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The specific heat of the two-dimensional $\pm J$ Ising model

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Abstract

The specific heat of the two-dimensional $\pm J$ Ising model has been investigated by the numerical transfer matrix method and Monte Carlo simulations from a new point of view. The region where a part of the specific heat takes a negative value has been investigated, which is characteristic of frustrated systems and reflects the non-trivial degeneracy of the ground state. The region mentioned above is found to be fairly large in the p - T plane (p is the concentration of the ferromagnetic bond and T is the temperature). Moreover, it includes the Nishimori line. Namely, it includes a part of the paramagnetic–ferromagnetic phase boundary, on which the specific heat cannot diverge. The present result indicates that the specific heat does not diverge at least on a part of the paramagnetic–ferromagnetic phase boundary above the multicritical point, which is in conflict with previous results.

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1. Introduction

To elucidate the nature of critical phenomena of two-dimensional disordered Ising models has been a subject of long-standing interest. Harris [1] concluded from a heuristic argument that the nature of critical phenomena of a disordered system becomes different from that of the corresponding pure system when the critical exponent of the specific heat, α , of the pure system is positive, while it remains the same when $\alpha < 0$. Since the two-dimensional pure ferromagnetic Ising model is the marginal case, namely $\alpha = 0$, many authors have investigated the properties of critical phenomena of the two-dimensional disordered Ising models [2–14].

For the two-dimensional unfrustrated random Ising models, many authors concluded that the specific heat diverges double logarithmically at the paramagnetic–ferromagnetic phase boundary [2–9], though there are several results which insist that the specific heat remains finite [1, 10–12].

For the two-dimensional $\pm J$ Ising model which corresponds to the two-dimensional frustrated random Ising model, a few results exist. Inoue [13] investigated the system-size dependence of the height of the peak of the specific heat at $p \geq 0.94$, where p is the concentration of the ferromagnetic bond ($0 \leq p \leq 1$), and concluded that the logarithmic divergence of the specific heat at the paramagnetic–ferromagnetic phase boundary is most probable in the same way as the pure case. Reis *et al* [14] investigated the system-size dependence of the correlation length at $p \geq 0.92$, and concluded that logarithmic corrections do not play a role in contrast with the unfrustrated disordered systems. They concluded, however, that the specific heat diverges at most logarithmically. Namely, they could not completely exclude the possibility of the double logarithmic divergence of the specific heat.

On the other hand, there exists the Nishimori line, which is defined by the equation $\exp(2J/k_B T) = p/(1-p)$. (k_B is the Boltzmann constant, which we put that $k_B = 1$ from now on.) On the Nishimori line, several rigorous results have been derived [15]. Particularly, it has been proved that the specific heat remains finite.

From the renormalization group approach, it is generally believed that, for the two-dimensional $\pm J$ Ising model, there exist two fixed points on the paramagnetic–ferromagnetic phase boundary above the multicritical point, namely the pure ferromagnetic fixed point and the multicritical fixed point [16, 17], and there seems to be no random fixed point in contrast with the three-dimensional case [18]. (In this paper, we use the phrase ‘multicritical point’ as the crossing point of the ferromagnetic–nonferromagnetic phase boundary and the Nishimori line, though there seems to be no spin glass phase in the two-dimensional case.) The pure ferromagnetic fixed point is stable, and the multicritical fixed point is unstable. Thus, the critical phenomena on the paramagnetic–ferromagnetic phase boundary above the multicritical point are governed by the pure ferromagnetic fixed point. Therefore, the critical exponent, α , should be zero on the whole paramagnetic–ferromagnetic phase boundary above the multicritical point. The fact mentioned above, however, does not help to determine the critical behaviour of the specific heat, since each of a logarithmic divergence, a double logarithmic divergence and a cusp-like behaviour belongs to the case $\alpha = 0$.

In this paper, we investigate the specific heat from a new point of view. We divide the specific heat of a system into two parts, C_1 and C_2 . (For detailed definitions of C_1 and C_2 , see section 2.) The value of C_1 is easily found to be non-negative and remains finite at finite temperature. On the other hand, the value of C_2 becomes negative at $T = 0$ when the system is frustrated and the ground state has non-trivial degeneracy. Since we can consider that the negative value of C_2 reflects the non-trivial ground state degeneracy, it is an interesting problem to make it clear up to what temperature the property persists. It is noted that in order that the specific heat may diverge, C_2 should become infinite.

