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Composition-tuned smeared phase transitions

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Phase transitions in random systems are smeared if individual spatial regions can order independently of the bulk system. In this paper, we study such smeared phase transitions (both classical and quantum) in substitutional alloys $A_{1-x}B_x$ that can be tuned from an ordered phase at composition $x = 0$ to a disordered phase at $x = 1$. We show that the ordered phase develops a pronounced tail that extends over all compositions $x < 1$. Using optimal fluctuation theory, we derive the composition dependence of the order parameter and other quantities in the tail of the smeared phase transition. We also compare our results to computer simulations of a toy model, and we discuss experiments.

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I. INTRODUCTION

When a phase transition occurs in a randomly disordered system, one of the most basic questions to ask is whether the transition is still sharp, i.e., associated with a singularity in the free energy. Naively, one might expect that random disorder rounds or smears any critical point because different spatial regions undergo the transition at different values of the control parameter. This expectation turns out to be mistaken, as classical (thermal) continuous phase transitions generically remain sharp in the presence of weak randomness. The reason is that a finite-size region cannot undergo a true phase transition at any nonzero temperature because its partition function must be analytic. Thus, true static long-range order can only be established via a collective phenomenon in the entire system (see, e.g., Ref. 1 for a pedagogical discussion).

Recent work has established, however, that some phase transitions are indeed smeared by random disorder. This can happen at zero-temperature quantum phase transitions when the order-parameter fluctuations are overdamped because they are coupled to an (infinite) heat bath.[2,3] As the damping hampers the dynamics, sufficiently large but finite-size regions can undergo the phase transition independently from the bulk system. Once several such regions have developed static order, their local order parameters can be aligned by an *infinitesimally small* mutual interaction. Thus, global order develops gradually, and the global phase transition is smeared. Classical thermal phase transitions can also be smeared provided the disorder is perfectly correlated in at least two dimensions. In these cases, individual "slabs" of finite thickness undergo the phase transition independently of the bulk system.[4,5]

The existing theoretical work on smeared phase transitions focuses on situations in which a sample with some fixed degree of randomness is tuned through the transition by changing the temperature (for classical transitions) or the appropriate quantum control parameter such as pressure or magnetic field (for quantum phase transitions). However, many experiments are performed on substitutional alloys such as $CePd_{1-x}Rh_x$ or $Sr_{1-x}Ca_xRuO_3$. These materials can be tuned from an ordered phase (ferromagnetic for the two examples given above) at composition $x = 0$ to a disordered phase at $x = 1$ while keeping the temperature and other external parameters fixed, i.e., they undergo a phase transition as a function of composition. The composition parameter x actually plays a dual role in these transitions. On the one hand, x is the control parameter of the phase transition. On the other hand, changing x also changes the degree of randomness. If such a composition-tuned phase transition is smeared, its behavior can therefore be expected to be different than that of smeared transitions occurring at fixed randomness.

In this paper, we investigate the properties of composition-tuned smeared phase transitions in substitutional alloys of the type $A_{1-x}B_x$. We show that the ordered phase extends over the entire composition range $x < 1$, and we derive the behavior of the system in the tail of the smeared transition. Our paper is organized as follows. In Sec. II, we consider a smeared quantum phase transition in an itinerant magnet. We use optimal fluctuation theory to derive the composition dependence of the order parameter, the phase boundary, and other quantities. In Sec. III, we briefly discuss how the theory is modified for smeared classical transitions in systems with correlated disorder. Section IV is devoted to computer simulations of a toy model that illustrate and confirm our theory. We conclude in Sec. V by comparing composition-tuned smeared transitions with those occurring at fixed randomness. We also discuss experiments.

