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2003 J. Phys. A: Math. Gen. 36 5699

(http://iopscience.iop.org/0305-4470/36/21/301)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **36** (2003) 5699–5706 PII: S0305-4470(03)59760-8

On the use of finite-size scaling to measure spin-glass exponents

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Received 18 February 2003, in final form 7 April 2003
Published 13 May 2003
Online at stacks.iop.org/JPhysA/36/5699

Abstract

Finite-size scaling (FSS) is a standard technique for measuring scaling exponents in spin glasses. Here we present a critique of this approach, emphasizing the need for all length scales to be large compared to microscopic scales. In particular we show that the replacement, in FSS analyses, of the correlation length by its asymptotic scaling form can lead to apparently good scaling collapses with the wrong values of the scaling exponents.

PACS numbers: 75.10.Jm, 75.50.Lk

(Some figures in this article are in colour only in the electronic version)

1. Introduction

This paper is a critique of finite-size scaling (FSS) methods as applied to spin glasses. We focus primarily on one- and two-dimensional Ising spin glasses, which order only at temperature $T = 0$, though the underlying ideas are quite general. The model is defined by the Hamiltonian $H = -\sum_{\langle i,j\rangle} J_{ij} S_i S_j - h \sum_i S_i$, where h is an external field which will be zero unless stated otherwise.

In dimension $d = 2$, a range of different methods for measuring exponents have led to widely differing quoted values, sometimes by as much as a factor of 2, for the same exponent [1–8]. Despite years of numerical study, these discrepancies have never been satisfactorily resolved. Here we present analytical and numerical results in dimension $d = 1$, for which exact analytical values for the scaling exponents are known. By applying standard FSS methods to the data, we find large discrepancies between the numerically determined exponents and the exact ones. We show that these discrepancies disappear if the data are plotted in a different way, using the exact correlation length in the FSS analysis instead of its leading scaling form. We conclude that the main cause of the discrepancies is large corrections to scaling in the expression for the correlation length, rather than corrections to FSS itself.

For the critical behaviour as $T \to 0$, there is only one independent exponent [9], except perhaps when the ground state has a non-trivial degeneracy. The exponent on which we focus our attention is the 'stiffness exponent' θ, which describes the dependence on length scale, l, of the energy, E, of an excitation from the ground state: $E \sim l^{\theta}$ [1, 2, 10, 11]. For $d \leqslant 2$, θ is

negative and large excitations are easily created by thermal fluctuations, destroying the ground-state order. Setting $E \sim T$ gives a characteristic length scale $\xi \sim T^{-\nu}$, with $\nu = -1/\theta$, above which the ground state is unstable against thermal fluctuations, i.e. ξ can be identified with the correlation length [1, 10].

The exponent θ describes the dependence on l of the energy of a 'droplet' of reversed spins, of linear size l. The energy is associated with the boundary of the droplet. A measurement of θ can be made through the numerical study of domain-wall energies, in which a wall, or 'interface', is imposed on a finite-size system by choice of boundary conditions [1]. One finds $\theta \approx -0.28$ in $d = 2$. It was recently shown that this result can be obtained in a way which is explicitly independent of the particular boundary conditions used to impose the interface [12]. The scaling result $\nu = -1/\theta$ then predicts $\nu \approx 3.6$ for the correlation length exponent.

There has been some debate as to whether the exponent θ (sometimes called θ_{DW}) extracted from domain-wall energies is identical to the exponent obtained by studying directly the size dependence of droplet energies. Droplet excitations can be created from the ground state by reversing a central spin holding the boundary spins fixed, where the scale l is the linear size of the system [13]. This approach gives $\theta \approx -0.42$, though the analysis has been criticized by Middleton who argues that only droplets whose area exceeds some fraction of l^2 should be included [14]. Hartmann and Moore [15] have shown how the apparent difference between the two values of θ can be explained by invoking a correction to scaling (a subdominant term of order $l^{-\omega}$, with $\omega > -\theta$, in the expression for the droplet energy), and that the corresponding value of θ is consistent with that obtained from domain-wall studies. Such corrections to scaling may also account for the value $\theta \approx -0.46$ obtained by Picco *et al* in their recent study of droplet energies [8].

