

## Boundary between Long-Range and Short-Range Critical Behavior in Systems with Algebraic Interactions

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We investigate phase transitions of two-dimensional Ising models with power-law interactions, using an efficient Monte Carlo algorithm. For slow decay, the transition is of the mean-field type; for fast decay, it belongs to the short-range Ising universality class. We focus on the intermediate range, where the critical exponents depend continuously on the power law. We find that the boundary with short-range critical behavior occurs for interactions depending on distance  $r$  as  $r^{-15/4}$ . This answers a long-standing controversy between mutually conflicting renormalization-group analyses.

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Many of the intermolecular forces that play a central role in large areas of chemistry, physics, and biology have a long-ranged nature. Well-known examples are electrostatic interactions, polarization forces, and van der Waals forces. Remarkably, there are still considerable deficiencies in our knowledge of the critical behavior induced by these interactions, which include the prominent case of Coulombic criticality (see Ref. [1] for a review).

But also for the simpler case of purely attractive, long-range interactions, there exists a smoldering controversy, which we aim to resolve in this work. The present understanding of critical behavior in systems with such algebraically decaying interactions is largely based on the renormalization-group (RG) calculations for the  $O(n)$  model by Fisher, Ma, and Nickel [2]. Their analysis revealed that different regimes can be identified for the universal critical properties, characterized by the decay power of the interactions. In view of the small number of global parameters determining the universality class, the location of the boundaries between these regimes is of considerable interest. It is, therefore, disturbing to note that there appears to be still no consensus on the theoretical side regarding the precise location of the boundary between short-range and long-range critical behavior.

In this Letter, we address this issue by means of numerical calculations, which allow us, with minimal prior assumptions, to decide between contradictory RG scenarios. Concretely, we demonstrate that the onset of the long-range regime occurs for interactions that decay more slowly than found in Ref. [2]. This result not only bears upon condensed-matter systems with long-range interactions, but also has implications for the renormalization-group treatment of competing fixed points in general, including random systems and gauge theories.

Our approach specializes to the Ising model,  $n = 1$ , in  $d$  dimensions, described by the reduced Hamiltonian,

$$\mathcal{H}/k_B T = -K \sum_{\langle ij \rangle} \frac{s_i s_j}{r_{ij}^{d+\sigma}}, \quad (1)$$

where the spins  $s_k = \pm 1$  are labeled by the lattice site  $k$ , the sum runs over all spin pairs, and the pair coupling depends on the distance  $r_{ij} = |\vec{r}_i - \vec{r}_j|$  between the spins. According to the analysis of Fisher *et al.* [2], universality classes are parametrized by  $\sigma$ , and the following three distinct regimes were identified: (a) The classical regime; the upper critical dimension is given by  $d_u = 2\sigma$ , so that mean-field-type critical behavior occurs for  $\sigma \leq d/2$ . (b) The intermediate regime  $d/2 < \sigma < 2$ ; here the critical exponents are *continuous functions* of  $\sigma$ . (c) The short-range regime; for  $\sigma \geq 2$ , the universal properties are those of the model with short-range interactions, e.g., between nearest neighbors only; thus one observes that, for  $d = 3$ , van der Waals interactions (decaying as  $1/r^6$ ) actually lie quite close to the boundary between regimes (b) and (c).

Although the general outline of these results has been widely accepted, one part of this picture has become the scene of a debate that appears, until now, to be unresolved. This concerns the situation close to  $\sigma = 2$ . In Ref. [2], it has been conjectured that, throughout the intermediate regime (b), the correlation-function exponent  $\eta$  is *exactly* given by  $2 - \sigma$ . On the other hand, in the short-range regime (c),  $\eta$  takes a constant (but  $d$ -dependent) value  $\eta_{sr} > 0$  for all  $d < 4$ , resulting in a *jump discontinuity* in  $\eta$  at the decay power  $\sigma = 2$ . While this remarkable phenomenon is not forbidden by thermodynamic arguments (which require only  $\eta \leq 2 + \sigma$ ), it has attracted considerable attention over the past decades and various efforts have been undertaken to reinvestigate the corresponding RG scenario [3–6]. In addition, it may be remarked that this scenario does not capture the one-dimensional case, where a phase transition is rigorously known to be absent [7] for  $\sigma > 1$ , rather than for  $\sigma > 2$  (see also Ref. [8] and references therein). The issue was first addressed by Sak [3], who pointed out that higher-order terms in the RG equations considered in Ref. [2] generate additional short-range interactions in the renormalization process, which affects the competition between the long-range and the short-range fixed points of the RG transformation. As