Thus, we investigate the region in the p – T plane where C_2 takes a negative value for the two-dimensional $\pm J$ Ising model. Our result shows that the region mentioned above is fairly large in the p – T plane. Moreover, it includes the Nishimori line. Namely, the region includes a part of the paramagnetic–ferromagnetic phase boundary above the multicritical point. In that region, the specific heat cannot diverge.

The present result indicates that the specific heat does not diverge at least on a part of the paramagnetic–ferromagnetic phase boundary near and above the multicritical point. The result is not directly in conflict with previous results [13, 14] which insist that the specific heat diverges at most logarithmically at the paramagnetic–ferromagnetic phase boundary near the pure ferromagnetic case ($p \geq 0.92$), since the range of the concentration of the calculations does not overlap. It is natural, however, to think that the nature of the phase transition does not change on the paramagnetic–ferromagnetic phase boundary above the multicritical point. Thus, we insist that the specific heat of the two-dimensional $\pm J$ Ising model does

not diverge on the whole paramagnetic–ferromagnetic phase boundary above the multicritical point, though we cannot exclude the possibility that there exists a singular point on the paramagnetic–ferromagnetic phase boundary which separates the nature of the specific heat.

2. The model and the method

We consider the two-dimensional $\pm J$ Ising model on a square lattice with only nearest neighbour interactions. The Hamiltonian is written as follows:

$$\mathcal{H} = - \sum_{(ij)} J_{ij} S_i S_j \quad (1)$$

where $S_i = \pm 1$, and the summation of (ij) runs over all the nearest neighbours. Each J_{ij} is determined according to the following probability distribution:

$$P(J_{ij}) = p\delta(J_{ij} - J) + (1 - p)\delta(J_{ij} + J). \quad (2)$$

In this paper, we put that $J = 1$.

The specific heat per bond, $C(p, T)$, is written as follows:

$$C(p, T) = \frac{1}{N_B} \frac{\partial}{\partial T} [\langle E \rangle_T]_p = \frac{1}{N_B} \frac{\partial}{\partial T} \sum_{(ij)} [\langle -J_{ij} S_i S_j \rangle_T]_p \quad (3)$$

where $\langle \dots \rangle_T$ denotes the thermal average in a given bond configuration, $\{J_{ij}\}$, at temperature T , $[\dots]_p$ denotes the configurational average at the ferromagnetic bond concentration, p , and N_B is the number of bonds.

Now, we divide the specific heat of the system, $C(p, T)$, into two parts, $C_1(p, T)$ and $C_2(p, T)$:

$$C(p, T) = C_1(p, T) + C_2(p, T) \quad (4)$$

where

$$C_1(p, T) = \frac{1}{N_B} \sum_{(ij)} \frac{\partial}{\partial T_{ij}} [\langle -J_{ij} \sigma_i \sigma_j \rangle_{\{T\}}]_p |_{\{T\}=T} \quad (5)$$

and

$$C_2(p, T) = \frac{1}{N_B} \sum_{(ij)} \sum_{lm \neq ij} \frac{\partial}{\partial T_{lm}} [\langle -J_{ij} \sigma_i \sigma_j \rangle_{\{T\}}]_p |_{\{T\}=T}. \quad (6)$$

Here, we introduce technically, T_{ij} , the local temperature of the bond, J_{ij} . Namely, $C_1(p, T)$ is considered to be the configurational average of the change of the local energy, $-\langle J_{ij} \sigma_i \sigma_j \rangle_{\{T\}}$, when we infinitesimally increase the corresponding local temperature, T_{ij} . On the other hand, $C_2(p, T)$ is considered to be the configurational average of the change of the local energy, $-\langle J_{ij} \sigma_i \sigma_j \rangle_{\{T\}}$, when we infinitesimally increase the temperature, T_{lm} , which surrounds the local bond, J_{ij} .

