Disorder-Induced Rounding of Certain Quantum Phase Transitions

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We study the influence of quenched disorder on quantum phase transitions in systems with overdamped dynamics. For Ising order-parameter symmetry disorder destroys the sharp phase transition by rounding because a static order parameter can develop on rare spatial regions. This leads to an exponential dependence of the order parameter on the coupling constant. At finite temperatures the static order on the rare regions is destroyed. This restores the phase transition and leads to a double-exponential relation between critical temperature and coupling strength. We discuss the behavior based on Lifshitz-tail arguments and illustrate the results by simulations of a model system.

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The influence of quenched disorder on phase transitions is an important problem in condensed matter physics. Initially it was suspected that disorder destroys any critical point [1]. However, it was soon found that classical continuous phase transitions generically remain sharp in the presence of weak disorder. If a clean critical fixed point (FP) fulfills the Harris criterion [2] $\nu \geq 2/d$, where ν is the correlation length exponent and d is the spatial dimensionality, weak disorder is renormalization group irrelevant. The system becomes asymptotically homogeneous at large length scales. Even if the Harris criterion is violated, the transition will generically be sharp. In this case the inhomogeneities either remain finite at all length scales, leading to a finite-disorder FP, or the relative magnitude of the disorder diverges under coarse graining corresponding to an infinite-randomness FP. A prominent example of the latter occurs in the McCoy-Wu model [3], a disordered 2D Ising model in which the disorder is perfectly correlated in one dimension. These correlations increase the effects of the disorder.

An important aspect of phase transitions in disordered systems are the Griffiths phenomena [4]. They are caused by large spatial regions that are devoid of any impurities and can be locally in the ordered phase even if the bulk system is in the disordered phase. Since these regions are of a finite size, no true static order develops. The fluctuations of these regions are very slow because they require changing the order parameter in a large volume. Griffiths [4] showed that this leads to a singular free energy. In generic classical systems this is a weak effect, since the singularity is only an essential one. An exception is the McCoy-Wu model [3]. Here, the disorder correlations lead to stronger effects, with the average susceptibility diverging in a finite region of the phase diagram.

Recently disorder effects have gained a lot of attention in the context of quantum phase transitions [5]. At these transitions order-parameter fluctuations in space *and* time have to be considered. Quenched disorder is time independent; it is thus always correlated in one of the relevant dimensions making disorder effects at quantum phase transitions generically stronger than at classical transitions. A prototypical model is the random quantum Ising ferromagnet. Its quantum phase transition in 1D [6–8] and 2D [9,10] is controlled by an infinite-randomness FP with activated rather than power-law dynamical scaling. The Griffiths singularities are enhanced, too: Several observables including the average susceptibility display power-law singularities with continuously varying exponents over a finite region of the disordered phase. Similar phenomena have also been found in quantum Ising spin glasses [11–13].

The systems in which infinite-randomness FPs and quantum Griffiths phenomena have been shown unambiguously all have undamped dynamics (a dynamical exponent $z = 1$ in the corresponding clean system). However, in itinerant electronic systems the order parameter couples to fermionic modes leading to overdamped dynamics (clean dynamical exponent $z > 1$). A prototype example is the itinerant quantum antiferromagnetic phase transition. The conventional perturbative renormalization group for this transition [14] yields a finite-disorder FP. However, by taking into account the effects of rare regions it was shown [15] that this FP is unstable, and the renormalization group flow is towards large disorder. The meaning of this runaway flow is presently not fully understood. In addition to the transition itself, quantum Griffiths phenomena in itinerant systems have also attracted much attention since they are of potential importance for a variety of heavy-fermion systems. It has been suggested [16] that overdamped systems show quantum Griffiths phenomena very similar to that of undamped systems. However, recently it has been argued [17] that for Ising symmetry the overdamping prevents the rare regions from tunneling leading to superparamagnetic rather than quantum Griffiths behavior [18].

In this Letter we reconsider the important question of disorder and rare regions at quantum phase transitions. We show that for Ising order-parameter symmetry and Landau overdamped dynamics, the sharp quantum phase transition is destroyed by rounding, because static order can develop on isolated rare regions. Our results can be summarized as follows: The relation between the order parameter m and the distance t from the clean critical point is exponential for small m. The precise form depends on the disorder distribution. For a Gaussian coupling constant distribution, m is finite for all t. Asymptotically it behaves as

$$\log(m) \sim -t^{2-d/\phi} \quad \text{for } t \to \infty. \tag{1a}$$

Here ϕ is the finite-size scaling shift exponent of the clean system. If the disorder is of a dilution type a finite order parameter starts to develop at the clean transition, i.e., for $t < 0$ [19]. For small $|t|$ it behaves as