a consequence, for  $d < 4$  the boundary between the intermediate and the short-range regime was found to shift from  $\sigma = 2$  to  $\sigma = 2 - \tilde{\eta}$ , where the  $\varepsilon$  expansion for  $\tilde{\eta}$  agrees to lowest orders with that of the short-range exponent  $\eta_{\text{sr}}$ . In a field-theoretic approach, Honkonen and Nalimov [6] proved, to all orders in perturbation theory, the stability of the short-range fixed point for  $\sigma > 2 - \eta_{\text{sr}}$  and of its long-range counterpart for  $\sigma < 2 - \eta_{\text{lr}}$ , where  $\eta_{\text{lr}}$  is the anomalous dimension of the field, evaluated at the *long-range* fixed point. Note that these authors also pointed out that the former result can be obtained from simple scaling arguments, but the latter *cannot*. Appealing aspects of these findings are, first, the continuous and monotonic  $\sigma$  dependence of the correlation-function exponent (provided that  $\eta_{\text{lr}}$  and  $\eta_{\text{sr}}$  coincide at  $\sigma = 2 - \eta_{\text{sr}}$ ), and, second, that the theory has now attained consistency with the exact results for the one-dimensional case.

However, the analysis of [3] has also been the subject of criticism. Van Enter [9] pointed out an apparent inconsistency in Sak's results. Three-dimensional *short-range*  $O(n)$  models exhibit a nonzero spontaneous magnetization below the critical temperature. Van Enter [9] derived that, for  $n \geq 2$ , this broken symmetry is inconsistent with the presence of a long-range perturbation with  $\sigma < 2$ . This contradicts Sak's finding that such perturbations are irrelevant in a nonvanishing range  $2 - \eta_{\text{sr}} < \sigma < 2$ . While this inconsistency emerges for  $n \geq 2$  and antiferromagnetic perturbations only, it may be taken as a sign that the renormalization scheme [3,6] is incomplete, which could thus also affect the purely ferromagnetic  $n = 1$  case. Another conflict with Sak's results arose from the analyses of Yamazaki [4]. A qualitative difference between his and Sak's result for the correlation-function exponent as a function of  $\sigma$  is the absence of a kink at  $\sigma = 2 - \eta_{\text{sr}}$ . However, we note a problem with the internal consistency of his results: The smoothly varying  $\eta(\sigma)$  was obtained by using a long-range (i.e.,  $k^\sigma$ -type, where  $k$  is the wave vector used in the Fourier representation) instead of a short-range ( $k^2$ -type) propagator in the RG calculations, despite the fact that, in the same calculation, it was found that the long-range term in the Landau-Ginzburg-Wilson Hamiltonian is irrelevant, and only the short-range term survives. A more serious objection was raised by Gusmão and Theumann [5] (but ignored in Ref. [6]), who argued that the parameter  $2 - \sigma$  (i.e.,  $2\alpha$  in the notation of Ref. [6]) is *not* a valid expansion parameter. They reconsidered the problem using renormalized perturbation theory in  $\varepsilon' = 2\sigma - d$ , and found that the long-range expansion in  $\varepsilon'$  is stable with respect to short-range perturbations up to  $\sigma = 2$ . This implies a restoration of the early result of Fisher *et al.* [2] that the boundary between the intermediate and the short-range regime lies at  $\sigma = 2$ . While, at least for  $d = 3$ , the difference between this value and  $\sigma = 2 - \eta_{\text{sr}}$  may be small, it indicates a fundamental dichotomy, which is also relevant for other systems with competing fixed points.

Until recently, it appeared not to be feasible to shed some light on this unsatisfactory situation by means of Monte Carlo simulations, for the following reasons. Since the problems reside in the transition region between the intermediate and the short-range regime, one expects corrections to scaling to converge only slowly with increasing system size. This necessitates the simulation of large systems. Since each spin interacts with all other spins in the system, the amount of work per Metropolis-type spin visit then becomes prohibitive. Use of a cluster Monte Carlo algorithm [10] that employs a number of operations per spin flip that is *independent of the system size*, and moreover suppresses critical slowing down, has now enabled us to obtain highly accurate data for sufficiently large system sizes.