A 'direct' measurement of the exponent ν, which describes the divergence of the correlation length, can be made by studying, for example, the spin-glass susceptibility

$$\chi_{\mathrm{SG}} = L^{-d} \sum_{i,j} \overline{\langle S_i S_j \rangle^2} \tag{1}$$

where the angular brackets represent a thermal average, the overbar is a disorder average, and L is the linear size of the system. At $T = 0$ every term in the sum is unity and $\chi_{\mathrm{SG}} = L^d$. For $T > 0$, $\overline{\langle S_i S_j \rangle^2} = f(r/\xi)$, where $f(x)$ is a scaling function with $f(0) = 1$, $f(x) \sim \exp(-x)$ for large x, giving [9] $\chi_{\mathrm{SG}} \sim \xi^d \sim T^{-\gamma}$ with $\gamma = d\nu$. FSS predicts $\chi_{\mathrm{SG}} = L^d F(L/\xi)$ for $L \to \infty, \xi \to \infty$ with L/ξ fixed but arbitrary. Using $\xi \sim T^{-\nu} = T^{1/\theta}$, one can determine θ by plotting $L^{-d}\chi_{\mathrm{SG}}$ against $LT^{-1/\theta}$, and choosing θ to give the best data collapse. Using this method, Kawashima *et al* [5] find $\nu \approx 2.0$, i.e. $\theta \approx -0.5$, which differs significantly from the value $\simeq -0.28$ inferred from the domain-wall studies.

A second method that has been used to extract θ numerically is to measure the magnetization per spin, $m(h) = L^{-d} \sum_i \overline{\langle S_i \rangle}$, induced by a small magnetic field h at $T = 0$ [6, 16–19]. Since in zero field we have $m(0) \sim L^{-d/2}$, a simple scaling argument for small h gives $m(h) = L^{-d/2} g[h(L)/J(L)]$, where $h(L) \sim hL^{d/2}$ is the effective field at scale L and $J(L) \sim L^{\theta}$ is the effective coupling at this scale. Hence $m(h) = L^{-d/2} M(L^{d/2-\theta}h)$. In the thermodynamic limit m should become independent of L, which implies $m \sim h^{1/\delta}$ with $\delta = 1 - 2\theta/d \approx 1.28$ for $d = 2$. An alternative way of writing the FSS form is

$$m_L(h) = L^{-d/2} G(L^{d/2} h^{1/\delta}) \tag{2}$$

with $G(0+) = \text{const}$ and $G(x) \sim x$ for $x \to \infty$. With this method, Rieger *et al* [6] obtained $\delta \approx 1.48$, which differs significantly from the scaling prediction ≈ 1.28 and, naively, predicts that $\theta \approx -0.48$ instead of the value ≈ -0.28 obtained from domain-wall studies.

To summarize, different ways of measuring θ give different, and seemingly incompatible, results. The value $\nu \approx 2$ obtained in [5] is equivalent to $\theta \approx -0.5$, which is similar to the

value $\theta \approx -0.48$ inferred from the $m(h)$ data of [6], and to the values ≈ -0.42 and ≈ -0.46 obtained by studying droplet excitation in [13] and [8] respectively, all of which differ from the value ≈ -0.28 obtained from domain-wall studies [1, 2, 12].

In an attempt to understand these differences, we have carried out analytical and numerical studies in space dimension $d = 1$, for which the corresponding exponent values are known exactly. We mimic the two-dimensional studies of Kawashima *et al* [5] and Rieger *et al* [6], and look at the T-dependence of χ_{SG} at $h = 0$ and the h-dependence of m at $T = 0$, respectively. We conclude that these quantities are affected by corrections to scaling so large that it is essentially impossible to extract the correct exponent values from system sizes that are accessible in $d = 2$.

