Finite-Size Scaling and Lack of Self-Averaging in Critical Disordered Systems

Shai Wiseman and Eytan Domany

Department of Physics of Complex Systems, The Weizmann Institute of Science, Rehovot 76100, Israel

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We simulated site dilute Ising models in $d = 3$ dimensions for several lattice sizes L. For each L singular thermodynamic quantities X were measured at criticality and their distributions $P(X)$ were determined for ensembles of several thousand random samples. For $L \to \infty$ the relative width of $P(X)$ tends to a universal constant: there is no self-averaging. The width of the distribution of the sample (i) dependent pseudocritical temperatures $T_c(i, L)$ scales as $\delta T_c(L) \sim L^{-1/\nu}$ and *not* as $\sim L^{-d/2}$. The sample dependence of $X_i(T, L)$ enters dominantly, but not exclusively, via $T_c(i, L)$. [S0031-9007(98)06491-6]

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Phase transitions in systems with quenched disorder are of considerable theoretical and experimental interest and have been the subject of intensive investigations. Nonetheless, there are only a few general exact results on such systems and some of these raised questions which were left unanswered for more than a decade. For example, the Harris criterion [1], which states the condition for stability of a pure fixed point against disorder as $1/\nu_{\text{pure}} \leq d/2$, was derived assuming that fluctuations of the local critical temperature $T_{c,L}$ of a region of size ξ_L^d scaled as $\delta T_c \sim \xi_L^{-d/2}$. Another result by Chayes *et al.* [2] stated that $1/\nu \leq d/2$ for any disordered system. This is identical with the Harris criterion for disordered systems governed by a pure fixed point. For systems governed by a random fixed point it raised the question as to whether the relation $\delta T_c \sim \xi^{-d/2}$ holds in this case as well.

Another important and relevant issue concerns the meaning of measurements done on disordered systems at or near their transition points. All measurements (experimental and numerical) are obtained for finite systems; moreover, each such system constitutes a particular realization of the quenched randomness. Hence, while taking the infinite system limit, increasing system size L, we also move between different realizations of the randomness. Thus the only meaningful objects for finite-size scaling are *distributions* of various properties in ensembles of random systems. Usually, measurements (experimental and numerical) are taken on a single (or a few) large system, and it is important to ascertain to what extent are the results obtained for a single system representative of the general class to which it belongs. The answer hinges on the important issue of self-averaging. If a quantity is not self-averaging, increasing L does not improve the statistics of its measurement (sample-to-sample fluctuations remain large). Whereas it has been known that for (spin and regular) glasses [3] there is no self-averaging in the ordered phase, the discovery [4] that there is no self-averaging for random *ferromagnets* at their critical point came as somewhat of a surprise (off criticality self-averaging does hold). The numerical work on which this claim was based has been backed up with a finite-size scaling ansatz [4] which seemed to fit the data quite well. Subsequently the issue has been investigated by Aharony and Harris (AH) [5], who provided a theoretical understanding of the absence of self-averaging in critical random ferromagnets. The central point of AH was that a random fixed point is characterized by a *distribution of nonzero width* of some measurable quantities (such as energies, susceptibilities, etc.), and hence if an ensemble of systems flows to this fixed point, its properties must also be distributed in a similar way. The argument was supported by a renormalization group calculation in $d = 4 - \epsilon$ dimensions. The AH work led to several predictions, some of which were in clear disagreement with the scaling theory [4]. Since neither the general arguments nor the results obtained by ϵ expansion can be viewed as definitive, independent confirmation is desired. Furthermore, recently claims were made [6] to the effect that the manner, in which the sample-to-sample fluctuations of the pseudocritical temperature scale with size, governs one's ability to observe the "true" critical exponents of random systems, quantum and classical.

In order to investigate these fluctuations, the extent to which our finite-size scaling ansatz holds and to test the AH results, we carried out extensive simulations of the $3 - d$ Ising model with site dilution. For the pure model the exponent $\alpha_p = 0.11 > 0$ [7], randomness is relevant, and the critical behavior is governed by a random fixed point. Various aspects of the critical properties of this model have been measured very carefully [8]. In particular, α, the specific heat exponent of the random model, is negative [8], consistent with [2].