$$\log(m) \sim -|t|^{-d/\phi} \quad \text{for } t \to 0- . \tag{1b}$$

At finite temperatures the static order on the rare regions is destroyed, and a finite interaction between them is required for long-range order. This restores a sharp phase transition. The dependence of the critical temperature on t is double exponential. For small T_c we obtain

$$\log(-a \log T_c) \sim t^{2-d/\phi} \qquad \text{Gaussian}, \tag{2a}$$

$$\log(-a \log T_c) \sim |t|^{-d/\phi} \qquad \text{dilution}. \tag{2b}$$

Moreover, in finite-size samples strong sample-to-sample fluctuations occur if the number of rare regions displaying static order becomes of the order of 1. Asymptotically for large linear system size L, the coupling strength t_L at which these fluctuations start behaves like

$$t_L \sim (\log L)^{1/(2-d/\phi)} \qquad \text{Gaussian}, \tag{3a}$$

$$|t_L| \sim (\log L)^{-\phi/d} \qquad \text{dilution}. \tag{3b}$$

Thus, finite-size effects are suppressed only logarithmically. In the remainder of this Letter, we sketch the derivation of these results, illustrate them by numerical results from a model system, and discuss their relevance for experiments as well as simulations.

For definiteness we consider the antiferromagnetic quantum phase transition of itinerant electrons with Ising spin symmetry. The Landau-Ginzburg-Wilson free energy functional of the clean transition reads [14,20]

$$S = \int dxdy m(x)\Gamma(x, y)m(y) + u \int dx m^4(x). \tag{4}$$

Here $x \equiv (\mathbf{x}, \tau)$ comprises position $\mathbf{x}$ and imaginary time τ, and $\int dx \equiv \int d\mathbf{x} \int_0^{1/T} d\tau$. $\Gamma(x, y)$ is the bare two-point vertex, whose Fourier transform is $\Gamma(\mathbf{q}, \omega_n) = (t + \mathbf{q}^2 + |\omega_n|)$. Here $t = (g - g_c)/g_c$ is the distance of the coupling constant g from the critical point. The dynamical part of Γ is proportional to $|\omega_n|$ reflecting the overdamping of the dynamics (undamped dynamics leads to ω_n^2). Quenched disorder is introduced by making t a random function of position, $t \to t + \delta t(\mathbf{x})$. We consider two different disorder distributions. The first is a Gaussian distribution with zero mean and a correlation function $\langle \delta t(\mathbf{x}) \delta t(\mathbf{y}) \rangle = \Delta^2 \delta(\mathbf{x} - \mathbf{y})$. The second disorder distribution is of a dilution type, $\delta t(\mathbf{x}) = 0$ everywhere except on randomly distributed finite-size islands (impurities) of spatial density c where $\delta t(\mathbf{x}) = W > 0$.

In the presence of disorder there are rare large spatial regions which are locally in the ordered phase while the bulk system is not. For the Gaussian disorder distribution which is unbounded, these regions exist for all t. For the dilution case they appear below the transition of the clean system, i.e., for $t < 0$. At zero temperature a single such region is equivalent to a classical Ising model in a rodlike geometry. It is finite in the d space dimensions but infinite in imaginary time. If the interaction in the time direction is short ranged, as is the case for undamped dynamics, true static order cannot develop on such a rare region. Instead, the order parameter displays slow fluctuations leading to quantum Griffiths phenomena. This is drastically different in a system with overdamped dynamics. The linear frequency dependence in Γ is equivalent to a long-range interaction in the time of the form $(\tau - \tau')^{-2}$. 1D Ising models with $1/r^2$ interaction are known to develop long-range order at finite temperatures [21]. Thus, in our quantum system, true static order develops on those rare regions which are locally in the ordered phase. In agreement with Ref. [17] we therefore do not find the usual quantum Griffiths phenomena. Once static order has developed on a few isolated rare regions, an infinitesimally small interaction or an infinitesimally small symmetry-breaking field are sufficient to align them. Consequently, a macroscopic order-parameter arises.

We now use Lifshitz-tail arguments [22] to derive the leading thermodynamic behavior for small order parameter m. In the dilution case, the probability w to find a region of linear size L_R devoid of any impurities ($\delta t = 0$) is given by $w \sim \exp(-cL_R^d)$ (up to preexponential factors). Such a rare region develops static order at some $t_c(L_R) < 0$. Finite-size scaling yields $|t_c(L_R)| \sim L_R^{-\phi}$ where ϕ is the finite-size scaling shift exponent of the clean system [23]. Thus, the probability for finding a rare region which becomes critical at t_c is given by

$$w(t_c) \sim \exp(-B|t_c|^{-d/\phi}) \quad \text{for } t \to 0- . \tag{5a}$$

For a Gaussian distribution similar arguments [24] give

$$w(t_c) \sim \exp(-\bar{B} t_c^{2-d/\phi}) \quad \text{for } t \to \infty. \tag{5b}$$

Here B and $\bar{B}$ are constants. The total order parameter m is obtained by integrating over all rare regions which are ordered at t, i.e., all rare regions having $t_c > t$. This leads to Eqs. (1a) and (1b). Note that the functional dependence on t of the order parameter on a given island is of a power-law type and thus only influences the preexponential factors.

