Lack of self-averaging of the specific heat in the three-dimensional random-field Ising model

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I. INTRODUCTION

The random-field Ising model (RFIM) [1] is one of the best studied glassy magnetic models [2, 3, 4], mainly because of its interest as a simple frustrated system. In fact, it has been a matter of conspicuous controversy over the last 15 years, mainly concerning the nature of its phase transitions. The RFIM Hamiltonian is given by:

$$\mathcal{H} = -J \sum_{<i,j>} S_i S_j - \sum_i h_i S_i$$

(1)

where $S_i = \pm 1$, $J > 0$ is the nearest-neighbors ferromagnetic interaction and the random-fields (RF's) are obtained from a discrete distribution $h_i = \pm \Delta$, where $\Delta = 2$ is the disorder strength, also called randomness of the system.

The notion of dimensional reduction [2] indicated that the critical behavior of the RFIM in $d$ dimensions, at sufficiently low randomness, should be identical to that of the well-known normal Ising model in $d - 2$ dimensions. On the other hand, the droplet theory of domain wall energies in the ferromagnetic state [8] suggested that a phase transition should exist in three-dimensions (3D), for finite-temperature and randomness. The puzzle has been cleared out by Imbrie [9], Schwartz [10] and Bricmont and Kupiainen [11]. Their arguments strongly support the view that a phase transition in 3D exists for sufficiently small randomness ($\Delta \approx 2.3$) [4].

From the experimental point of view, a true realization of the RFIM is hardly conceived. However, it has been shown that dilute antiferromagnets in uniform external field (DAFF) represent physical realizations of the RFIM [12] and a number of experiments investigated the phase transitions of such 3D systems [11]. These experiments have proven to be very difficult and their interpretation doubtful due to the slow, glassy dynamics of the system.

Although there exist several open questions about the phase transition in the RFIM, it is now generally accepted that a new fixed point controls the behavior of RF ferromagnets [12, 13]. The significance of this for the RFIM (in $d > 2$) is that this new zero-temperature random fixed point controls the whole critical line ($T_c(\Delta)$) and that the RF's are always relevant. For disordered systems with weak randomness which couples to the local energy (such as random-site impurity or random-bond models) the crossover to a new random fixed point, depends on the Harris criterion [13, 17]. According to this, the disorder is relevant if the correlation length exponent of the pure model ($\nu = \nu_{pure}$) satisfies the condition $\nu > 2$ and this condition may be stated, with the help of the hyperscaling relation ($\alpha = 2 - d\nu$, as $\alpha > 0$). Since the specific heat exponent of the 3D Ising model is positive [12], weak disorder should be expected to be relevant. In the case of the RFIM the type of disorder is much more severe, since the randomness couples to the local order parameter and the crossover renormalization group eigenvalue is always positive [13]. The inequality $\nu > 2/d$, derived by Chayes et al. [12], for the correlation length exponent of a generic disordered system ($\nu = \nu_{random}$) would imply, using again hyperscaling, a negative specific heat exponent ($\alpha < 0$). However, it is believed that hyperscaling is violated in the RFIM and the specific heat exponent $\alpha$ is related to $\nu$ by a modified hyperscaling law $2 - \alpha = (d - d\nu)$. The exponent $\theta$ characterizes the scaling of the stiffness of the ordered phase at the critical point [16]. Thus, the specific heat exponent of the RFIM is not restricted, by the above theoretical considerations, to be negative [12].

The inconsistency of various estimations in the literature concerning the critical exponent $\alpha$ is the origin of a long lasting lively controversy, leaving open, so far, even the question of divergence or saturation of the specific heat. The specific heat of the RFIM can be experimentally measured and is of considerable theoretical interest. Several Monte Carlo methods at finite temperatures but also methods using ground state configurations have been used to estimate the critical exponent $\alpha$. Some of the
ground state studies came up with strongly negative values, ranging from $\alpha = -1.5$ to $\alpha = -0.5$, whereas Middleton and Fisher estimated marked disagreement $\alpha = -0.01 \pm 0.09$. Experiments on DAFF provided evidence of a second order phase transition and a logarithmic singularity for the specific heat [21]. Recently, Barber and Belanger in their Monte Carlo study of a DAFF model reported also that their specific heat curve closely mimics a logarithmic peak. Moreover, it has been pointed out that a strongly negative value of $\alpha$ causes serious difficulties when it comes to finding a consistent set of scaling relations to describe the critical behavior of the RFIM. These scaling relations are consistent if one uses $\alpha \approx 0$ [13], which is also close to the experimental value [11]. Clearly more work is needed to understand the specific heats behavior of the model. This important issue may be intimately linked to the violation of self-averaging of the specific heat, illustrated below in Sec. III.

