LETTER

Wang–Landau study of the random bond square Ising model with nearest- and next-nearest-neighbor interactions

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Abstract. We report results from a Wang–Landau study of the random bond square Ising model with nearest-neighbor ($J_{nn}$) and next-nearest-neighbor ($J_{nnn}$) antiferromagnetic interactions. We consider the case $R = J_{nn}/J_{nnn} = 1$ for which the competitive nature of interactions produces a sublattice ordering known as superantiferromagnetism and the pure system undergoes a second-order transition with a positive specific heat exponent $\alpha$. For a particular disorder strength we study the effects of bond randomness and we find that, while the critical exponents of the correlation length $\nu$, magnetization $\beta$, and magnetic susceptibility $\gamma$ increase as compared to the pure model, the ratios $\beta/\nu$ and $\gamma/\nu$ remain unchanged. Thus, the disordered system obeys weak universality and hyperscaling similarly to other two-dimensional disordered systems. However, the specific heat exhibits an unusually strong saturating behavior which distinguishes the present case of competing interactions from other two-dimensional random bond systems studied previously.

Keywords: classical Monte Carlo simulations, classical phase transitions (theory), finite-size scaling, disordered systems (theory)
In the last three decades, the effect of quenched randomness on the critical behavior of statistical models in two (2D) and three dimensions (3D) has been the subject of intensive study. First-order transitions are known to be dramatically softened in the presence of quenched randomness [1]–[5], while continuous transitions may have their exponents altered under random fields or for random bonds [3, 6, 7]. There are some very useful phenomenological arguments and some, perturbative in nature, theoretical results, pertaining to the occurrence and nature of phase transitions in the presence of quenched randomness [3], [8]–[12]. The most celebrated criterion is that suggested by Harris [6]. This criterion relates directly the persistence, for random bonds, of the non-random behavior to the specific heat exponent $\alpha_p$ of the corresponding pure system. If $\alpha_p$ is positive, then the disorder will be relevant, i.e., under the effect of the disorder, the system will reach a new critical behavior. Otherwise, if $\alpha_p$ is negative, disorder is irrelevant and the critical behavior will not change. The value $\alpha_p = 0$ gives an inconclusive, marginal case. The 2D Ising model falls into this category and although it is the most studied case, it is still controversial [13]–[27]. In general and despite the intensive efforts of the last few years on several different models, our current understanding of the quenched randomness effects is rather limited and the situation appears still unclear for both cases, of first- and second-order phase transitions.

The present letter is the first investigation of the bond disorder effects on an interesting 2D model with competing interactions. We consider the square Ising model with nearest-neighbor ($J_{nn}$) and next-nearest-neighbor ($J_{nnn}$) antiferromagnetic interactions for a certain value of the coupling ratio $R = J_{nn}/J_{nnn} = 1$. For this value of $R$, the pure system undergoes a clear second-order phase transition (from the superantiferromagnetic (SAF) state to the paramagnetic state) and accurate estimates of critical exponents have recently been reported [28, 29]. Since the value for the critical exponent $\alpha_p$ of the specific heat of this generalized Ising model is very close (almost identical; see the discussion below) to that of the 2D three-state Potts model ($\alpha_p = 1/3$) our choice of studying this case closely follows the motivation of similar numerical studies performed earlier by Kim [30] and Picco [31] on the 2D random bond three-state Potts ferromagnet. In other words, due to the difficulties and possible crossover effects in the marginal case of $\alpha_p = 0$ (2D Ising model) it is desirable to study here the critical behavior induced by disorder in a case where the pure model has a positive specific heat exponent and according to the Harris criterion [6] is expected to reach a new critical behavior. Our results will be therefore profitably compared to those of Kim [30] and Picco [31] for the 2D random bond three-state Potts ferromagnet and possible interesting differences may reflect aspects that are due to the different microscopic interactions.