In the remainder of the paper, therefore, we consider the $d = 1$ Ising spin glass in two situations: (i) $T > 0$ and $h = 0$. We calculate χ_{SG} and use the FSS form $\chi_{\mathrm{SG}} = Lf(LT^{-1/\theta})$ to determine θ. We show that the exact value of θ gives a very poor data collapse for the system sizes studied, and that a reasonable data collapse is obtained with a significantly different value of θ; (ii) $T = 0, h > 0$. We calculate $m_L(h)$ and use the FSS form $m_L(h) = L^{1/2}g(L^{1/2}h^{1/\delta})$ to determine δ. Again, the exact δ gives a poor collapse, and the best collapse is obtained with a very different δ. To facilitate comparison with the $d = 2$ data of Kawashima *et al* and of Rieger *et al* we choose, for the $h = 0$ results, a bond distribution $P(J)$ engineered to give $\theta = -0.282$, i.e. a value equal to that of the $d = 2$ system, while for the $h > 0$ data we choose the distribution such that $\delta = 1.282$ is equal to the value predicted in $d = 2$ for $\theta = -0.282$. These choices are imposed by using a bond distribution of the form

$$P_\alpha(J) \propto |J|^\alpha \exp(-J^2/2). \tag{3}$$

For any distribution satisfying $P(J) \sim |J|^\alpha$ for $J \to 0$ it may be shown [10] that $\theta = -1/(1+\alpha)$ for $d = 1$, so the choice $\alpha = 2.546$ gives $\theta = -0.282$, while $\alpha = 6.042$ gives $\delta = 1.282$.

2. Results

(i) $T > 0, h = 0$. The Ising Hamiltonian for $d = 1$ can be written as $H = -\sum_i J_i S_i S_{i+1}$, and we use free boundary conditions. It is straightforward to show that (for $j \geqslant i$) $\langle S_i S_j \rangle = \prod_{r=i}^{j-1} \tanh(\beta J_i)$ and

$$\overline{\langle S_i S_j \rangle^2} = a^{|j-i|} \tag{4}$$

where $a = \overline{\tanh^2(\beta J_r)}$ is independent of r. Finally

$$\chi_{\mathrm{SG}} = \frac{1}{L} \sum_{i,j=1}^{L} \overline{\langle S_i S_j \rangle^2} = \frac{1+a}{1-a} - \frac{2a(1-a^L)}{L(1-a)^2}. \tag{5}$$

The quantity $a = \int \mathrm{d}J\, P_\alpha(J) \tanh^2(\beta J)$ may be evaluated numerically for any temperature T. The resulting χ_{SG} is plotted in figure 1, in the scaling form χ_{SG}/L against $LT^{-1/\theta}$, for lattice sizes up to $L = 320$. In the upper figure, we use the exact value, $\theta = -0.282$, while in the lower we use $\theta = -0.36$, which is our 'best fit by eye'. Comparing these two plots one observes that (i) the exact value of θ gives a good collapse only at small values of the scaling variable, where χ_{SG}/L is close to its $T = 0$ value of unity; (ii) the 'best fit by eye' is a much better fit over a large part of the plot, especially for the larger systems. Small but systematic departures from perfect scaling are evident in the low T region, but these are only observable because we have perfect data (no statistical errors). In real (i.e. noisy) data such small effects could easily be obscured by the noise, and might lead one to suppose that the correct value of θ were close to -0.36.