II. SMEARED QUANTUM PHASE TRANSITION

A. Model and phase diagram

In this section, we investigate the ferromagnetic or antiferromagnetic quantum phase transition of itinerant electrons with Ising-order-parameter symmetry. In the absence of quenched randomness, the Landau-Ginzburg-Wilson free-energy functional of this transition in d space dimensions reads[6,7]

$$S = \int dy dz \psi(y)\Gamma(y,z)\psi(z) + u\int dy \psi^4(y)\,. \qquad (1)$$

Here, ψ is a scalar order-parameter field, $y \equiv (\mathbf{y},\tau)$ comprises imaginary time τ and d-dimensional spatial position $\mathbf{y}$, $\int dy \equiv \int d\mathbf{y} \int_0^{1/T} d\tau$, and u is the standard quartic coefficient. $\Gamma(y,z)$ denotes the bare inverse propagator (two-point vertex) whose Fourier transform reads

$$\Gamma(\mathbf{q},\omega_n) = r + \xi_0^2\mathbf{q}^2 + \gamma_0(\mathbf{q})|\omega_n|. \qquad (2)$$

Here, r is the distance from criticality,[8] ξ_0 is a microscopic length scale, and ω_n is a Matsubara frequency. The dynamical part of $\Gamma(\mathbf{q},\omega_n)$ is proportional to $|\omega_n|$. This overdamped dynamics reflects the Ohmic dissipation caused by the coupling between the order-parameter fluctuations and the gapless fermionic excitations in an itinerant system. The damping coefficient $\gamma_0(\mathbf{q})$ is $\mathbf{q}$-independent for an antiferromagnetic transition but proportional to $1/|\mathbf{q}|$ or $1/|\mathbf{q}|^2$ for ballistic and diffusive ferromagnets, respectively.

We now consider two materials, A and B. Substance A is in the magnetic phase, implying a negative distance from criticality, $r_A < 0$, while substance B is nonmagnetic with $r_B > 0$. By randomly substituting B atoms for the A atoms to form a binary alloy $A_{1-x}B_x$, we can drive the system through a composition-driven magnetic quantum phase transition.

A crucial role in this transition is played by rare A-rich spatial regions. They can be locally in the magnetic phase even if the bulk system is nonmagnetic. In the presence of Ohmic dissipation, the low-energy physics of each such region is equivalent to that of a dissipative two-level system, which is known to undergo, with increasing dissipation strength, a phase transition from a fluctuating to a localized phase.[9] Therefore, the quantum dynamics of sufficiently large rare regions completely freezes,[10] and they behave as classical superspins. At zero temperature, these classical superspins can be aligned by an *infinitesimally small* residual interaction, which is always present as they are coupled via the fluctuations of the paramagnetic bulk system. The order parameter is thus spatially very inhomogeneous, but its average is nonzero for any $x < 1$, implying that the global quantum phase transition is smeared by the disorder inherent in the random positions of the A and B atoms.[2,11,12]

At small but nonzero temperatures, the static magnetic order on the rare regions is destroyed, and a finite interaction of the order of the temperature is necessary to align them. This restores a sharp phase transition at some transition temperature $T_c(x)$, which rapidly decreases with increasing x but reaches zero only at $x = 1$. If the temperature is raised above T_c, the locally ordered rare regions act as independent classical moments, leading to super-paramagnetic behavior. A sketch of the resulting phase diagram is shown in Fig. 1.

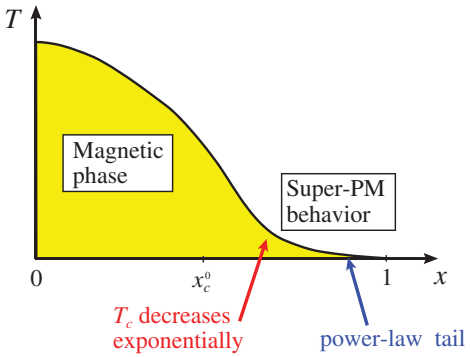

FIG. 1. (Color online) Schematic temperature-composition phase diagram of a binary alloy $A_{1-x}B_x$ displaying a smeared quantum phase transition. In the tail of the magnetic phase, which stretches all the way to $x = 1$, the rare regions are aligned. Above T_c, they act as independent classical moments, resulting in super-paramagnetic (PM) behavior. x_c^0 marks the critical composition in the average-potential approximation defined in Eq. (3).

B. Optimal fluctuation theory

In this section, we use optimal fluctuation theory[13,14] to derive the properties of the tail of the smeared quantum phase transition. This is the composition range where a few rare regions have developed static magnetic order but their density is so small that they are very weakly coupled.