In zero field, the pure system under consideration is governed by the Hamiltonian

$$\mathcal{H}_p = J_{nn} \sum_{(i,j)} S_i S_j + J_{nnn} \sum_{(i,j)} S_i S_j,$$

where here both nearest-neighbor ($J_{nn}$) and next-nearest-neighbor ($J_{nnn}$) interactions are assumed to be positive. It is well known that the model develops at low temperatures SAF order for $R = J_{nn}/J_{nnn} > 0.5$ [32, 33] and by symmetry the critical behavior associated with the SAF ordering is the same under $J_{nn} \to -J_{nn}$. We will consider here only the case $R = J_{nn}/J_{nnn} = 1$, with $J_{nn} = J = 1$. For this case ($R = 1$), the system undergoes a second-order phase transition, in accordance with the commonly accepted...
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scenario for many years of a non-universal critical behavior with exponents depending on the coupling ratio $R$ \cite{32}--\cite{36}. The recent Wang–Landau \cite{37} study of Malakis \textit{et al} \cite{28} has refined earlier estimates \cite{33,35} for the correlation length exponent $\nu$ and values very close to those of the 2D three-state Potts model $\nu_p$ (Potts) = $5/6$ \cite{38} were obtained. From the finite size scaling (FSS) of the pseudocritical temperatures \cite{28} it was found that $\nu_p(\text{SAF}; R = 1) = 0.8330(30)$ and the subsequent study of Monroe and Kim \cite{29}, using the Fisher zeros of the partition function, yielded a quite closely matching estimate: $\nu_p(\text{SAF}; R = 1) = 0.848(1)$. Furthermore, from the FSS of the specific heat data an estimate for the ratio $\alpha_p/\nu_p = 0.412(5)$ was also found \cite{28}. Finally, from the magnetic data and in accordance with an earlier conjecture of Binder and Landau \cite{33}, Malakis \textit{et al} \cite{28} found additional evidence of the weak universality scenario \cite{39} and obtained the values $\beta_p/\nu_p = 0.125$ and $\gamma_p/\nu_p = 1.75$. The values of the above three ratios of exponents satisfy the Rushbrook relation, assuming that $\nu_p = 0.8292$, which is very close to the estimate obtained from the shift behavior of the SAF $R = 1$ model, thus providing self-consistency to the estimation scheme. From these results, it is tempting to conjecture that the SAF model with $R = 1$ obeys the same thermal exponents with the 2D three-state Potts model ($\nu_p = 5/6 = 0.833\cdots$ and $\alpha_p = 1/3 = 0.333\cdots$ \cite{38}), but the respective values of the magnetic critical exponents are different ($\beta_p/\nu_p = 2/15 = 0.133\cdots$ and $\gamma_p/\nu_p = 26/15 = 1.733\cdots$ \cite{38}).

In the present study, we consider a particular type of bond disorder, the same for both nearest- and next-nearest-neighbor spins $i$ and $j$ according to the following bimodal distribution:

$$P(J_{ij}) = \frac{1}{2}[\delta(J_{ij} - J_1) + \delta(J_{ij} - J_2)]; \quad \frac{J_1 + J_2}{2} = 1; \quad r = \frac{J_2}{J_1} = 0.6.$$ \hspace{1cm} (2)

The resulting disordered (random bond) version of the Hamiltonian defined in equation (1) reads now as

$$\mathcal{H} = \sum_{(i,j)} J_{ij} S_i S_j + \sum_{(i,j)} J_{ij} S_i S_j.$$ \hspace{1cm} (3)

This particular choice of the disorder strength $r = 0.6$ is strong enough, as will be shown below, for observing dramatic saturation effects on the originally diverging behavior of the specific heat of the pure model. Only this case will be considered in this letter; the more general case for other values of the disorder strength together with a comparative study with the 2D random bond Ising model and also details of our numerical scheme will be presented in a longer paper. The present Wang–Landau study \cite{37} closely follows our recent implementations of an energy restricted sampling, known as critical minimum energy subspace (CrMES) \cite{40} appropriately adapted to the study of systems with complicated free-energy landscapes, such as the random-field Ising model \cite{41}. We impose periodic boundary conditions on square lattices with linear sizes $L$ in the range $L = 20–120$ and simulate relatively large ensembles of 100 disorder realizations.

