Evaluation of an Efficient Monte Carlo Algorithm to Calculate the Density of States

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***Abstract*—Phase transitions and critical phenomena are the most universal phenomena in nature. To understand the phase transitions and critical phenomena of a given system as a continuous function of temperature and to obtain the partition function zeros in the complex temperature plane indicating most effectively phase transitions and critical phenomena, we need to calculate the density of states. Currently, Wang-Landau Monte Carlo algorithm is one of the most efficient Monte Carlo methods to calculate the approximate density of states. Using Wang-Landau Monte Carlo algorithm, the density of states for the Ising model on $L \times L$ square lattices ($L = 4 \sim 32$) with periodic boundary conditions is obtained, and the partition function zeros of the Ising model are evaluated in the complex temperature plane. By examining the behavior of the first partition function zero (partition function zero closest to the positive real axis), phase transitions and critical phenomena can be much more accurately analyzed. The approximate first zeros of the Ising ferromagnet, obtained from Wang-Landau algorithm, are quite close to the exact ones, indicating that it is a reliable method for calculating the density of states and the first partition function zeros.**

***Index Terms*—Phase transition, density of states, Ising model, partition function zeros.**

I. Introduction

Phase transitions and critical phenomena are the most universal phenomena in nature. The two-dimensional Ising model is the simplest system showing phase transitions and critical phenomena at finite temperatures. Since the Onsager (Nobel prize winner in 1968) solution [1] of the square-lattice Ising model with periodic boundary conditions in the absence an external magnetic field, the two-dimensional Ising model has played a central role in our understanding of phase transitions and critical phenomena [2].

To understand phase transitions and critical phenomena, various theoretical methods (such as mean-field theory, power-series expansion and analysis, renormalization group, and transfer matrix) have been developed. Recently, computer simulations, in particular, Monte Carlo computer simulations have been the most popular method in studying phase transitions and critical phenomena. To understand the phase transition and critical phenomena of a given system as a continuous function of temperature, to obtain the partition function zeros indicating most effectively phase transitions and critical phenomena, and to perform microcanonical analysis of phase transitions and critical phenomena, we need to calculate the density of states. Currently, Wang-Landau Monte Carlo algorithm [3] is one of the most efficient Monte Carlo methods to calculate the approximate density of states. In Wang-Landau Monte Carlo algorithm, the inverse of the density of states is employed as the sampling probability function, and the real values for the density of states can be obtained quickly due to its modification factor.

Phase transitions and critical phenomena can also be understood based on the concept of partition function zeros. Fisher introduced the partition function zeros in the complex temperature plane utilizing the Onsager solution of the square-lattice Ising model in the absence of an external magnetic field [4]. Fisher also showed that the partition function zeros in the complex temperature plane of the square-lattice Ising model determine its ferromagnetic and antiferromagnetic critical temperatures at the same time in the absence an external magnetic field. By calculating the partition function zeros and examining the behavior of the first partition function zero (partition function zero closest to the positive real axis) in the thermodynamic limit, phase transitions and critical phenomena can be much more accurately analyzed than examining the behavior of the specific heat per volume for real values of the temperature, which is plagued by the noise due to the subleading terms containing zeros other than the first ones [5−20].

In the next section, the density of states and the partition function of the square-lattice Ising model are defined. In Section III, Wang-Landau Monte Carlo algorithm to calculate the approximate density of states is briefly explained. In Section IV, the concept of the partition function zeros in the complex temperature plane is introduced, the partition function zeros of the square-lattice Ising model are evaluated in the complex temperature plane using the exact density of states and the approximate density of states, and both results are compared.

