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Study on the Square-lattice Ising Model with Self-dual Boundary Conditions

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The exact specific heats of the Ising ferromagnet on $L \times L$ square lattices ($L = 3 \sim 16$) with self-dual boundary conditions are evaluated using the microcanonical transfer matrix and high-performance massive computing. From the specific heats, we obtain the shift exponent $\lambda = 1.879(9)$ for the square-lattice Ising ferromagnet with self-dual boundary conditions in the thermodynamic limit ($L \to \infty$) for the first time.

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I. INTRODUCTION

Phase transitions are the most universal phenomena in nature. The two-dimensional Ising ferromagnet is the simplest system showing phase transitions at finite temperatures. Since the Onsager solution of the square-lattice Ising ferromagnet with periodic boundary conditions, the two-dimensional Ising ferromagnet has played a central role in our understanding of phase transitions [1].

In the thermodynamic limit, the specific heat (per volume) of the square-lattice Ising ferromagnet becomes infinite at the critical temperature where the phase transition emerges. In a finite system, the specific heat shows a finite, sharp peak. The location (the so-called effective critical temperature) of the sharp peak for the specific heat in a finite system approaches the critical temperature for the infinite system as the system size increases. The characteristic of the approach to the critical temperature is determined by the shift exponent.

For the first time, Ferdinand and Fisher [2] found the value of the shift exponent λ for the square-lattice Ising ferromagnet with periodic boundary conditions and that value was equal to the thermal scaling exponent ($y_t = 1$). The coincidence of λ and y_t is not a result of finite-size scaling; rather, λ is a free parameter [2–5]. However, the properties of λ are not well known. Even the behavior of λ for the square-lattice Ising ferromagnet is not yet understood. Hoelbling and Lang [4] estimated approximately the shift exponent for the square-lattice Ising ferromagnet with sphere-like boundary conditions by using Monte Carlo simulations and obtained $\lambda = 1.76(7)$ and $\lambda = 1.71(10)$, completely different from $\lambda = 1$. Recently, Janke and Kenna [5] obtained the shift exponent $\lambda = 2$ for the square-lattice Ising ferromagnet with Brascamp-Kunz boundary conditions. In this work, for the first time, we obtain the exact specific heats of the Ising ferromagnet on $L \times L$ square lattices ($L = 3 \sim 16$) with self-dual boundary conditions by using the microcanonical transfer matrix [6–10] and estimate the shift exponent for the square-lattice Ising ferromagnet with self-dual boundary conditions in the thermodynamic limit ($L \to \infty$).

II. NUMBER OF STATES AND SELF-DUAL BOUNDARY CONDITIONS

The Ising model on a lattice with N_s sites and N_b bonds is defined by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \tag{1}$$

where J is the coupling constant, $\langle i,j \rangle$ indicates a sum over all nearest-neighbor pairs of lattice sites, and $\sigma_i = \pm 1$. We define the number of states, $\Omega(E)$, with a given energy $E = -\sum_{\langle i,j \rangle} \sigma_i \sigma_j$, where E is integers ($-N_b \leq E \leq N_b$). Then, the partition function of the Ising model at temperature T is written as

$$Z(T) = \sum_E \Omega(E) e^{-\beta J E}, \tag{2}$$

where $\beta = 1/k_B T$ (k_B is the Boltzmann constant).

Duality relations are most important in understanding the exact properties of spin systems and field theory. In particular, self-duality determines the critical point of the two-dimensional Ising model [1]. A spin model with self-dual boundary conditions satisfies self-duality even

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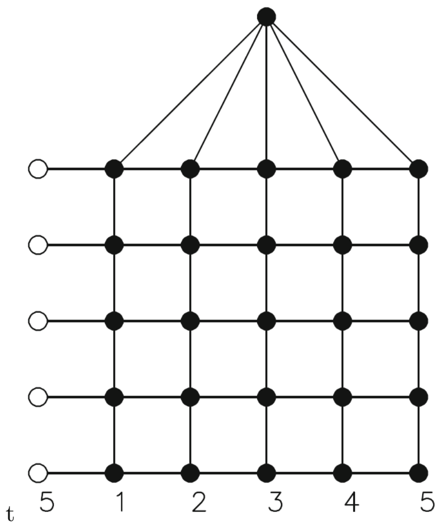

Fig. 1. 5×5 square lattice with self-dual boundary conditions.

in a finite system, and these conditions are very useful in obtaining exact information on a spin system [11]. The square lattices with self-dual boundary conditions used in this work are periodic in the horizontal direction, and another site above the $L \times L$ square lattice is connected to L sites on the last (Lth) row [8,9], as shown in Fig. 1. The number of lattice sites is $N_s = L^2 + 1$, and the number of bonds is $N_b = 2L^2$.

