Self-averaging and criticality: A comparative study
in 2d random bond spin models

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Abstract. We investigate and contrast, via the Wang-Landau (WL) algorithm, the effects of quenched bond randomness on the self-averaging properties of two Ising spin models in 2d. The random bond version of the superantiferromagnetic (SAF) square model with nearest- and next-nearest-neighbor competing interactions and the corresponding version of the simple ferromagnetic Ising model are studied. We find that, the random bond SAF model shows a strong violation of self-averaging, much stronger than that observed in the case of the random bond Ising model. Our analysis of the asymptotic scaling behavior of the variance of the distribution of the sample-dependent pseudocritical temperatures is found to be consistent with the renormalization group prediction of Aharony and Harris. Using this alternative approach, we find estimates of the correlation length exponent $\nu$ in agreement with results obtained from the usual finite-size scaling (FSS) methodology.

Keywords: Classical Monte Carlo simulations, Classical phase transitions (Theory), Finite-size scaling, Disordered systems (Theory)
1. Introduction

Phase transition in systems with quenched disorder are of considerable theoretical and experimental interest and have been the subject of intensive investigations \cite{1, 2, 3}. Nowadays, the effect of disorder coupled to the energy density on second-order phase transitions is well understood. The phase transition remains second-order and the eventual modification of the universality class is governed by the specific heat divergence exponent $\alpha_p$, as stated by the Harris criterion \cite{4}. According to this criterion, if $\alpha_p$ is positive, disorder is relevant, i.e. the system will reach a new critical behavior under the presence of quenched randomness. Otherwise, if $\alpha_p$ is negative, disorder is irrelevant and the critical behavior will not change. The value $\alpha_p = 0$ of the 2d Ising model is an inconclusive, marginal case \cite{5}.

In the present paper we simulate two different 2d random bond Ising spin systems, the marginal case of the simple 2d Ising model ($\alpha_p = 0$) and the non-marginal case of the square SAF model with nearest- ($J_{nn}$) and next-nearest-neighbor ($J_{nnn}$) competing interactions on the square lattice \cite{6, 7} for $R = J_{nn} / J_{nnn} = 1$ ($\alpha_p > 0$ \cite{8}). Several aspects of the critical behavior of these two models have been elucidated in references \cite{9, 10} and will be also briefly reviewed in the following Section. Our aim here is to study and contrast the dependence of the self-averaging properties of the systems and use these properties for an alternative investigation of their critical behavior. Self-averaging is an important issue when studying phase transitions in disordered systems. Although it has been known for many years now that for (spin and regular) glasses there is no self-averaging in the ordered phase \cite{11}, for random ferromagnets such a behavior was first observed for the random field Ising model in a paper by Dayan et al \cite{12} and some years later for the random versions of the Ising and Ashkin-Teller models by Wiseman and Domany \cite{13}. These latter authors proposed a FSS ansatz describing the absence of self-averaging and the universal fluctuations of random systems near critical points that was refined and put on a more rigorous basis by the intriguing renormalization group work of Aharony and Harris \cite{14}. Ever since, the subject of breakdown of self-averaging is an important aspect in several numerical investigations of disordered spin systems \cite{15, 16, 17, 18, 19, 20, 21, 22, 23, 24}.

In the next Section we define the models under study and we review their critical behavior. Basic analytical predictions on the issue of self-averaging in disordered systems are also presented in this Section. In Section 3 we briefly outline our entropic sampling scheme and we present our results on the self-averaging properties of both models. Finally, we summarize our conclusions in Section 4.
2. Models and theoretical aspects on self-averaging

The general form of the Hamiltonian of the random bond versions of both models considered here is given by

\[ H = \sum_{<i,j>} J_{ij}^{(nn)} S_i S_j + \sum_{(i,j)} J_{ij}^{(nnn)} S_i S_j, \]  

where \( S_i = \pm 1 \) are Ising spins, the superscripts \((nn)\) and \((nnn)\) stand for nearest- and next-nearest-neighbor interactions, and the implementation of bond disorder follows the binary distribution

\[ P(J_{ij}) = \frac{1}{2} \left[ \delta(J_{ij} - J_1) + \delta(J_{ij} - J_2) \right]; \quad \frac{J_1 + J_2}{2} = 1; \quad r = \frac{J_2}{J_1}, \]

where the ratio \( r \) is the disorder strength and throughout the paper takes the value \( r = 3/5 = 0.6 \). From equation (1) we obtain:

- The random bond ferromagnetic Ising model for \( J_{ij}^{(nn)} < 0 \) and \( J_{ij}^{(nnn)} = 0 \). Note here that, with this distribution the random Ising system exhibits a unique advantage that its critical temperature \( T_c \) is exactly known \[25\] as a function of the disorder strength \( r \) through: \( \sinh(2J_1/T_c)\sinh(2rJ_1/T_c) = 1 \) \((k_B = 1)\). This provides an excellent check for the accuracy of the numerical scheme, by comparing the estimated critical temperature with the exact result, as illustrated in reference [9].