The RFIM has been studied numerically using traditional [17, 19, 23, 24] but also more sophisticated Monte Carlo techniques [4]. However, the nature of the model demands enormous computer resources. The equilibration of the system at low temperatures is exponentially slow for large systems. Furthermore, in order to get a good estimate of the mean properties of the system, it is necessary to repeat the simulations for a large number of realizations of RF’s. In the present work we have applied the new and popular Wang-Landau (WL) [25] and broad histogram (BH) [26] methods to estimate the density of states (DOS), $G(E)$, of the model. These methods have been employed in a unified implementation using the Schulz et al. N-fold version of the WL scheme [23, 28] and the energy space was restricted using the recent critical minimum energy subspace (CMES) technique [12].

The rest of the paper is organized as follows. In Sec. III we provide an outline of the numerical methods which are involved in our calculations, including a brief description of the WL and BH methods. The recently developed CMES restriction is properly adapted and illustrated for the RFIM and useful technical details are provided. In Sec. III we discuss the main conclusion of our work: the violation of self-averaging of the specific heat of the RFIM by studying the relevant probability distributions. The scaling behavior of the pseudocritical temperatures and their sample-to-sample fluctuations are also presented. Our conclusions are summarized in Sec. IV.

II. A NUMERICAL APPROACH

We proceed to describe and appropriately adapt to the RFIM a recently developed Monte Carlo approach, based on the WL algorithm for estimating the DOS and using the idea of dominant energy subspaces (CMES technique). Consider a particular RF realization. Then, the specific heat and its peak are easily obtained with the help of the usual statistical sums. The CMES scheme [13] uses only a small but dominant part $(\tilde{E}_-, \tilde{E}_+)$ of the energy space $(E_{\text{min}}, E_{\text{max}})$ to determine the specific heat peaks. Let $\tilde{E}$ denote the value of energy producing the maximum term in the partition function at the pseudocritical temperature (corresponding to the specific heat peak) and $S(E) = \ln(G(E))$ the microcanonical entropy. Then, Eq. (2) defines the CMES approximation:

$$C_L(\tilde{E}_-, \tilde{E}_+) = N^{-1}T^{-2} \left\{ \bar{Z}^{-1} \sum_{\tilde{E}_-} E^{2} \exp \left[ \bar{\Phi}(E) \right] - \left( \bar{Z}^{-1} \sum_{\tilde{E}_-} E \exp \left[ \bar{\Phi}(E) \right] \right)^2 \right\}$$

(2a)

$$\bar{\Phi}(E) \equiv \left[ S(E) - \beta \tilde{E} \right] - \left[ S(\tilde{E}) - \beta \tilde{E} \right], \quad \tilde{E} = \sum_{\tilde{E}_-} \exp \left[ \bar{\Phi}(E) \right]$$

(2b)

where $N = L^3$ and $(\tilde{E}_-, \tilde{E}_+)$ is the minimum dominant subspace satisfying the following accuracy criterion:

$$\left| \frac{C_L(\tilde{E}_-, \tilde{E}_+)}{C_L(E_{\text{min}}, E_{\text{max}})} - 1 \right| \leq r$$

(3)

with $r = 10^{-6}$. This accuracy is extremely demanding compared to the statistical errors produced by the DOS method and to the large sample-to-sample fluctuations of the RFIM. An algorithmic approach for specifying the CMES is described in Ref. [13].