We start by recapitulating a few definitions. Consider an ensemble of systems of linear size L, denoting a particular realization of the randomness by i. For each such system we measure, at temperature T, various thermodynamic densities $X_i(T, L)$ (such as the susceptibility per site $X = \chi$, magnetization M, etc.). Denote by $T_c(i, L)$ the pseudocritical temperatures of each of these samples

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[obtained, for example, by locating the maximum of χ (see Fig. 1)]. The sample-averaged pseudocritical temperature $T_c(L) = [T_c(i,L)]$ approaches, for $L \to \infty$, the asymptotic limit $T_c(L) \to T_c$. Our main results can be summarized as follows:

(i) *Lack of self-averaging.*—The values of χ, measured at T_c for many samples of size L, are distributed with mean $[\chi(L)]$ and variance $V_\chi(L)$. The normalized square width

$$R_\chi = V_\chi/[\chi]^2 \to C \text{ as } L \to \infty,$$

i.e., goes to a constant, for large L, as predicted by AH, in contradiction to our prediction $R \sim L^{\alpha/\nu}$. The distributions of various thermodynamic quantities do not become sharp in the thermodynamic limit and the system is not self-averaging.

(ii) *Universality.*—We studied different dilutions and two random ensembles, one with a fixed *concentration* of magnetic sites (grand canonical) and the other with a fixed *number* of spins, placed at random on the lattice (canonical). For grand-canonical ensembles with different concentrations, AH predicted that the constant C is universal and indeed we find the same asymptotic width. However, their predicted (to order ϵ^0) universal value is $R_M/R_\chi = 0.25$; we find 0.35(2). Two different ensembles *seem* to asymptote to different values of R [9,10] (even when the concentration in one equals the fraction of spins of the other).

(iii) The pseudocritical temperatures $T_c(i,L)$ are distributed with a width $\delta T_c(L)$ which scales as

$$\delta T_c(L) \sim L^{-1/\nu}. \tag{1}$$

This behavior was suggested by AH, reasoning that when combined with the finite-size scaling theory of [4] it gave rise to the lack of self-averaging discussed in item (i). However, this reasoning depends on the validity of the finite-size scaling theory. Here we establish the validity of (1) independently of any additional assumptions. We rule out the possibility that $\delta T_c(L) \sim L^{-d/2}$ as was assumed by us [4] and listed by others [6] as "the most likely scenario." The latter behavior occurs only in systems governed by a pure fixed point [1]. Note that the critical concentration in percolation [11] behaves as in (1) (see also a similar phenomenon in the random-field Ising model [12]).

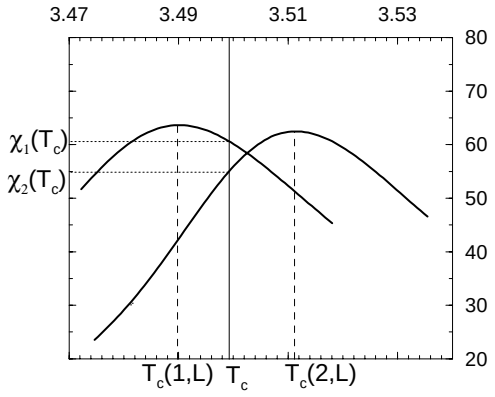

FIG. 1. Susceptibility per spin of two systems of size $L = 32$, generated with site occupation probability $p = 0.8$ versus temperature. $T_c(i,L)$ denotes the pseudocritical temperature of sample i, identified by the maximum of the susceptibility. T_c is the value approached by the mean of these in the $L \to \infty$ limit.

(iv) The finite-size scaling form assumed in [4],

$$X_i(T,L) \approx L^\rho Q_i(\dot{t}_i L^{1/\nu}), \tag{2}$$

$$\dot{t}_i = [T - T_c(i,L)]/T_c, \tag{3}$$

where $\dot{t}_i$ is a sample-dependent reduced temperature, is correct. The sample dependence of X_i is predominantly due to the sample dependence of $\dot{t}_i$.

(v) Different realizations with the same $\dot{t}_i$ and L still have slightly different X_i; the scaling function $Q_i(x)$ *does* depend on the realization i via some intrinsic variable not yet understood.

(vi) It may be computationally advantageous to measure various quantities, for instance, to find critical exponents, at the sample-dependent pseudocritical point $T_c(i,L)$ (where $\dot{t}_i = 0$), rather than at T_c. This is so since, as a consequence of item iv, the variance at $T_c(i,L)$ is much smaller.