Two main and mutually excluded scenarios \[5\] exist for the description of the critical behavior of the random version of the Ising model. The first, is the logarithmic corrections scenario, which, based on quantum field theory results \[26, 27, 28, 29\], states that the presence of quenched disorder changes the critical properties of the system only through a set of logarithmic corrections to the pure system behavior. The second scenario of the so-called weak universality \[30, 31, 32, 33\], assumes that critical quantities, such as the zero field susceptibility, magnetization, and correlation length display power law singularities, with the corresponding exponents \( \gamma, \beta, \) and \( \nu \) changing continuously with the disorder strength; however this variation is such that the ratios \( \gamma/\nu \) and \( \beta/\nu \) remain constant at the pure system’s value. The specific heat of the disordered system is, in this case, expected to saturate. Overall, for the random Ising model, the results of most studies \[34, 35, 36, 37, 38\], including our recent investigation \[9\], support the scenario of logarithmic corrections. Here, additional evidence in favor of this scenario are presented, via an alternative route that involves the asymptotic scaling behavior of the sample-to-sample fluctuations of the susceptibility’s pseudocritical temperature.

- The random bond square \((R = 1)\) SAF model for \( J_{ij}^{(nn)} = J_{ij}^{(nnn)} > 0 \). It is well-known that the pure square SAF model develops at low temperatures SAF order for \( R = J_{nn}/J_{nnn} > 0.5 \) \[6, 7\]. For the case \( R = 1 \), that we deal with, the pure system undergoes a second-order phase transition, in accordance with the commonly accepted scenario of a non-universal critical behavior with exponents depending on the coupling ratio \( R \) \[6, 7\]. In fact, recent numerical studies of the
model indicated that the $R = 1$ model undergoes, at its pure version [8, 39], a clear second-order transition with an exponent $\nu_p$ very close to that of the 2d three-state Potts model $\nu_p(Potts) = 5/6$ [40], and at its random bond version [9, 10], a transition governed by a random fixed point with a correlation length exponent $\nu = 1.080(20)$ and magnetic exponents that satisfy the weak universality scenario for disordered systems as stated by Kim [41]. Furthermore, a strong saturating behavior of the specific heat was observed that distinguished this case of competing interactions from other 2d random bond ferromagnetic systems studied previously [41, 42].

Our numerical studies of disordered systems are carried out near their critical points using finite samples; each sample $i$ is a particular random realization of the quenched disorder. A measurement of a thermodynamic property $X$ yields a different value for the exact thermal average $X_i$ of every sample $i$. In an ensemble of disordered samples of linear size $L$ the values of $X_i$ are distributed according to a probability distribution $P(X)$. In most Monte Carlo studies, see also our recent investigations [9, 10], one considers the ensemble averages $[X]_{av}$ and their scaling properties. However, here, we will focus on obtaining direct evidence about the nature of the governing fixed points and the self-averaging properties of the disordered systems via the distribution $P(X)$, where $X$ may be the sample-dependent pseudocritical temperatures $T_c(i, L)$ and the corresponding magnetic susceptibility peaks $\chi_{max}(i, L)$. The behavior of this distribution is directly related to the issue of self-averaging mentioned in the introduction. In particular, by studying the behavior of the width of $P(X)$ with increasing the system size $L$, one may address qualitatively the issue of self-averaging, as has already been stressed by previous authors [17]. In general, we characterize the distribution $P(X)$ by its average $[X]_{av}$, and also by the relative variance $R_X = V_X/[X]_{av}^2$, where $V_X = [X^2]_{av} - [X]_{av}^2$. Suppose now that $X$ is a singular density of an extensive thermodynamic property, such as $M$ or $\chi$, or the singular part of $E$ and $C$. The system is said to exhibit self-averaging if $R_X \to 0$ as $L \to \infty$. If $R_X$ tends to a non-zero value, i.e. $R_X \to const \neq 0$ as $L \to \infty$, then the system exhibits lack of self-averaging. The importance of the above concept has been illustrated by Aharony and Harris [14] and their main conclusions are summarized below:

- **Away from the critical temperature:** $R_X = 0$. In a finite geometry, the correlation length $\xi$ is finite for $T \neq T_c$ and it can be found, using general statistical arguments, originally introduced by Brout [43], that $R_X \propto (\xi/L)^d \to 0$, as $L \to \infty$. This is called strong self-averaging.