We present numerical results for the critical exponent  $\eta$  and the Binder cumulant [11] as a function of  $\sigma$ , which allow us to distinguish between the different theories. The simulated systems are defined on  $L \times L$  lattices with periodic boundaries and sizes from  $L = 4$  to  $L = 1000$ . We chose to study two-dimensional systems not only to maximize the attainable linear system size, but, in particular, because there the exponent  $\eta_{\text{sr}} = \frac{1}{4}$  has a much larger value than for  $d = 3$  ( $\eta_{\text{sr}} \approx 0.037$ ); this maximizes both the size of the disputed region  $(2 - \eta_{\text{sr}}, 2)$  and the magnitude of the supposed jump in  $\eta(\sigma)$ . The length of the simulations was such that (for the largest system sizes) typically a relative uncertainty of one part in a thousand was reached for the Binder cumulant. The precise form of the pair interaction was taken as

$$\tilde{K}(|\vec{r}|) = K \int_{r_x-(1/2)}^{r_x+(1/2)} dx \int_{r_y-(1/2)}^{r_y+(1/2)} dy \frac{1}{(x^2 + y^2)^{(d+\sigma)/2}}, \quad (2)$$

where  $\vec{r} = (r_x, r_y)$  denotes the difference between the integer coordinates of the two interacting spins. It is important to note that this interaction, which was adopted for purely technical reasons [10], differs from the interaction in Eq. (1) only in powers of  $r$  that decay faster than  $r^{-d-\sigma}$ ; these terms are irrelevant and will affect only nonuniversal terms, such as the location of the critical point. The critical exponents and boundaries of the regimes (a)–(c) will not be altered. As mentioned, we have adopted periodic boundary conditions, which are expected to speed up the approach to the thermodynamic limit. No artificial cutoff was imposed on the interaction range: Interactions take place between all periodic images.

We have carried out simulations for decay powers  $\sigma = 1.2, 1.4, 1.6, 1.75, 1.85, 1.95, 2.0, 2.05, 2.25, 2.5, 2.75$ , and  $3.0$ . For each value of  $\sigma$ , we have determined the critical coupling  $K_c$  on the basis of a finite-size scaling analysis of the susceptibility-like quantity  $\langle m^2 \rangle$  and of the dimensionless amplitude ratio  $Q \equiv \langle m^2 \rangle^2 / \langle m^4 \rangle$ , where  $m$  is the magnetization density.  $Q$  is a variant of the fourth-order cumulant introduced by Binder [11]. For Ising-like

systems above the upper critical dimension, i.e., in the classical regime, it has been predicted [12] to take the universal critical value  $8\pi^2/\Gamma^4(\frac{1}{4}) \approx 0.456947$ , the same value as in the mean-field model [10]; this has been confirmed numerically in Ref. [13]. In the short-range regime, it takes a universal value close to  $Q = 0.856216\dots$  [14,15]. In the intermediate regime, finally,  $Q$  has been calculated by means of a singular expansion in  $\varepsilon'$ , up to second order in  $\sqrt{\varepsilon'}$  [16,17]. From the magnetic susceptibility, which diverges as  $L^{\gamma/\nu}$  at criticality,  $\eta$  can be extracted using the scaling law  $\gamma = (2 - \eta)\nu$ . An important issue in these finite-size analyses is the fact that the correction-to-scaling exponents are essentially unknown, and actually depend on the borderline value of  $\sigma$ . In particular, there will be logarithmically decaying finite-size corrections at the borderline itself. Considerable effort has been exercised to encompass all such uncertainties in the quoted margins for our estimates for  $K_c$ ,  $Q$ , and  $\eta$  (see Table I).

While the detailed least-squares analysis depended on the value of  $\sigma$ , the following general procedure was applied. An (effective) leading correction-to-scaling exponent  $y_i$  was obtained from a fit of the amplitude ratio  $Q$ , in which also temperature-dependent terms were taken into account. Subsequently,  $\gamma/\nu$  was extracted from an analysis of  $\langle m^2 \rangle$  in which  $y_i$  was kept fixed. This allowed us to include higher-order corrections. The analysis was then repeated with  $y_i$  varied within its uncertainty margins, in order to determine the uncertainty in  $\gamma/\nu$ . Finally, the entire analysis was repeated for different minimum system sizes. For  $\sigma = 1.75$ , a consistent analysis could be obtained only by allowing for logarithmic corrections to scaling, as would be expected if the crossover from long-range to short-range criticality occurs at  $\sigma = 2 - \eta_{sr}$ .

