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Critical scaling of the mutual information in two-dimensional disordered Ising models

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Abstract. Rényi mutual information, computed from second Rényi entropies, can identify classical phase transitions from their finite-size scaling at critical points. We apply this technique to examine the presence or absence of finite temperature phase transitions in various two-dimensional models on a square lattice, which are extensions of the conventional Ising model by adding a quenched disorder. When the quenched disorder causes the nearest neighbor bonds to be both ferromagnetic and antiferromagnetic, (a) a spin glass phase exists only at zero temperature, and (b) a ferromagnetic phase exists at a finite temperature when the antiferromagnetic bond distributions are sufficiently dilute. Furthermore, finite temperature paramagnetic-ferromagnetic transitions can also occur when the disordered bonds involve only ferromagnetic couplings of random strengths. In our numerical simulations, the 'zero temperature only' phase transitions are identified when there is no consistent finite-size scaling of the Rényi mutual information curves, while for finite temperature critical points, the curves can identify the critical temperature T_c by their crossings at T_c and $2\,T_c$.

Keywords: classical Monte Carlo simulations, classical phase transition, disordered spin chains

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Contents

1. Introduction 2
2. Models 3
3. Method 4
4. Results 6
5. Discussion and concluding remarks 7
   Acknowledgments 8
   References 8

1. Introduction

A system with quenched disorder is one where some of the parameters defining its behaviour are random variables that do not evolve with time, and as such they are quenched or frozen. One such example is a spin glass, which is a disordered magnetic system. Although the interactions between the magnetic moments in a spin glass are frustrated, nevertheless it exhibits a transition from the paramagnetic phase to a novel ordered phase—the spin glass phase—where the spins are frozen in an irregular pattern. Since randomness and frustration are the necessary ingredients for the emergence of a spin glass, quenched disorder in a classical spin system can lead to frustration, and thus generate spin glasses. In two-dimensional (2d) lattices, there have been extensive studies of such systems and all the results point to the fact that no spin glass phase exists for nonzero temperatures [1]. In fact, the lower critical dimension for Ising spin glasses is believed to be two, which indicates that the critical temperature for 2d is zero. However, finite temperature paramagnetic-ferromagnetic transitions are possible in such disordered systems if the frustration is reduced [2, 3], or removed altogether [4–7]. This can be achieved either by sufficiently reducing the number of antiferromagnetic bonds, or having only ferromagnetic couplings in the model.

In this work, we study a variety of classical spin-1/2 models on square lattices, which are extensions of the Ising model with some kind of quenched disorder. We reexamine the presence or absence of finite temperature phase transitions for these models using the method of classical Monte Carlo simulations, which, via a replica-trick scheme, can detect finite temperature critical points, even identifying their universality classes without any *a priori* knowledge of an order parameter or associated broken symmetry [8–10]. The method involves computation of Rényi mutual information (RMI) derived from the second Rényi entropies. The critical scaling of this mutual information with system size can detect and classify phase transitions. This method has been successfully applied in a number of classical systems [11–19]. The physical reason for information quantities being able to detect phase transitions is the deep connection between certain measurable thermodynamic quantities and principles of information theory. In fact, information can be quantified in terms of entropy, which in turn can be defined from thermodynamic observables [20, 21]. For classical phase transitions, correlation lengths diverge at the critical points, indicative of the existence of long-range channels for information transfer. Furthermore, the usefulness of the mutual information was demonstrated in a striking way by Stéphan *et al* [12], where simple classical Monte Carlo simulations of the 2d Ising model at its phase transition could compute the central charge of the associated $(1+1)$-dimensional conformal field theory (CFT) [21–25], thus identifying its universality class.

The paper is structured as follows: In section 2, we discuss the models for which the RMI is calculated as a function of system size and temperature. In section 3, we describe the numerical techniques employed to get the RMI curves. Section 4 describe our numerical results. We conclude with a discussion and some outlook in section 5.

2. Models

In this section, we describe the 2d classical spin models on a square lattice of a linear dimension L, for which we probe the critical temperature $T_{\rm c}$. Throughout this work, we will set the energy scale $J = 1$.