Using an ensemble of $M (m = 1,...,M)$ macroscopic samples of linear size $L$ corresponding to different RF realizations we have applied the described scheme in a broad energy space that covers the overlap of the dominant energy subspaces for all RF’s of the ensemble. For a RF realization, say $m$, let us denote by $(\tilde{E}_-, m, \tilde{E}_+, m)$ the location of the dominant energy subspace defined by the above restriction, and by $\Delta \tilde{E}_m = \tilde{E}_+ m - \tilde{E}_- m$ its extension. Our simulations were carried out in the broad energy subspace, which covers at least the union of the individual subspaces, i.e. $(E_{\text{min}} M, E_{\text{max}} M) \equiv \bigcup_{m} (\tilde{E}_-, m, \tilde{E}_+ m)$, of total extension $(\Delta \tilde{E} M) = E_{\text{max}} M - \tilde{E}_- M$. Note that, the total extension may be for large lattices several times larger than the individual extensions. This practice has the advantage that the approximation of the specific heat for a particular RF is accurate in a wide temperature range, including its pseudocritical temperature. Thus, the present implementation is not the most efficient for the purposes of locating only the specific heat peaks. However, this usage provides a more reliable alternative for comparing the statistics of the specific heat peaks to the averaged specific heat curve used in the literature (see for example Ref. [17] and also Sec. III) and for discussing the pathology of this quite common choice. Despite the strong fluctuations of the
energy value corresponding to the maximum term of the partition function $Z$, the union of the CMES for large samples of RF’s is a relatively small subspace, compared to that of the normal Ising model. Consider the case $L = 16$. Then, the energy levels used in Ref. [14] for the normal Ising model, counting from the ground state ($ie = 1$), are the levels ($ie = 1220 - 2410$). Using an ensemble of 1000 RF’s the union of the CMES was found to be the range of levels ($ie = 1 - 950$), while our simulations were performed in a wider range ($ie = 1 - 1200$). This is of the same order with that of the normal Ising model and at least five times smaller than that of the total energy space.

There are some points that one should observe from this figure. Firstly, in both cases the extension of the CMES for a particular RF is much smaller than the broad energy space used in the simulations. Specifically, for the $RF_a$ the dominant energy subspace is approximately of the order of 850 energy levels ($ie = 800 - 1650$), which is almost three times smaller than the 2500 levels of the total union space. Secondly, the fluctuations of the extension $\Delta E_b$ of the $RF_a$ are more pronounced and this is related to the existence of a secondary peak in the left of the main peak. This secondary peak causes a stronger fluctuation in the estimation of the end points of the corresponding dominant subspaces. In any case, we could improve the efficiency of our scheme by a factor of at least two (for the case $L = 24$), by carefully individualizing the used energy space for simulating a particular RF. In fact, the fast early stages of the WL process may be used as a prognostic method to approximately locate the CMES of a particular RF, and this strategy may be an indispensable ingredient in analogous future studies. Finally, an entropic sampling study of the magnetic properties of the RFIM using the CMES restrictive entropic scheme based on the high-levels of the WL algorithm [29] would be greatly facilitated by such a strategy.

To determine the density of states, we have used the N-fold version of the WL method as presented by Schulz et al. [27], using 20 iterations for the reduction ($f_{j+1} = \sqrt{f_j}$, $f_1 = e$) of the WL modification factor. Our implementation is analogous to that presented in Ref. [28], where the first 13 iterations follow the simple WL scheme and the rest iterations ($j = 14 - 20$) use the N-fold version of Schulz et al. [27]. We have used a flatness criterion of 5% for the energy histogram [25, 28]. For RF’s $h_i = \pm 2$ the classes for the N-fold process are specified by the energy changes $\Delta E_n = -16 + 4 \cdot (n - 1)$, $n = 1, 2, ..., 9$. Using the part of the simulation corresponding to the N-fold iterations ($j = 14 - 20$), we have accumulated data corresponding to non-zero energy changes in order to apply the well-known BH equation [26]:

$$
G(E) = G(E + \Delta E_n) \frac{N(E + \Delta E_n)}{N(E)} E = G(E + \Delta E_n) \cdot \left(1 + \frac{N(E + \Delta E_n)}{N(E)} - 1\right)
$$

$N(E)$ is the number of possible spin flip moves from a microstate of energy $E$ to a macrostate with energy $E + \Delta E_n$, which are known during the N-fold process. In this way we have produced 4 BH ($n = 1, 2, 3, 4$) approximations for the DOS and the specific heat for each RF of the ensemble.