Each disorder realization is repeatedly simulated up to four times with different initial conditions. Furthermore, in our implementation of the Wang–Landau repetition process thermal properties are calculated at two different Wang–Landau levels and this practice enabled us to estimate statistical errors. The statistical errors of the Wang–Landau method (WL errors) used for the estimation of thermal and magnetic properties of a particular realization were found much smaller than the statistical errors coming from the
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fact that we used, for disorder averaging, a finite number of 100 realizations. Therefore, 
the WL errors are not shown in our graphs, since in all cases, they are much smaller 
than the symbol sizes, whereas the latter errors of ‘finite disorder sampling’ (fds errors) 
are considerable and are presented in all our figures as error bars. The mean values over 
disorder are denoted as [
\ldots\]_{av}, the corresponding maxima as [
\ldots\]^*_{av}, and the individual 
maxima as [
\ldots\]^*_{av}. Since in our fitting attempts we have used mainly data from the peaks 
of the disorder averaged curves (i.e. [C]^*_{av}), their fds errors are the relevant statistical 
errors and have been determined by two similar methods. Using our runs, organized 
in four groups of 25 realizations for each lattice size, an application of the jackknife 
method [42] and a straightforward four-point variance calculation (blocking method) [42] 
were undertaken using the corresponding four peaks of the averaged curves, for all thermal 
and magnetic properties studied. It appears that the jackknife method yields some 
reasonably conservative errors, that are about 15–20% larger than the corresponding 
calculated standard deviations. These jackknife errors are shown as error bars in all 
our figures and have been used in all our fits. Finally, let us point out that sample-to-
sample fluctuations for the individual maxima (such as [\chi]^*_{av}) become very large with 
the lattice size. The definition of the order parameter follows reference [28], using the four 
sublattice magnetizations: 

\[ M = \sum_{i=1}^{4} |M_i|/4. \]

Let us start the presentation of our results with the most striking effect of the bond 
randomness on the specific heat of the square SAF model. In figure 1 we contrast the 
size dependence of the specific heat maxima of the pure (filled squares) and the random 
bond models (filled circles). The suppression of the specific heat maxima is clear for the 
disordered case, even for the smaller sizes shown, and this behavior should be compared 
with the behavior of the specific heat of the above mentioned previous studies concerning 
the 2D random bond three-state Potts ferromagnet [30,31]. It will then be observed 
from these comparisons that, in full disagreement with our finding of a strong saturating 
specific heat for the SAF \( R = 1 \) model, in the case of the 2D random bond three-state

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**Figure 1.** Size dependence of the maxima of the specific heat for the pure (filled 
squares; data taken from reference [28]) and the random bond models (filled 
circles).
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Figure 2. (a) Simultaneous fitting of the pseudocritical temperatures of the average specific heat (filled squares) and magnetic susceptibility (filled circles). (b) Log–log plot of the maxima of the average logarithmic derivatives defined in equation (5). Linear fits are applied for $L \geq 30$. Error bars are explained in the text.

Potts model one obtains a still diverging behavior for disorder strengths $r = 0.9, 0.5,$ and $0.25$ [30] and an increasing but progressively saturating behavior is obtained only for the very strong disorder $r = 0.1$ [31]. On the other hand, for the random bond SAF $R = 1$ model, it is evident from figure 1 that the data for the average specific heat saturate to a value already, from the size of $L = 40$, and any small variation around this value is mainly coming from the fds errors. Therefore the estimation of the ratio $\alpha/\nu$ for this model is not possible from the specific heat data, and the alternative route via the Rushbrook relation will be implemented later.