The Edwards–Anderson spin glass model [26], described by the Hamiltonian:

$$H = -\sum_{\langle ij\rangle} J_{ij}\, S_i^z\, S_j^z\,, \tag{1}$$

has a glassy phase below $T_{\rm c}$. Here $S_i^z = \pm 1$ represents the L^2 Ising spins and $\langle ij\rangle$ denotes nearest neighbor sites. The coupling strength J_{ij} between the nearest neighbors is a random (quenched) variable. The values of J_{ij} are drawn from a continuous Gaussian distribution with zero mean and unit variance:

$$P(J_{ij}) = \frac{\exp\left(-J_{ij}^2/2\right)}{\sqrt{2\,\pi}}, \tag{2}$$

or from a discrete bi-modal distribution:

$$P(J_{ij}) = \frac{1}{2}\left[\delta(J_{ij}+1) + \delta(J_{ij}-1)\right], \tag{3}$$

such that $J_{ij} = \pm 1$ with equal probability. For 2d, all studies found $T_{\rm c}$ to be zero.

When the values of J_{ij} in equation (1) are drawn from the probability distribution

$$P(J_{ij}) = p\,\delta(J_{ij}+1) + (1-p)\,\delta(J_{ij}-1),\ \text{with}\ 0 \leqslant p \leqslant 1, \tag{4}$$

then we get a random-bond Ising model, where the probabilities p and $(1-p)$ are associated with antiferromagnetic and ferromagnetic couplings, respectively. It was shown in [2, 3] that although the spin glass phase does not exist in 2d for $T > 0$ (at $T = 0$, the model has a spin glass phase), but for a sufficiently small concentration of antiferromagnetic bonds ($p < p_{\rm c}$), there exists a finite temperature phase transition from the paramagnetic to the ferromagnetic phase. At $p = 0$, we have the standard ferromagnetically coupled 2d Ising model with $T_{\rm c} \simeq 2.269$. For $p > 0$, this $T_{\rm c}$ is reduced by frustration induced by the antiferromagnetic couplings, until it vanishes at $p_{\rm c} \simeq 0.12$ [27].

J. Stat. Mech. (2018) 043301

We also consider a variation of the Hamiltonian in equation (1) by adding a second nearest neighbor interaction of uniform strength J', such that the Hamiltonian is given by:

$$H = -\sum_{\langle ij\rangle} J_{ij}\, S_i^z\, S_j^z - J' \sum_{\langle\langle ij\rangle\rangle} S_i^z\, S_j^z\,. \tag{5}$$

Here $\langle\langle ij\rangle\rangle$ denotes next nearest neighbor sites with distance $\sqrt{2}$ lattice spacing units apart. The system, with $J' = 1$ and $J_{ij} = \pm\lambda$ (dubbed as 'randomly coupled ferromagnet' or RCF), was predicted to have a finite temperature phase transition from numerical analysis [28–30]. The authors estimated the ordering temperatures to be close to 2 for $\lambda = 0.5$, 0.7 and dropping to zero near $\lambda = 1$.

We also study a 2d random-bond Ising model only with ferromagnetic couplings, such as that in the Hamiltonian in equation (1), we now have [4–7]:

$$P(J_{ij}) = p\,\delta(J_{ij} - 1) + (1-p)\,\delta(J_{ij} - \tilde{J}), \text{ with } 0 \leqslant p \leqslant 1. \tag{6}$$

For $\tilde{J} = 0$, the resulting 'dilute ferromagnet' is a disorder model where nonzero exchange interactions exist only between a fraction p of neighboring pairs of Ising spins. This system shows a finite temperate paramagnetic-ferromagnetic phase transition for $1/2 < p \leqslant 1$. The dependence of $T_{\rm c}$ on p can be found in figure 2 of [5, 6] and table 2 of [7]. Furthermore, for $p = 1/2$, the model is self-dual and $T_{\rm c}$ is determined exactly by the relation [4, 31]:

$$\tanh\left(\frac{J}{k_{\rm B}\, T_{\rm c}}\right) = {\rm e}^{-\frac{2\,\tilde{J}}{k_{\rm B}\,T_{\rm c}}}, \tag{7}$$

where we have restored the dimension-full quantities $(J, k_{\rm B})$ for convenience of illustration. Although this is not a spin glass system as it has no frustration, nevertheless it will be used to demonstrate that our method captures the $T_{\rm c}$ even for a disordered system.

