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Abstract

We study the two-dimensional $\pm J$ Ising model, three-state Potts model and four-state Potts model by the numerical transfer matrix method to investigate the behaviour of the sample-to-sample fluctuations of the internal energy on the Nishimori line. The result shows a maximum at the multicritical point in all the models we investigated. The large sample-to-sample fluctuations of the internal energy as well as the existence of a singularity in these fluctuations imply that the bond configuration (or, equivalently, the distribution of frustrated plaquettes) may be experiencing a non-trivial change in its behaviour at the multicritical point. This observation is consistent with the picture that the phase transition at the multicritical point is of geometry-induced nature.

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1. Introduction

Two-dimensional spin glasses, especially the $\pm J$ Ising model and the random q-state Potts model, have been studied using both theoretical and numerical methods. Some exact results have been derived [1], the phase diagram has been drawn [1, 2] and recently the exact location of the multicritical point has been predicted [3]. However, the characteristics of the multicritical point are not well understood except that the critical exponents have different values from those along the ferro–para critical curve [2, 4]. The properties of the multicritical point are of great interest because this point represents one of the simplest non-trivial renormalization group fixed points in random spin systems [5] and also because we may be able to understand the significance of the Nishimori line from the study of the multicritical point.

In the present paper we investigate the sample-to-sample fluctuations of the internal energy near the multicritical point. The thermal average of the Hamiltonian, namely the internal energy, has different values from one bond configuration to another, given a fixed probability parameter (p for the ferromagnetic bonds in the $\pm J$ model, for example). Although the internal energy is self-averaging, the variance of its distribution is of order N, the system size.

If the variance is anomalously large and singular at some point, it would mean that a non-trivial (and possibly drastic) change happens in the bond configuration at that point because the value of the internal energy fluctuates strongly from sample to sample. This is exactly what we shall show in the present paper to exist at the multicritical point by observing the system along the Nishimori line.

The Nishimori line plays an important role in the determination of the phase diagram. In particular, it is believed that the multicritical point lies on the line [1]. We have another advantage to study the sample-to-sample fluctuations along the Nishimori line: these fluctuations are directly related to the average specific heat on the line. This fact reduces numerical efforts considerably because it is not necessary to generate very many samples to calculate the variance. Only the average of the specific heat needs to be computed. We shall make full use of this relation later.

In the next section, we show that the sample-to-sample fluctuations of the internal energy are very simply related to the specific heat on the Nishimori line. This facilitates numerical calculations enormously as mentioned above. In section 3 we investigate numerically the behaviour of these fluctuations near the multicritical point on the Nishimori line for three models: the $\pm J$ Ising model, three-state Potts model and four-state Potts model. We will see that these fluctuations show a maximum at the multicritical point. The physical significance of the results is discussed in the final section.

2. Average fluctuations of the internal energy

Let us consider the random Z_q model with gauge symmetry which includes the $\pm J$ Ising model and the random q-state Potts model. The general Hamiltonian is written as follows:

$$H = -\sum_{\langle ij \rangle} V(S_i - S_j + J_{ij}) \tag{1}$$

where $S_i = 0, 1, \ldots, q - 1$ is the q-state spin variable, $J_{ij} = 0, 1, \ldots, q - 1$ is the quenched random bond variable and V is an interaction function of period q. The summation is taken over the first-neighbouring sites of the square lattice. The J_{ij} variable follows the probability distribution

$$P(J_{ij}; \beta_p) = \frac{e^{\beta_p V(J_{ij})}}{\sum_{\eta=0}^{q-1} e^{\beta_p V(\eta)}}. \tag{2}$$

The Hamiltonian (1) is invariant under the gauge transformation $S_i \rightarrow S_i - \sigma_i$, $J_{ij} \rightarrow J_{ij} + \sigma_i - \sigma_j$, where $\sigma_i = 0, 1, \ldots, q - 1$, but $P(J_{ij}; \beta_p)$ is not. Using the gauge theory [1], some exact results can be derived such as the average internal energy on the so-called Nishimori line defined by $\beta \equiv 1/T = \beta_p$,

$$[E] \equiv [\langle H \rangle] = -N_B \frac{\sum_\eta V(\eta) e^{\beta V(\eta)}}{\sum_\eta e^{\beta V(\eta)}}. \tag{3}$$