II. Exact Density of States

The Ising model [1, 2] on a lattice with Ns sites and Nb bonds is defined by the Hamiltonian

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j , \tag{1}$$

where J is the coupling constant between two neighboring magnetic spins (positive value of J for a ferromagnetic interaction and negative value of J for an antiferromagnetic

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interaction), $< i, j >$ indicates a sum over all nearest-neighbor pairs (i and j) of lattice sites, and $\sigma_i = \pm 1$ (positive value for the upward magnetic spin on a lattice site i and negative value for the downward magnetic spin). For the Ising model on $L \times L$ square lattice with periodic boundary conditions, the number of spins is $N_s = L^2$ and the number of bonds is $N_b = 2L^2$. If we define the density of states, $\Omega(E)$, with a given energy

$$E = \frac{1}{2} \sum_{<i,j>} (1 - \sigma_i \sigma_j), \tag{2}$$

where E is a positive integer ($0 \le E \le N_b$), the Hamiltonian can be written as

$$H = 2J(E - L^2) \tag{3}$$

for the square-lattice Ising model.

Finally, the partition function of the square-lattice Ising model (a sum 2^{L^2} over possible spin configurations)

$$Z = \sum_{\{\sigma_n\}} \exp(-\beta H), \tag{4}$$

where $\beta = 1/k_B T$, k_B is the Boltzmann constant, and T is temperature, is expressed as

$$Z(y) = \exp(2\beta J L^2) \sum_{E=0}^{2L^2} \Omega(E) y^E, \tag{5}$$

where $y = \exp(-2\beta J)$. For a ferromagnetic interaction, the physical interval is $0 \le y \le 1$ ($0 \le T \le \infty$). That is, y is a convenient temperature variable, confined to a short interval [0, 1]. Given the density of states $\Omega(E)$, the partition function is a polynomial in y. Naturally, we obtain the entropy as a function of energy according to the Boltzmann formula

$$S(E) = k_B \ln \Omega(E) \tag{6}$$

from the density of states. Therefore, the partition function of the square-lattice Ising model can be written as

$$Z(y) = \exp(2\beta J L^2) \sum_{E=0}^{2L^2} \exp[S(E)/k_B] y^E. \tag{7}$$

The states with $E = 0$ are the ferromagnetic ground states (where all spins align in the same direction), whereas the states with $E = 2L^2$ correspond to the antiferromagnetic ground states (where all nearest-neighbor spins of any spin on the lattice are oppositely oriented to it). Also, the density of states satisfies the following relation

$$\Omega(E) = \Omega(2L^2 - E) \tag{8}$$

due to the symmetry of the square-lattice Ising model. Table I shows the exact integer values for the density of states of the Ising model on the 8×8 square lattice with periodic boundary conditions, obtained from the Onsager solution [1].

TABLE I: EXACT INTEGER VALUES FOR THE DENSITY OF STATES $\Omega(E)$ OF THE ISING MODEL ON THE 8 X 8 SQUARE LATTICE WITH PERIODIC BOUNDARY CONDITIONS, AS A FUNCTION OF ENERGY E (= 0 ~ 64)

E	$\Omega(E)$
0	2
4	128
6	256
8	4672
10	17920
12	145408
14	712960
16	4274576
18	22128384
20	118551552
22	610683392
24	3150447680
26	16043381504
28	80748258688
30	396915938304
32	1887270677624
34	8582140066816
36	36967268348032
38	149536933509376
40	564033837424064
42	1971511029384704
44	6350698012553216
46	18752030727310592
48	50483110303426544
50	123229776338119424
52	271209458049836032
54	535138987032308224
56	941564975390477248
58	1469940812209435392
60	2027486077172296064
62	2462494093546483712
64	2627978003957146636

The values of the density of states for $66 \le E \le 128$ are easily obtained using the relation $\Omega(E) = \Omega(2L^2 - E)$. As shown in the table, we notice that

$$\Omega(E) = 0 \tag{9}$$

for E = odd numbers. It is a general result for periodic boundary conditions, independent of the system size L. For other kinds of boundary conditions, we obtain non-zero values for the density of states even in the case of E = odd numbers. Also, we have

$$\sum_{E=0}^{2L^2} \Omega(E) = 2^{L^2} = 18446744073709551616 \tag{10}$$

for L = 8.

