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Modification of smeared phase transitions by spatial disorder correlations

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Abstract. Phase transitions in disordered systems can be smeared if rare spatial regions develop true static order while the bulk system is in the disordered phase. Here, we study the effects of spatial disorder correlations on such smeared phase transitions. The behaviors of observables are determined within optimal fluctuation theory. We show that even short-range correlations can qualitatively modify smeared phase transitions. For positive correlations (like impurity atoms attract each other), the order parameter is enhanced, while it is suppressed for repulsive correlations (like atoms repel each other). We use computer simulations to generate various types of disorder correlations, and to verify our theoretical predictions.

Keywords: spatial disorder correlations, smeared phase transitions, optimal fluctuation theory

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INTRODUCTION

Phase transitions occur between different macroscopic states of many-particle systems when control parameters such as temperature, pressure, magnetic field, chemical composition, *etc.* are varied. Phase transitions occurring at nonzero temperatures are called *thermal or classical* transitions. They are driven by thermal fluctuations. Another type of transitions, the so-called *quantum* phase transitions occur at absolute zero temperature, when a nonthermal external parameter is changed [1]. They are driven by quantum rather than thermal fluctuations. The study of observable quantities at quantum phase transitions is an important subject of modern condensed matter theory.

Since materials often feature considerable amounts of quenched disorder, the study of phase transitions in the presence of imperfections or randomness has received much attention. Initially, it was thought that any kind of disorder can destroy sharp phase transitions because (in the presence of disorder) the system divides itself up into regions which can undergo the transition at different values of the control parameter. Later, it became clear that phase transitions are generically sharp in the presence of weak disorder. However, under special conditions, rare finite-size spatial regions can indeed undergo the phase transition independently, leading to a smearing of the transition. This happens, for example, at quantum phase transitions with overdamped order parameter dynamics [2, 3, 4] or at thermal phase transitions with extended defects [5, 6].

Theories of disordered systems often assume the randomness to be uncorrelated in space even though real systems contain some amount of disorder correlations. At critical points, this assumption is justified as long as the correlations are not too long-ranged. This can be understood, e.g., by looking at the Harris criterion [7] for the stability of a clean critical point against weak disorder. Harris divided up the system into

regions whose linear size is the correlation length ξ . The variation of the local critical temperatures from region to region can be estimated using central limit theorem, yielding $\delta T_c \sim \xi^{-d/2}$, where d is the space dimension. Harris observed that the critical behavior of the clean transition can be unchanged if the fluctuations δT_c between the regions are smaller than the global distance $t = T - T_c$ from criticality, *i.e.*, $\delta T_c < t$. Because $\xi \sim t^{-\nu}$, this leads to the inequality $t^{d\nu/2} < t$ for $t \rightarrow 0$, where ν is the correlation length critical exponent of the clean system. Thus, for stability of the clean critical behavior we must have $d\nu > 2$. This inequality is called the Harris criterion.

Weinrib *et al.*, [8] generalized the Harris criterion to long-range correlated disorder. They considered power-law correlations, $C(\mathbf{x} - \mathbf{y}) = [(T_c(\mathbf{x}) - T_c)(T_c(\mathbf{y}) - T_c)]_{\text{av}} \sim |\mathbf{x} - \mathbf{y}|^{-\alpha}$, where $[\dots]_{\text{av}}$ is the disorder average. To estimate fluctuations between correlation volumes ξ^d , the central limit theorem estimate has to be replaced by

$$(\delta T_c)^2 = \frac{1}{\xi^{2d}} \int_{\xi^d} d\mathbf{x}^d \int_{\xi^d} d\mathbf{y}^d C(\mathbf{x} - \mathbf{y}) \sim \xi^{-\min(\alpha, d)}. \quad (1)$$

For $\alpha = d$, we find $(\delta T_c)^2 \sim \xi^{-d} \log \xi$. Then, the stability criterion for clean critical behavior takes the form $d\nu - 2 > 0$ for $\alpha \geq d$ or $\alpha\nu - 2 > 0$ for $\alpha < d$.

