2012 4th International Conference on Computer Modeling and Simulation (ICCMS 2012)
IPCSIT vol.22 (2012) © (2012) IACSIT Press, Singapore

Evaluation of Wang-Landau Monte Carlo Simulations

Seung-Yeon Kim

School of Liberal Arts and Sciences Chungju National University Chungju, Korea 380-702

Abstract. Efficiency of Wang-Landau Monte Carlo algorithm is evaluated by calculating the partition function zeros of the square-lattice Ising model. The partition function zeros of the square-lattice Ising ferromagnet with periodic boundary conditions are calculated from the density of states generated by Wang-Landau Monte Carlo computer simulations. The approximate first zeros, which determine the critical temperature and the critical exponents of a given system with phase transition, obtained from Wang-Landau algorithm, are compared with the exact first zeros. We find that the errors of the approximate first zeros from the exact ones are remarkably small, indicating that Wang-Landau algorithm is a quite reliable method for calculating the first zeros.

Keywords: Monte Carlo computer simulations, Wang-Landau Monte Carlo algorithm, Partition function zeros

1. Introduction

Phase transitions and critical phenomena are the most universal phenomena in nature. The two-dimensional Ising ferromagnet is the simplest system showing phase transitions and critical phenomena at finite temperatures. Since the Onsager (Nobel prize winner in 1968) 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 and critical phenomena [1].

The most important method in studying phase transitions and critical phenomena is computer simulations, in particular, Monte Carlo computer simulations. A importance sampling Monte Carlo method, Metropolis Mote Carlo algorithm [2], has been used extensively in science and engineering. In Metropolis Mote Carlo algorithm, the natural canonical distribution function, $\mathrm{Exp}[- H / k_B T]$, where H is the Hamiltonian of a given system and k_B is the Boltzmann constant, is employed as the sampling probability function at a given temperature T. The canonical distribution function can be written as $g(E)\ \mathrm{Exp}[- E / k_B T]$, as a function of energy E, where $g(E)$ is the density of states and $\mathrm{Exp}[- E / k_B T]$ 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 properties of a given system as a continuous function of temperature, Metropolis Mote Carlo algorithm is not useful. To understand the properties of a given system as a continuous function of temperature, a new computer simulation method, Wang-Landau Monte Carlo algorithm [3], has been introduced recently. In Wang-Landau Monte Carlo algorithm, the density of states $g(E)$ is employed as the sampling probability function. In this work, we evaluate efficiency of Wang-Landau Monte Carlo algorithm by calculating the partition function zeros of the square-lattice Ising model.

2. 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.

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 [4]. 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 [5].

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 [6]. 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 [7−31].

For a system with the phase transition at the critical point T_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) $C(T)$ appears in this limit. It is clear from $C(T)$ that the leading behavior of such a singularity is due to the pair of partition function zeros closest to the real axis, called the first zeros [23]. Therefore, by calculating the partition function zeros and examining the behavior of the first zeros 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.

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. Next, we evaluate efficiency of Wang-Landau Monte Carlo algorithm by calculating the partition function zeros of the square-lattice Ising model.

3. Exact First Zeros

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 $y = \mathrm{Exp}[-2J/k_B T]$ plane where J is the coupling constant between two neighboring magnetic spins. Among the partition function zeros, the first zero is most important because it determines the critical temperature and the critical exponents. Tab.1 shows the exact first zeros of the Ising ferromagnet on $L \times L$ square lattices ($L = 4 \sim 20$) with periodic boundary conditions. As shown in the table, as the system size increases, the real part of the first zero approaches the exact critical temperature $y_c = -1 + \sqrt{2} = 0.4142135623730950$, and the imaginary part of the first zero decreases quickly.

Tab.1: Exact first zero as a function of the system size

System Size L	Exact First Zero
4	0.4444395319800772 + 0.1872942080259974 i
6	0.4361842497526979 + 0.1206869428519625 i
8	0.4313561367685625 + 0.0893746869542861 i
10	0.4282572974955254 + 0.0710431382436936 i
12	0.4261054598770712 + 0.0589791409518722 i
14	0.4245251434294016 + 0.0504286870623749 i
16	0.4233155229514006 + 0.0440487351863922 i
18	0.4223598990614609 + 0.0391045195675401 i
20	0.4215858813328893 + 0.0351597456080490 i

4. Approximate First Zeros

We have calculated the partition function zeros of the square-lattice Ising ferromagnet with periodic boundary conditions from the density of states $g(E)$, generated by Wang-Landau Monte Carlo computer simulations with the 20 % flatness criteria [3] for histograms. We have used a Linux PC with one Intel E6600 CPU for Wang-Landau Monte Carlo computer simulations. The CPU time for the Ising model on 4 x 4 square lattice is just 57 seconds. Also, the CPU time is 9 minutes and 20 seconds on 12 x 12 square lattice, and 26 minutes and 27 seconds on 20 x 20 square lattice. Therefore, Wang-Landau Monte Carlo algorithm is quite fast with a modern computer.

