the same diffusive spin dynamics leads to the $|\mathbf{q}|^{d-2}$ term, which dominates the usual gradient squared term as long as $d < 4$. In the original treatment of quantum FMs by Hertz [18], loop corrections would have been required to find this term, while the method of Ref. [14] builds it into the bare theory. Consequently, the correlations between the spin density fluctuations are effectively long-ranged, a feature that is well known to stabilize the Gaussian critical behavior [19]. Indeed, it was shown in Ref. [14] that the Gaussian critical behavior, with $\eta = 4 - d$, $\nu = 1/(d-2)$, $\gamma = 1$, and $z = d$, is stable for $2 < d < 4$. Here η, ν, and γ are the usual critical exponents, and z is the dynamical critical exponent. They can all be simply read off Eq. (5). The exponents β and δ were also determined in Ref. [14], their values in $d = 3$ are $\beta = 2$, $\delta = 3/2$. The remarkable claim of Ref. [14] was that these exponent values, which in $d = 3$ are very different from both mean-field values and classical Heisenberg values, constitute the *exact* critical behavior of itinerant quantum FMs.

An obvious question is whether this claim survives the consideration of rare regions. To answer this, we perform an analysis analogous to the one for AFMs above. A simple way to incorporate the rare regions into the action is to write the quenched disorder or Δ-term in the action as a random mass in the Gaussian vertex (i.e., to 'undo' the integrating-out of the random mass), to construct inhomogeneous saddle-point solutions and expand about them, and then to integrate over the manifold of saddle points as in the AFM case. Clearly, this leads to a w-term in the action, like in Eq. (3). We have derived the same result starting from a more microscopic formulation. We will report the details of the derivation elsewhere [16], here we mention only one important point: After Eq. (3) we mentioned that w is proportional to u^2. Since u in the FM case is wavenumber dependent and diverges in the short-wavelength limit (i.e., its bare scale dimension is negative) [14], this raises the question whether the bare value of w is finite. The answer is affirmative, since the w-term arises from field configurations that are nonzero only on islands. The u that contributes to the bare value of w therefore has to be taken at wavenumbers that are on the order of a typical inverse island size, and hence is finite. Once again it is important here that the island size distribution falls off exponentially for large sizes. We can thus treat w as a number.

Now let us perform a power counting analysis to determine the stability properties of the Gaussian FP. Assigning a length L a scale dimension $[L] = -1$, the scale dimension of the imaginary time is $[\tau] = -z = -d$. For the scale dimension of the field we find $[\boldsymbol{\varphi}(x)] = (d+2)/2$. The scale dimensions of both w and Δ then become $[w] = [\Delta] = 4 - d$, i.e. they are irrelevant with respect to the Gaussian FP for $d < 4$, and marginal in $d = 4$. Terms of higher than quartic order in $\boldsymbol{\varphi}$ that are produced by a technical derivation of the effective action [16] turn out to also be irrelevant. We thus conclude that the FM critical behavior determined previously [14] is *stable* against rare regions physics, in sharp contrast to the AFM case. The reason for this qualitative difference is the effective long-ranged interaction between the order parameter fluctuations (as expressed in Eq. (5) and in the value of the exponent η), which is sufficient to suppress all disorder fluctuations, including the ones due to rare regions. By the same arguments, the FM Gaussian FP is also stable against replica symmetry breaking.

We conclude with one additional remark. One might ask why the rare regions or local moments don't cut off the singular wavenumber dependences $|\mathbf{q}|^{d-2}$ and $|\omega_n|/\mathbf{q}^2$ in the Gaussian vertex, Eq. (5). The reason why this does not happen is that both singularities are consequences of spin diffusion, which in turn is a consequence of the spin conservation law. The rare regions ultimately derive from a spin-independent disorder potential, which clearly cannot destroy spin conservation. We note, however, that the above arguments are restricted to a tree-level analysis of our effective field theory. Although the effective theory is a sophisticated one, which at tree level contains many effects that would require loops in more standard treatments, we of course cannot exclude the possibility that loop corrections might lead to qualitatively new terms in the action. If such new terms included a RG-generated spin dependent potential, then this might change our conclusions. However, at such a level of analysis one would also have to include effects due to interactions between the rare regions, which we have mostly neglected. Such interactions are known to weaken the effects of the rare region [11], but in general it is not known by how much.

We gratefully acknowledge helpful discussions with Ferdinand Evers and John Toner. This work was supported by the NSF under grant Nos. DMR-98-70597 and DMR–96–32978, and by the DFG under grant No. SFB 393/C2.

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