Here the square brackets denote the configurational average, the angular brackets are for the thermal average and N_B is the number of bonds. If we denote

$$\{V\} = \sum_{\eta=0}^{q-1} V(\eta) P(\eta; \beta)$$

equation (3) is expressed as

$$[E] = -N_B \{V\}. \tag{4}$$

In the case of the $\pm J$ Ising model, $q = 2$, $V(0) = +J$ and $V(1) = -J$, the average internal energy (3) reduces to

$$[E] = -N_B J \tanh(\beta J).$$

In the case of the q-state Potts model with $V(0) = +J$ and $V(1) = V(2) = \cdots = V(q-1) = 0$,

$$[E] = -N_B J \frac{1}{1 + (q-1)\,\mathrm{e}^{-\beta J}}.$$

We also find from the gauge theory that

$$[\langle H^2 \rangle] = N_B\{V^2\} + N_B(N_B - 1)\{V\}^2 \tag{5}$$

when $\beta = \beta_p$; thus, with equation (4),

$$N_B(\{V^2\} - \{V\}^2) = [\langle H^2 \rangle] - [\langle H \rangle]^2. \tag{6}$$

Since the specific heat is defined by

$$T^2[C] = [\langle H^2 \rangle - \langle H \rangle^2] \tag{7}$$

we obtain, combining equations (6) and (7),

$$N_B(\{V^2\} - \{V\}^2) - T^2[C] = [E^2] - [E]^2 \ (\geqslant 0). \tag{8}$$

The right-hand side of equation (8) is the sample-to-sample fluctuations of the internal energy, $[(\Delta E)^2]$. Note that equation (8) holds only on the Nishimori line $\beta = \beta_p$. In the case of the $\pm J$ Ising model, equation (8) reduces to the well-established inequality

$$T^2[C] \leqslant N_B J^2 \operatorname{sech}^2(\beta J).$$

Equation (8) indicates that the sample-to-sample fluctuations of the internal energy can be evaluated from the average of the specific heat because the quantity $\{V^2\} - \{V\}^2$ is trivially calculated. This fact is a great advantage since it eliminates the necessity to evaluate the variance directly by using a large number of samples; the specific heat is a self-averaging quantity and therefore can be calculated with high precision from a small number of samples with sufficiently large system size. Away from the Nishimori line, we do not have such a simple relation because equations (4) and (5) do not hold.

Since the actual distribution of bond values (and therefore of frustration) changes from sample to sample in finite-size systems with given β_p, the internal energy takes various values from one set of bonds to another around the average value. Relation (8) helps us to estimate the variance of the internal energy $[(\Delta E)^2]$ and directly depends on the distribution of frustration, which has a geometrical nature: the sample-to-sample fluctuations of the internal energy should reflect the geometrical structure of the distribution of frustration, which is a quantity independent of thermal variables but depends only on the bond configuration. This argument suggests that we may be able to investigate the properties of the distribution of frustration by looking at the sample-to-sample fluctuations of the internal energy, or equivalently, the average specific heat on the Nishimori line. It is believed that the Nishimori line intersects the phase boundary between paramagnetic and ferromagnetic phases [1] (see figure 1). If the distribution of frustration undergoes a sharp change in its behaviour, it would be reflected in anomalously large sample-to-sample fluctuations of physical quantities including the internal energy. Such an anomaly, if it exists on the right-hand side of equation (8), is related to the singularity of the specific heat at the multicritical point on the Nishimori line due to equation (8). Since the specific heat is singular at the multicritical point, we may conclude that the sample-to-sample fluctuations are also singular there. Hence, by calculating the average specific heat near the multicritical point, we are able to investigate the structure of the distribution of frustration, which is of purely geometrical nature. A similar argument has been used to relate the free
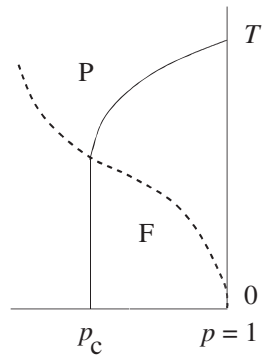
Figure 1. Phase diagram of the $\pm J$ Ising model in two dimensions. There exist ferromagnetic (F) and paramagnetic (P) phases, and no spin glass phase exists. The Nishimori line is shown as a dashed line.

energy and the entropy of frustration [6]. The next section gives us some numerical support to confirm this idea.

