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Specific Heat Exponent of Random–Field ising Magnets

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Abstract Zero – temperature simulations of the $d=3$ random–fieldIsing model (RFIM) with a bimodal distribution suggest that the specificheat's critical behaviour is consistent with an exponent $\alpha \simeq 0$. Thisis compatible with experimental measurements on random – field anddiluted – antiferromagnetic systems and, together with previoussimulations on the Gaussian RFIM, settles a clear picture for thecurrently controversial issue of the value of the criticalexponent α in the random–field problem.

Keywords Random– FieldIsing Model, Critical Exponents, Optimization Methods

1. Introduction

The RFIM has been extensively studied due to its interest as asimple frustrated system, as well as its close connection toexperiments[1]. Its beauty is that the mixture ofrandom fields and the standard Ising model creates rich physicsand leaves many still unanswered problems. The Hamiltonian describing the model is

$$H^{(RFIM)} = -J\sum_{<i,j>}\sigma_i\sigma_j - \sum_i h_i\sigma_i, \qquad (1)$$

where $\sigma_i = \pm 1$ are Ising spins, $J>0$ is thenearest-neighbour's ferromagnetic interaction, and h_i areindependent quenched random fields obtained from a relevantdistribution $P(h_i)$. Although the existence of anordered ferromagnetic phase for the $d>2$ RFIM is wellestablished, many years now[2], a clear resolution ofits critical behaviour is still lacking, in many terms.Historically, one of the main puzzles has been the mean-fieldprediction of a tricritical point in the phase diagram of thebimodal RFIM[3]. Currently, although we know thatthe phase transition of the RFIM is of second – orderwith a verysmall value of the exponent β, irrespective of $P(h_i)$[3-7], alarge controversy on the scaling behaviour of the specific heatcontinues to castdoubts[4,8-13].

In particular, the specific heat of the RFIM can be experimentallymeasured[8] and is, for sure, of great theoreticalimportance. Yet, it is well known that it is one of the mostintricate thermodynamic quantities to deal with in numerical simulations,even when it comes to pure systems. For the RFIM, Monte Carlomethods at positive temperatures $(T>0)$ have been used to estimate the value of itscritical exponent α, but were restricted to rather smallsystems sizes and have also revealed many serious problems, i.e.,severe violations ofself-averaging[9,10,13]. On the other handa better picture emerged throughout the years from zero–temperature $(T=0)$ computations, suggesting estimates of $\alpha \simeq 0$, at leastfor the Gaussian model[4,14]. However, evenby using the same numerical techniques, but different scalingapproaches, some inconsistencies have been recorded in the literature.The most prominent was that of Ref.[4], where a strongly negative value of the critical exponent $\alpha$was estimated. On the other hand, experiments on random field anddiluted antiferromagnetic systems suggest a clear logarithmic divergence of the specific heat, corresponding to an exponent $\alpha = 0$ [8], as also expected from scaling.

In this work we shed some light on this issue by providingnumerical results at zerotemperature for the RFIM with abimodal distribution of the form

$$P(h_i) = (1/2)\left[\delta(h_i - h) + \delta(h_i + h)\right], \qquad (2)$$

where h defines the disorder (field) strength. Our effort benefitsfrom (i) the existence of robust computational methods of graphtheory at $T=0$ and (ii) the work of Hartmann andNowak[15] that have suggested accurate estimates ofthe critical field $h_c = 2.20(2)$ and the correlation length's exponent $\nu = 1.67(11)$ of the bimodal RFIM using theseground–statecalculations and linear sizes up to $L=80$. Although Ref.[15] is the most thorough one in the literatureof the bimodal RFIM, we should note here that also other previousworks in the field have provided estimates for the set (h_c,ν) that compare well to these values[16,17].

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2. Simulation at Zero Temperature

As it is well known, the random field is a relevant perturbationat the pure fixed point, and the random-field fixed point is at zero temperature[2]. We can therefore determine the critical behaviour, staying at $T = 0$ and crossing the phase boundary at $h = h_c$. This is a convenient approach because we candetermine the ground states exactly using efficient optimizationalgorithms[18-21] through an existing mapping of the ground state to the maximum–flowoptimization problem[22-24]. A clearadvantage of this approach is the ability to simulate large system sizes and disorder ensembles avoiding at the same time statisticalerrors and equilibration problems, which are the two majordrawbacks encountered in positive – temperature simulations of systems with rough free–energy landscapes [25]. The application of optimization algorithms to the RFIM is nowadays well established[25]. Here, we have implemented the Push–Relabelalgorithm of Goldberg and Tarjan[26], including also an interesting modification proposed by Middleton and Fisher[4].