We now present numerical evidence for each of the statements made above.

The site-dilute Ising model.—Each site of a cubic lattice is either occupied by an Ising spin or empty. Here we report results obtained for a grand-canonical ensemble of samples in which the occupation of each site was determined independently with probability $p = 0.8$. At this probability Heuer found the fastest crossover to the asymptotic (random) critical behavior [8]. We used the Wolff [13] single cluster algorithm [14] with skewed periodic boundary conditions [15] on lattices of sizes $L = 4$, 8, 16, 32, and 64. For each of these sizes we simulated, respectively,

$$n_L = 10\,000,\ 4000,\ 32\,000,\ 4000, \text{ and } 1479$$

different random samples. High-precision measurements of various critical properties yielded $T_c = 3.49921(3)$, $\alpha/\nu = -0.066(9)$, $\beta/\nu = 0.505(2)$, $\gamma/\nu = 1.990(4)$, $1/\nu = 1.467(5)$, in good agreement with [8].

Lack of self-averaging, distribution of the critical susceptibility.—Curves of $\chi(T) = ([\langle M^2\rangle - \langle|M|\rangle^2])/pL^3T$ are presented in Fig. 1 for two samples of size $L = 32$.

From measuring $\chi_i(T_c) = [\langle M^2\rangle]/pL^3T_c$ (without subtraction of $[\langle M^2\rangle]$) for an ensemble of samples we constructed the histogram of Fig. 2, for various sizes L.

As evident from the histograms and from the inset, the widths of these distributions approach a constant for increasing L. This is the result of AH, whereas our scaling theory [4] would predict $R_\chi \sim L^{\alpha/\nu}$. The source of the discrepancy is an assumption we made regarding the distribution of the pseudocritical temperatures; had we assumed that (1) holds, our scaling ansatz would have also

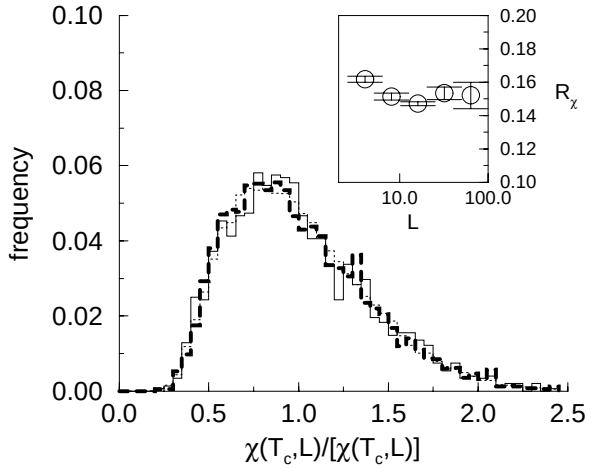

FIG. 2. Distribution of the critical susceptibilities, measured at T_c for different samples and different sizes $L = 16$ (thin dotted line), $L = 32$ (thick dashed line), and $L = 64$ (thin solid line). For each L the values of $\chi_i(T_c, L)$ were normalized by the ensemble average of all samples of that size. The inset shows the second moment of the distribution as a function of L; evidently $R_\chi \to C$.

produced the correct result $R_\chi \sim$ const. Therefore confirmation of this result may serve as an indication of the validity of (1) as well. Nevertheless, since this interpretation depends on the validity of further assumptions implicit in our scaling theory, it is important to verify independently and directly scaling and (1).

Universality.—We studied two more random ensembles: another grand-canonical one, but with occupation probability $p = 0.6$, and a canonical one with a fixed number of $0.6L^d$ spins, randomly placed in each sample. We found that the limiting values of both R_χ and R_m are the same for the two grand-canonical ensembles (with $p = 0.8, 0.6$), indicating universality, but for the canonical ensemble different values were obtained. These results will be presented and explained elsewhere [9].

Distribution of the pseudocritical temperatures.—We estimated, using the histogram reweighting method [16], the pseudocritical temperature $T_c(i, L)$ of every sample of our ensembles. This was done in an iterative way; the first guess for $T_c(i, L)$ was T_c—from data collected at this point we calculated the susceptibility as a function of T; the temperature at which it had its maximum was our next estimate for $T_c(i, L)$, where more data were collected, and so on. The procedure converged in less than ten iterations within the resolution imposed by the statistical error in determining the temperature of the maximal χ. The resulting histograms for several sizes are collapsed on Fig. 3 using the value of $y_t = \frac{1}{\nu} = 1.467(5)$ which was determined independently [10] by simulations at T_c.