III. LACK OF SELF-AVERAGING OF THE SPECIFIC HEAT

For a disordered system we have to perform two distinct kinds of averaging. For each sample, the usual thermal average has to be carried out and then we have to average over the random parameters. Let $C_m(T)$ denote the specific heat of a particular realization $m$ in the ensemble of $M$ realizations of RF’s. The pseudocritical temperature $T_{m,c}$ will, of course, depend on the realization of the RF. The location of the corresponding peak

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**FIG. 1:** The specific heat for two characteristic examples of RF’s, $RF_a$ (dotted line) and $RF_b$ (solid line). The specific heat curves were obtained using the average DOS over the 50 runs for each RF. The inset shows the fluctuation of the extension of the individual dominant subspaces over 50 runs.
is denoted by \((C_m^*, T_{L,m}^*)\) and the respective probability distributions by \(P_L(C_m^*)\) and \(P_L(T_{L,m}^*)\).

FIG. 2: Averaged curves for various samples of RF’s.

Rieger and Young \[17, 19\] have studied the following sample summation for the specific heat curves:

\[ [C]_{av} = \frac{1}{M} \sum_{m=1}^{M} C_m(T) \]  \hspace{1cm} (4)

and the finite-size scaling behavior of the peak of this averaged curve has been studied by assuming that the maximum \([C]_{av} = \max_T [C]_{av}\) and the corresponding pseudocritical temperature \(T_{L}^*\) obey the scaling laws:

\[ [C]_{av}^* \approx p + cL^{\alpha/\nu} \]  \hspace{1cm} (5a)
\[ T_{L}^* \approx T_c + bL^{-1/\nu} \]  \hspace{1cm} (5b)

Here we shall also examine the scaling of the sample averages of the specific heat maxima and the pseudocritical temperatures, defined by:

\[ [C_m^*]_{av} = \frac{1}{M} \sum_{m} C_m^* \approx \tilde{p} + \tilde{c}L^{\tilde{\alpha}/\tilde{\nu}} \]  \hspace{1cm} (6a)
\[ [T_{L,m}^*]_{av} = \frac{1}{M} \sum_{m} T_{L,m}^* \approx \tilde{T}_c + \tilde{b}L^{-1/\tilde{\nu}} \]  \hspace{1cm} (6b)

The possibility of different exponents may be ultimately related to the functional form of the distributions \(P_L(C_m^*)\) and \(P_L(T_{L,m}^*)\), whose behavior is decisive for the comprehension of the critical behavior of the RFIM.

For a small number of RF’s the averaged curve \([C]_{av}\) has several local maxima reflecting a very strong sample-to-sample fluctuation of the individual pseudocritical temperature. Fig. 2 shows how the smoothness of this curve develops, as we increase the number of RF’s. Fig. 3 presents an example of the probability distribution \(P_L(T_{L,m}^*)\). Since the peaks are found in different locations, the averaging in Fig. 1 wipes the particular peaks out. This explains why the averaged curve does not represent the behavior of the most probable, say \(x\), realization of the RF’s: \([C]_{av}(T) \neq C_x(T)\). It also suggests the absence of self-averaging for the specific heat of the present model, at least for the randomness studied here. Fig. 3 illustrates the finite-size behavior of the distribution \(P_L(C_m^*)\). Although for \(L = 4\) the distribution is sharp, as \(L\) increases the distribution broadens so that there is a significant number of RF’s having their peaks higher, or lower, than the expected sample mean, defined in Eq. 6a. The above observations provide very strong evidence that the real behavior of the RFIM is not appropriately described by a possible misleading saturation of \([C]_{av}\). The source of this problem is the severe fluctuation of the pseudocritical temperatures and the lack of self-averaging may be an important statement.