3. Method

Let us consider the Hamiltonian of a classical spin system defined on a square lattice. We divide the lattice into two regions, A and B, with the spin configurations within each subsystem denoted by i_A and $i_{\rm B}$ respectively. The probability of the state i_A occurring in subregion A is $p_{i_A} = \sum_{i_{\rm B}} p_{i_A, i_{\rm B}}$, where $p_{i_A,i_{\rm B}} = \frac{{\rm e}^{-\beta E(i_A, i_{\rm B})}}{Z[T]}$ is the probability of existence of any arbitrary state of the entire system, obtained from the Boltzmann distribution. We have denoted the energy associated with the states i_A and $i_{\rm B}$ by $E(i_A, i_{\rm B})$, and the partition function for $A \cup B$ by $Z[T] = \sum_{i_A, i_{\rm B}} {\rm e}^{-\beta E(i_A, i_{\rm B})}$, where $\beta^{-1} = k_{\rm B}\, T$. We will use the units where $k_{\rm B}$ is set to 1.

In the partitioned system, the second Rényi entropy for subregion A is defined by [8]:

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J. Stat. Mech. (2018) 043301

$$
\begin{aligned}
S_2(A) &= -\ln\left(\sum_{i_A} p_{i_A}^2\right) \\
&= -\ln\left(\sum_{i_A} \frac{\sum_{i_\mathrm{B}} \mathrm{e}^{-\beta E(i_A, i_\mathrm{B})} \sum_{j_\mathrm{B}} \mathrm{e}^{-\beta E(i_A, j_\mathrm{B})}}{Z^2[T]}\right) \\
&= -\ln\left(Z[A,2,T]\right) + 2\ln\left(Z[T]\right),
\end{aligned} \tag{8}
$$

where $Z[A,2,T] = \sum_{i_A, i_\mathrm{B}, j_\mathrm{B}} \mathrm{e}^{-\beta\{E(i_A, i_\mathrm{B}) + E(i_A, j_\mathrm{B})\}}$ can be interpreted as the partition function of a new 'replicated' system, such that the spins in subregion A are restricted to be the same in both the replicas, while the spins in subregion B are unconstrained for the two copies. Due to the constraint for the spins in the replicas of the subregion A, there the spins in the bulk behave as if their effective temperature is $T/2$ for local interactions. Using the second Rényi entropies, RMI is defined as the symmetric function:

$$
I_2(A,B) = S_2(A) + S_2(B) - S_2(A \cup B) = -\ln\left(\frac{Z[A,2,T]\, Z[B,2,T]}{Z^2[T]\, Z[T/2]}\right). \tag{9}
$$

The data is obtained by thermodynamic integration and imposing periodic boundary conditions on the lattice.

The RMI scales as [9]:

$$
\frac{I_2(A,B)}{L} = a_2(\beta) + \frac{d_2(\beta)}{L} + \mathcal{O}\left(L^{-2}\right), \tag{10}
$$

where the term $d_2(\beta)$ is related to the symmetry breaking of the lattice. When the symmetry breaking causes $d_2(\beta)$ to change sign, it passes through zero and the function $\frac{I_2(A,B)}{L}$ is then independent of system size up to order $\mathcal{O}\left(L^{-2}\right)$. One can show that $d_2(\beta) < 0$ for $T_\mathrm{c} < T < 2T_\mathrm{c}$, and is positive elsewhere. This leads to the crossings in $\frac{I_2(L/2,L/2)}{L}$ at the temperatures T_c and $2T_\mathrm{c}$ for different system sizes. Thus the RMI as a function of temperature reveals a continuous phase transition at critical temperature T_c. This method has been successfully applied for detecting finite temperature phase transitions with great accuracy in a variety of classical systems [9, 10, 11, 19].