TABLE II: APPROXIMATE VALUES FOR THE DENSITY OF STATES $\Omega(E)$ OF THE ISING MODEL ON THE 8 X 8 SQUARE LATTICE WITH PERIODIC BOUNDARY CONDITIONS, AS A FUNCTION OF ENERGY E, OBTAINED FROM WANG-LANDAU MONTE CARLO ALGORITHM

E	$\Omega(E)$
0	2.0
4	127.4
6	255.1
8	4656.6
10	17893.1
12	144522.0
14	711580.2
16	4246933.2
18	21930324.7
20	117959662.0
22	607864844.6
24	3141196764.1
26	16031280614.1
28	80763014316.9
30	397547867401.4
32	1896126034244.0
34	8616391282913.0
36	37010388229450.7
38	149497396152612.3
40	564138451122736.3
42	1974546436062731.0
44	6361612074395794.0
46	18848286897649970.0
48	50748192131679070.0
50	124052697782181100.0
52	272702357160341300.0
54	538833615118266100.0
56	950195978440535000.0
58	1482917293139119000.0
60	2044706519336103000.0
62	2480176354118822000.0
64	2647205100816658000.0
66	2481685597611912000.0
68	2045217128048957000.0
70	1482774804531565000.0
72	950073686197236000.0
74	539916556625655100.0
76	273497776072990000.0
78	124382702728906700.0
80	50914788916632710.0
82	18903473835185660.0
84	6425496048611473.0
86	1997172631232223.0
88	570664400401192.8
90	151012039783018.9
92	37342836397764.3
94	8650942216058.1
96	1896807076900.0
98	398414563513.1
100	81043609427.3
102	16130155148.4
104	3167278999.3
106	613397094.4
108	118983233.4
110	22149806.8
112	4274929.4
114	714107.5
116	145441.5
118	17815.8
120	4648.6
122	253.1
124	127.1
128	2.0

III. APPROXIMATE DENSITY OF STATES

One of the most important methods in studying phase transitions and critical phenomena is computer simulation, in particular, Monte Carlo computer simulation. The importance sampling Monte Carlo method, Metropolis Mote Carlo algorithm [21], has been used extensively in science and engineering. In Metropolis Mote Carlo algorithm, the natural canonical distribution function,

$$\exp(-\beta H), \tag{11}$$

where H is the Hamiltonian of a given system, is employed as the sampling probability function at a given temperature T. The canonical distribution function can be written as

$$\Omega(E)\exp(-\beta E), \tag{12}$$

as a function of energy E, where $\Omega(E)$ is the density of states and $\exp(-\beta E)$ is the Boltzmann-Gibbs factor. As energy E increases, the density of states increases sharply and the Boltzmann-Gibbs factor decreases sharply. Therefore, the canonical distribution function is a needle-shaped function around E_T, which becomes the delta function in the thermodynamic limit.

Metropolis Mote Carlo algorithm is the most efficient method for understanding the properties of a given system at a fixed temperature. However, if we want to understand the phase transitions and critical phenomena of a given system as a continuous function of temperature, to obtain the partition function zeros in the complex temperature plane indicating most effectively phase transitions and critical phenomena, and to perform microcanonical analysis of phase transitions and critical phenomena, Metropolis Mote Carlo algorithm is not useful. To understand the transition properties of a given system as a continuous function of temperature, to obtain the partition function zeros, and to perform microcanonical analysis, we need to calculate the density of states. Currently, Wang-Landau Monte Carlo algorithm is one of the most efficient Monte Carlo methods to calculate the approximate density of states [3].

In Wang-Landau Monte Carlo algorithm, the reciprocal of the density of states, $1/\Omega(E)$, is also employed as the sampling probability function. That is, the transition probability from a state with energy E_1 to another state with energy E_2 is defined by

$$p(E_1 \to E_2) = \min[\Omega(E_1)/\Omega(E_2), 1], \tag{13}$$

where E_1 and E_2 are energies before and after a random spin flip. Because this definition means a random walk in energy space with a probability proportional to the reciprocal of the density of states, $1/\Omega(E)$, a truly flat histogram for the energy distribution can be obtained after an infinite number of random Monte Carlo moves.

