Nonmonotonic Crossover of the Effective Susceptibility Exponent

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We have numerically determined the behavior of the magnetic susceptibility upon approach of the critical point in two-dimensional spin systems with an interaction range that was varied over nearly 2 orders of magnitude. The full crossover from classical to Ising-like critical behavior, spanning several decades in the reduced temperature, could be observed. Our results convincingly show that the effective susceptibility exponent γ_{eff} changes *nonmonotonically* from its classical to its Ising value when approaching the critical point in the ordered phase. In the disordered phase the behavior is monotonic. Furthermore, the hypothesis that the crossover function is universal is supported. [S0031-9007(97)03721-6]

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At a continuous phase transition, several thermodynamic observables diverge as a power of the temperature distance to the critical point. These powers, or critical exponents, have universal values which are identical for large classes of systems. For example, uniaxial ferromagnets, binary alloys, simple fluids, binary mixtures, ionic solutions, and polymer mixtures all belong to the three-dimensional Ising universality class. However, the corresponding power-law behavior is only observed asymptotically close to the critical point. As stated by the Ginzburg criterion [1], classical or mean-field-like critical behavior may be observed at temperatures farther away from the critical temperature T_c. The explanation of this *crossover* in terms of competing fixed points of a renormalization-group transformation is one of the great achievements of Wilson's renormalization theory. Nevertheless, the precise nature of the crossover between these two universality classes is still subject to debate. Theoretically, several attempts have been made to approximately calculate crossover functions. For instance, Nicoll and Bhattacharjee [2] solved the renormalization equations in d dimensions to second order in $\epsilon = 4 - d$ by applying a specific matching condition, whereas Bagnuls and Bervillier [3] used massive field theory in $d = 3$. The results of Belyakov and Kiselev [4] are phenomenological generalizations of first-order ϵ expansions. All these results are only valid in the symmetric phase $(T > T_c)$ and suggest that the crossover behavior is universal. However, Anisimov *et al.* [5] claimed that, while at criticality microscopic cutoff effects may be neglected compared to the infinite correlation length, this is no longer the case in the crossover region. This implies that the crossover functions cannot be represented as universal functions of one variable. A particular question concerns the variation of the so-called effective exponents describing the continuous change from one type of power-law behavior to another in the crossover region. Whereas some calculations predict a strictly monotonical variation, others indicate that a *nonmonotonical* variation might be possible. While on the theoretical side several important open questions remain, the experimental situation is hardly better. Measurements in the critical region are difficult, and accurate results are scarce. Fisher [6] has discussed experiments on micellar solutions (expected to belong to the Ising universality class) [7] that yielded values for the susceptibility exponent γ that lie below the classical value $\gamma_{MF} = 1$, while the Ising value is given by $\gamma_I = 1.237$ [8]. He argues that these results can be incorporated in a standard scaling description of crossover behavior if one allows for an effective susceptibility exponent that varies nonmonotonically as a function of the reduced temperature $t = (T - T_c)/T_c$. More recently, Anisimov *et al.* [9] measured a susceptibility χ for which they found that the logarithmic derivative $\gamma_{\text{eff}} \equiv -d \ln \chi / d \ln |t|$ approached the Ising value from *above* upon approach of the critical point. As this implies a nonmonotonical variation of γ_{eff}, Bagnuls and Bervillier subsequently suggested that the measurements might have been taken outside the critical region, see Refs. [10,11]. Indeed, since the crossover region is expected to span several decades in the reduced temperature [5,6], in many experiments the full crossover behavior cannot be observed. At the same time, the large extent of the crossover region reinforces its experimental relevance: Many measurements of critical exponents are actually made *within* the crossover region, and thus only a detailed knowledge of the crossover behavior guarantees a correct interpretation of the data.