In figure 2(a) we present the FSS behavior of two pseudocritical temperatures of the model $T[Z]_{\text{av}}$, i.e. the temperatures corresponding to the average specific heat ($Z = C$: filled squares) and the average magnetic susceptibility ($Z = \chi$: filled circles). Solid lines show a simultaneous fit to both data sets according to the relation

$$T[Z]_{\text{av}} = T_c + bL^{-1/\nu},$$

(4)
giving $T_c = 1.980(9)$ for the critical temperature of the disordered model, which is to be compared with the corresponding critical temperature $T_{c\text{p}} = 2.0823(17)$ of the pure system [28]. The value for $\chi^2/\text{DoF}$ of the above fit, using the jackknife errors, is 0.11. Correspondingly, the values of $\chi^2/\text{DoF}$ for all our fits vary in the range 0.1–0.4. On the other hand, using the smaller simple standard deviation errors, one would obtain for $\chi^2/\text{DoF}$ values in the range 0.2–0.7. The above ranges for the ratios $\chi^2/\text{DoF}$ reflect the goodness of our fits. One could also use the FSS of the pseudocritical temperatures defined with the help of the average of the individual maxima of the specific heat and

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susceptibility, i.e. the $T^{[Z^*_\text{av}]}$, but this choice gives similar results and it is not shown here for brevity. A first estimation of the critical exponent $\nu$ of the correlation length is obtained from the above shift behavior and is $\nu = 1.080(20)$, as illustrated in the graph. An alternative estimation of the exponent $\nu$ is attempted now from the FSS analysis of the logarithmic derivatives of several powers of the order parameter with respect to the temperature $[4, 43]$:

$$\frac{\partial \ln \langle M^n \rangle}{\partial T} = \frac{\langle M^n E \rangle}{\langle M^n \rangle} - \langle E \rangle,$$

which scale as $L^{1/\nu}$ with the system size. In figure 2(b) we consider on a double-logarithmic scale the size dependence of the first-order (filled squares), second-order (filled circles), and fourth-order (filled triangles) maxima of the average over the ensemble of realizations logarithmic derivatives. The solid lines shown are corresponding linear fits whose slopes provide respectively estimates for $1/\nu$. The estimates in figure 2(b) have an average for the correlation length exponent of the order of $\nu = 1.089$. Combining all the above estimates we propose an error bound for $\nu$ of the order of 0.015. Thus, in comparison with its value for the pure model, the exponent $\nu$ for the disordered model shows an increase of the order of 30%, reflecting the strong influence of the disorder on the thermal properties of the system. It is important to point our here that our estimate is in agreement with the inequality $\nu \geq 2/D$ derived by Chayes et al [7] for disordered systems.

Turning now the magnetic properties of the model we begin by presenting the behavior of the order parameter at the critical temperature. We present in figure 3(a) on a log–log scale the FSS behavior of the average order parameter at the estimated critical temperature $T_c = 1.98$. The straight line shows a linear fit for $L \geq 30$ with a slope of 0.126(5) which is a first manifestation that the ratio $\beta/\nu$ has within error bars the value of the pure model. Furthermore, in the inset of panel (a) we plot in a log–log plot the size dependence of the maxima of the average absolute order parameter derivative, defined as

$$\frac{\partial \langle |M| \rangle}{\partial T} = \langle |M| E \rangle - \langle |M| \rangle \langle E \rangle,$$