For the Ising ferromagnet, the total number of states is 2^{N_s}; for example, $2^{257} \approx 2.316 \times 10^{77}$ for $L = 16$. Using the microcanonical transfer matrix [7–10] and high-performance massive computing, we have classified all spin states according to their energy values up to $L = 16$, yielding the exact integer values for the number of states. It was an enormous work. Table 1 shows the number of states $\Omega(E)$ for the Ising model on a 6×6 square lattice with self-dual boundary conditions. Furthermore, the largest numbers of states $\Omega_{\max}$ are

$$\Omega(L = 10) = 143935158797600457686468505150 \quad (3)$$

for $L = 10$ (approximately 1.439×10^{29}),

$$\begin{aligned} \Omega(L = 12) \;=\; & 2106084520935378672696130204259 \\ & 997726780736 \end{aligned} \quad (4)$$

for $L = 12$ (approximately 2.106×10^{42}), and

$$\begin{aligned} \Omega(L = 14) \;=\; & 8120632774635057597958513098173 \\ & 576736311942388810048556546 \end{aligned} \quad (5)$$

for $L = 14$ (approximately 8.121×10^{57}). Finally, the largest number of states for $L = 16$ is

$$\begin{aligned} \Omega(L = 16) \;=\; & 818603299865509640399073379902 \\ & 971626964573669807611467789097 \\ & 4465522341887874, \end{aligned} \quad (6)$$

which corresponds to 3.5% of all spin states and is approximately 8.186×10^{75}.

Table 1. Number of states $\Omega(E)$ for the Ising model on a 6×6 square lattice with self-dual boundary conditions.

E	$\Omega(E)$	E	$\Omega(E)$
−72	2	−66	12
−64	72	−62	24
−60	186	−58	492
−56	2016	−54	1996
−52	9510	−50	15732
−48	55300	−46	81000
−44	274764	−42	447240
−40	1321350	−38	2184480
−36	5901808	−34	10031436
−32	24252342	−30	41571284
−28	90186954	−26	153308088
−24	298616774	−22	493936476
−20	864567822	−18	1367793812
−16	2155390824	−14	3203812320
−12	4550631200	−10	6243613848
−8	7991696814	−6	9941306464
−4	11453398440	−2	12702682608
0	13144257580	2	12839428308
4	11895839742	6	10200191404
8	8430481140	10	6396320580
12	4695353794	14	3207281580
16	2082104556	18	1308299752
20	746939436	22	442132008
24	220065538	26	125851968
28	54186960	30	30875660
32	11385318	34	6688764
36	2123358	38	1320720
40	362166	42	247316
44	60810	46	42732
48	8600	50	7440
52	1416	54	984
56	120	58	192
60	24	62	12
66	4		

III. SPECIFIC HEAT AND SHIFT EXPONENT

Given $\Omega(E)$, we can evaluate the exact specific heat (per volume) as

$$\begin{aligned} C(T) &= (N_s k_B T^2)^{-1} \frac{\partial^2}{\partial \beta^2} \ln Z(T) \\ &= \frac{J^2}{N_s k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2). \end{aligned} \quad (7)$$

For the Ising ferromagnet on $L \times L$ square lattices ($L = 3 \sim 16$) with self-dual boundary conditions, we obtain the exact specific heats per volume ($V = N_s = L^2 +$

Table 2. Effective critical temperature $T_c(L)$ and effective shift exponent $\lambda(L)$ for various system sizes L.