Although it is tempting to apply numerical simulations to shed some light on these issues, in practice one encounters difficulties comparable to those experienced by experimentalists. In particular the size of the crossover region constitutes a towering hurdle. A major effort has been undertaken in Ref. [12] for three-dimensional polymer mixtures, in which crossover occurs as a function of the polymer chain length. These systems offer the advantage that the crossover can be influenced both by varying the temperature and by changing the chain length. Despite chain lengths of up to 512 monomers, the results did not span the full crossover region. Mon and Binder [13] examined the two-dimensional Ising model with an extended range of interaction R, where crossover from Ising to classical behavior occurs when R is increased. They studied crossover in finite systems at $T = T_c$. Even in these systems the mean-field regime could hardly be reached. In Ref. [14] we showed that a new Monte Carlo (MC) cluster algorithm for long-range interactions [15] could be applied to this model, leading to a speed increase of many orders of magnitude compared to conventional algorithms.

In this Letter we use this algorithm to study two-dimensional Ising systems with a variable interaction range and present results for the crossover behavior of the magnetic susceptibility at temperatures below and above T_c. Although two-dimensional systems are simpler than their three-dimensional counterparts, this model exhibits a surprising behavior. In particular, a qualitative difference between $T < T_c$ and $T > T_c$ is found. The advantage of examining two-dimensional instead of three-dimensional systems is the much larger variation of the critical exponents in the crossover region and the accessibility of larger interaction ranges, which makes it feasible to cover the full crossover region.

The model under investigation was introduced in Ref. [13] and is defined by the following Hamiltonian:

$$\mathcal{H}/k_BT = -\sum_{ij} K_d(\mathbf{r}_i - \mathbf{r}_j)s_i s_j\,, \qquad (1)$$

where the spins s take the values ± 1, the sum runs over all spin pairs, and the spin-spin coupling depends on the distance $|\mathbf{r}|$ between the spins as $K_d(\mathbf{r}) = cR_m^{-d}$ for $|\mathbf{r}| \leq R_m$ and $K_d(\mathbf{r}) = 0$ for $|\mathbf{r}| > R_m$. For finite R_m the critical behavior of this model will be Ising-like, but for $R_m \to \infty$ it will be classical. This implies a singular dependence of the critical amplitudes on R_m, which was first derived on phenomenological grounds in Ref. [13]. In Ref. [14] a renormalization derivation of these singular dependences was given, which, in addition, revealed logarithmic corrections for $d = 2$. To avoid lattice effects we formulate range dependences in terms of an effective interaction range R, which is directly related to R_m [13]. The Ginzburg criterion introduces a parameter $G \propto R^{-2d/(4-d)}$ (the Ginzburg number) which determines whether the critical behavior will be Ising-like ($t \ll G$) or classical ($t \gg G$). In the latter case, care must be taken that t is still within the critical region. For many experimental systems the Ginzburg number is not small, and one has left the critical region before observing the full crossover to classical critical behavior. In our model system, G is adjustable so that we can vary t/G over the full crossover region while keeping t sufficiently small. On the other hand, for a too small Ginzburg number, the critical point must be approached very closely to access the Ising regime. The diverging correlation length is then, in our simulations, truncated by the finite system size L. Therefore we construct the crossover function by studying systems with various values of G (interaction ranges) such that t has to be varied only within a limited range (but in such a way that the results for several different G overlap at fixed t/G).

We have carried out MC simulations of square systems with periodic boundary conditions containing up to 1000×1000 spins in which each spin interacts with up to 31 416 neighbors. This corresponds to an effective interaction range R of 71 lattice spacings or intermolecular distances. To avoid systematic errors in the determination of the crossover behavior, an accurate estimate of T_c as a function of R is required. For systems with interaction ranges up to $R \approx 8.3$, results for $T_c(R)$ have been obtained in Ref. [14]. For larger ranges the critical temperature can be calculated to a comparable accuracy from a renormalization expression for $T_c(R)$ [14]. Further simulational details will be presented elsewhere [16].