It is easily calculated that

$$C_1(p, T) = \frac{1}{N_B T^2} \sum_{(ij)} \left(1 - [\langle \sigma_i \sigma_j \rangle_T^2]_p \right). \quad (7)$$

Namely, $C_1(p, T)$ has an upper bound;

$$C_1(p, T) \leq \frac{1}{T^2}. \quad (8)$$

Therefore, at finite temperature, in order that the specific heat may diverge, $C_2(p, T)$ should become infinite.

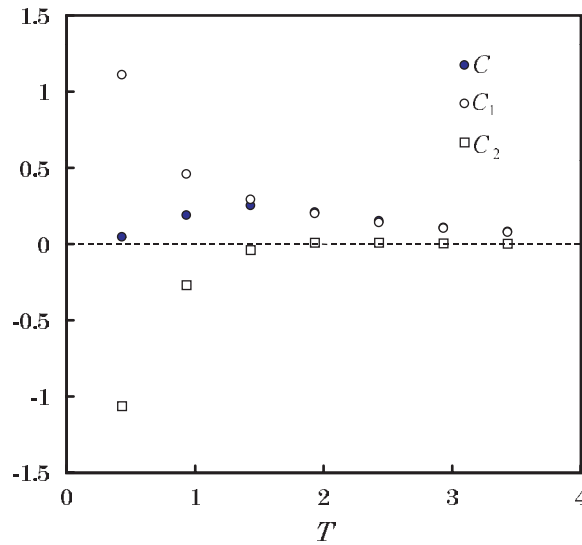


Figure 1. The temperature dependence of $C(p, T)$, $C_1(p, T)$ and $C_2(p, T)$ for $L = 4$ at $p = 0.8$.

Now, we consider the case at zero temperature. At zero temperature, the specific heat $C(p, 0)$ becomes zero. When there is no non-trivial degeneracy in the ground state of the system, each $[\langle \sigma_i \sigma_j \rangle_T^2]_p = 1$. Namely, $C_1(p, 0)$ becomes zero. Thus, $C_2(p, 0)$ also becomes zero. On the other hand, when the ground state has non-trivial degeneracy, some of $[\langle \sigma_i \sigma_j \rangle_T^2]_p$ become less than 1. Namely, $C_1(p, 0)$ becomes positive infinite. Thus, $C_2(p, 0)$ becomes negative infinite in this case. The negative value of $C_2(p, T)$ at finite temperature may be considered to be one of the influences of the non-trivial ground state degeneracy of the frustrated system. Thus, it is an interesting problem to make it clear up to what temperature the property persists. Therefore, in the following sections, we investigate the region in the p - T plane where $C_2(p, T)$ takes the negative value for the two-dimensional $\pm J$ Ising model.

In the actual calculations, it is rather difficult to estimate the value of $C_2(p, T)$ directly. On the other hand, $C(p, T)$ can be estimated from the fluctuation of the energy of the system, namely $[\langle E^2 \rangle_T - \langle E \rangle_T^2]_p$, and $C_1(p, T)$ can be estimated from the nearest neighbour correlations. Therefore, we have estimated the values of $C(p, T)$ and $C_1(p, T)$ directly by the transfer matrix method and Monte Carlo simulations, and the value of $C_2(p, T)$ has been estimated indirectly from the equation $C_2(p, T) = C(p, T) - C_1(p, T)$.

3. Results by the numerical transfer matrix method

In this section, we investigate the region in the p - T plane where $C_2(p, T)$ takes a negative value by the numerical transfer matrix method. We have calculated for the lattice size, $L = 4$ – 16 , at the bond concentration, $p = 0.65$ – 0.95 . In the calculations, we take the free boundary condition, and the configurational average for 10^4 – 10^5 bond configurations.

Figure 1 shows the temperature dependence of $C(p, T)$, $C_1(p, T)$ and $C_2(p, T)$ for $L = 4$ at $p = 0.8$. We can see that $C_2(p, T)$ takes a negative value in the low temperature region. We have estimated the temperature, $T_0(L, p)$, where $C_2(p, T)$ takes the value zero for $L = 4$ – 16 at $p = 0.65$ – 0.95 . Figure 2 shows the temperature dependence of $C_2(p, T)$ near the zero point for $L = 14$ at $p = 0.9$. From the figure, we have estimated the temperature of the zero point, $T_0(L = 14, p = 0.9) = 1.2764(14)$. The estimated values of $T_0(L, p)$ for various L

