ISSN: 2350-0328
International Journal of Advanced Research in Science, Engineering and Technology
Vol. 5, Issue 2 , February 2018

Calculations of the Partition Function Zeros for the Ising Ferromagnet on 6 x 6 Square Lattice with Periodic Boundary Conditions

Seung-Yeon Kim

School of Liberal Arts and Sciences, Korea National University of Transportation, Chungju, South Korea

ABSTRACT: Phase transitions and critical phenomena occur universally in nature. The theory of partition functions zeros is very powerful and efficient method to investigate phase transitions and critical phenomena. Ferromagnet is greatly popular material in modern science, engineering, and technology. The Ising ferromagnet has played a central role in developing modern theory of phase transitions and critical phenomena. We study systematically the calculations of the partition function zeros from the complete partition function and from the partial partition functions of the square-lattice Ising ferromagnet with periodic boundary conditions. In particular, we compare the partition function zeros from the complete partition function of the Ising ferromagnet on 6 x 6 square lattice with the partition function zeros from the partial partition functions.

KEYWORDS: Partition function zeros, Phase transitions.

I. INTRODUCTION

Phase transitions occur universally in nature such as the ice-water phase transition. Modern theory of phase transition is based on the understanding of the ferromagnet-paramagnet phase transition [1]. Ferromagnet is the most popular magnet in modern industrial society [2]. In higher temperature, ferromagnet changes into paramagnet, and it loses its macroscopic magnetic force due to large thermal fluctuation. A specific magnetic material changes from ferromagnet into paramagnet at a fixed temperature, the so-called critical temperature. The critical temperature is the most important inherent property of a given material. At the critical temperature, phase transitions and critical phenomena emerge.

The theory of partition functions zeros [3-10] in the complex temperature plane is the most powerful and efficient method to investigate phase transitions and critical phenomena. The partition function Z(T), as a function of temperature T, is the most fundamental quantity from which all kinds of thermodynamic functions such as free energy, internal energy, entropy, and specific heat are obtained. To calculate rigorously the partition function zeros, the complete partition function is required. However, it is very difficult to obtain the complete partition function. Therefore, the partition function zeros have been usually calculated from the partial partition functions.

The Ising ferromagnet has played a central role in developing modern theory of phase transitions and critical phenomena [1]. The partition function of the square-lattice Ising ferromagnet with periodic boundary conditions has been obtained by Nobel prize laureate Onsager [11] and his colleague Kaufman [12]. Nowadays, it is called the Onsager revolution [1]. It was the starting point for understanding phase transitions and critical phenomena correctly. In this work, we study systematically the calculations of the partition function zeros from the complete partition function and from the partial partition functions of the square-lattice Ising ferromagnet with periodic boundary conditions by using the Onsager-Kaufman exact solution. In particular, we compare the partition function zeros from the complete partition function of the square-lattice Ising ferromagnet with the partition function zeros from the partial partition functions. Even though this kind of comparison is very important, it has never been performed systematically.

ISSN: 2350-0328
International Journal of Advanced Research in Science, Engineering and Technology
Vol. 5, Issue 2 , February 2018

II. ISING FERROMAGNET AND THE DENSITY OF STATES

The Hamiltonian H of the Ising ferromagnet is defined by

$$H = J \sum_{<i,j>} [1 - S(i)\, S(j)],$$

where J is the coupling constant, <i,j> indicates the sum over all nearest-neighbor pairs of lattice sites, and S(i) is the microscopic magnetic spin on the lattice site (i), taking 1 (upward direction) or -1 (downward direction). Then, the energy E of the Ising ferromagnet can be conveniently written as

$$E = \frac{1}{2} \sum_{<i,j>} [1 - S(i)S(j)].$$

Now, the partition function Z(y) of the Ising ferromagnet on L x L square lattice with periodic boundary conditions can be expressed as

$$Z(y) = \sum_{E=0}^{2L^2} g(E)\, y^E,$$

where g(E) is the density of states and $y=e^{-2J/kT}$ is the so-called low-temperature variable with k being the Boltzmann constant.

Table 1 shows the exact integer values for the density of states g(E), as a function of energy E, of the Ising ferromagnet on 6 x 6 square lattice with periodic boundary conditions, obtained from the Onsager-Kaufman exact solution [11,12]. The partition function Z(y) is a polynomial in the low-temperature variable y with the integer coefficients g(E). As shown in the table, the density of ground states is g(E = 0) = 2. One is the all-spin-up state, and the other is the all-spin-down state. The sum over all the densities of states is 2^{36} = 68719476736 ≈ 6.87 x 10^{10}. The maximum density of states is g(E = 36) = 13172279424 ≈ 1.32 x 10^{10}, corresponding to completely random states. The maximum density of states accounts for 19 % of states.

Table 1. Exact integer values for the density of states g(E), as a function of energy E, of the Ising ferromagnet on 6 x 6 square lattice with periodic boundary conditions. The density of states is zero, g(E)=0, for other values of energy, not shown in the table.