In the two-dimensional Ising model $\gamma_I = 7/4$, and the susceptibility χ diverges for $t \uparrow 0$ as $A_I^-(-t)^{-7/4}$ and for $t \downarrow 0$ as $A_I^+ t^{-7/4}$. The critical amplitudes for the nearest-neighbor model are known exactly [17], $A_I^- = 0.025537\ldots$, and $A_I^+ = 0.96258\ldots$. Note the very large asymmetry, $A_I^+/A_I^- \approx 38$. Mean-field theory predicts a susceptibility that for $t \uparrow 0$ diverges as $1/(-2t)$ and for $t \downarrow 0$ as $1/t$, i.e., a susceptibility exponent $\gamma_{MF} = 1$ and a much smaller ratio $A_{MF}^+/A_{MF}^- = 2$. As derived in Refs. [13,14], the Ising critical amplitude of the susceptibility is proportional to $R^{-3/2}$. Thus, in a graph displaying the results for various ranges as a function of the crossover variable $t/G \propto tR^2$, a data collapse is obtained for χ/R^2. The susceptibility is related to the average magnetization per spin m. In our simulations we have, for $t < 0$, sampled the connected susceptibility given by the fluctuation relation $\tilde{\chi} = L^d(\langle m^2\rangle - \langle|m|\rangle^2)/k_BT$, whereas for $t > 0$ we have used $\chi = L^d\langle m^2\rangle/k_BT$.

In Fig. 1 we show the magnetic susceptibility below T_c for various system sizes and interaction ranges. This graph exhibits several interesting features. For very small values of $|t|$ the curves lie almost horizontal; this is the finite-size regime, where the correlation length is truncated by the system size. For somewhat larger values of $|t|$ the curves start following the Ising asymptote with slope [i.e., the logarithmic derivative $d\ln\chi/d\ln|t|$] $-7/4$. This is the critical behavior as it is experimentally measured close to T_c. Also, the critical amplitude A_I^- is accurately reproduced by the simulations. At even lower T, we see that the curves for systems with small interaction ranges start to deviate from the Ising asymptote toward the mean-field asymptote (slope -1) without actually reaching it. These systems have left the critical region and the order

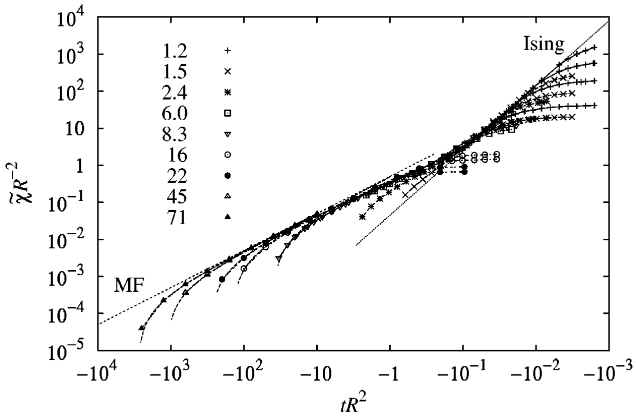

FIG. 1. Crossover behavior of the connected susceptibility $\tilde{\chi}$ for various ranges and system sizes. In this and all following figures, the numbers in the key refer to values for the interaction range R.

parameter shows strong saturation effects (which decreases the susceptibility). However, systems with a larger interaction range clearly cross over to the mean-field asymptote, reproducing the mean-field critical amplitude A^-_{MF}. For even lower temperatures these systems also exhibit saturation effects, which for $R \gtrsim 8.3$ are accurately described by mean-field theory (dashed curves). However, the outstanding feature of this graph is the region between the Ising and the mean-field asymptote. Namely, before settling at the latter asymptote, the curve describing the susceptibility first has (in this double-logarithmic plot) a slope that is *less steep* than in the mean-field regime. That is, $\gamma^-_{\text{eff}} < 1$ (the superscript minus sign indicates that we are considering the case $t < 0$). To illustrate this effect more clearly we have reproduced Fig. 1 without the data that are plagued by finite-size effects or lie outside the critical region. Furthermore, we have corrected for the saturation effects for systems with large ranges. While this is a real physical effect, it can be removed by applying a correction factor accounting for the difference between the asymptotic mean-field susceptibility and the mean-field susceptibility affected by saturation. The resulting graph is shown in Fig. 2. The nonmonotonical variation of the