The means and widths of these distributions are

$$T_c(L) \approx T_c - 0.532 \cdot L^{-1/\nu}, \qquad \delta T_c(L) \approx 2.13 \cdot L^{-1/\nu}. \tag{4}$$

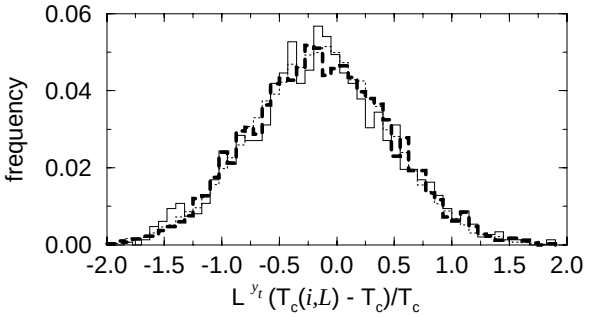

FIG. 3. Distribution of scaled pseudocritical temperatures obtained for sizes $L = 16$ (thin dotted line), $L = 32$ (thick dashed line), and $L = 64$ (thin solid line), using $y_t = 1/\nu = 1.467$ and $T_c = 3.4992$.

The width of the distribution exceeds by a factor of nearly 4 the shift of its average from T_c. Hence, the large fluctuations in $\chi(T_c)$ are due to the large value of $\delta T_c(L)$; when we perform measurements at the fixed temperature T_c, some samples we deal with will be considerably above their pseudocritical temperature and some below (see Fig. 1). We have also made straightforward fits of the variance $\delta T_c(L)^2$ to the form $\delta T_c(L)^2 \sim L^{-2\rho}$, and fits of the shift of $T_c(L)$ to $T_c(L) - T_c \sim l^{-\lambda}$; we found $\rho = 1.449(8)$ and $\lambda = 1.42(4)$. ρ is within errors of the shift exponent λ (its error bar is small); we believe that we can conclude $\rho \neq d/2 = 1.5$. Since one expects that $\lambda = y_t$ and we have also determined independently $y_t = 1.467(5)$, our results strongly suggest that all of these exponents are actually the same $\rho = \lambda = 1/\nu$.

Testing the scaling ansatz.—Replacing Q_i by Q in Eq. (2) constitutes an assumption that the dependence on the realization of the randomness can be absorbed in the pseudocritical temperature of the particular sample. Our first task was to check the extent to which this holds, i.e., to what extent can one collapse data obtained at different sizes and temperatures for different samples. Figure 4 presents the magnetization for two system sizes. The data collapse well onto two branches of a function, one below and one above $T_c(i, L)$, lending support to the validity of the scaling ansatz. We succeeded in fitting thousands of data points at three different sizes to two scaling functions (corresponding to the two branches). This may be interpreted as supporting a *strong scaling hypothesis*, e.g., that for large L,

$$X_i(T, L) \approx L^\rho \tilde{Q}(\dot{t}_i L^{1/\nu}). \tag{5}$$

Here we modified (2) by dropping the sample dependence of the scaling function, i.e., assuming that the *entire* sample dependence can be absorbed in $\dot{t}_i$. On the other hand, as evident from Fig. 4, the data points do exhibit considerable scatter about the main trend. To investigate the extent of violation of such a strong scaling relation, we studied the distribution of the susceptibility maxima.

Sample dependence of the scaling function.—If, instead of $\chi_i(T_c, L)$, we measure for each sample and

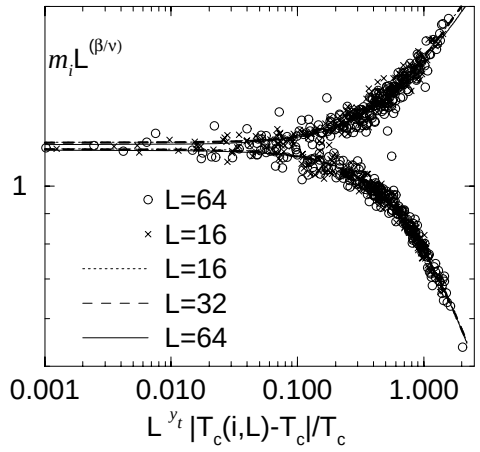

FIG. 4. Scatter plot of the scaled modulus of the magnetization, measured at T_c for ensembles of samples of two different sizes, plotted (on log-log scale) versus the scaled temperature $\dot{t}_i = \{T_c - T_c(i,L)\}/T_c$. The lines are the scaling functions fitted separately for three different sizes, showing remarkable agreement. The scatter of the points from the lines is due partially to measurement error (thermal) and partly to genuine sample dependence of the scaling function.