Thus, for $\alpha \geq d$, the original short-range Harris criterion is recovered. However, for $\alpha < d$, long-range correlations lead to a new inequality. Thus, as long as the correlations decay faster than x^{-d} with distance, correlated and uncorrelated disorder have the same effect on the stability of the clean critical behavior.

In Ref. [9], we studied the effects of spatially correlated disorder on *smear*ed phase transitions, and we showed that even short-range correlations qualitatively modify the behavior of observable quantities. Here, we summarize this theory. We then report the results of new computer simulations for which we have generated spatially correlated atom distributions using Kawasaki Monte Carlo simulations [10].

CORRELATED DISORDER AT SMEARED PHASE TRANSITIONS

In this section, we summarize the theory of Ref. [9] for the behavior of observables in the tail of smeared phase transitions. We consider a material consisting of substances A and B. Material A is in the magnetic phase characterized by a negative distance from criticality $t_A < 0$. Material B is in the paramagnetic phase with $t_B > 0$. The quantum phase transition from a non-magnetic to a magnetic phase can be tuned by substituting magnetic atoms A for nonmagnetic atoms B in the binary alloy $A_{1-x}B_x$.

Due to statistical fluctuations in the atom distribution, there can be large (rare) spatial regions which show local order because they have a high local concentration of A atoms even if the bulk system is in the non-magnetic phase. If the order parameter fluctuations are overdamped, the quantum dynamics of these regions freezes. This leads to inhomogeneous magnetic order and a smearing of the phase transition [2].

We now explore the effects of disorder correlations on smeared phase transitions within optimal fluctuation theory. Assume that there are attractive short-range correlations between like atoms, with disorder correlation length ξ_{dis} . Like atoms tend to form clusters of typical volume $V_{\text{dis}} \approx 1 + a\xi_{\text{dis}}^d$. Roughly, the transition point x_c^0 where the

phase transition would happen without having any rare regions effects, can be found by setting the average distance from criticality to zero. This gives $x_c^0 = -t_A/(t_B - t_A)$. A rare region of linear size L_{RR} can show local static order if the local concentration of non-magnetic B atoms is smaller than some critical concentration $x_c(L_{RR})$ which can be estimated from finite size scaling [11], $x_c = x_c^0 - DL_{RR}^{-\phi}$. Here, D is a non-universal constant, and ϕ is the shift exponent which takes the value of $1/2$ within mean-field approximation. As the concentration x_c must be positive, we obtain the condition $L_{\min} = (D/x_c^0)^{1/\phi}$ for the minimum size of a locally ordered rare region.

The probability $P(N, N_B)$ for a rare region with $N = L_{RR}^d$ sites to have $N_B = N x_{\text{loc}}$ sites occupied by B atoms is equal to the probability $P_{\text{clus}}(N/V_{\text{dis}}, N_B/V_{\text{dis}})$ of finding N_B/V_{dis} B-clusters among N/V_{dis} clusters. It is given by the binomial distribution

$$P_{\text{clus}}(N/V_{\text{dis}}, x_{\text{loc}}/V_{\text{dis}}) = \binom{N/V_{\text{dis}}}{N_B/V_{\text{dis}}} (1-x)^{\frac{N-N_B}{V_{\text{dis}}}} x^{\frac{N_B}{V_{\text{dis}}}}. \quad (2)$$

To calculate the total magnetization, we can simply integrate the binomial distribution (2) over all rare regions showing local order. In the regime where the concentration x is somewhat larger than x_c^0 , we find (up to power-law prefactors)

$$M \sim \exp \left[-\frac{C}{(1 + a\xi_{\text{dis}}^d)} \frac{(x - x_c^0)^{2-d/\phi}}{x(1-x)} \right], \quad (3)$$

where C is a non-universal constant. In this regime, the magnetization drops exponentially with x , and spatial disorder correlations modify the prefactor in the exponent.