Tab.2 shows the approximate first zeros of the Ising ferromagnet on L x L square lattices (L = 4 ~ 20) with periodic boundary conditions, obtained from Wang-Landau Monte Carlo computer simulations. The third column of the table shows the errors of the approximate first zeros from the exact ones. It should be noted that the errors are remarkably small. Hence, we conclude that Wang-Landau Monte Carlo algorithm is a quite reliable method for calculating the partition function zeros, in particular, the first zeros.

Tab.2: Approximate first zero as a function of the system size

System Size L	Approximate First Zero	Error (%)
4	0.4443746227827420 + 0.1875279524143367 i	0.050
6	0.4361708330499551 + 0.1204563922748490 i	0.051
8	0.4311015629498683 + 0.0891428713930486 i	0.078
10	0.4286219008962024 + 0.0705746715478227 i	0.137
12	0.4261963705955438 + 0.0589390738277786 i	0.023
14	0.4242806729227413 + 0.0504547673888370 i	0.058
16	0.4234407520086122 + 0.0442294013769738 i	0.052
18	0.4224314416543388 + 0.0389508716198877 i	0.040
20	0.4213463155523976 + 0.0351986300295024 i	0.057

5. Acknowledgments

This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (grant number 2011-0014994).

6. References

[1] DOMB Cyril. The Critical Point (Taylor and Francis, London, 1996).

[2] METROPOLIS Nicholas; ROSENBLUTH Arianna W.; ROSENBLUTH Marshall N.; TELLER Augusta H.; TELLER Edward. Equation of State Calculations by Fast Computing Machines, Journal of Chemical Physics [J], 1953, VOL:21, PP:1087-1092.

[3] WANG Fugao; LANDAU David P. Efficient, Multiple-Range Random Walk Algorithm to Calculate the Density of States, Physical Review Letters [J], 2001, VOL:86, PP:2050-2053.

[4] YANG Chen-Ning; LEE Tsung-Dao. Statistical Theory of Equations of State and Phase Transitions. I. Theory of Condensation, Physical Review [J], 1952, VOL:87, PP:404-409.

[5] LEE Tsung-Dao; YANG Chen-Ning. Statistical Theory of Equations of State and Phase Transitions. II. Lattice Gas and Ising Model, Physical Review [J], 1952, VOL:87, PP:410-419.

[6] FISHER Michael E. The Nature of Critical Points, in Lectures in Theoretical Physics, edited by W. E. Brittin (University of Colorado Press, Boulder, CO, 1965), VOL:7C, PP:1-159.

[7] KIM Seung-Yeon; CRESWICK Richard J. Yang-Lee Zeros of the Q-State Potts Model in the Complex Magnetic Field Plane, Physical Review Letters [J], 1998, VOL:81, PP:2000-2003.

[8] KIM Seung-Yeon; CRESWICK Richard J. Density of States, Potts Zeros, and Fisher Zeros of the Q-State Potts Model for Continuous Q, Physical Review E [J], 2001, VOL:63, ARTICLE:066107, PP:1-12.

[9] KIM Seung-Yeon. Partition Function Zeros of the Q-State Potts Model on the Simple-Cubic Lattice, Nuclear Physics B [J], 2002, VOL:637, PP:409-426.

[10] KIM Seung-Yeon. Density of the Fisher Zeros for the Three-State and Four-State Potts Models, Physical Review E [J], 2004, VOL:70, ARTICLE:016110, PP:1-5.

[11] KIM Seung-Yeon. Yang-Lee Zeros of the Antiferromagnetic Ising Model, Physical Review Letters [J], 2004, VOL:93, ARTICLE:130604, PP:1-4.

[12] KIM Seung-Yeon. Yang-Lee Zeros of the One-Dimensional Q-State Potts Model, Journal of the Korean Physical Society [J], 2004, VOL:44, PP:495-500.

[13] KIM Seung-Yeon. Fisher Zeros and Potts Zeros of the Q-State Potts Model in a Magnetic Field, Journal of the Korean Physical Society [J], 2004, VOL:45, PP:302-309.