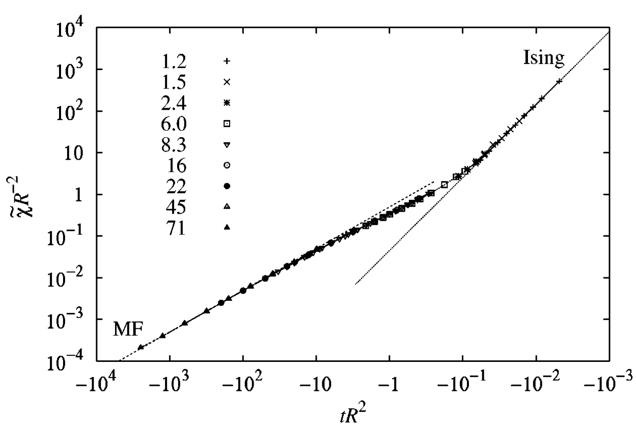

FIG. 2. Crossover curve for the connected susceptibility $\tilde{\chi}$.

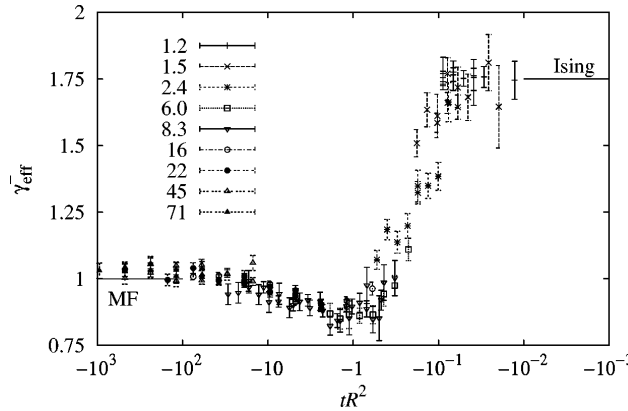

FIG. 3. The effective susceptibility exponent γ^-_{eff} below T_c.

slope is now clearly visible. The data for different interaction ranges $1 \lesssim R \lesssim 70$ overlap for considerable intervals of tR^2. The perfect collapse of these data lends strong support to the hypothesis that the crossover curve is universal and spans several decades in the reduced temperature. In addition, it follows from the renormalization treatment in Ref. [14] that the correlation length ξ decreases as $t^{-\nu}$ with an amplitude which is for $d = 2$ to leading order independent of R. Thus, at a fixed value of tR^2 the curves for different ranges have *different* values for ξ, and the fact that they collapse implies that the ratio between ξ and the lattice spacing a does not affect the crossover curve. This is markedly different from the results of Ref. [5] for $d = 3$. Also, the influence of irrelevant fields is not visible in the data collapse. To connect to experimental results, we have plotted the effective exponent γ^-_{eff} (obtained by numerical differentiation) in Fig. 3. Starting from T_c, γ^-_{eff} first steeply decreases to a minimum below γ_{MF} and then gradually rises to the asymptotic mean-field value.