In the far tail of the smeared transition at $x \rightarrow 1$, the composition dependence of the order parameter is given by a non-universal power law $M \sim (1-x)^\beta$ with $\beta = (aL_{\min}^d + a\xi_{\text{dis}}^d)/V_{\text{dis}}$. For small disorder correlation length $\xi_{\text{dis}} \ll L_{\min}$, earlier results for uncorrelated disorder [12] are recovered, $\beta \approx L_{\min}^d$. In the limit of large correlation lengths $\xi \gg L_{\min}$, all clusters show local order, and all magnetic A atoms contribute to the magnetization. This leads to $\beta = 1$. Thus, in the far tail, disorder correlations modify the exponent of the order parameter. In both regimes, for attractive correlations as considered here, the magnetization M at a given concentration x increases with increasing correlation length ξ_{dis} .

COMPUTER SIMULATIONS

To illustrate the theory we now show results of numerical simulations of a toy model. Motivated by the quantum-classical mapping [1] we consider a classical Ising model with infinite-range interaction in one (timelike) dimension and short-range interaction in three spacelike dimensions. The Hamiltonian has the form [9]

$$H = -\frac{1}{L_\tau} \sum_{\langle \mathbf{y}, \mathbf{z} \rangle, \tau, \tau'} J_0 S_{\mathbf{y}, \tau} S_{\mathbf{z}, \tau'} - \frac{1}{L_\tau} \sum_{\mathbf{y}, \tau, \tau'} J_{\mathbf{y}} S_{\mathbf{y}, \tau} S_{\mathbf{y}, \tau'}. \quad (4)$$

Here, \mathbf{y} and \mathbf{z} are space coordinates, τ is the timelike coordinate. L_τ is the system size in the time direction. $\langle \mathbf{y}, \mathbf{z} \rangle$ denotes pairs of nearest neighbors in space. $J_{\mathbf{y}}$ is a binary-

random variable, which takes values J_l or J_h depending on the type of atom on the given lattice site \mathbf{y} . The concentration of sites with J_l and J_h are x and $1 - x$, respectively. The values of J_y at different lattice sites are not independent, but they are correlated.

Because the interaction is infinite-ranged in the timelike direction, this dimension can be treated within mean-field theory. This leads to coupled mean-field equations for the local magnetization at site \mathbf{y}

$$m_{\mathbf{y}} = \tanh \beta (J_{\mathbf{y}} m_{\mathbf{y}} + \sum_{\mathbf{z}} J_0 m_{\mathbf{z}} + h), \quad (5)$$

where $h = 10^{-10}$ is a small symmetry-breaking field and the sum is over all nearest neighbors of site \mathbf{y} . $\beta = 1/T_{cl}$ is the inverse classical temperature (not related to the physical temperature of the quantum system which is encoded in L_{τ}) [1]. The smeared phase transition can be tuned by changing the composition x in the temperature range $T_h > T_{cl} > T_l$, where $T_h = J_h + 6J_0$ and $T_l = J_l + 6J_0$ are the phase transition temperatures for pure systems with all $J_{\mathbf{y}} = J_h$ and $J_{\mathbf{y}} = J_l$, respectively.

In order to generate correlated binary random variables we use a more realistic method than the one used in Ref. [9]. We consider a model of A and B atoms with short-range interactions. This model is equivalent to an Ising model

$$H' = -J_{KW} \sum_{\langle \mathbf{y}, \mathbf{z} \rangle} n_{\mathbf{y}} n_{\mathbf{z}}, \quad (6)$$

where $n_{\mathbf{y}} = \pm 1$ corresponds to A and B atoms and $J_{KW} > 0$ for attractive correlations. To obtain correlated atom distributions with a well-defined concentration x , we use Monte Carlo simulations by the Kawasaki method [10]. We can control the correlations between the atoms by changing the ‘‘Kawasaki’’ temperature T_{KW} in these simulations. At $T_{KW} = 4.5$, atoms are correlated with power-law correlation, while at higher T_{KW} correlations are short-ranged (decay exponentially). Correlation length increases from 0 to ∞ with decreasing T_{KW} from ∞ to 4.5. Figure 1 show examples of the atom configurations for two T_{KW} and several concentrations x .