A crude estimate of the transition point in the binary alloy $A_{1-x}B_x$ can be obtained by simply averaging the distance from criticality, $r_{\rm av} = (1-x)r_A + xr_B$. The transition point corresponds to $r_{\rm av} = 0$. This gives the critical composition in the "average-potential approximation,"

$$x_c^0 = -r_A/(r_B - r_A). \tag{3}$$

Let us now consider a single A-rich rare region of linear size L_{RR} embedded in a nonmagnetic bulk sample. If the concentration $x_{\rm loc}$ of B atoms in this region is below some critical concentration $x_c(L_{RR})$, the region will develop local magnetic order. The value of the critical concentration follows straightforwardly from finite-size scaling,[15,16]

$$x_c(L_{RR}) = x_c^0 - DL_{RR}^{-\phi}, \tag{4}$$

where ϕ is the finite-size shift exponent and D is a constant. Within mean-field theory (which should be qualitatively correct in our case because the clean transition is above its upper critical dimension[6]), one finds $\phi = 2$ and $D = \xi_0^2/(r_B - r_A)$. Since $x_c(L_{RR})$ must be positive, Eq. (4) implies that a rare region needs to be larger than $L_{\rm min} = (D/x_c^0)^{1/\phi}$ to develop local magnetic order.

As the last ingredient of our optimal fluctuation theory, we now analyze the random distribution of the atoms in the sample. For simplicity, we assume that the lattice sites are occupied *independently* by either A or B atoms with probabilities $1-x$ and x, respectively. Modifications due to deviations from a pure random distribution (i.e., clustering) will be discussed in the concluding Sec. V. The probability of finding $N_B = Nx_{\rm loc}$ sites occupied by B atoms in a spatial region with a total of $N \sim L_{RR}^d$ sites is given by the binomial distribution

$$P(N,x_{\rm loc}) = \binom{N}{N_B}(1-x)^{N-N_B}x^{N_B}. \tag{5}$$

We are interested in the regime $x > x_c^0$ where the bulk system will not be magnetically ordered but $x_{\rm loc} = N_B/N < x_c(L_{RR})$ such that local order is possible in the region considered.

To estimate the total zero-temperature order parameter M in the tail of the smeared transition (where the rare regions are very weakly coupled), we can simply sum over all rare regions displaying local order

$$M \sim \int_{L_{\rm min}}^{\infty} dL_{RR} \int_0^{x_c(L_{RR})} dx_{\rm loc}\, m(N,x_{\rm loc})P(N,x_{\rm loc}). \tag{6}$$

Here, $m(N,x_{\rm loc})$ is the order parameter of a single region of N sites and local composition $x_{\rm loc}$, and we have suppressed a combinatorial prefactor. We now analyze this integral in two parameter regions: (i) the regime where x is somewhat larger

than x_c^0 but not by too much and (ii) the far tail of the transition at $x \to 1$.

If x is not much larger than x_c^0, the rare regions are expected to be large, and we can approximate the binomial distribution (5) by a Gaussian,

$$P(N,x_{\rm loc}) = \frac{1}{\sqrt{2\pi N(1-N)}} \exp\left[-N\frac{(x_{\rm loc}-x)^2}{2x(1-x)}\right]. \quad (7)$$

To exponential accuracy in x, the integral (6) can now be easily performed in the saddle-point approximation. Neglecting $m(N,x_{\rm loc})$, which only modifies power-law prefactors, we find that large rare regions of size $L_{RR}^{\phi} = D(2\phi - d)/[d(x - x_c^0)]$ and maximum possible B concentration $x_{\rm loc} = x_c^0 - DL_{RR}^{-\phi}$ dominate the integral. Inserting these saddle-point values into the integrand yields the composition dependence of the order parameter as[17]

$$M \sim \exp\left[-C\frac{\left(x-x_c^0\right)^{2-d/\phi}}{x(1-x)}\right], \quad (8)$$

where $C = 2(D/d)^{d/\phi}(2\phi - d)^{d/\phi-2}\phi^2$ is a nonuniversal constant.