The algorithm starts by assigning an excess x_i to each latticesite i, with $x_i = h_i$. Residual capacity variables r_{ij} between neighbouring sites are initially set to J. A height variable u_i is then assigned to each node via a global updatestep. In this global update, the value of u_i at each site inthe set $T = \{ j \mid x_j < 0 \}$ of negative excesssites is set to zero. Sites with $x_i \geq 0$ have u_i set to thelength of the shortest path, via edges with positive capacity from i to T. The ground state is found by successively rearranging the excesses x_i, via *push* operations, and updating the heights, via*relabel* operations. When no more pushes or relabels are possible, a final global update determines the ground state, sothat sites which are path connected by bonds with $r_{ij} > 0$ to Thave $\sigma_i = -1$, while those which are disconnected from T have $\sigma_i = +1$.

A push operation moves excessfrom a site i to a lower height neighbour j, if possible, thatis, whenever $x_i > 0$, $r_{ij} > 0$, and $u_j = u_i - 1$. In a push,the working variables are modified according to $x_i \to x_i - \delta$; $x_j \to x_j + \delta$; $r_{ij} \to r_{ij} - \delta$; $r_{ji} \to r_{ji} + \delta$, where $\delta = \min(x_i, r_{ij})$. Push operations tend to move thepositive excess towards sites in T. When $x_i > 0$ and nopush is possible, the site is relabelled, with u_i increased to $1 + \min_{\{j | r_{ij} > 0\}} u_j$. In addition, if a set ofhighest sites U becomes isolated, with $u_i > u_j + 1$, forall $i \in U$ and all $j \notin U$, the height u_i forall $i \in U$ is increased to its maximum value, N, asthese sites will always be isolated from the negative excessnodes. Periodic global updates are often crucial to the practicalspeed of the algorithm[4]. Following thesuggestions of Middleton and Fisher[4],we have also applied global updates here every N relabels, a practise found to be computationally optimum.Using this scheme, we performed simulations of the bimodal RFIMfor systems containing up to $N = 128^3$ spins, for 5 candidate h_c -values ofthe field strength in the range[2.18 - 2.22] with a step 0.01, following the proposed critical value $h_c = 2.20(2)$ of Ref.[15]. For each pair (L, h_c) an extensive disorder averaging has beenundertaken by sampling over 5×10^4 random– fieldrealizations.

3. Results and Discussion

In general, one expects that the finite – temperature definition of the specific heat C can be extended to zero temperature, with the second derivative of $\langle E \rangle$ with respect to temperature being replaced by the second derivative of the ground–stateenergy density E_{gs} with respect to the random field h[4,12]. The first derivative $\partial E_{gs} / \partial J$ is just

$$E_J = -(1/N) \sum_{<i,j>} \sigma_i \sigma_j \,. \tag{3}$$

The general finite – size scaling form assumed is that the singular part of the specific heat C_s behaves as

$$C_s \simeq L^{\alpha/\nu} \tilde{C} \{ (h - h_c) L^{1/\nu} \} \,. \tag{4}$$

Thus, one may estimate α by studying the behaviour of $[E_J]_{av}$ at $h = h_c$[4]. The computation from the behaviour of $[E_J]_{av}$ is based on integrating Eq. (4) up to h_c, which gives a dependence of the form

$$[E_J]_{av} (h = h_c) = c_1 + c_2 L^{-(\alpha - 1)/\nu} \,, \tag{5}$$

with c_i constants. Alternatively, following the prescription of Ref.[12], one may calculate the second derivative by finite differences of $E_J(h)$ for values of h near h_c and determine α by fitting to the maximum of the peaks in C_S, which occur at $h_L - h_c \approx L^{-1/\nu}$. However, this latter approach may be more strongly affected by strong finite – size corrections, since the peaks in C_s found by numerical differentiation are somewhat above h_s, and furthermore is computationally more demanding since one must have the values of $[E_J]_{av}$ in a wide range of $h$values. In the present case, where the critical value h_c is known with good accuracy[15], the first approach seems to be more suitable to follow.