- **At the critical temperature** there exist two possible scenarios: (i) models in which according to the Harris criterion the disorder is relevant ($\alpha_p > 0$): $R_X \neq 0$. Then, the system at the critical point is not self-averaging and (ii) models in which according to the Harris criterion disorder is irrelevant ($\alpha_p < 0$): $R_X = 0$. In this case $R_X$ scales as $L^{\alpha/\nu}$, where $\alpha$ and $\nu$ are the critical exponents of the pure system, which are the same in the disordered one. This is called weak self-averaging.
The pseudocritical temperatures $T_c(i, L)$ of the disordered system are distributed with a width $\delta[T_c(L)]_{av}$, whose square scales with the system size as $\delta^2[T_c(L)]_{av} \sim L^{-n}$, where $n = d$ or $n = 2/\nu$, depending on whether the disordered system is controlled by the pure or the random fixed point, respectively. The above behavior is now well established by the pioneering works of Aharony and Harris [14] and Wiseman and Domany [13, 17].

In the following Section, we will test the above theoretical predictions for the two disordered models under study and extract useful information for some aspects of their critical behavior, as these emerge from the above described theory.

3. Simulations and results

The numerical scheme used to estimate here the self-averaging properties of the random versions of the Ising and the SAF models has been presented in detail in references [9, 10], where a two stage strategy of an energy-restricted [45] implementation of the WL algorithm [44] was proposed and successfully applied on the above random models. In these papers our analysis focused on the averaged curves $[\ldots]_{av}$ and in particular on the scaling behavior of their maxima $[\ldots]_{max}^{av}$, which as discussed above is the common practise in disordered systems. Here, we follow a different averaging process, namely that of averaging over the individual maxima $\chi_{max}^{i, L}_{av}$ of the random realizations. Within this practise, apart from having an also accurate, as will be seen below, estimator of mean values, one has the advantage of estimating directly the corresponding sample-to-sample fluctuations of a thermodynamic quantity $X$, that may be defined with the help of the variance of the corresponding distribution $P(X)$, as defined in the discussion of self-averaging in Section 2. In particular, we consider square lattices with periodic boundary conditions and linear sizes $L$ in the range $L = 20 – 120$. For each lattice size we present results of ensembles of up to 200 - for the larger sizes - bond disorder realizations. Note here that, the statistical errors of the WL method have been omitted from all our figures below, since they were found to be much smaller than the errors due to the finite number of disorder averaging, shown in figure 2 and even smaller than the sample-to-sample fluctuations, shown in figure 3.

We start the presentation of our results with figure 1 where we show the normalized fluctuation of (a) the pseudocritical temperature of the magnetic susceptibility $T_c(i, L)/[T_c(L)]_{av}$ and (b) the susceptibility maxima $\chi_{max}^{i, L}/[\chi_{max}^{L}]_{av}$ for both random bond models considered, for a lattice size $L = 60$ and a subset of 100 disorder realizations. It is clear from this figure that for both quantities, $T_c(i, L)$ and $\chi_{max}^{i, L}$, the variance of the data for the case of the random bond SAF model is much larger, compared to the simple random bond Ising model. This strong sample-dependence for the random bond SAF model is reflected in figure 2, where we illustrate the FSS behavior of the ratio $R_{[\chi_{max}]}_{av}$, defined in Section 2, as a function of the inverse linear size for both models considered. From the main panel and the corresponding inset we observe a definite approach to a non-zero limiting value, indicating a strong violation of
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Figure 1. Normalized fluctuation of (a) the pseudocritical temperature and (b) the susceptibility maxima for both random bond models considered for a lattice size \( L = 60 \) in a subset of 100 disorder realizations.

self-averaging \([14, 17, 24]\) of both the random Ising and SAF models. However, for the case of the random SAF model this limiting value is much larger, by a factor of \( \sim 100 \).

Let us point out here that, for the magnetic susceptibility, the lack of self-averaging may be present even for pure systems \([47]\). The results shown in the figures above verify this expectation in a definite way and reveal an interesting aspect, which is the sensitivity of the microscopic interactions to bond randomness.