3. Numerical calculations

We have tested the ideas of the previous section by numerically calculating the average specific heat on long strips by the transfer matrix method. We have studied three models: the $\pm J$ Ising model, three-state Potts model and four-state Potts model. We have used long strips of length 5000 and of various widths with free boundary conditions and without an external field. By the transfer matrix method we calculated the free energy along the Nishimori line. The specific heat was obtained from the numerical second derivative of the free energy by the inverse of the temperature. We averaged the specific heat over ten samples.

For the $\pm J$ Ising model the widths of the lattice are $3 \leqslant L \leqslant 14$. The lattice size (up to 5000×14) and number of samples (ten) are much smaller than those in the existing numerical transfer matrix studies [4, 7]. However, since our purpose is much more modest than these investigations (not trying to evaluate the critical exponents, for instance), our system size turns out to be sufficient as we shall show. Another reason for the small scale of our computation is that the use of formula (8) greatly reduces the necessary number of samples as discussed in the previous section.

We define the parameter p for the $\pm J$ Ising model by

$$e^{2\beta_p J} = \frac{p}{1-p}.$$

Thus p is the probability that $J_{ij} = 0$, i.e. $V(J_{ij}) = +J$.[1] Each bond follows the probability distribution

$$P(J_{ij}) = p\delta(J_{ij}) + (1-p)\delta(J_{ij} - 1)$$

and we restrict our studies to $0.5 < p < 1$. For the three-state Potts model, $3 \leqslant L \leqslant 9$ and for the four-state Potts model, $3 \leqslant L \leqslant 7$. For the q-state Potts model, we define

$$e^{\beta_p J} = \frac{1}{p} - (q-1)$$

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[1] Note that we use the Hamiltonian (1) where J_{ij} takes the values 0 and 1. This notation is completely equivalent to the usual Hamiltonian $H = -\sum J_{ij} S_i S_j$ where S_i, S_j and J_{ij}/J take the values ± 1.
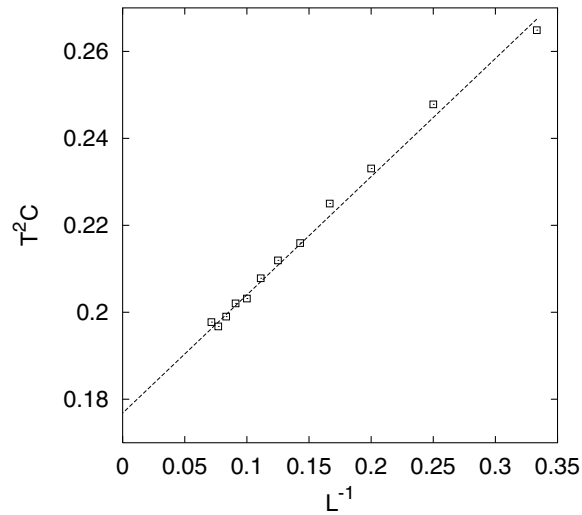
Figure 2. Extrapolation of T^2C near the multicritical point for the $\pm J$ Ising model, $p = 0.8900$.
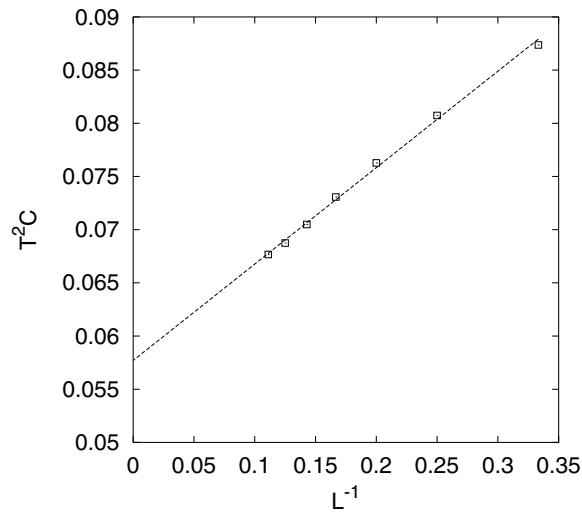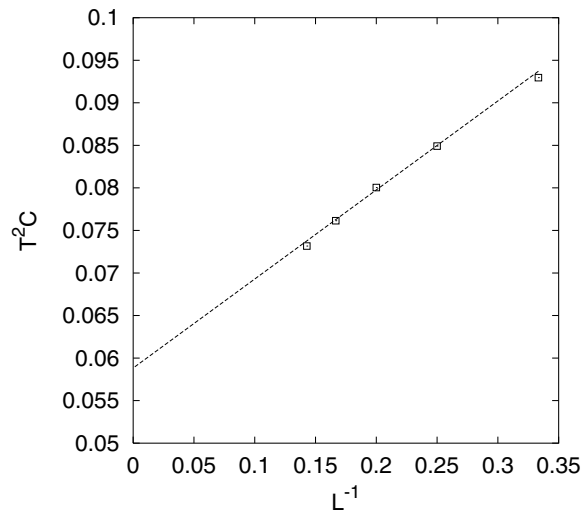