The critical coupling exhibits a very smooth but also remarkable, almost parabola-shaped dependence on  $\sigma$ , with

TABLE I. Results of detailed finite-size-scaling analyses for two-dimensional systems with power-law interactions, for several values of the decay parameter  $\sigma$ . The results for the critical coupling  $K_c$ , the fourth-order amplitude ratio  $Q$ , and the correlation-function exponent  $\eta$  are followed by the estimated error in the last decimal places. The last column lists the predicted values for  $\eta$  (see the text).

$\sigma$	$K_c$	$Q$	$\eta$	$\eta$ [predicted]
1.20	0.114966 (3)	0.559 (4)	0.798 (18)	0.80
1.40	0.125300 (4)	0.650 (3)	0.616 (10)	0.60
1.60	0.133397 (5)	0.752 (7)	0.410 (24)	0.40
1.75	0.137872 (2)	0.840 (10)	0.286 (24)	0.25
1.85	0.140073 (3)	0.85 (3)	0.30 (6)	0.25 or 0.15
1.95	0.141644 (3)	0.849 (14)	0.24 (4)	0.25 or 0.05
2.00	0.142198 (3)	0.850 (6)	0.266 (16)	0.25
2.05	0.142610 (8)	0.857 (7)	0.260 (14)	0.25
2.25	0.142831 (9)	0.856 (7)	0.248 (12)	0.25
2.50	0.140401 (8)	0.860 (3)	0.246 (8)	0.25
2.75	0.135636 (11)	0.855 (3)	0.250 (10)	0.25
3.00	0.129267 (12)	0.857 (3)	0.248 (8)	0.25

a maximum around  $\sigma = 2.17$ . This nonmonotonic variation may be due to our use of the integrated coupling (2) which tends to enhance the close-neighbor couplings, in particular for large  $\sigma$ . For  $\sigma > 2$ , both  $Q$  and  $\eta$  are fully consistent with the known values for the two-dimensional Ising universality class. On the other hand, for  $\sigma \leq 1.60$ ,  $\eta$  is in excellent agreement with the RG prediction  $2 - \sigma$  [2];  $Q$  exhibits a remarkably linear deviation from its mean-field value [16]. However, in the disputed region  $1.75 \leq \sigma < 2.0$ , where we invested most of our computing efforts, the uncertainties are still considerable; this is by itself already indicative of the occurrence of a crossover between two fixed points.

In the absence of accurate predictions for the amplitude ratio  $Q$  (depicted in Fig. 1), this quantity does not provide much further evidence to distinguish between the different theoretical scenarios. However, there is no evidence for a jump in  $Q$  at  $\sigma = 2$ ; this fails to support the Gusmão and Theumann analysis [5]. For  $\sigma = 1.85$  and  $\sigma = 1.95$ , we find that  $Q$  is compatible with the 2D Ising value, and the deviation of about 1.5 standard errors at  $\sigma = 1.75$  is still within acceptable limits.

On the other hand, the exponent  $\eta$  offers clear evidence in order to distinguish between the different scenarios (cf. Fig. 2). While also this quantity suffers from relatively large uncertainties in the crossover region, these uncertainties are small enough to exclude the scenario of Ref. [5] which implies that a transition to short-range critical behavior occurs at  $\sigma = 2$  and that  $\eta = 2 - \sigma$  for  $\sigma < 2$ . Indeed, instead of the 2D Ising value  $\eta = \frac{1}{4}$ , this exponent should then take the values 0.15 at  $\sigma = 1.85$  and 0.05 at  $\sigma = 1.95$ . However, at these two values of  $\sigma$ , our results for  $\eta$  lie within one standard deviation from the 2D Ising value, and two-and-a-half, respectively almost five, standard deviations above  $2 - \sigma$ .