Broad distributions, with lack of self-averaging have been studied also in other physical problems, such as in the well-known case of the scaling theory of Anderson localization. There, it has been shown that for a disordered electronic sample the conductance distribution at the point of the metal-insulator transition (the mobility edge) is so broad, that the conductance is not a self-averaging quantity. Noteworthy that, the lack of self-averaging appears to be a common property of disordered systems at criticality and that besides the above mentioned paradigm, one can find several examples of magnetic systems where this feature is present \[31, 32, 33, 34\]. Actually, when dealing with physical quantities that are characterized by broad distributions, one must be mindful when attempting to define a transition in terms of related averaged quantities. In this sense, it seems that for the present model the common use of \([C]_{av}\) may be a “meaningless” choice for a proper description. In order to discuss the significance of the above broad probability...
distributions and to present a more convincing finite-size scaling argument for the violation of self-averaging in the thermodynamic limit, we have included as an inset in Fig. 4 the ratio $R_c = V_c / [C_n^{\text{av}}]^2$, where $V_c$ is the sample-to-sample variance of the mean. Both the WL and BH estimates are shown with their errors. The variance $V_c$ was reduced, by eliminating the statistical (DOS) errors, assumed to be of the order of the difference between multiple measurements and also a separation $S = 16$ between successive recordings of the accepted microstates of the WL process. The separation refinement is generally believed to improve the accuracy of the WL method [24,36]. Fig. 4 illustrates its effect in a repeated application using the RF, that appears also in Fig. 1 From Fig. 4 we observe that the effect of separation is to increase the mean value of the maximum of the specific heat by an amount which is of the same order with the standard deviation of the statistical errors that one obtains by using multiple measurements (100 independent WL runs) without separation. The standard deviation of the new sample of multiple measurements (25 independent WL runs using separation) is also of the same order, as shown in Fig. 5. We note that, the WL sampling in these two figures (Fig. 1 and Fig. 5) one can detect the effects of different restrictions on the energy space which is slightly wider than the CMES of the RF. From these two figures (Fig. 1 and Fig. 5) one can detect the effects of different restrictions on the energy space. The observed sudden decrease of the right tail of the specific heat (a similar comment applies also for the left tail) in Fig. 1 is an effect induced by the restriction imposed on the energy space and appears in the neighborhood of
T \approx 3$. The further restriction imposed in the new samplings (appearing in Fig. 4) is now reflected in the shift of the observed sadden decrease in the neighborhood of T \approx 2.5. Before attempting to simulate larger samples of RF’s, other refinements should be also tested, in order to obtain a more accurate and efficient scheme. In any case, our study shows that there is a large number of RF’s with sharp peaks strongly fluctuating in their pseudocritical temperatures and this generic property makes the proposed CMES scheme the most appropriate alternative, despite the accuracy and slowing down problems observed at the larger sizes. Sharp peaks are usually missed by importance sampling, due to an inadequate temperature scanning often used.

![Graph](image)

**FIG. 6:** Illustration of the separation effect in the specific heat of the RF\(_{a}\). The specific heat curves shown were calculated from the average DOS over the runs, while the horizontal lines represent the mean values of the independent runs for the specific heat peaks. The dotted line shows the case S = 16, while the solid line the case S = 0. The error bars illustrate the standard deviation (of the independent peaks) over the 25 (dotted) and 100 (solid) WL runs, corresponding to S = 16 and S = 0.