which is expected to scale as $L^{(1-\beta)/\nu}$ with the system size $[4, 43]$. Thus, the slope of the straight line, which is again a linear fit for $L \geq 30$, provides the estimate $(1 - \beta)/\nu = 0.791(11)$. This estimate when combined with the value for $\nu = 1.089$ gives a value for $\beta/\nu$ of the order of 0.127 and using the earlier error bars for $\nu$ we propose again an error bound of the order of 0.015. Thus, the two estimations are self-consistent and our results indicate that although the exponent $\beta$ increases in the disordered case, the ratio $\beta/\nu$ remains unchanged to its pure value, i.e. $\beta/\nu = \beta_p/\nu_p = 0.125$ [28]. In the sequel, we show in panel (b) of figure 3 the behavior of the magnetic susceptibility of the model in order to provide estimates for the ratio $\gamma/\nu$. We present two data points: the filled squares refer to the maxima of the average curve $[\chi^*_\text{av}]$, while the filled circles refer to the average of the individual maxima $[\chi^*_\text{av}]$. In the latter case the error bars shown reflect the sample-to-sample fluctuations, which are, as already pointed out, larger than the fds errors of the corresponding averaged curves and of course much larger than the statistical errors. The solid and dotted lines are linear fits for $[\chi^*_\text{av}]$ and $[\chi^*_\text{av}]$ respectively, giving the values $\gamma/\nu = 1.751(10)$ and $\gamma/\nu = 1.757(11)$, thus providing convincing...
Figure 3. (a) Log–log plot of the average magnetization at the estimated critical temperature. The inset shows the log–log plot of the maxima of the average absolute order parameter derivative. (b) Log–log plot of the size dependence of the maxima of the magnetic susceptibilities: $\chi^*_\text{av}$ (filled squares) and $\chi^*_\text{av}$ (filled circles). Sample-to-sample fluctuations of $\chi^*_\text{av}$ become much larger than the fds errors of $\chi^*_\text{av}$.

evidence that $\gamma/\nu = \gamma_p/\nu_p = 1.75$ [28], i.e. the ratio $\gamma/\nu$ maintains the value of the pure model. Thus, the ratios $\beta/\nu$ and $\gamma/\nu$ for the disordered square SAF model appear to be the same as the corresponding ratios of the pure square SAF model but different from those of the 2D three-state Potts model. Therefore, our results reinforce both the weak universality scenario for the pure SAF model, as first predicted by Binder and Landau [33], and the generalized statement of weak universality in the presence of bond randomness, given by Kim [30] and concerning also the 2D random bond three-state Potts ferromagnet.

Finally, as discussed above, it is not possible to directly estimate the specific heat exponent from FSS of the specific heat data. Yet, having estimated the values for $\beta/\nu$, $\gamma/\nu$, and $\nu$, we may estimate $\alpha$ using either the Rushbrook ($\alpha+2\beta+\gamma = 2$) or equivalently, since $2\beta/\nu + \gamma/\nu = 2$, the hyperscaling $(2-\alpha = D\nu)$ relation. Both relations provide a negative value for the specific heat exponent $\alpha = 2 - D\nu = 2 - 2\beta - \gamma = -0.173(40)$, reflecting the early saturation effect. This value of $\alpha$ differs significantly from the values estimated for relevant cases in the 2D random bond Potts ferromagnet [30, 31]. One may attribute this strongly saturating behavior of the specific heat to the competitive nature of interactions which is supposedly responsible for the observed sensitivity of the SAF model to bond randomness, since the disorder effects in this case are much more dramatic in comparison with the effects observed in other 2D models with simple ferromagnetic interactions, such as the 2D three-state Potts ferromagnet [30, 31].
In conclusion, we have applied the Wang–Landau algorithm to investigate the interesting effects caused by the presence of quenched bond randomness on the critical behavior of the square Ising model with nearest- and next-nearest-neighbor interactions. Using standard finite size scaling techniques, on high accuracy numerical data, we have estimated the critical temperature of the disordered model to be well below the value of the corresponding pure model and we have extracted values for all critical exponents of the random bond square SAF model. These values verify hyperscaling and also satisfy the Chayes et al inequality [7] and the weak universality scenario for disordered systems, as stated by Kim [30]. The observed unusual strong saturating behavior of the specific heat with a negative exponent $\alpha$, distinguishes the present case of competing interactions from other 2D random bond systems studied previously.

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