L	$T_c(L)$	$\lambda(L)$
3	2.121521537422514	1.834290766266961
4	2.182068897979543	1.751501565668740
5	2.210251851180947	1.723925755430902
6	2.226146591667633	1.716182390122910
7	2.236150910583562	1.716443825631383
8	2.242917341796927	1.720133780587815
9	2.247734816686384	1.725276501091982
10	2.251300145283003	1.730952774915163
11	2.254020249660602	1.736716211006934
12	2.256147155691615	1.742308818754875
13	2.257844351235055	1.747784428329883
14	2.259222132659822	1.752856325357665
15	2.260357019581940	1.757676037460046
16	2.261303768427133	

Table 3. Peak height $C_p(L)$ of the specific heat and effective thermal scaling exponent $y_t(L)$.

L	$C_p(L)$	$y_t(L)$
3	0.591963049934772	1.340871294581897
4	0.720229087304665	1.275446701152670
5	0.814437465382729	1.240964593711301
6	0.889236943493654	1.220193646845132
7	0.951699876038500	1.206320750097926
8	1.005610725510630	1.196324012822146
9	1.053209659767338	1.188704563966745
10	1.095933312874473	1.182645906440382
11	1.134761355238459	1.177668500125062
12	1.170394335379823	1.173473192170668
13	1.203352316252394	1.169863967001735
14	1.234033172366205	1.166707047126323
15	1.262748889405431	1.163907939039329
16	1.289749166428292	

1). Table 2 shows the (dimensionless) effective critical temperature $T_c(L)$, corresponding to the peak location of the specific heat $C(T, L)$, for various system sizes L. Clearly, as the system size increases, the effective critical temperature approaches the exact critical temperature $T_c = -2J/k_B \ln(\sqrt{2}-1) = 2.269185314213022(J/k_B)$ in the thermodynamic limit.

The shift exponent λ is defined by the scaling law [2–6]

$$\Delta T_c(L) = T_c - T_c(L) \sim L^{-\lambda}, \tag{8}$$

from which the effective shift exponent $\lambda(L)$ is evaluated by combining the scaling laws with respect to two effective critical temperatures, $T_c(L)$ and $T_c(L+1)$, as

$$\lambda(L) = -\frac{\ln[\Delta T_c(L+1)/\Delta T_c(L)]}{\ln[(L+1)/L]}. \tag{9}$$

Table 2 shows the effective shift exponent $\lambda(L)$ for various system sizes L. By using the Bulirsch-Stoer (BST) method [12,13], we have extrapolated the values for finite lattices to infinite size ($L \to \infty$), and the extrapolated value of the shift exponent is $\lambda = 1.879(9)$ for the square-lattice Ising ferromagnet with self-dual boundary conditions. The error estimates are twice the difference between the ($n-1$,1) and the ($n-1$,2) approximants [14]. Our value is completely different from $\lambda = 1$ for periodic boundary conditions [2], but close to $\lambda = 1.76(7)$ and $\lambda = 1.71(10)$ for sphere-like boundary conditions [4] and to $\lambda = 2$ for Brascamp-Kunz boundary conditions [5].

Similarly, the peak height $C_p(L)$ of the specific heat scales as [6]

$$C_p(L) \sim L^{2y_t - d}, \tag{10}$$

where y_t is the thermal scaling exponent and $d = 2$ in two dimensions. Therefore, the effective thermal scaling exponent can be defined as

$$y_t(L) = \frac{1}{2}\left(d + \frac{\ln[C_p(L+1)/C_p(L)]}{\ln[(L+1)/L]}\right). \tag{11}$$