The density of states is *a priori* unknown. Therefore, at the first time, we generate a crude version of the density of states, $\Omega_0(E)$, by accepting all $L^2 \times 10^6$ Monte Carlo steps. Now,

the initial density of states $\Omega_0(E)$ is employed as the sampling probability function, and then the density of states is changed after a Monte Carlo step. Each Monte Carlo step, the density of states is updated according to the following rule

$$\Omega(E) \rightarrow f\Omega(E), \tag{14}$$

where f (> 1) is the modification factor [3]. Owing to this factor, an improved version of the density of states can be obtained quickly. At the first time, the modification factor is conveniently chosen as

$$f_1 = e. \tag{15}$$

During a finite number of Monte Carlo steps with f_1, the initial density of states $\Omega_0(E)$ evolves into the new density of states $\Omega_1(E)$. Next, the modification factor is reduced according to the following rule

$$f_i = \sqrt{f_{i-1}}. \tag{16}$$

Therefore, during a finite number of Monte Carlo steps with

$$f_2 = \exp(1/2), \tag{17}$$

the density of states $\Omega_1(E)$ evolves into $\Omega_2(E)$. If we repeat these processes thirty times, we have the final modification factor

$$f_{30} = \exp(2^{-29}) = 1.00000000186, \tag{18}$$

and reach an accurate version of density of states $\Omega_{30}(E)$, quite close to the true density of states, for example, the exact integer values in Table I.

Every $L^2 \times 10^6$ Monte Carlo steps, we check the flatness of the energy histogram distribution $h_i(E)$. If the maximum histogram value is less than 1.2 times the average value of histogram $< h_i(E) >$ and the minimum histogram value is larger than $0.8 < h_i(E) >$ (the so-called 20% flatness criterion), we reduce the modification factor from f_i to f_{i+1}, and reset the histogram to zero. If not, we repeat $L^2 \times 10^6$ Monte Carlo steps again and again until the 20% flatness criterion is satisfied without changing the value of the modification factor.

Table II shows the approximate values for the density of states of the Ising model on the 8×8 square lattice with periodic boundary conditions, obtained from Wang-Landau Monte Carlo algorithm. As shown in the table, the approximate values are quite close to the exact integer ones in Table I.

IV. Partition Function Zeros

In the thermodynamic limit, the specific heat (per volume) of the square-lattice Ising ferromagnet becomes infinite at the critical temperature where the transition between the paramagnetic phase and the ferromagnetic phase emerges. In finite systems, the specific heat per volume shows a sharp peak but is not infinite. At the same time, the location (the so-called effective critical temperature) of the sharp peak of the specific heat in a finite system is different from the critical temperature at the inifinite system. As the system size increases, the effective critical temperature approaches the critical temperature.

Given the density of states $\Omega(E)$, the free energy (per volume) of the square-lattice Ising model is given by

$$\begin{aligned} f(y) &= -(k_B T L^{-2}) \ln Z(y) \\ &= -(k_B T L^{-2})[2\beta J L^2 + \ln \sum_{E=0}^{2L^2} \Omega(E) y^E]. \end{aligned} \tag{19}$$

Therefore, the specific heat (per volume) is expressed as

$$\begin{aligned} C(y) &= (k_B T^2 L^2)^{-1} \frac{\partial^2}{\partial \beta^2} \ln Z(y) \\ &= (k_B L^{-2})(\ln y)^2 (< E^2 > - < E >^2). \end{aligned} \tag{20}$$

In the thermodynamic limit, the specific heat (per volume) of the square-lattice Ising ferromagnet diverges at the critical temperature

$$\begin{aligned} y_c &= \exp(-2J / k_B T_c) = \sqrt{2} - 1 \\ &= 0.4142135623730950. \end{aligned} \tag{21}$$

The ordered ferromagnetic phase appears below y_c, whereas the disordered paramagnetic phase appears above y_c. The properties of the phase transition of the Ising model are completely equivalent to those of the gas-liquid phase transition for a simple system [22, 23].