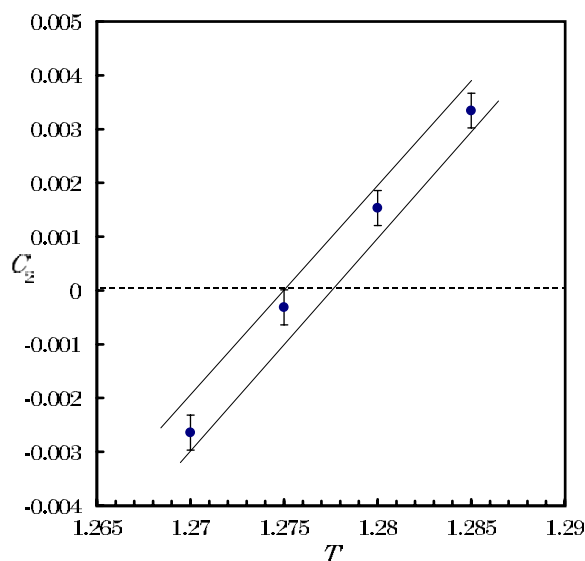


Figure 2. The temperature dependence of $C_2(p, T)$ near the zero point for $L = 14$ at $p = 0.9$.

Table 1. The estimated value of $T_0(L, p)$. $T_N(p)$ is the temperature of the Nishimori line at p .

L	$p = 0.65$	$p = 0.7$	$p = 0.75$	$p = 0.8$	$p = 0.85$	$p = 0.9$	$p = 0.95$
4	3.88(6)	2.85(5)	2.222(16)	1.803(8)	1.4968(28)	1.2553(13)	1.0303(20)
6	3.88(6)	2.845(35)	2.220(12)	1.8045(45)	1.5025(25)	1.2672(12)	1.0517(12)
8	3.88(12)	2.835(65)	2.234(22)	1.8065(85)	1.5020(40)	1.2722(22)	1.0650(20)
10	3.90(10)	2.885(45)	2.230(12)	1.8035(75)	1.5045(30)	1.2744(26)	1.0650(20)
12	3.88(4)	2.83(5)	2.220(14)	1.8035(65)	1.5038(25)	1.2759(19)	1.0823(18)
14	3.88(4)	2.862(42)	2.225(14)	1.8055(35)	1.5050(25)	1.2764(14)	1.0880(20)
16	3.89(7)	2.845(30)	2.225(15)	1.803(7)	1.5047(19)	1.2768(18)	1.0932(12)
$T_N(p)$	3.2308	2.3604	1.8205	1.4427	1.1530	0.9102	0.6792

and p are shown in table 1. The accuracy of the values of $T_0(L, p)$ becomes worse as the concentration, p , becomes small, since the gradient of $C_2(p, T)$ near the zero point becomes small.

We can see that, at each concentration, p , the size dependence of the values of $T_0(L, p)$ is very small, and the values are fairly large compared to the value of $T_N(p)$, the temperature of the Nishimori line at p .

We have no definite principle to estimate the value of $T_0(p)$ which is the extrapolated value of $T_0(L, p)$ to $L \rightarrow \infty$. No clear size dependence, however, can be seen at $p = 0.65$ – 0.8 . Thus, we perform naive extrapolation to $L \rightarrow \infty$ in this region. It can be seen that the value of $T_0(L, p)$ slightly increases as L increases at $p = 0.85$ – 0.95 . We have found that the extrapolation by the L^{-2} -law works fairly well at $p = 0.85$ and $p = 0.9$. Figure 3 shows a plot of $T_0(L, p)$ versus $1/L^2$ at $p = 0.9$, where we have estimated that $T_0(p = 0.9) = 1.278(3)$. We have also found that the extrapolation by the $L^{-1/2}$ -law works fairly well at $p = 0.95$. The estimated values of $T_0(p)$ for various p are shown in table 2. Strictly speaking, we cannot justify the above extrapolation at each p . We can say, however, that the extrapolated values, $T_0(p)$, might not change drastically even if we use other extrapolation laws, and there seems to be no possibility that the value of $T_0(p)$ becomes equal to or smaller than the temperature of the Nishimori line at each p .