In our numerical simulations, we compute the RMI using classical Monte Carlo algorithm coupled with the transfer-matrix ratio trick [32–34], from the expression

$$
\frac{Z[A,2,T]}{Z^2[T]} = \prod_{i=0}^{N-1} \frac{Z[A_{i+1},2,T]}{Z[A_i,2,T]}, Z[A_0,2,T] = Z^2[T], \tag{11}
$$

where A_i denotes a series of N blocks of increasing size, the consecutive blocks differing by a one-dimensional strip of spins running parallel to the boundary separating A and B. While A_0 labels the empty region, $A_N = A$. The details of the algorithm can be found in [12]. In addition to implementing this procedure, we supplement it by parallel tempering to ensure that the states used in the estimation of the ratios of the partition

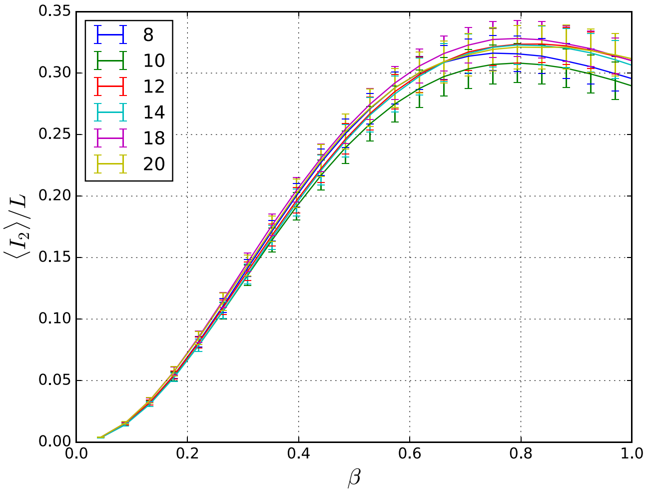


Figure 1. RMI for Edwards–Anderson model with J_{ij} drawn from the continuous Gaussian bond distribution of equation (2) and averaged over 250 disorder realizations.

functions, $\left\{ \frac{Z[A_{i+1},2,T]}{Z[A_i,2,T]} \right\}$, are efficiently sampled. Finally, we find $\langle I_2 \rangle$ by averaging over a reasonable number of disorder realizations.

4. Results

In this section, we will demonstrate the behavior of the RMI curves for the different models described in section 2. The error bars for averaging over disorder realizations are indicated in each plot.

For the Edwards–Anderson model, we consider only the continuous bond distribution class given by equation (2). Consistent with the literature [1], the RMI curves in figure 1 do not show any single crossing point, indicating the absence of any finite temperature transition to the glassy phase. The RCF model in equation (5) was predicted to have a nonzero T_c [28–30], but the geometry of the problem prevented certain Monte Carlo optimizations. We have used a cluster update algorithm for the Monte Carlo updates for interactions involving nearest neighbors. It is nontrivial to design such an algorithm for next nearest neighbor interactions, and hence it is beyond the scope of the current work. Without such cluster updates, the efficiency of the Monte Carlo simulations is an order of magnitude less, and with the computation power available to us, this did not lead to convergent results.

For the random-bond Ising model with the distribution given in equation (4), we can clearly identify the T_c associated with the presence of the ferromagnetic-paramagnetic phase transition for a representative case with $p = 0.04$, as shown in figure 2. The β_c is found to be in the range $[0.49, 0.51]$, consistent with the literature [27].