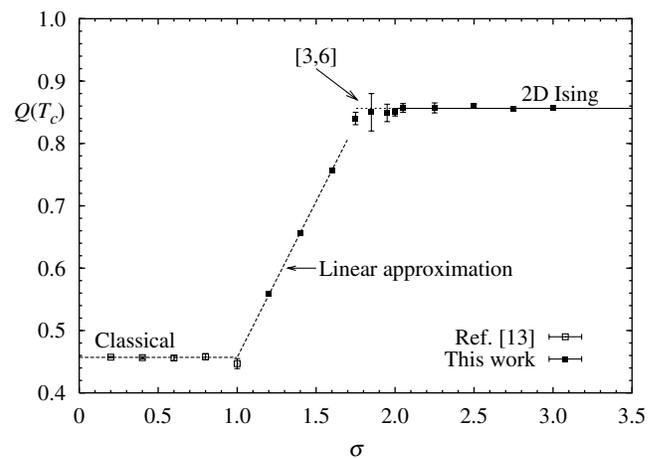


FIG. 1. The amplitude ratio  $Q$  as a function of the decay parameter  $\sigma$ . The behavior is consistent with a crossover from long-range to short-range critical behavior around  $\sigma = 1.75$ , as predicted in Refs. [3,6].

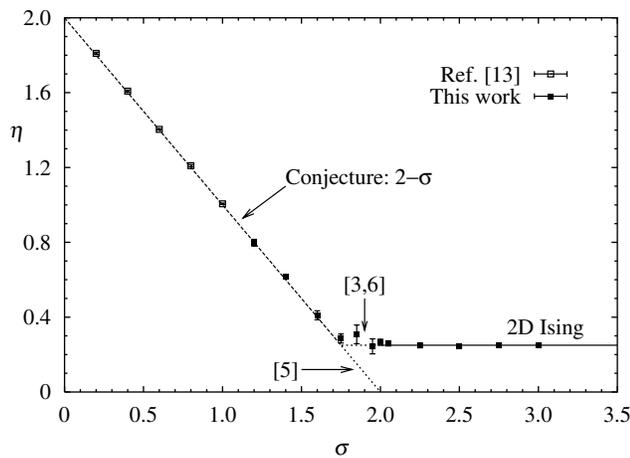


FIG. 2. The correlation-function exponent  $\eta$  as a function of the decay parameter  $\sigma$ . For  $\sigma < 1.75$  the data are in excellent agreement with the conjecture  $\eta = 2 - \sigma$  [2], whereas for  $\sigma > 1.75$  they agree with the  $d = 2$  short-range Ising universality class. A crossover at  $\sigma = 2$  [5] is clearly excluded.

In summary, we have demonstrated that both the correlation-function exponent  $\eta$  and the fourth-order amplitude ratio  $Q$  take their (universal) short-range Ising values for  $\sigma > 2 - \eta_{\text{sr}}$ . For  $\sigma > 2$  this could be shown with high numerical accuracy, but also for  $2 - \eta_{\text{sr}} < \sigma < 2$  the results are precise enough to convincingly exclude a crossover from long-range to short-range critical behavior at  $\sigma = 2$ . Instead, they support a crossover at  $\sigma = 2 - \eta_{\text{sr}}$ , in agreement with Refs. [3,6]. This provides a clear answer to the dilemma posed by conflicting renormalization-group scenarios.

Furthermore, our findings for  $\eta$  are in excellent agreement with  $\eta = 2 - \sigma$  in the intermediate range  $d/2 < \sigma < 2 - \eta_{\text{sr}}$ , supporting the conjecture that all higher-order contributions vanish in the  $\varepsilon'$  expansion for  $\eta$  [2] and in contrast with the scenario proposed in Ref. [4].

The amplitude ratio  $Q$  depends approximately linearly on  $\sigma$  for  $d/2 < \sigma < 2 - \eta_{\text{sr}}$ . Remarkably, the most prominent deviations from linearity occur near  $\sigma = 2 - \eta_{\text{sr}}$ , while the  $\varepsilon'$  expansion predicts a square-root-like singularity at the opposite end of the intermediate range [16].

Finally, we quote a plausible explanation for the breakdown of the description of Ref. [5] in the range  $2 - \eta_{\text{sr}} < \sigma < 2$  [18]. If the validity of the  $\varepsilon'$  expansion is not uniform in  $\sigma$ , the region of convergence may shrink to zero when  $\sigma$  approaches 2. Then one cannot fix  $\varepsilon'$  and take

the limit  $\sigma \rightarrow 2$ , as is done in Ref. [5]. This would also explain why the long-range ( $\varepsilon'$ ) expansion does not provide any indication of a change to short-range behavior at  $\sigma = 2 - \eta_{\text{sr}}$ .

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