Phase transitions and critical phenomena can also be understood based on the concept of partition function zeros. Yang and Lee (Nobel prize winners in 1957) proposed a rigorous mechanism for the occurrence of phase transitions in the thermodynamic limit and yielded an insight into the unsolved problem of the ferromagnetic Ising model at arbitrary temperature (T) in an external magnetic field (B) by introducing the concept of the zeros of the partition function *Z(T,B)* in the *complex* magnetic-field plane [22]. They also formulated the celebrated circle theorem, which states that the partition function zeros of the Ising ferromagnet lie on the unit circle in the complex fugacity plane [23].

Following Yang and Lee's idea, Fisher introduced the partition function zeros in the complex *temperature* plane utilizing the Onsager solution of the square-lattice Ising model in the absence of an external magnetic field [4]. Fisher also showed that the partition function zeros in the complex temperature plane of the square-lattice Ising model determine its ferromagnetic and antiferromagnetic critical temperatures at the same time for $B = 0$. In finite systems no zero cut the

positive real axis in the complex temperature plane, but some zeros for a system showing a phase transition approach the positive real axis as the system size increases, determining the critical temperature and the related critical exponents in the thermodynamic limit.

Since the properties of the partition function zeros of a given system provided the valuable information on its exact solution, the earlier studies on partition function zeros were mainly performed in the fields of mathematics and mathematical physics. Nowadays, the concept of partition function zeros is applied to all fields of science from elementary particle physics to protein folding, and they are used as one of the most effective methods to determine the critical temperatures and exponents [5−20].

The partition function $Z(y)$ of the square-lattice Ising model can be expressed as its zeros $\{y_i\}$ in the complex temperature (y) plane:

$$Z(y) = \exp(2\beta JL^2)\sum_{E=0}^{2L^2} \Omega(E) y^E = A\prod_{i=1}^{2L^2} (y - y_i), \qquad (22)$$

where A is constant. In terms of the partition function zeros, the free energy is given by

$$f(y) = -(k_B T L^{-2})[\ln A + \sum_{i=1}^{2L^2} \ln(y - y_i)], \qquad (23)$$

and the specific heat by

$$C(y) = (k_B L^{-2})(\ln y)^2 \sum_{i=1}^{2L^2} \left[\frac{y}{y - y_i} - \left(\frac{y}{y - y_i} \right)^2 \right]. \qquad (24)$$

For a system with the phase transition at the critical temperature y_c, the loci of the partition function zeros close in toward the real axis to intersect it in the thermodynamic limit, and the singularity of the specific heat (per volume) $C(y)$ appears in this limit. It is clear from $C(y)$ that the leading behavior of such a singularity is due to the pair of partition function zeros closest to the positive real axis, called the first zeros (y_1). Therefore, by calculating the partition function zeros and examining the behavior of the first zero in the thermodynamic limit, the critical behavior can be much more accurately analyzed than examining the behavior of the specific heat per volume for real values of the temperature, which is plagued by the noise due to the subleading terms containing zeros other than the first ones.

TABLE III: EXACT FIRST ZERO $y_1(L)$ OF THE ISING FERROMAGNET ON L x L SQUARE LATTICE ($L = 4 \sim 32$) WITH PERIODIC BOUNDARY CONDITIONS

L	$y_1(L)$
4	0.4444395319800772 + 0.1872942080259974 *i*
8	0.4313561367685625 + 0.0893746869542861 *i*
12	0.4261054598770712 + 0.0589791409518722 *i*
16	0.4233155229514006 + 0.0440487351863922 *i*
20	0.4215858813328893 + 0.0351597456080490 *i*
24	0.4204086628321746 + 0.0292591011649791 *i*
28	0.4195556551626489 + 0.0250556995741284 *i*
32	0.4189091317852369 + 0.0219089496918388 *i*