Lastly, we show the results for the random-bond Ising model of equation (6) only with ferromagnetic couplings in figure 3. Again, the presence or absence of a nonzero T_c is consistent with the literature [4–7, 31]. For the $p = 1/2$ self-dual case, an analytic

J. Stat. Mech. (2018) 043301

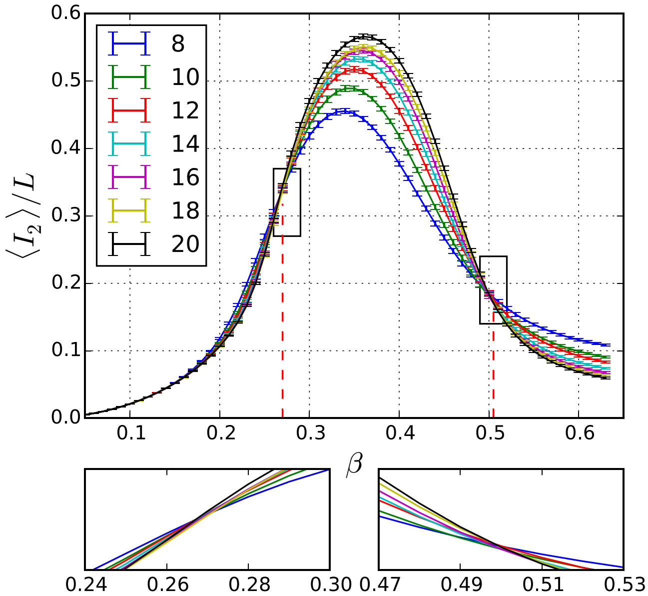
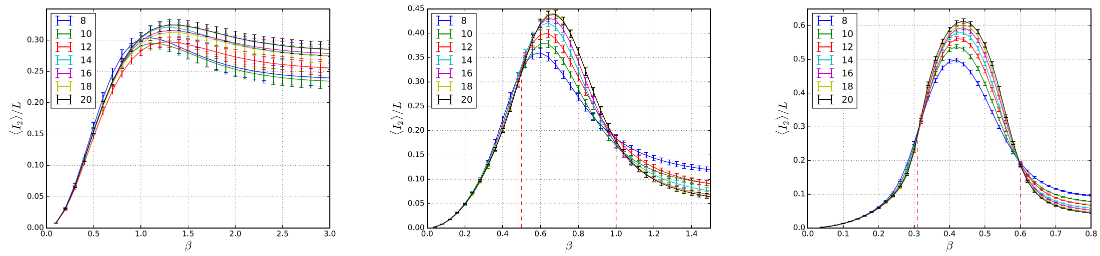


Figure 2. RMI with $p = 0.04$ for the distribution given in equation (4), averaged over 150 disorder realizations. The crossings occur in the ranges $\beta \in [0.25, 0.28]$ and $\beta \in [0.49, 0.51]$.



(a) (b) (c)

Figure 3. RMI for three different scenarios from equation (6), averaged over 100 disorder realizations. (a) For $\tilde{J} = 0$ and $p = 0.4$, no crossing is seen implying a zero-temperature phase transition. (b) For $\tilde{J} = 0$ and $p = 0.6$, crossings occur at $\beta \approx 0.5 \pm 0.04$ and $\beta \approx 1.0 \pm 0.04$. (c) For $\tilde{J} = 0.5$ and $p = 0.5$ (self-dual point), crossings occur at $\beta \approx 0.31 \pm 0.005$ and $\beta \approx 0.609 \pm 0.005$.

expression for the critical point exists (see equation (7)). Solving equation (7) for $J = 1$ and $\tilde{J} = 0.5$, we obtain $\beta_c = 0.609 \pm 0.005$ which matches well with our numerical estimate of $\beta_c = 0.61$. These values are within the error bars and greater accuracy is achievable with a smaller grid and more disorder realizations, which is limited by computational power available to us.

5. Discussion and concluding remarks

We have shown that the detection of classical phase transition points by the RMI method works seamlessly even for disordered systems. It was not at all clear *a priori* that one would be able to see the precise I_2/L crossings at T_c and $2T_c$, given the fact

J. Stat. Mech. (2018) 043301

that the curves have finite error bars due to disorder averaging. Nonetheless, the method has successfully identified the T_c's predicted in the literature for all the models considered, except the RCF.

Given the success of the RMI techniques to identify the phase transitions in these disordered models, in future works, one can apply an extension of this technique [12, 19] to extract the central charges of the CFTs associated with the corresponding critical points, which in many cases are either unknown or do not have an analytic expression. The universality class can be identified if we can extract the central charge c by using geometric mutual information.

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