Thus, using our numerical data we have constructed the disorder – averaged curves $[E_J]_{av}(h)$ shown in Fig. 1 for all 5 values of the candidate critical field h_c, as also indicated in the figure. The error bars shown reflect the sample – to – samplefluctuations in the ensemble of the

disorder realizations. The solid lines are power – lawfittings of the form $\left[E_J\right]_{av}(h=h_c)=c_1+c_2L^{-x}$, where $x=(\alpha-1)/\nu$. The estimates for the exponent x are also shown in Figure 1, each one next to the corresponding curve. Using now the estimate $\nu=1.67(11)$ of Ref.[15] and the relation $x=(\alpha-1)/\nu$ we calculate the critical exponent α of the specific heat and its error bars and we plot its dependence on h_c in Fig. 2. Note that the rather large error bars come mainly from the error of the critical exponent ν used $\delta\nu=0.11$. The dotted line in this figure is a guide for the eye and marks the case $\alpha=0$. From Fig. 2 it is clear that the critical exponent α is very close to zero (especially for the value $h_c=2.20$ that has been proposed as the exact critical disorder strength of the bimodal RFIM we get $\alpha=-0.03(8)$. All this set of α–values is in accordance with the experimental prediction of a diverging specific heat[8] and also with the most extensive numerical works on the Gaussian RFIM that have predicted $\alpha=-0.01(6)$ [4] and $0.1(1)$ [14] using similar techniques.

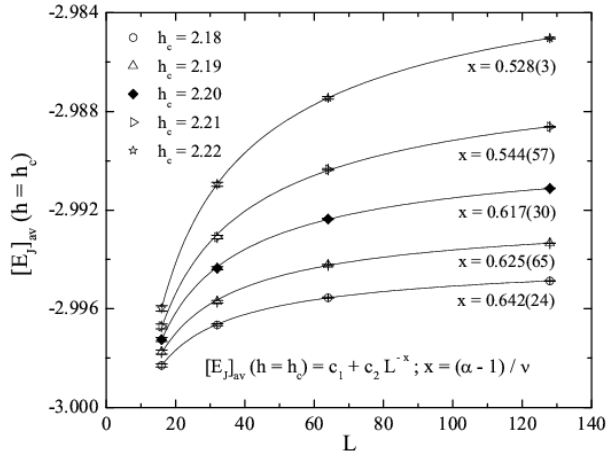

Figure 1. Finite – size scaling behaviour of the bond part of the energy density at the 5 candidate values of the critical random – fieldstrength

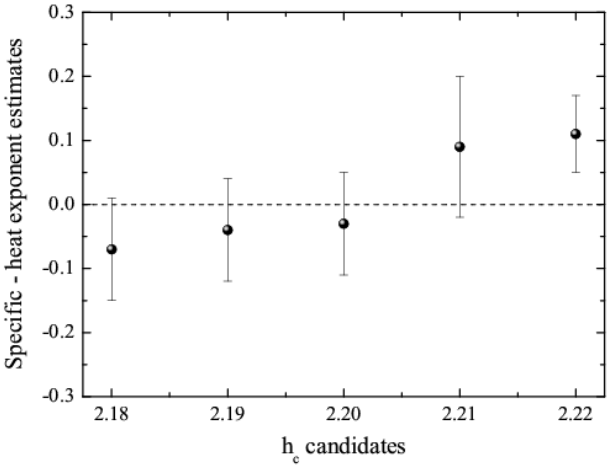

Figure 2. Specific – heat exponent estimates as a function of the 5 candidate values for the critical field

4. Conclusions

In summary, we have presented an independent estimation of the critical exponent α of the bimodal RFIM. The scaling behaviour of the bond part of the energy density at the critical field indicated that $\alpha\simeq 0$, thus pointing at a logarithmic divergence of the specific heat, in agreement with experimental data[8], and also in agreement with the most important studies of the corresponding Gaussian model[4,14]. Our effort became feasible through the implementation of a modified version of the Push – Relabelalgorithm[4] that enabled us to simulate very large system sizes, up to $N=128^3$ spins, and disorder ensembles of the order of 5×10^4 , for several values of the field strength. Clearly, such a computational task goes beyond the limits of any kind of positive – temperatureMonte Carlo scheme.

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