At finite temperatures the static order on the rare regions is destroyed, and a finite interaction of the order of the temperature is necessary to align them. This means a sharp phase transition is recovered. To estimate the transition temperature we note that the interaction between two rare regions depends exponentially on their spatial distance r, $E_{\mathrm{int}} \sim \exp(-r/\xi_0)$, where ξ_0 is the bulk correlation length. The typical distance r itself depends exponentially on t via $r \sim w^{-1/d}$. The leading dependence of the critical temperature T_c on t is thus

$$T_c \sim \exp(-r/\xi_0) \sim \exp(-aw^{-1/d}/\xi_0), \tag{6}$$

where a is a constant. Inserting Eqs. (5a) and (5b) for w leads to Eqs. (2a) and (2b). Above this exponentially small critical temperature the rare regions essentially behave classically.

We now turn to finite-size effects at zero temperature. Since the total order parameter is the sum of contributions of many independent islands, finite-size effects in a macroscopic sample are governed by the central limit theorem. However, for $t \to \infty$ (Gaussian distribution) or $t \to 0-$ (dilution) very large and thus very rare regions are responsible for the order parameter. The number N of rare regions which start to order at t_c in a sample of size L behaves like $N \sim L^d w(t_c)$. When N becomes of the order of 1, strong sample-to-sample fluctuations arise. Using Eqs. (5a) and (5b) for $w(t_c)$ leads to Eqs. (3).

To illustrate the rounding of the transition we now show numerical data for a model system, viz., a classical Ising model with two spatial and one timelike dimensions. The disorder is of a dilution type and totally correlated in the time direction. The interaction is short ranged in space but infinite ranged in time. This simplification retains the crucial property of static order on the rare regions but permits system sizes large enough to study exponentially rare events. The Hamiltonian reads

$$H = -\frac{1}{L_\tau}\sum_{\langle \mathbf{x},\mathbf{y}\rangle,\tau,\tau'} S_{\mathbf{x},\tau}S_{\mathbf{y},\tau'} - \frac{1}{L_\tau}\sum_{\mathbf{x},\tau,\tau'} J_{\mathbf{x}}S_{\mathbf{x},\tau}S_{\mathbf{x},\tau'}. \tag{7}$$

Here $\mathbf{x}$ and τ are the space and time coordinates, respectively. L_τ is the system size in the time direction and $\langle \mathbf{x}, \mathbf{y}\rangle$ denotes pairs of nearest neighbors. $J_{\mathbf{x}}$ is a quenched binary random variable with the distribution $P(J) = (1-c)\delta(J-1) + c\delta(J)$. In this classical model L_τ takes the role of the inverse temperature in the corresponding quantum system and the classical temperature takes the role of the coupling constant g. Because the interaction is infinite ranged in time, the timelike dimension can be treated in mean-field theory. For $L_\tau \to \infty$, this leads to a set of coupled mean-field equations (one for each $\mathbf{x}$)

$$m_{\mathbf{x}} = \tanh\beta\left[J_{\mathbf{x}}m_{\mathbf{x}} + \sum_{\mathbf{y}(\mathbf{x})}' m_{\mathbf{y}} + h\right], \tag{8}$$

where $h = 10^{-8}$ is a small symmetry-breaking magnetic field. Equation (8) is solved numerically in a self-consistency cycle.

Figure 1 shows the total magnetization and the susceptibility (corresponding to the inverse energy gap of the quantum system) as functions of temperature for linear size $L = 100$ and impurity concentration $c = 0.2$. The data are averages over 200 disorder realizations [25]. At first glance these data suggest a sharp phase transition close to $T = 4.88$. However, a closer investigation, Fig. 2, shows that the singularities are rounded. If this rounding were a conventional finite-size effect the magnetization curve should become sharper with increasing L and the susceptibility peak should diverge. This is not the case here; instead the transition remains rounded for $L \to \infty$.