[14] KIM Seung-Yeon. Fisher Zeros of the Ising Antiferromagnet in an Arbitrary Nonzero Magnetic Field Plane, Physical Review E [J], 2005, VOL:71, ARTICLE:017102, PP:1-4.

[15] KIM Seung-Yeon. Density of Yang-Lee Zeros and Yang-Lee Edge Singularity for the Antiferromagnetic Ising Model, Nuclear Physics B [J], 2005, VOL:705, PP:504-520.

[16] KIM Seung-Yeon. Honeycomb-Lattice Antiferromagnetic Ising Model in a Magnetic Field, Physics Letters A [J], 2006, VOL:358, PP:245-250.

[17] KIM Seung-Yeon. Density of Yang-Lee Zeros for the Ising Ferromagnet, Physical Review E [J], 2006, VOL:74, ARTICLE:011119, PP:1-7.

[18] MONROE James L.; KIM Seung-Yeon. Phase Diagram and Critical Exponent for Nearest- Neighbor and Next-Nearest-Neighbor Interaction Ising Model, Physical Review E [J], 2007, VOL:76, ARTICLE:021123, PP:1-5.

[19] KIM Seung-Yeon; HWANG Chi-Ok; KIM Jin Min. Partition Function Zeros of the Antiferromagnetic Ising Model on Triangular Lattice in the Complex Temperature Plane for Nonzero Magnetic Field, Nuclear Physics B [J], 2008, VOL:805, PP:441-450.

[20] KIM Seung-Yeon. Specific Heat of the Square-Lattice Ising Antiferromagnet in a Nonzero Magentic Field, Journal of Physical Studies [J], 2009, VOL:13, ARTICLE:4006, PP:1-3.

[21] KIM Seung-Yeon. Partition Function Zeros of the Square-Lattice Ising Model with Nearest- and Next-Nearest-Neighbor Interactions, Physical Review E [J], 2010, VOL:81, ARTICLE:031120, PP:1-7.

[22] KIM Seung-Yeon. Partition Function Zeros of the Honeycomb-Lattice Ising Antiferromagnet in the Complex Magnetic-Field Plane, Physical Review E [J], 2010, VOL:82, ARTICLE:041107, PP:1-7.

[23] LEE Jae Hwan; KIM Seung-Yeon; LEE Julian. Exact Partition Function Zeros and the Collapse Transition of a Two-Dimensional Lattice Polymer, Journal of Chemical Physics [J], 2010, VOL:133, ARTICLE:0114106, PP:1-6.

[24] LEE Jae Hwan; SONG Hyun Suk; KIM Jin Min; KIM Seung-Yeon. Study of a Square-Lattice Ising Superantiferromagnet Using the Wang-Landau Algorithm and Partition Function Zeros, Journal of Statistical Mechanics [J], 2010, VOL:10, ARTICLE:P03020, PP:1-9.

[25] KIM Seung-Yeon. Honeycomb-lattice Ising Model in a Nonzero Magentic Field: Low-temperature Series Analysis and Partition Function Zeros, Journal of the Korean Physical Society [J], 2010, VOL:56, PP:1051-1054.

[26] HWANG Chi-Ok; KIM Seung-Yeon. Yang-Lee Zeros of Triangular Ising Antiferromagnets, Physica A [J], 2010,

VOL:389, PP:5650-5654.

[27] KIM Seung-Yeon. Triangular-lattice Ising Model in a Nonzero Magentic Field, Journal of the Korean Physical Society [J], 2011, VOL:58, PP:5-8.

[28] KIM Seung-Yeon. Yang-Lee Edge Singularity of the Square-lattice Ising Ferromagnet, Journal of the Korean Physical Society [J], 2011, VOL:59, PP:2205-2208.

[29] KIM Seung-Yeon. Specific Heat and Partition Function Zeros of the Three-state Potts Model, Journal of the Korean Physical Society [J], 2011, VOL:59, PP:2980-2983.

[30] LEE Jae Hwan; KIM Seung-Yeon; LEE Julian. Parallel Algorithm for Calculation of the Exact Partition Function of a Lattice Polymer, Computer Physics Communications [J], 2011, VOL:182, PP:1027-1033.

[31] LEE Jae Hwan; KIM Seung-Yeon; LEE Julian. Collapse Transition of a Square-Lattice Polymer with Next Nearest-Neighbor Interaction, Journal of Chemical Physics [J], 2011, VOL:135, ARTICLE:204102, PP:1-4.