size the *maximal* value of the susceptibility $\chi_i^{\max} = \chi[T_c(i,L),L]$, we accumulate all of our data at the same value of the scaling variable $\dot{t}_i L^{1/\nu} = 0$. Hence, if for large L the scaling function goes to a sample-independent form, the distribution of $\chi_i^{\max}$ should approach a δ function. This distribution is presented in Fig. 5: Even though it is much narrower (by a factor of $\approx$70) than the distribution of Fig. 2, as the inset shows, its width also *goes to a constant*. Hence, a strong scaling hypothesis such as (5) can be viewed only as an approximation.

Consequences for efficient simulations.—In order to acquire data for large systems with high precision (say to estimate exponents from finite-size scaling analysis), the commonly accepted procedure is to perform, for all sizes, simulations at one temperature T_c. The error inherent in doing this, due to sample-to-sample fluctuations, is much larger than that of taking measurements at $T_c(i,L)$. The latter procedure involves a different computational overhead, that of determining $T_c(i,L)$. Clearly, this may be advantageous if the width of the quantities measured at the pseudocritical temperature of each sample is much smaller than that of the data taken at T_c.

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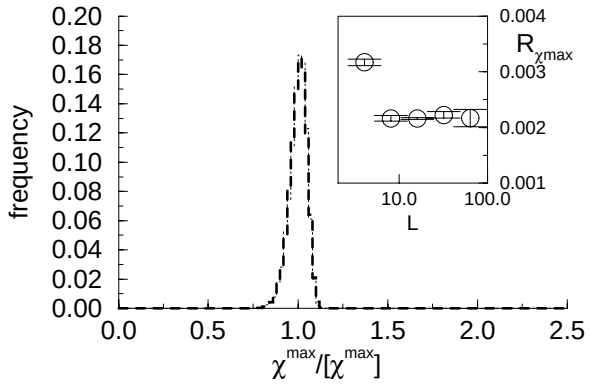

FIG. 5. Distribution of the normalized maximal susceptibilities for samples of sizes $L = 16$ (thin dotted line) and $L = 32$ (thick dashed line). The horizontal scale is the same as Fig. 2, to emphasize how small the width of this distribution is, which also goes to a constant (see inset).

[1] A. B. Harris, J. Phys. C **7**, 1671 (1974).
[2] J. T. Chayes, L. Chayes, D. S. Fisher, and T. Spencer, Phys. Rev Lett. **57**, 2999 (1986).
[3] K. Binder and A. P. Young, Rev. Mod. Phys. **58**, 837 (1986), and references therein.
[4] S. Wiseman and E. Domany, Phys. Rev E **52**, 3469 (1995).
[5] A. Aharony and A. B. Harris, Phys. Rev. Lett. **77**, 3700 (1996).
[6] F. Pázmándi, R. T. Scalettar, and G. T. Zimányi, Phys. Rev. Lett. **79**, 5130 (1997).
[7] M. E. Fisher, Rev. Mod. Phys. **46**, 597 (1974).
[8] H. O. Heuer, J. Phys. A **26**, L333 (1993).
[9] A. Aharony, A. B. Harris, and S. Wiseman (unpublished).
[10] S. Wiseman and E. Domany (unpublished).
[11] D. Stauffer and A. Aharony, *Introduction to Percolation Theory* (Taylor & Francis, London, 1992), p. 74.
[12] J. C. Angeles D'Auriac and N. Sourlas, Europhys. Lett. **39**, 473 (1997).
[13] U. Wolff, Phys. Rev. Lett. **62**, 361 (1989).
[14] S. Wang and R. H. Swendsen, Physica (Amsterdam) **167A**, 565 (1990).
[15] K. Binder and D. W. Heermann, *Monte Carlo Simulations in Statistical Physics* (Springer-Verlag, Berlin, 1988).
[16] R. H. Swendsen, Physica (Amsterdam) **194A**, 53 (1993).