Using the Onsager solution of the square-lattice Ising ferromagnet with periodic boundary conditions, we can obtain the exact partition function zeros of the square-lattice Ising model in the complex y plane. Among the partition function zeros, the first zero (y_1) is most important because it determines the critical temperature and the critical exponents. Table III shows the exact first zeros $y_1(L)$ of the Ising ferromagnet on L x L square lattices ($L = 4 \sim 32$) with periodic boundary conditions. As shown in the table, as the system size L increases, the real part of the first zero $\mathrm{Re}[y_1(L)]$ approaches the exact critical temperature $y_c = -1 + \sqrt{2}$ following the finite-size scaling law

$$\Delta \mathrm{Re}[y_1(L)] = \mathrm{Re}[y_1(L)] - y_c \sim L^{-1}. \qquad (25)$$

Also, the imaginary part of the first zero $\mathrm{Im}[y_1(L)]$ decreases quickly following the similar finite-size scaling law

$$\mathrm{Im}[y_1(L)] \sim L^{-1}. \qquad (26)$$

However, it is impossible to calculate the partition function zeros by using popular Metropolis Monte Carlo computer simulations. That is why the concept of the partition function zeros has not been used popularly and extensively in science and engineering. Now, with new Wang-Landau Monte Carlo computer simulations, it is possible to calculate the partition function zeros. We have calculated the partition function zeros of the square-lattice Ising ferromagnet with periodic boundary conditions from the density of states $\Omega(E)$, generated by Wang-Landau Monte Carlo computer simulations with the 20 % flatness criterion for histograms. We have used one core of a Linux PC with one Intel i7-2600K CPU for Wang-Landau Monte Carlo computer simulations. The CPU time for the Ising model on 10 x 10 square lattice is just 3 minutes and 19 seconds. Also, the CPU time is 14 minutes and 8 seconds on 20 x 20 square lattice, and 48 minutes and 26 seconds on 32 x 32 square lattice. Therefore, Wang-Landau Monte Carlo algorithm is quite fast with a modern computer.

TABLE IV: APPROXIMATE FIRST ZERO $y_1(L)$ OF THE ISING FERROMAGNET ON L x L SQUARE LATTICE ($L = 4 \sim 32$) WITH PERIODIC BOUNDARY CONDITIONS, OBTAINED FROM WANG-LANDAU MONTE CARLO ALGORITHM

L	$y_1(L)$
4	0.4443746227827420 + 0.1875279524143367 *i*
8	0.4311015629498683 + 0.0891428713930486 *i*
12	0.4261963705955438 + 0.0589390738277786 *i*
16	0.4234407520086122 + 0.0442294013769738 *i*
20	0.4213463155523976 + 0.0351986300295024 *i*
24	0.4205150208576107 + 0.0294455914640483 *i*
28	0.4195652085874216 + 0.0250443689758780 *i*
32	0.4190968920648668 + 0.0220230300146012 *i*

Table IV shows the approximate first zeros $y_1(L)$ of the Ising ferromagnet on L x L square lattices ($L = 4 \sim 32$) with periodic boundary conditions, obtained from Wang-Landau Monte Carlo computer simulations. As shown in the table, the approximate first zeros are quite close to the exact ones in Table III.

TABLE V: ERRORS OF THE APPROXIMATE FIRST ZEROS FROM THE EXACT ONES FOR THE ISING FERROMAGNET ON L X L SQUARE LATTICE

L	Error (%) for $\mathrm{Re}[y_1(L)]$	Error (%) for $\Delta\mathrm{Re}[y_1(L)]$	Error (%) for $\mathrm{Im}[y_1(L)]$
4	0.015	0.215	0.125
8	0.059	1.485	0.259
12	0.021	0.764	0.068
16	0.030	1.376	0.410
20	0.057	3.250	0.111
24	0.025	1.717	0.637
28	0.002	0.179	0.045
32	0.045	3.999	0.521

Table V shows the errors (%) of the approximate first zeros from the exact ones. The second column of the table shows the error of the real part of the approximate first zero from the exact one, and the errors are less than 0.06%. The third column shows the error for the difference, as in (25), between the real part and the critical temperature, and the errors are less than 4.0%. The fourth column of Table V shows the error of the imaginary part of the approximate first zero from the exact one, and the errors are less than 0.64%. Overally, the errors are quite small, indicating that Wang-Landau Monte Carlo algorithm is a reliable method for calculating the density of states and the first partition function zeros.

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