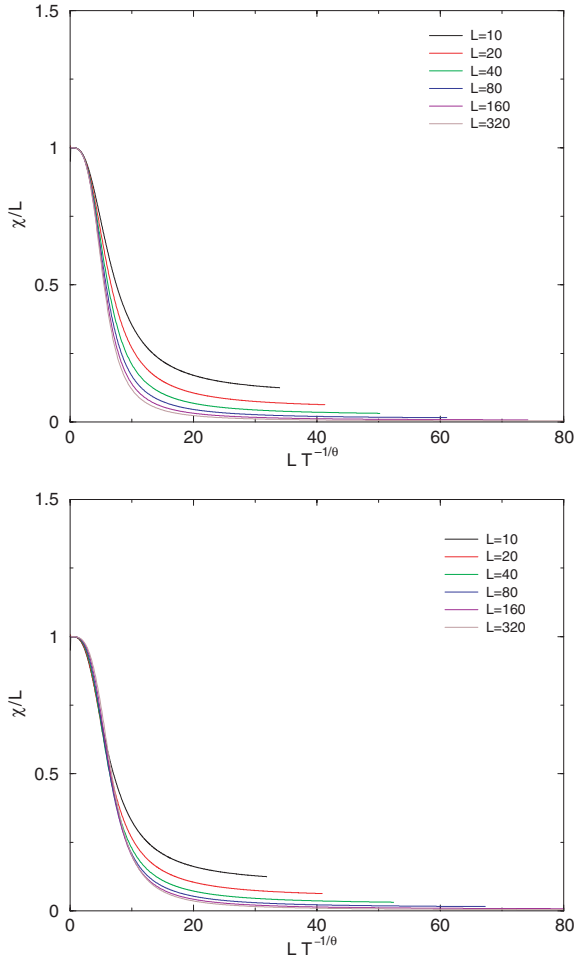

Figure 1. Susceptibility scaling plot. From top to bottom: $\theta = -0.28$ (theoretical) and $\theta = -0.36$ (best fit by eye).

This tells us that the relation $\xi \sim T^{-\nu}$, where $\nu = -1/\theta$, is only valid for rather small T. Corrections to this form are important over most of the regime presented in figure 1. A striking confirmation of this is provided by figure 2, where the same data are plotted against L/ξ_{exact}, where ξ_{exact} is the exact correlation length for each temperature. From equation (2) we can identify this length scale as $\xi_{\text{exact}} = -1/\ln a$. The data in figure 2 collapse almost perfectly for all sizes $L \geqslant 40$.

The lesson here is that it is not FSS itself which is breaking down, but the use of the relation $\xi \sim T^{-\nu}$ over the whole temperature range explored. We suspect that similar problems affect the interpretation of the data of Kawashima *et al* [5].

(ii) $T = 0, h > 0$. For non-zero magnetic field, the 1D problem cannot be solved analytically in closed form for general system size, L. One can, however, determine the relevant correlation length, ξ, numerically. Here ξ is to be interpreted as the length scale over which the ground state for $h > 0$ locally resembles the $h = 0$ ground state. We define it as the average 'domain length', where a domain is a cluster of spins completely aligned with one of

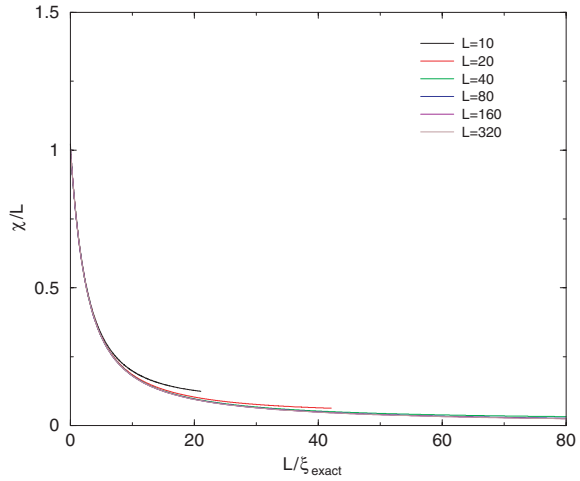

Figure 2. Data collapse with scaling variable L/ξ_{exact}.

the two $h = 0$ ground states. This definition corresponds to the scaling argument $L^{d/2}h^{1/\delta}$ in equation (2), i.e. this argument $\sim(L/\xi)^{d/2}$ with $\xi \propto h^{-2/d\delta}$.