Let us now analyze the far tail of the smeared transition, $x \to 1$. In this regime, the binomial distribution cannot be approximated by a Gaussian. Nonetheless, the integral (6) can be estimated in the saddle-point approximation. We find that for $x \to 1$, the integral is dominated by pure-A regions of the minimum size that permits local magnetic order. This means $L_{RR} = L_{\rm min} = (D/x_c^0)^{1/\phi}$ and $x_{\rm loc} = 0$. Inserting these values into the integrand (6), we find that the leading composition dependence of the order parameter in the limit $x \to 1$ is given by a nonuniversal power law,

$$M \sim (1-x)^{L_{\rm min}^d} = (1-x)^{(D/x_c^0)^{d/\phi}}. \quad (9)$$

We thus find that M is nonzero in the entire composition range $0 \leqslant x < 1$, illustrating the notion of a smeared quantum phase transition.

So far, we have focused on the zero-temperature order parameter. Other quantities can be found in an analogous manner. Let us, for example, determine the phase boundary, i.e., the composition dependence of the critical temperature, T_c. As was discussed in Sec. II A, the static magnetism of the rare regions is destroyed at nonzero temperatures. Consequently, magnetic long-range order in the sample can only develop, if the rare regions are coupled by an interaction of the order of the temperature. The typical distance between neighboring locally ordered rare regions can be estimated from their density, ρ, as $r_{\rm typ} \sim \rho^{-1/d} \sim M^{-1/d}$. Within the Landau-Ginzburg-Wilson theory (see Refs. 1 and 2), the interaction between two rare regions drops off exponentially with their distance r, $E_{\rm int} \sim \exp(-r/\xi_b)$, where ξ_b is the bulk correlation length. This leads to a double-exponential dependence of T_c on x for compositions somewhat above x_c^0, i.e., $\ln(1/T_c) \sim \exp\{C(x-x_c^0)^{2-d/\phi}/[dx(1-x)]\}$. For $x \to 1$, we find $\ln(1/T_c) \sim (1-x)^{-L_{\rm min}^d/d}$. However, in a real metallic magnet, the locally ordered rare regions are coupled by an Ruderman-Kittel-Kasuya-Yosida (RKKY) -type interaction that decays as a power law with distance, $E_{\rm int} \sim r^{-d}$, rather than exponentially.[18] [This interaction is not contained in the long-wavelength expansion implied in Eq. (2).] Therefore, the composition dependence of the critical temperature takes the same form as that of the magnetization,

$$T_c \sim \exp\left[-C\frac{\left(x-x_c^0\right)^{2-d/\phi}}{x(1-x)}\right] \quad (10)$$

for compositions somewhat above x_c^0 and

$$T_c \sim (1-x)^{L_{\rm min}^d} = (1-x)^{(D/x_c^0)^{d/\phi}} \quad (11)$$

in the far tail of the smeared transition, $x \to 1$.

We now turn to the order-parameter susceptibility. It consists of two different contributions, one from the paramagnetic bulk system and one from the locally ordered rare regions. The bulk system provides a finite, noncritical background throughout the tail of the smeared transition. Let us discuss the rare-region contribution in more detail. At zero temperature, the total order parameter M is nonzero for all $x < 1$. The rare regions therefore always feel a symmetry-breaking effective field which cuts off any possible divergence of their susceptibilities. We conclude that the zero-temperature susceptibility does not diverge anywhere in the tail of the smeared transition. If the temperature is raised above T_c, the relative alignment of the rare regions is lost, and they behave as independent large (classical) moments, leading to a super-paramagnetic temperature dependence of the susceptibility, $\chi \sim 1/T$ (see Fig. 1). At even higher temperatures, when the damping of the quantum dynamics becomes unimportant, we expect the usual nonuniversal quantum Griffiths power laws, $\chi \sim T^{\lambda-1}$, where λ is the Griffiths exponent.[11,12,19]

III. SMEARED CLASSICAL PHASE TRANSITION

Classical (thermal) phase transitions with uncorrelated disorder cannot be smeared because all rare regions are of finite size and thus can not undergo a true phase transition at any nonzero temperature. However, perfect disorder correlations in one or more dimensions lead to rare regions that are infinitely extended in the thermodynamic limit. If the number of correlated dimensions is high enough, these infinitely large rare regions can undergo the phase transition independently of the bulk system, leading to a smearing of the global phase transition.[4] This happens, for example, in a randomly layered Ising magnet, i.e., an Ising model with disorder correlated in two dimensions.[5]