Figure 3. Extrapolation of T^2C near the multicritical point for the three-state Potts model, $p = 0.0795$.

and the probability distribution (2) is then

$$P(J_{ij}) = (1 - (q - 1)p)\delta(J_{ij}) + \sum_{l=1}^{q-1} p\delta(J_{ij} - l)$$

with $0 < p < 1/(q - 1)$.

For each point on the Nishimori line $\beta = \beta_p$ we extrapolate the specific heat to the limit $L \to \infty$. We have found that the extrapolation by the L^{-1} law works quite well in almost all cases (see figures 2–4). This is natural because we are mostly treating values of p away from the multicritical point. Exactly at the multicritical point, the extrapolation needs some care, in particular if one wishes to estimate the critical exponents [4]. However, for our purpose to

Figure 4. Extrapolation of T^2C near the multicritical point for the four-state Potts model, $p = 0.0615$.
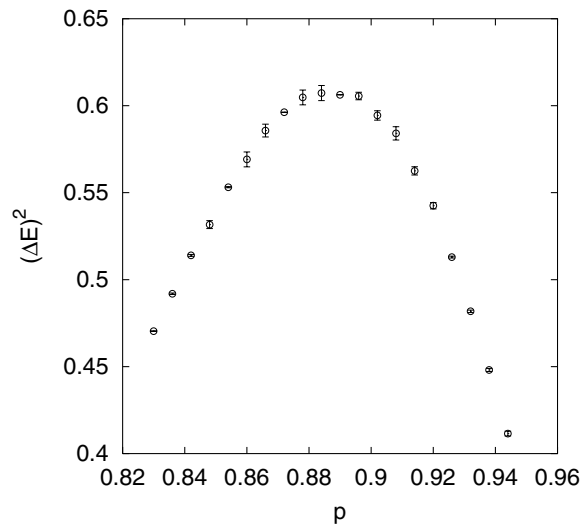
Figure 5. Sample-to-sample fluctuations of the internal energy for the $\pm J$ Ising model.

confirm the existence of a peak in the sample-to-sample fluctuations of the internal energy at the multicritical point, the method of extrapolation is rather irrelevant, which we confirmed by using other powers such as $L^{-1.5}$ in some cases. The error bars in the extrapolated values have been estimated by changing the range of extrapolation fitting, for example, from comparison of extrapolation using $3 \leqslant L \leqslant 14$ with that using $6 \leqslant L \leqslant 14$.