To study the smeared phase transition we then solve the mean-field equations (5) numerically. Figure 1 show the magnetization M as a function of concentration x for several disorder correlations (several T_{KW}). The data show that at a given x , the magnetization M increases with decreasing T_{KW} from ∞ to 4.5 (*i.e.* with increasing correlation length). Thus, the magnetization is enhanced compared to uncorrelated case. We also consider repulsive (anti-)correlations. To obtain repulsively correlated atoms, we set $J_{KW} < 0$ when generating the atom distribution. The solution of (5) shown in Figure 1 demonstrates that the magnetization is suppressed compared to the uncorrelated case.

CONCLUSIONS

We have studied the effects of spatial correlations between impurity atoms on smeared phase transitions. We have shown that even short-range correlations between atoms have dramatic effects and qualitatively modify the behavior of observables. Attractive disorder correlations enhance the magnetization in the tail of the smeared transition, while repulsive correlations suppress it. This is in contrast to conventional critical behavior, at

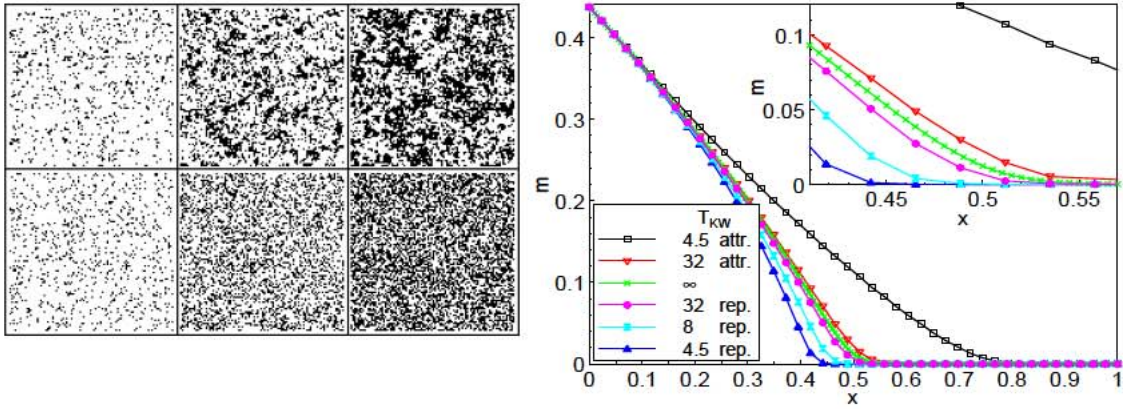


FIGURE 1. Left: Examples of the atom configuration on a square lattice of 96^2 sites generated by Kawasaki Monte Carlo simulations with attractive interactions $J_{KW} = 1$. The Kawasaki temperature T_{KW} is 4.5 in the top row and 32.0 in the bottom row. The concentration x takes values 0.1, 0.3 and 0.5 (left to right). Right: Magnetization M versus composition x for correlated disorder ranging from strong attractive correlations to strong repulsive (anti-)correlations. The data stem from one disorder realization of 256^3 sites for each case, using $J_h = 20$, $J_l = 8$, $J_0 = 1$, $h = 10^{-10}$, and $T_{cl} = 24.25$.

which correlations that decay sufficiently fast lead to the same critical behavior as uncorrelated disorder. We have verified our theoretical predictions by performing computer simulations. To this end, we have generated both attractively and repulsively correlated disorder by means of Kawasaki Monte Carlo simulations. We have found that the resulting data qualitatively agree with our theory. We emphasize that our results do apply not only to the quantum phase transitions considered here, but to all disorder induced smeared phase transitions.

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