In this section, we discuss how the theory of Sec. II is modified for these smeared classical phase transitions. For definiteness, we consider a classical Landau-Ginzburg-Wilson free energy in d dimensions,

$$S = \int d\mathbf{y}\psi(\mathbf{y})\left[r - \partial_{\mathbf{y}}^2\right]\psi(\mathbf{y}) + u\int d\mathbf{y}\psi^4(\mathbf{y}). \quad (12)$$

As in the quantum case, we now consider a binary alloy $A_{1-x}B_x$ of two materials A and B. The atoms are arranged randomly in $d_\perp$ dimensions, while they are perfectly correlated in $d_\parallel = d - d_\perp$ dimensions. For example, if $d_\perp = 1$ and $d_\parallel = 2$, the system would consist of a random sequence of layers, each made up of only A atoms or only B atoms.

If the correlated dimension $d_\parallel$ is sufficiently large, the alloy undergoes a smeared classical phase transition as the

composition x is tuned from 0 to 1 at a (fixed) temperature at which the material A is magnetically ordered, $r_A < 0$, while the material B is in the nonmagnetic phase, $r_B > 0$. The optimal fluctuation theory for the behavior in the tail of the smeared transition can be developed along the same lines as the theory in Sec. II. The only important difference stems from the fact that the randomness is restricted to $d_\perp$ dimensions. The dimensionality d in Eqs. (8) and (9) therefore needs to be replaced by $d_\perp$, leading to

$$M \sim \exp\left[-C\frac{\left(x - x_c^0\right)^{2-d_\perp/\phi}}{x(1-x)}\right] \tag{13}$$

for compositions somewhat above x_c^0 and

$$M \sim (1-x)^{L_{\min}^{d_\perp}} = (1-x)^{(D/x_c^0)^{d_\perp/\phi}} \tag{14}$$

for $x \to 1$. The same substitution of d by $d_\perp$ was also found for smeared classical transitions tuned by temperature rather than composition.[4]

IV. COMPUTER SIMULATIONS

To verify the predictions of the optimal fluctuation theory in Sec. II and to illustrate our results, we have performed computer simulations of a toy model, viz., a classical Ising model with d spacelike dimensions and one timelike dimension. The interactions are between nearest neighbors in the spacelike directions but infinite-ranged in the timelike ones. This $(d+1)$-dimensional toy model retains the possibility of static order on the rare regions (which is crucial for the transition being smeared) but permits system sizes large enough to study exponentially rare events. The Hamiltonian reads

$$H = -\frac{1}{L_\tau}\sum_{\langle \mathbf{y},\mathbf{z}\rangle,\tau,\tau'} S_{\mathbf{y},\tau}S_{\mathbf{z},\tau'} - \frac{1}{L_\tau}\sum_{\mathbf{y},\tau,\tau'} J_{\mathbf{y}}S_{\mathbf{y},\tau}S_{\mathbf{y},\tau'}. \tag{15}$$

Here, $\mathbf{y}$ and $\mathbf{z}$ are d-dimensional spacelike coordinates and τ is the timelike coordinate. L_τ is the system size in the time direction and $\langle \mathbf{y},\mathbf{z}\rangle$ denotes pairs of nearest neighbors on the hypercubic lattice in space. $J_{\mathbf{y}}$ is a quenched random variable having the binary distribution $P(J) = (1-x)\delta(J - J_h) + x\delta(J - J_l)$ with $J_h > J_l$. In this classical model, L_τ plays the role of the inverse temperature in the corresponding quantum system and the classical temperature plays the role of the quantum tuning parameter. 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 for the local magnetizations $m_{\mathbf{y}} = (1/L_\tau)\sum_\tau S_{\mathbf{y},\tau}$; they read

$$m_{\mathbf{y}} = \tanh\beta\left[J_{\mathbf{y}}m_{\mathbf{y}} + \sum_{\mathbf{z}} m_{\mathbf{z}} + h\right], \tag{16}$$

where the sum is over all nearest neighbors of site $\mathbf{y}$ and $h \to 0$ is a very small symmetry-breaking magnetic field which we typically set to 10^{-12}. If all $J_{\mathbf{y}} \equiv J_h$, the system undergoes a (sharp) phase transition at $T_h = J_h + 2d$, and if all $J_{\mathbf{y}} \equiv J_l$, it undergoes the transition at $T_l = J_l + 2d$. In the temperature range $T_h > T > T_l$, the phase transition can therefore be tuned by composition x.