Data for system sizes up to $L = 680$ are displayed in figure 3, where each data point represents an average of 50 000 samples. As explained above, we choose $\alpha = 6.042$ in (3), corresponding to the value $\delta = 1.282$ predicted by the scaling theory in $d = 2$ for $\theta = -0.282$. The plots are double-logarithmic plots based on the asymptotic scaling form (2) with $d = 1$. It is found, however, that if (2) is used as it stands, i.e. $L^{1/2}m_L(h)$ is plotted against $L^{1/2}h^{1/\delta}$, it is difficult to get a perfect data collapse at small h, for any value of δ. This is because the magnetization per spin in zero field has a binomial distribution, and its average over samples, $m_L(0)$, is not exactly proportional to $L^{-1/2}$ for small L (for $L \to \infty$, the binomial distribution approaches the normal distribution and the $L^{-1/2}$ dependence becomes asymptotically exact). An alternative FSS form can, however, be obtained by simply replacing the factors $L^{1/2}$ in (2) by $1/m_L(0)$. This has been done in figure 3. In this way, the ordinate is identically zero at $h = 0$ and data collapse at small h is greatly improved.

In the upper plot in figure 3, the exact value $\delta = 1.282$ is used, while the lower plot shows the 'best fit by eye' obtained with $\delta \approx 1.37$. The curves saturate at large h, when all spins are aligned with the field. The scaling region extends to, and somewhat beyond, the visible 'elbow' in the data. It is remarkable that a very good fit by eye (lower plot) is obtained for the *wrong* value, $\delta = 1.37$, of the scaling exponent, while the exact value, $\delta = 1.282$, is visibly worse (upper plot).

This paradox, that the best collapse appears to be obtained with the *wrong* exponent value, is resolved in a similar manner to the $h = 0$ case. In figure 4 we show the same data replotted against $\ln[(L/\xi)^{1/2}]$, where ξ is the average domain length for a given h, as defined above. It is calculated numerically using transfer matrix methods and taking systems long enough that the mean domain length converges (which requires longer systems at smaller h).

The collapse is very good, up to and a little beyond the elbow, as expected. The disappearance, in the new scaling variable, of the plateau from figure 3 is a consequence of the saturation of ξ, at the value 2, in this regime, i.e. the plateau gets compressed to a single point in these variables. As in the zero-field case, the failure of the data to collapse with the correct scaling exponent, when naive FSS is employed, indicates an inappropriate choice

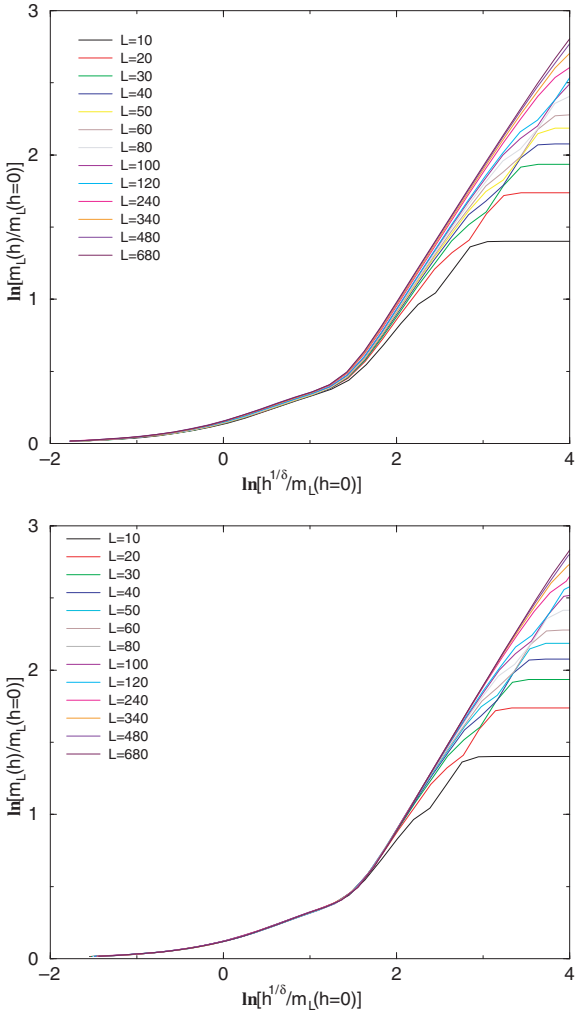

Figure 3. Magnetization versus field, scaled by the numerically determined zero-field magnetization. Top: theoretical, $\delta = 1.282$ and bottom: best collapse by eye, $\delta_{\rm col} = 1.37$.