Now we turn to the symmetric phase, for which a data collapse of the susceptibility χ is shown in Fig. 4. Just as below T_c, finite-size effects occur for very small t. Outside the finite-size regime the data for various R nicely collapse on the Ising asymptote, again with slope

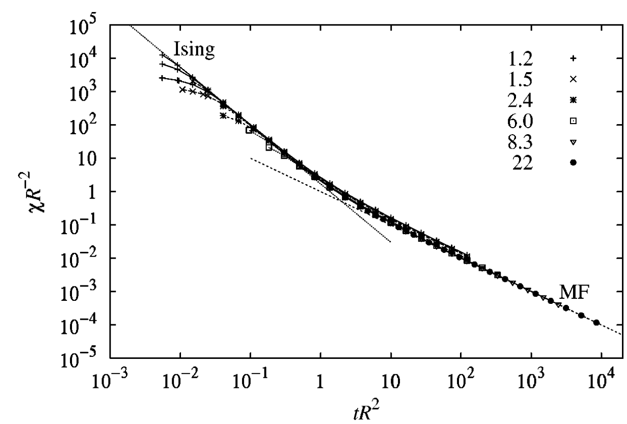

FIG. 4. Crossover behavior of the susceptibility χ for various ranges and system sizes.

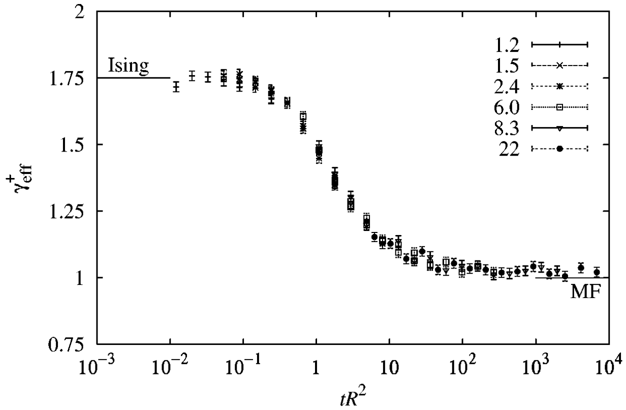

FIG. 5. The effective susceptibility exponent γ^+_{eff} above T_c.

$-7/4$ but with a much larger amplitude. For higher temperatures the curves appear to gradually approach the mean-field asymptote. However, the critical amplitude A^+_{MF} is reproduced only for larger interaction ranges. This stresses an important point: Above T_c no saturation of the order parameter occurs, marking the end of the critical region, but the system smoothly passes over to regular (noncritical) behavior. In this high-temperature region the susceptibility decreases proportional to $1/T$. It is this behavior that is seen in the graph at high temperatures for systems with small interaction ranges. As rightfully stressed by Bagnuls and Bervillier [10], this behavior should be clearly distinguished from classical *critical* behavior. Thus, it is by no means disturbing that the curves for small R deviate from the mean-field asymptote, and this does not imply a nonuniversal character of the crossover curve in the critical region. Disregarding these systems that have left the critical region, we note that above T_c the susceptibility smoothly crosses over from Ising-like to classical critical behavior and that the effective exponent γ^+_{eff} decreases monotonically from $7/4$ toward 1, as visualized in Fig. 5.

In conclusion, we have presented crossover curves for the magnetic susceptibility in two-dimensional Ising models with medium-range interactions, both for $t < 0$ and $t > 0$. Unlike previous treatments, which all suffered from some systematic limitations (like extrapolating low-order ϵ expansions to physical dimensions), the present approach, for the first time, gives an explicit description of crossover scaling functions for critical phenomena. At least in principle, these curves could be directly compared to experimental results. The large interaction ranges that could be accessed allowed us to observe the crossover between Ising-like and classical critical behavior for nearly six decades in the crossover variable. This has yielded, for the first time, strong numerical evidence that below T_c the effective susceptibility exponent γ_{eff} varies nonmonotonically between its Ising value and its classical value. Above T_c, on the other hand, the exponent shows a monotonical variation between the two limiting values. Thus, the plausibility of the occurrence of a minimum in γ_{eff} in three-dimensional systems, at least in the phase of broken symmetry, has been greatly increased. Furthermore, the fact that the crossover curves for many different interaction ranges collapse supports the hypothesis that this curve is universal.

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