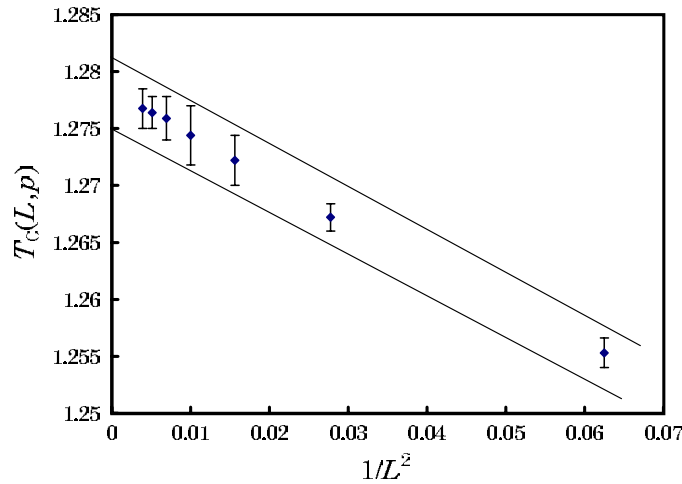


Figure 3. A plot of $T_0(L, P)$ versus $1/L^2$ at $p = 0.9$.

Table 2. The estimated value of $T_0(p)$ for various p . $T_N(p)$ is the temperature of the Nishimori line at p .

p	$T_0(p)$	$T_N(p)$
0.65	3.88(6)	3.2308
0.7	2.845(65)	2.3604
0.75	2.217(19)	1.8205
0.8	1.805(9)	1.4427
0.85	1.506(3)	1.1530
0.9	1.278(3)	0.9102
0.95	1.154(3)	0.6792

Figure 4 shows the estimated values of $T_0(p)$ for various p in the p – T plane, which are denoted by black squares. The dashed line denotes the Nishimori line, and the open circles denote the paramagnetic–ferromagnetic phase boundary above the multicritical point [19]. We can see that the region where $C_2(p, T)$ takes the negative value is fairly large. We can also see that the region mentioned above contains the Nishimori line. There are several numerical calculations about the paramagnetic–ferromagnetic phase boundary of the two-dimensional $\pm J$ Ising model [13, 19–22, 27]. It is noted that all the calculations are almost consistent with each other and they show that, above the multicritical point, the concentration, p , of the phase boundary increases as the temperature increases. Thus, a part of the paramagnetic–ferromagnetic phase boundary is included in the region where $C_2(p, T)$ takes a negative value. In that region, the specific heat cannot diverge. Namely, the specific heat does not diverge at least on a part of the paramagnetic–ferromagnetic phase boundary above the multicritical point.

4. Monte Carlo simulations near the paramagnetic–ferromagnetic phase boundary

In order to elucidate the region where $C_2(p, T)$ takes a negative value near the paramagnetic–ferromagnetic phase boundary, we have performed Monte Carlo simulations for larger lattices, $L = 31$ – 121 , at $p = 0.88$ – 0.92 . In the calculations, we take the skew boundary condition in one direction and the periodic boundary condition in the other direction.

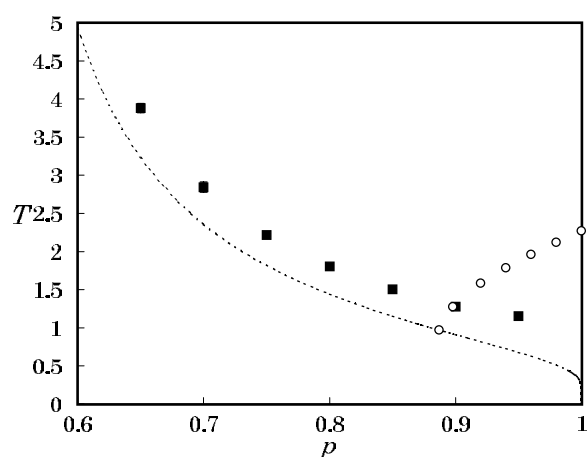


Figure 4. The estimated values of $T_0(p)$ for various p in the p - T plane, which are denoted by black squares. The dashed line denotes the Nishimori line, and the open circles denote the paramagnetic-ferromagnetic phase boundary above the multicritical point.