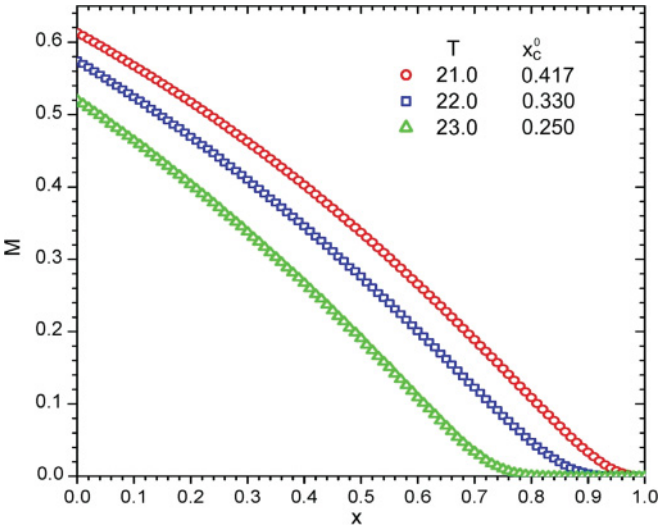

FIG. 2. (Color online) Magnetization M vs composition x for a $(3+1)$-dimensional system having $J_h = 20$, $J_l = 8$, and several values of the classical temperature T. The data represent averages over 100 samples of size $L = 100$. The values of the critical concentration in the average-potential approximation, x_c^0, are shown for comparison.

The mean-field equations (16) can be solved efficiently in a self-consistency cycle. Using this approach, we studied systems in one, two, and three space dimensions. The system sizes were up to L = 10 000 in one dimension, and up to $L = 100$ in two and three dimensions. For each parameter set, the data were averaged over a large number of disorder realizations. Details will be given with the individual results below.

Figure 2 shows an overview over the magnetization M as a function of composition x for a $(3+1)$-dimensional system at several values of the classical temperature in the interval $T_h > T > T_l$. The figure clearly demonstrates that the magnetic phase extends significantly beyond the average-potential value $x_c^0 = (T_h - T)/(T_h - T_l)$. In this sense, the magnetic phase in our binary alloy benefits from the randomness. In agreement with the smeared-phase-transition scenario, the data also show that $M(x)$ develops a pronounced tail toward $x = 1$. (By comparing different system sizes, we can exclude that the tail is due to simple finite-size rounding.[4]) We performed similar simulations for systems in one and two space dimensions with analogous results.

To verify the theoretical predictions of the optimal fluctuation theory developed in Sec. II, we now analyze the tail of the smeared phase transition in more detail. Figure 3 shows a semilogarithmic plot of the magnetization M versus the composition x for a $(1+1)$-dimensional system, a $(2+1)$-dimensional system, and a $(3+1)$-dimensional one. In all examples, the data follow the theoretical prediction of Eq. (8) over at least two orders of magnitude in M in a transient regime of intermediate compositions x.

We also check the behavior of the magnetization for compositions very close to $x = 1$. Since Eq. (9) predicts a nonuniversal power law, we plot $\log(M)$ versus $\log(1-x)$ for a $(3+1)$-dimensional system in Fig. 4. The figure shows that the magnetization tail indeed decays as a power of $(1-x)$ with $x \to 1$. The exponent increases with increasing temperature in