Fig. 7 illustrates that the two pseudocritical temperatures, \([T_{L,m}^*]_{av}\) and \(T_L^*\), tend to the same limit (\(T_c = T_c\)). The behavior of \([T_{L,m}^*]_{av}\) is smoother than the behavior of \(T_L^*\), which is more sensitive to the sample size. Using our data for \([T_{L,m}^*]_{av}\) we found a reasonably good fit with \(\bar{T}_c = 2.03(18)\) and \(\bar{\nu} = 1.31(18)\). This value is very close to the value \(\nu = 1.37(9)\) found in Ref. 16 and lies between the values 1.0(1) of Ref. 20 and the estimates 1.6(3) and 1.4(2) of Ref. 17. The inset in Fig. 7 illustrates the scaling of the sample-to-sample variance of the average \([T_{L,m}^*]_{av}\) of Eq. (6a). Assuming that the square of these sample-to-sample fluctuations scales with the linear size \(L\) according to \(\delta^2([T_{L,m}^*]_{av}) \sim L^{-2/\nu}\), we obtain, from the fit shown in the inset, the value \(\nu = 1.18(15)\). This estimate is slightly smaller than the value found above, which is in good agreement with the best estimate in literature 10. The rather slow approach of the fluctuations to zero is also an interesting finding. According to Aharony and Harris 33 and Wiseman and Domany 34, the fact that the square width of the distribution of the sample dependent pseudocritical temperatures scales with \(L^{-2/\nu}\) and not with \(L^{-d}\), when combined with finite-size scaling 34, is an indication of lack of self-averaging of the random system. Therefore, our main conclusion is reinforced and is also in conformity with the results of Parisi and Sourlas 35. The numerical study of these authors showed that the strong fluctuations of the 3D RFIM produce a maximal violation of self-averaging for the correlation length. It appears that the disorder present in the RFIM brings about drastic effects and its strong non self-averaging behavior includes also the specific heat, as suggested in this paper.

It is quite possible that the above relevant aspect was overlooked in previous finite-temperature studies but also in ground state calculations. We think that, at least partly, this practice is behind the existing controversial situation in the literature concerning the behavior of the specific heat. For instance, the saturation of \([C^*]_{av}\) is evident from the very small sizes and its behavior does not admit a finite-size scaling, but rather appears as a random fluctuation around the value 0.84, as shown by the dashed line in Fig. 5. The negative value for the exponent \(\alpha\) found, from the study of \([C^*]_{av}\) in previous finite-temperature studies 17, 10 seems to us questionable. In addition to all the reasons mentioned above, the very early and clear saturation observed here and the possibility of a crossover behavior of the model at larger lattice sizes are strong indications that make us question the meaning of such a scaling prediction. It appears that the behavior of \([C^*]_{av}\) incorporates more of the physical content of the model, although its asymptotic behavior seems unsettled at the lattice sizes studied here. As pointed out earlier, the systematic errors
of the WL scheme for large lattice sizes are due to the practical \((j = 20)\) but not fully converged usage of this algorithm in our simulations. This option was dictated by the need of studying large samples of RF’s. We assume that the decline of the estimates observed here for \(L > 24\) is stronger, as pointed out earlier, from the underestimation observed by studying smaller samples of RF’s and using longer \((j = 24)\) runs. Then, it is quite obvious from Fig. 5 that the true asymptotic behavior cannot be observed at these lattice sizes, although its saturation seems to be now plausible. In order to obtain a safe and sound estimation of the large \(L\)-behavior, larger systems of at least of the order of \(L = 60\) should be considered. This is an extremely demanding computer project and will have to be postponed, until further tests make available a more accurate and optimum refinement of the presented scheme. Finally, let us point out that, our first attempts to observe the behavior of the susceptibility of the 3D RFIM via a recently proposed entropic scheme \[29\], suggested also an even stronger violation of self-averaging for the magnetic properties of the system.

IV. CONCLUSIONS

In spite of many years of study, the conflicting situation in literature concerning the divergence or saturation of the specific heat of the RFIM is still an open important topic, necessary for a better comprehension of the model. This problem was considered in a completely new basis in this paper. The property of self-averaging of the specific heat was addressed in a concise way and its violation was explicitly shown by studying the relevant probability distributions. This finding may lead to a better theoretical and numerical approach of the problem. The scaling behavior of the pseudocritical temperatures and their sample-to-sample fluctuations were also presented, and found to support a strong violation of the self-averaging property of the system. The new ideas and numerical techniques utilized to tackle the RFIM use as an essential ingredient the critical minimum energy subspace scheme. We hope that the combination of algorithms and techniques applied here will be useful in further numerical studies of this and other similarly challenging problems.

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