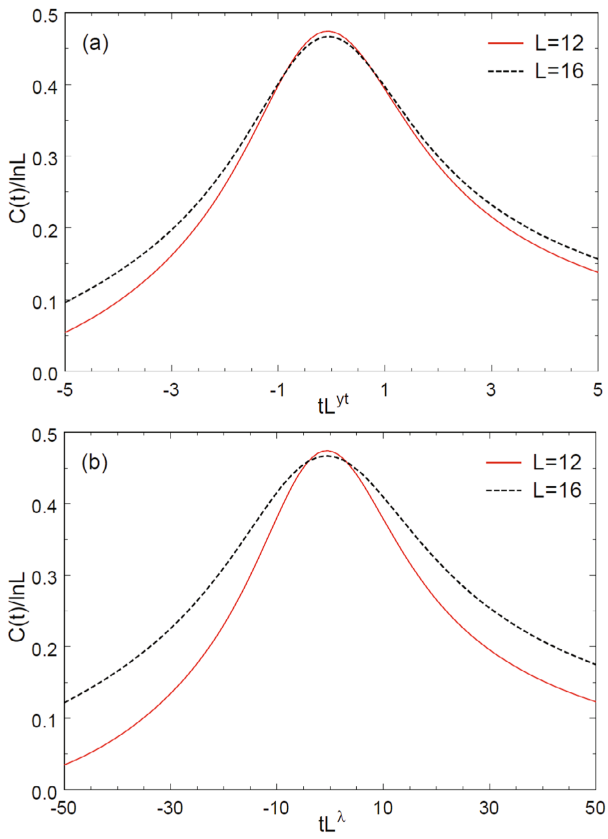

Fig. 2. (Color online) Scaling plot for the specific heats of the Ising model with the scaling variables (a) tL^{y_t} and (b) tL^{λ}, where $t = (T - T_c)/T_c$.

Table 3 shows the peak height $C_p(L)$ of the specific heat and the effective thermal scaling exponent $y_t(L)$. The BST estimate for the thermal scaling exponent is $y_t = 1.084(6)$, in agreement with the known exact value of $y_t = 1$.

In the critical region ($t = (T-T_c)/T_c \approx 0$), the specific heat can be written as

$$C(t, L) \sim (\ln L) C(tL^{y_t}) \tag{12}$$

due to the logarithmic divergence of the specific heat for the square-lattice Ising ferromagnet [1–4]. Figure 2(a) shows the scaling plot for the specific heats ($L = 12$ and 16) of the Ising model with self-dual boundary conditions according to Eq. (12). As expected, in the critical region, the scaled specific heats, $C(t, L)/\ln L$, collapse with the scaling variable tL^{y_t}. As shown in Fig. 2(b), we also try the scaling variable tL^{λ}, for which no collapse is implied.

IV. CONCLUSION

We have evaluated the exact specific heats of the Ising ferromagnet on $L \times L$ square lattices ($L = 3 \sim 16$) with self-dual boundary conditions by using the microcanonical transfer matrix. For the first time, we have obtained the shift exponent $\lambda = 1.879(9)$ for the specific heat of the square-lattice Ising ferromagnet with self-dual boundary conditions in the limit $L \to \infty$. Our value is completely different from $\lambda = 1$ for periodic boundary conditions, but is close to $\lambda = 1.76(7)$ and $\lambda = 1.71(10)$ for sphere-like boundary conditions and to $\lambda = 2$ for Brascamp-Kunz boundary conditions.

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REFERENCES

[1] C. Domb, *The Critical Point* (Taylor and Francis, London, 1996).
[2] A. E. Ferdinand and M. E. Fisher, Phys. Rev. **185**, 832 (1969).
[3] M. N. Barber, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic Press, New York, 1983), Vol. 8, p. 145.
[4] C. Hoelbling and C. B. Lang, Phys. Rev. B **54**, 3434 (1996).
[5] W. Janke and R. Kenna, Phys. Rev. B **65**, 064110 (2002).
[6] S.-Y. Kim, J. Korean Phys. Soc. **59**, 2980 (2011).
[7] S.-Y. Kim and R. J. Creswick, Phys. Rev. Lett. **81**, 2000 (1998).
[8] S.-Y. Kim and R. J. Creswick, Phys. Rev. E **63**, 066107 (2001).
[9] S.-Y. Kim, Phys. Rev. E **70**, 016110 (2004).
[10] S.-Y. Kim, Phys. Rev. Lett. **93**, 130604 (2004).
[11] F. Y. Wu, Rev. Mod. Phys. **54**, 235 (1982).
[12] R. Bulirsch and J. Stoer, Numer. Math. **6**, 413 (1964).
[13] W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, *Numerical Recipes in Fortran 77*, 2nd edition (Cambridge University Press, Cambridge, 1992), p. 104.
[14] J. H. Lee, S.-Y. Kim and J. Lee, J. Chem. Phys. **133**, 114106 (2010); J. Chem. Phys. **135**, 204102 (2011); Phys. Rev. E **86**, 011802 (2012); Phys. Rev. E **87**, 052601 (2013).