of scaling variable rather than a failure of FSS itself, i.e. the scaling variable $L^{1/2}h^{1/\delta}$ is only useful at very small values of h.

Finally we have studied the 'domain-wall' and 'droplet' energies directly for the model with bond distribution (3), choosing $\alpha = 2.546$, corresponding to $\theta = -0.282$. The system has L bonds and free boundaries. The domain-wall energy, E, is given by the magnitude of the weakest bond in the system. Averaging over 10^5 samples, with $10 \leqslant L \leqslant 320$, and plotting $\ln\langle E\rangle$ against $\ln L$ gives the exponent $\theta = -0.297(2)$, which is again different from the exact value for this model, $\theta = -0.282$, but the difference is much smaller than that in the studies described earlier in this paper. There is also a small curvature in the data: extracting the exponent from the last two data points, $L = 160$ and 320, gives $\theta = -0.288$, even closer to the exact value.

One can create a droplet excitation by fixing the boundary spins in the ground-state configuration and reversing the central spin. The droplet that forms around the reversed spin is

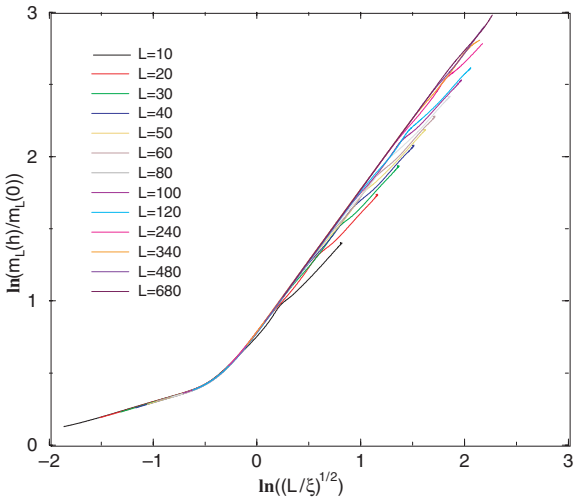

Figure 4. Magnetization scaling plot using the numerically determined correlation length.

bounded by the weakest bonds to its left and right. Computing the droplet energy numerically, averaging over 10^5 samples for $10 \leqslant L \leqslant 320$, and plotting $\ln\langle E_{\text{droplet}}\rangle$ against $\ln L$ as before gives $\theta = -0.303(3)$. Using only the last two data points gives $\theta = -0.290$. The discrepancy between the values of θ obtained from domain-wall and droplet energies is not statistically significant, in contrast to what is observed in $d = 2$ [8]. In the latter case, the boundary of a droplet forms a closed loop, which may tend to raise its energy due to an effective repulsion between different parts of the interface, leading to large corrections to scaling [15]. In $d = 1$ the 'interface' consists of two isolated points and this effect is absent.

3. Conclusion

In summary, we have demonstrated by exact calculations in $d = 1$ that a naive use of FSS, in which the asymptotic form of the scaling variable is employed, can lead to erroneous estimates of the scaling exponents, while FSS itself works rather well. We note that the discrepancies between the exact exponents and those obtained using FSS have the same sign in $d = 1$ and $d = 2$ when one uses the domain-wall estimate of θ to estimate the 'exact' exponents in $d = 2$. This suggests that a similar mechanism may be involved in both cases. We conclude by restating our view that domain-wall studies provide the most reliable determination of the exponent θ in spin glasses.

Acknowledgment

ACC thanks EPSRC for a Research Studentship.

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