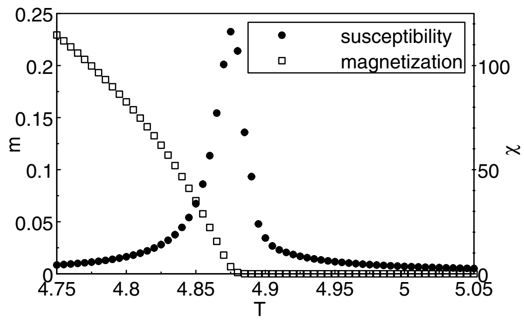

FIG. 1. Magnetization and susceptibility ($L = 100$, $c = 0.2$).

For comparison with the analytical results, Fig. 3 shows the logarithm of the average magnetization as a function of $1/(T_c^0 - T)$ where $T_c^0 = 5$ is the critical temperature of the clean system ($c = 0$). The data follow Eq. (1b) over almost 4 orders of magnitude in m with the expected shift exponent of $\phi = 2$. This figure also shows "typical," i.e., logarithmically averaged magnetization data for different system sizes. Deviations between the typical and the average values (which are essentially size independent) reflect strong sample-to-sample fluctuations. The data show that the onset T_L of these fluctuations shifts to larger temperatures with increasing system size. A more detailed analysis shows that $t_L = (T_L - T_c^0)$ follows Eq. (3b) in good approximation.

In the remaining paragraphs we discuss the generality of the results and their consequences for experiments and simulations. The rounding of the transition is due to the fact that at zero temperature static order can develop on a finite spatial region in a Landau-damped system. We thus expect all quantum phase transitions with discrete order-parameter symmetry and overdamped dynamics (i.e., a low frequency dependence $\sim|\omega|$ or slower in the Gaussian propagator) to be rounded by disorder. Systems with continuous symmetry behave differently. It is known

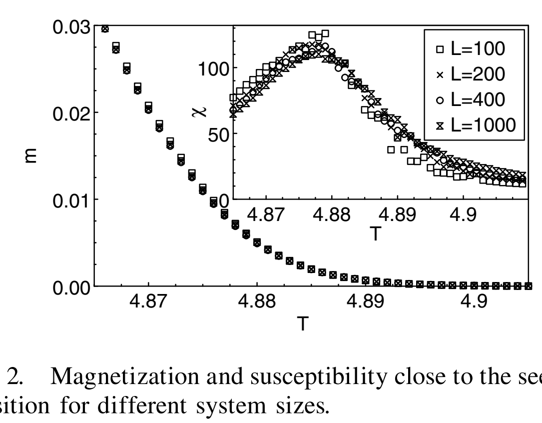

FIG. 2. Magnetization and susceptibility close to the seeming transition for different system sizes.

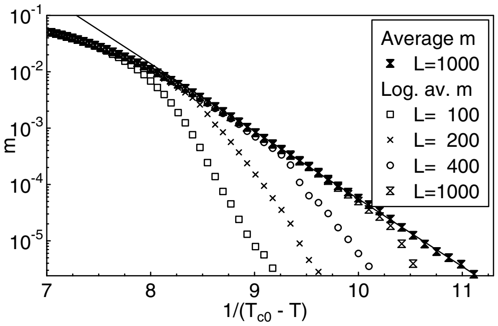

FIG. 3. $\log(m)$ as a function of distance from the clean critical point. The solid line is a fit of the average magnetization to Eq. (1b) with $\phi = 2$. The logarithmically averaged data show the onset of the sample-to-sample fluctuations.

[26] that classical 1D XY and Heisenberg systems develop long-range order at finite T only if the interaction falls off more slowly than $1/r^2$. Consequently, in a quantum system at zero temperature static order on a rare region develops only if the frequency dependence in the Gaussian propagator is slower than $|\omega|$. The itinerant ferromagnetic or antiferromagnetic quantum phase transitions with XY or Heisenberg symmetries will thus remain sharp in the presence of disorder [27].

The rounding of the quantum phase transition leads to an unusual phenomenology in experiments. Data at larger order parameter and not too low temperature do not resolve the exponentially small order-parameter tail but probe the rounded transition. With increasing precision and decreasing temperature the apparent critical point shifts towards the disordered phase, accompanied by strong sample-sample fluctuations. Similar effects will also occur in simulations. In a recent Monte Carlo simulation of a related model [28] a sharp transition was found controlled by an infinite-randomness fixed point. However, in this simulation the linear system sizes are below $L = 30$, thus it likely probes the rounded transition rather than the exponential magnetization tail.

In this Letter we have concentrated on the behavior of the system for very small order-parameter values, i.e., in the "tail region" of the rounded transition. The above arguments suggest that the properties of the rounded transition itself are experimentally also very important because they control the behavior in a wide preasymptotic region. However, these properties are likely to be nonuniversal, and so far they are not very well understood.

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