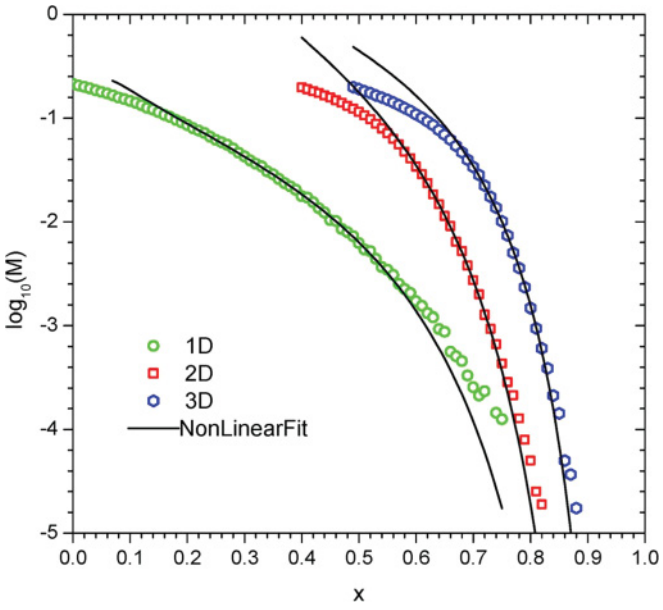

FIG. 3. (Color online) $\log(M)$ vs x in the tail of the transition for three example systems: (i) $(3+1)$-dimensional system with $L=100$, $J_h=20$, $J_l=8$, and $T=23$, (ii) $(2+1)$-dimensional system with $L=100$, $J_h=15$, $J_l=8$, and $T=18$, and (iii) $(1+1)$-dimensional system with $L=10\,000$, $J_h=11$, $J_l=8$, and $T=12.8$. All data are averages over 100 disorder configurations. The solid lines are fits to Eq. (8) with the fit intervals restricted to $x\in(0.25,0.55)$ in $(1+1)$ dimensions, $(0.6,0.72)$ in $(2+1)$ dimensions and (0.7,0.82) for the $(3+1)$-dimensional example.

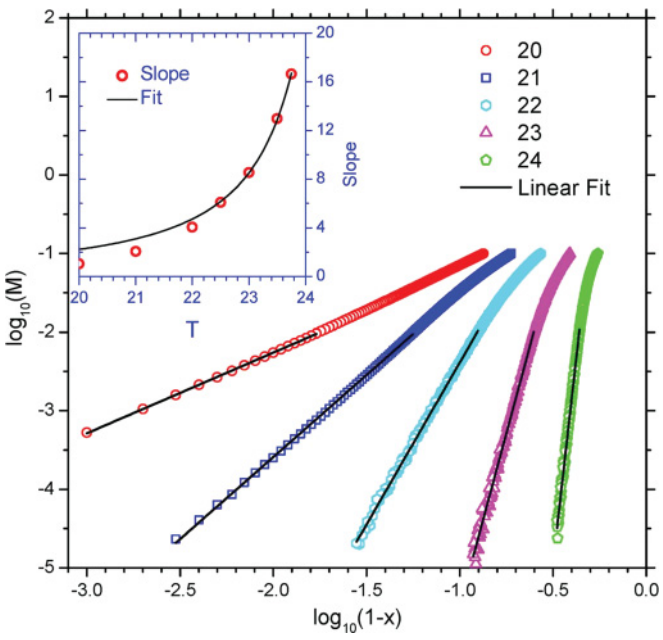

FIG. 4. (Color online) $\log(M)$ vs $\log(1-x)$ for a $(3+1)$-dimensional system with $L=100$, $J_h=20$, and $J_l=8$ and several temperatures. All data are averages over 100 disorder configurations. The solid lines are fits to the power law, Eq. (9). The inset shows the exponent as a function of temperature with the solid line being a fit to $[x_c^0(T)]^{-3/2}$.

agreement with the prediction that it measures the minimum size, $N_{\min}\sim L_{\min}^d$, a rare region needs to have to undergo the transition independently. The inset of Fig. 4 shows a fit of the exponent to $L_{\min}^d\sim[x_c^0(T)]^{-3/2}=[(T_h-T)/(T_h-T_l)]^{-3/2}$. The equation describes the data reasonably well; the deviations at small exponents can be explained by the fact that our theory assumes the rare-region size to be a continuous variable which is not fulfilled for rare regions consisting of just a few lattice sites.

Our computer simulation thus confirm the theoretical predictions in both composition regions in the tail of the transition. In a transient regime above x_c^0, we observe the exponential dependence, Eq. (8), while the magnetization for $x\to 1$ follows the nonuniversal power law, Eq. (9).

V. CONCLUSIONS

In summary, we have investigated phase transitions that are tuned by changing the composition x in a random binary alloy $A_{1-x}B_x$, where pure A is in the ordered phase while pure B is in the disordered phase. If individual, rare A-rich spatial regions develop true static order, they can be aligned by an infinitesimal residual interaction. This results in the smearing of the global phase transition, in agreement with the classification put forward in Ref. 20.