Table 3. The condition of the Monte Carlo simulation.

p	L	MCS	N_b
0.88	31	400 000	240
	61	800 000	96
	121	800 000	120
0.89	31	600 000	240
	61	5 000 000	120
	121	16 000 000	80
0.9	31	800 000	320
	61	14 000 000	160
	91	30 000 000	64
0.91	31	1 400 000	480
	61	10 000 000	96
	121	20 000 000	32
0.92	31	600 000	720
	61	1 400 000	120
	121	800 000	64

The condition of the simulation is shown in table 3. MCS denotes the Monte Carlo step of the simulation, which is chosen to be larger than 20τ , where the relaxation time, τ , is evaluated by the statistical time-independent method [23], and N_b is the number of bond configurations.

The temperature dependence of $C_2(p, T)$ near the zero point for $L = 91$ at $p = 0.9$ is shown in figure 5, where we have estimated that $T_0(L = 91, p = 0.9) = 1.2765(45)$. The estimated values of $T_0(L, p)$ for various L and p are shown in table 4.

Though $T_0(L, p)$ takes similar values even if the lattice size, L , changes, we have extrapolated the values of $T_0(L, p)$ to $L \rightarrow \infty$ by the L^{-2} -law. We show the estimated values of $T_0(p)$ for various p in table 5 with the temperature of the Nishimori line, $T_N(p)$.

The results are also shown in figure 6. The black circles and squares denote $T_0(p)$ evaluated by the Monte Carlo simulations and by the numerical transfer matrix method, respectively. The dashed line denotes the Nishimori line, and the open circles denote the

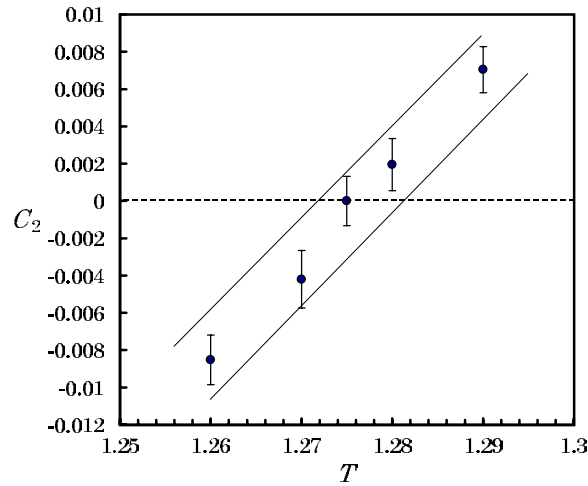


Figure 5. The temperature dependence of $C_2(p, T)$ near the zero point for $L = 91$ at $p = 0.9$.

Table 4. The estimated values of $T_0(L, p)$ for various L and p .

p	$L = 31$	$L = 61$	$L = 91$	$L = 121$
0.88	1.3485(55)	1.3535(45)		1.3555(35)
0.89	1.3075(45)	1.303(5)		1.3055(55)
0.9	1.286(4)	1.2775(45)	1.2765(45)	
0.91	1.269(4)	1.2665(45)		1.2685(45)
0.92	1.249(4)	1.2485(45)		1.2485(35)

Table 5. The values of $T_0(p)$ for various p . $T_N(p)$ is the temperature of the Nishimori line at p .

p	$T_0(p)$	$T_N(p)$
0.88	1.355(5)	1.0038
0.89	1.3045(55)	0.9566
0.9	1.275(5)	0.9102
0.91	1.267(5)	0.8644
0.92	1.2485(55)	0.8188

paramagnetic–ferromagnetic phase boundary above the multicritical point [16]. It can be seen that both results by the numerical transfer matrix method and Monte Carlo simulations are consistent with each other.

The crossing point of the paramagnetic–ferromagnetic phase boundary and the boundary of the region where $C_2(p, T)$ takes a negative value has been estimated to be 0.8985(15). Therefore, we conclude that the specific heat cannot diverge on the paramagnetic–ferromagnetic phase boundary at least for $p_c \leq p \leq 0.8985(15)$, where p_c is the concentration of the multicritical point. There are many numerical estimates of p_c : 0.8905(5) [14], 0.8872(8) [24], 0.886(3) [25], 0.8906 [26] and 0.8907(2) [27]. Recently, there has been a conjecture about the exact value of p_c , which insists that $p_c = 0.889\,972$ [28].