In the main panels of figure 2 we illustrate the shift behavior of the individual averaged pseudocritical temperatures \([T_c(L)]_{av}\) of the magnetic susceptibility for (a) the random bond Ising model and (b) the random bond SAF model. The error bars shown in this figure, as was already mentioned above, are the sample-to-sample fluctuations of the two disordered models \( \delta T_c(L) \). The shift behavior of these pseudocritical temperatures is expected to provide estimates for both the critical temperature and the correlation length exponent, via the relation

\[
[T_c(L)]_{av} = T_c + bL^{-1/\nu}.
\]

The solid lines shown in both panels are fits of the form (3) giving the values: \( T_c = 2.2243(6) \) and \( \nu = 1.010(12) \) for the random bond Ising model and \( T_c = 1.978(8) \) and \( \nu = 1.084(22) \) for the random bond SAF model. For the case of the random Ising model, the estimated value \( T_c = 2.2243(6) \) of the critical temperature is in excellent agreement with the value 2.2245(7), obtained in reference \([9]\) from the scaling
Figure 2. Behavior of the ratio \( R_{\chi_{\text{max}}^{\text{av}}} \), defined in the text, as a function of the inverse lattice size for both models in the main panel and only for the random bond Ising model in the inset. The statistical error bars shown are due to the finite number disorder sampling and have been estimated using the jackknife method [46].

of the ensemble average \([\ldots]_{\text{av}}^{\text{max}}\), via a simultaneous fitting of the specific heat’s and magnetic susceptibility’s pseudocritical temperatures, and also with the exact value \( T_c = 2.22419 \ldots \). Note that, this latter comparison consists a concrete reliability test in favor of the accuracy of our numerical data. Also, for the correlation length exponent, our results indicate that it maintains, within error bars, the value of the pure model, i.e. \( \nu = 1 \), in agreement with reference [9]. Turning now to the random bond square SAF model, the results obtained here for the critical temperature, \( T_c = 1.978(8) \), and correlation length exponent, \( \nu = 1.084(22) \), are also in good agreement with our recent study of this model [10], where from the shift behavior of various pseudocritical temperatures, the values \( T_c = 1.980(9) \) and \( \nu = 1.080(20) \) were obtained.

In the corresponding insets of figure 3 we illustrate the scaling of the sample-to-sample fluctuations of the sample-averaged pseudocritical temperatures of the magnetic susceptibility, shown in the main panel of this figure, in a log-log scale. Following Aharony and Harris [14] (see also the discussion in Section 2), we assume that the square of these sample-to-sample fluctuations scales with the linear size \( L \) according to \( L^{-n} \) we obtain, from the excellent fittings for both models, the values \( n = 1.98(3) \) and \( n = 1.83(4) \), respectively. For the case of the random bond SAF model the situation is quite clear. The system is described by a new random fixed point, so that \( n = 2/\nu \), and the estimate for \( \nu \) is 1.093(24), in agreement with the estimation 1.084(22) provided above from the shift behavior of the corresponding pseudocritical temperature and also with the traditional estimations presented in reference [10]. The result \( n = 1.98 \) for
FIGURE 3. Shift behavior of the pseudocritical temperatures of the magnetic susceptibility for (a) the random bond Ising model and (b) the random bond square SAF model. The error bars show the sample-to-sample fluctuations of the models in the ensembles of the simulated realizations. The corresponding insets show the FSS of the square of these sample-to-sample fluctuations in a log-log scale for the larger sizes studied ($L \geq 50$). The solid lines shown are linear fits giving estimates for the exponent $n$.

the random Ising model has within error bars the value of the space dimension $d = 2$ and thus provides further strong indications that, the random bond version of the Ising model is governed by the pure fixed point. An analogous study has been performed by Tomita and Okabe [19] for the 2d site diluted Ising model, where also an exponent $n \approx 2$ has been estimated via the scaling of the sample-to-sample fluctuations of the pseudocritical temperatures. Thus, figure 3 illustrates an important aspect of the critical behavior of disordered systems that can be determined by studying their self-averaging properties.

4. Conclusions

In the present paper we have investigated the effects induced by the presence of quenched bond randomness on the critical self-averaging properties of two Ising spin models in 2d, namely the regular Ising model and the case of competing interactions in a generalized square Ising model. Our comparative study uncovered the sensitivity of the microscopic competing interactions, responsible for the SAF ordering, to bond randomness. This is manifested in the much stronger violation of self-averaging of the magnetic susceptibility and the large fluctuations of the individual corresponding pseudocritical temperatures. Moreover, a detailed finite-size scaling analysis of the width of the distribution of the
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Sample-dependent pseudocritical temperatures of the magnetic susceptibility verified the theoretical expectations of Aharony and Harris and provided an alternative approach of extracting the value for the correlation length exponent. Thus, the generally undesirable feature of lack of self-averaging in quenched random systems has been turned here into a useful tool that contributes to our understanding of the nature of phase transitions of these systems by providing an alternative approach to criticality.

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