The resulting values of the energy fluctuations are plotted in figures 5–7 for the $\pm J$ Ising model, three-state Potts model and four-state Potts model, respectively. The positions of the multicritical points are predicted in [3]: for the $\pm J$ Ising model $p_c = 0.889\,972$, for the three-state Potts model $p_c = 0.079\,7308$ and for the four-state Potts model $p_c = 0.063\,0965$.
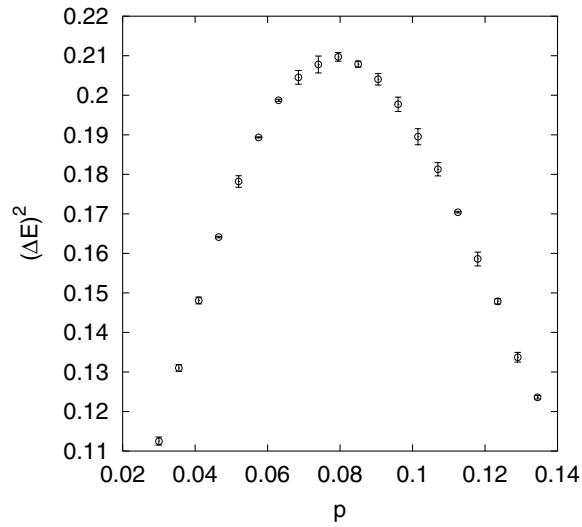
Figure 6. Sample-to-sample fluctuations of the internal energy for the three-state Potts model.
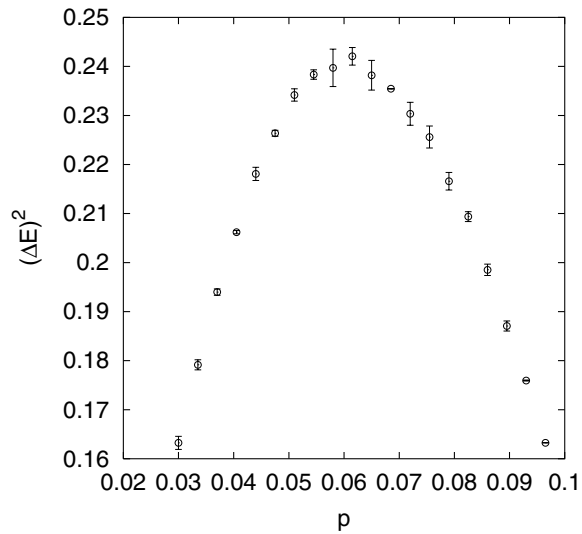

Figure 7. Sample-to-sample fluctuations of the internal energy for the four-state Potts model.

By comparison of these values with those in figures 5–7 we clearly see that the sample-to-sample fluctuations of the internal energy have a maximum at (or at least very near) the multicritical point for each model. It seems reasonable to expect similar behaviour in other random models with Z_q symmetry.

4. Conclusion

We have studied the $\pm J$ Ising model, three-state Potts model and four-state Potts model by the numerical transfer matrix method. We have first shown that the sample-to-sample fluctuations

of the internal energy are, on the Nishimori line, related to the specific heat and are expected to have a peculiar behaviour at the multicritical point. It was found indeed from numerical calculations that the sample-to-sample fluctuations become anomalously large at or very near the multicritical point in all the models we investigated. Since these fluctuations are related to the specific heat by equation (8), they should have a singularity at the multicritical point (as the specific heat is singular there) although it is difficult to see this effect within our numerical precision. The existence of a peak at the multicritical point in conjunction with the existence of a singularity, anyway, suggests that the bond distribution and the distribution of frustration undergo an anomalous change in behaviour at $p = p_c$. This point of view is in agreement with the argument in [6] that the phase transition at the multicritical point along the Nishimori line is induced by a geometrical anomaly[2]. Since the rate of thermal excitations ($e^{-\beta J}/e^{\beta J}$) coincides with the ratio of the bond configurations ($(1 - p)/p$) on the Nishimori line, the physical situations are very special there, which may be one of the reasons for the existence of a maximum in the configurational variance of the thermal quantity at the multicritical point along the Nishimori line. It is an interesting future problem to investigate what happens on the sample-to-sample fluctuations of physical quantities away from the Nishimori line.

Note added in proof. We have found after submission of the paper that the sample-to-sample fluctuations of the energy, equation (8), is proportional to the derivative of the energy by K_p with K fixed. Thus a maximum in these fluctuations means that the energy changes most dramatically at the multicritical point as K_p changes. The exact upper bound on the specific heat is the sum of two derivatives by K and K_p and corresponds to the derivative along the Nishimori line.

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[2] This never implies that the critical exponents should coincide with those of the simple conventional percolation transition.