At first glance, the value 0.8985 is very close to several estimated values of p_c . The values of $T_0(p)$ and $T_N(p)$, however, are distinctly different at any value of p , which can be seen from tables 2 and 5. Thus, there seems to be no possibility that the value of $T_0(p)$ becomes

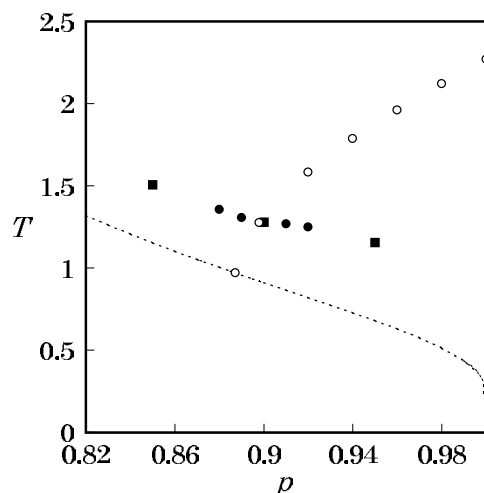


Figure 6. The estimated values of $T_0(p)$ for various p in the p - T plane. The black circles and squares denote the values of $T_0(p)$ by the Monte Carlo simulations and by the numerical transfer matrix method, respectively. The dashed line denotes the Nishimori line, and the open circles denote the paramagnetic-ferromagnetic phase boundary above the multicritical point.

equal to or smaller than the value of $T_N(p)$ at each p , even if, for example, other extrapolation laws have been used. Therefore, we stress that the boundary of the region where $C_2(p, T)$ takes a negative value has to cross the paramagnetic-ferromagnetic phase boundary distinctly above the multicritical point in the p - T plane, namely, the concentration of the crossing point mentioned above is definitely larger than the value of p_c .

5. Conclusions

We have investigated the property of the specific heat of the two-dimensional $\pm J$ Ising model by the numerical transfer matrix method and Monte Carlo simulations from a new point of view. We have estimated the region where $C_2(p, T)$ takes a negative value in the p - T plane, which is one of the characteristics of the frustrated system, and reflects the non-trivial degeneracy of the ground state. By the numerical transfer matrix method for $L = 4$ -16, and the Monte Carlo simulations for $L = 31$ -121, the region has been found to be fairly large in the p - T plane, which includes the Nishimori line. At present, we have no idea why the region becomes so large and the boundary of the region follows closely the Nishimori line. It must be noted, however, that the same feature is also seen in the three-dimensional $\pm J$ Ising model from the preliminary result by Monte Carlo simulations.

Moreover, the region mentioned above includes a part of the paramagnetic-ferromagnetic phase boundary, on which the specific heat cannot diverge. Thus, our results indicate that the specific heat cannot diverge on the paramagnetic-ferromagnetic phase boundary at least near and above the multicritical point. On the other hand, there are several works in the literature which claim that, near the pure ferromagnetic point ($p \geq 0.92$), the specific heat diverges at most logarithmically [13, 14]. Both results are not directly in conflict with each other, since the range of the concentration of the calculations does not overlap. It is natural, however, to think that the nature of the phase transition does not change on the paramagnetic-ferromagnetic phase boundary above the multicritical point. In the literature, where the divergence of the specific heat is insisted on, the change of the peak height of the specific heat of various

lattice sizes was investigated [13, 14]. It is a very subtle problem whether the specific heat diverges or remains finite, when the divergence is so weak as the logarithmic divergence. Our extrapolation, however, is straightforward and the values of $T_0(p)$ might not change drastically even when there exist other system-size corrections, and there seems to be no possibility that the value of $T_0(p)$ becomes equal to or smaller than the temperature of the Nishimori line at each p . Thus, we insist that the specific heat of the two-dimensional $\pm J$ Ising model does not diverge on the whole range of the paramagnetic–ferromagnetic phase boundary above the multicritical point, though we cannot exclude the possibility that a singular point exists on the paramagnetic–ferromagnetic phase boundary, which separates the nature of the specific heat.

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