As an example, we have studied the quantum phase transition of an itinerant Ising magnet of the type $A_{1-x}B_x$. At zero temperature, the ordered phase in this binary alloy extends over the entire composition range $x<1$, illustrating the notion of a smeared quantum phase transition. Upon raising the temperature, a sharp phase transition is restored, but the transition temperature $T_c(x)$ is nonzero for all $x<1$ and reaches zero only right at $x=1$ (see Fig. 1). Using optimal fluctuation theory, we have derived the functional forms of various thermodynamic observables in the tail of the smeared transition. We have also briefly discussed smeared classical phase transitions that can occur in systems with correlated disorder, and we have performed computer simulations of a toy model that confirm and illustrate the theory.

Although our results are qualitatively similar to those obtained for smeared phase transitions occurring at fixed randomness as a function of temperature or an appropriate quantum control parameter, the functional forms of observables are not identical. The most striking difference can be found in the far tail of the transition. In the case of composition tuning, the order parameter vanishes as a nonuniversal power of the distance from the end of the tail ($x=1$), reflecting the fact that the minimum rare-region size required for local magnetic order is finite. In contrast, if the transition occurs at fixed composition as a function of temperature or some quantum control parameter, the order parameter vanishes exponentially[2,4] because the minimum size of an ordered rare region diverges in the far tail. These differences illustrate the fact that the behavior of observables at a smeared phase transition is generally *not* universal in the sense of critical phenomena; it depends on details of the disorder distribution and how the transition is tuned. Only the question of whether or not a particular phase transition is smeared is universal, i.e., determined only by symmetries and dimensionalities.

Let us briefly comment on the relation of our theory to percolation ideas. The optimal fluctuation theory of Sec. II B applies for compositions x larger than the percolation threshold of the A atoms. Because the A clusters are disconnected in this composition range, percolation of the A atoms does not play a role in forming the tail of the ordered phase at large x. Instead, distant rare regions are coupled via the fluctuations of the paramagnetic bulk phase and, in metallic magnets, via the RKKY interaction. Percolation does play a role, though, in the crossover between the inhomogeneous order in the tail of the transition and the bulk order at lower x.

We note in passing that the behavior of a diluted system (where B represents a vacancy) with *nearest-neighbor* interactions is not described by our theory. In this case, the A clusters are not coupled at all for compositions x larger than the A-percolation threshold. Therefore they cannot align, and long-range order is impossible. As a result, the superparamagnetic behavior of the locally ordered clusters extends all the way down to zero temperature. This was recently discussed in detail on the example of a diluted dissipative quantum Ising model.[21]

In the present paper, we have assumed that the A and B atoms are distributed independently over the lattice sites, i.e., we have assumed that there are no correlations between the atom positions. It is interesting to ask how the results change if this assumption is not fulfilled, for example, because like atoms tend to cluster. As long as the correlations of the atom positions are short-ranged (corresponding to a finite, microscopic length scale for clustering), our results will not change *qualitatively*. All arguments in the optimal fluctuation theory still hold using a typical cluster of like atoms instead of a single atom as the basic unit. However, such clustering will lead to significant *quantitative* changes (i.e., changes in the nonuniversal constants in our results), as it greatly increases the probability of finding large locally ordered rare regions. We thus expect that clustering of like atoms will enhance the tail and move the phase boundary $T_c(x)$ toward larger x. A quantitative analysis of this effect requires explicit information about the type of correlations between the atom positions and is thus relegated to future work.

Let us, finally, turn to experiment. Tails of the ordered phase have been observed at many quantum phase transitions. However, it is often not clear whether these tails are an intrinsic effect or due to experimental difficulties such as macroscopic concentration gradients or other macroscopic sample inhomogeneities. Recent highly sensitive magneto-optical experiments on $Sr_{1-x}Ca_xRuO_3$ have provided strong evidence for a smeared ferromagnetic quantum phase transition.[22] The behavior of the magnetization and critical temperature in the tail of the smeared transition agree well with the theory developed here. Moreover, the effects of clustering discussed above may explain the wide variation of the critical composition between about 0.5 and 1 reported in earlier studies.[23–25] We expect that our smeared-quantum-phase-transition scenario applies to a broad class of itinerant systems with quenched disorder.

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