E	g(E)	E	g(E)	E	g(E)
0	2	4	72	6	144
8	1620	10	6048	12	35148
14	159840	16	804078	18	3846576
20	17569080	22	71789328	24	260434986
26	808871328	28	2122173684	30	4616013408
32	8196905106	34	11674988208	36	13172279424
38	11674988208	40	8196905106	42	4616013408
44	2122173684	46	808871328	48	260434986
50	71789328	52	17569080	54	3846576
56	804078	58	159840	60	35148
62	6048	64	1620	66	144
68	72	72	2		

III. PARTITION FUNCTION ZEROS

The partition function zeros are the roots of the polynomial Z(y). Because the coefficients g(E) of the polynomial Z(y) are not negative, as shown in the table, the partition function zeros are complex in the low-temperature variable y. The partition function zero closest to the positive real axis is called the first partition function zero, shortly, the first zero.

ISSN: 2350-0328
International Journal of Advanced Research in Science, Engineering and Technology
Vol. 5, Issue 2 , February 2018

The first partition function zero causes phase transitions and critical phenomena [3-10]. Analyzing the behavior of the first partition function zero, phase transitions and critical phenomena can be understood precisely and accurately.

Figure 1 shows the partition function zeros in the low-temperature variable y of the Ising ferromagnet on 6 x 6 square lattice with periodic boundary conditions. Open circles indicate the partition function zeros obtained from the complete partition function with the density of states g(E) from E = 0 to E = 72. Plus symbols indicate the partition function zeros obtained from the partial (that is, the first half) partition function with the density of states g(E) from E = 0 to E = 36. As shown in the figure, the number of the partition function zeros for the first-half partition function is reduced to half. Remarkably, the locations of the most important zeros, the first partition function zeros, are almost same. The first partition function zero for the complete partition function is

$$y_1 = 0.4361842 + 0.1206869\, i.$$

And the first partition function zero for the first-half partition function is

$$y_1 = 0.4361895 + 0.1206819\, i.$$

The difference between these two first partition function zeros is negligible.

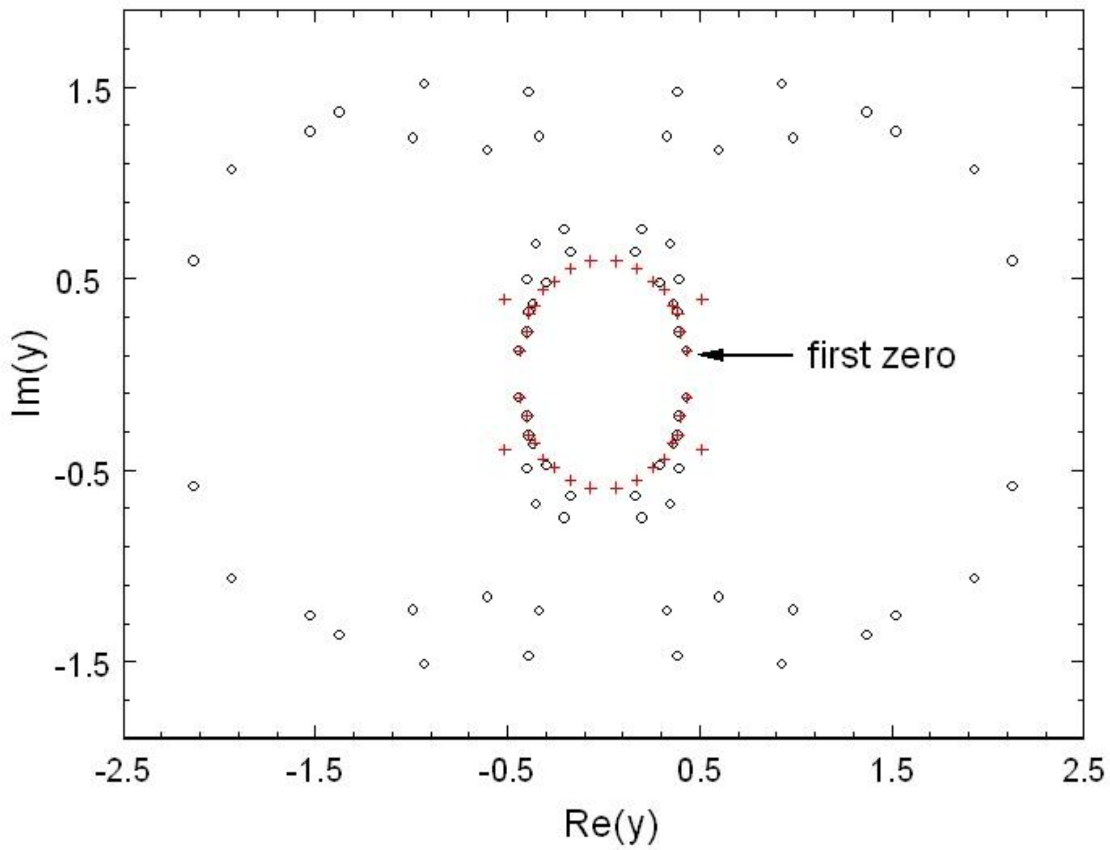

Figure 1. Partition function zeros in the low-temperature variable y of the Ising ferromagnet on 6 x 6 square lattice with periodic boundary conditions. Open circles indicate the partition function zeros obtained from the complete partition function with the density of states g(E) from E = 0 to E = 72. Plus symbols indicate the partition function zeros obtained from the partial partition function with the density of states g(E) from E = 0 to E = 36. The first zero is the first partition function zero closest to the positive real axis, causing phase transitions and critical phenomena.

Figure 2 shows again the partition function zeros in the low-temperature variable y of the Ising ferromagnet on 6 x 6 square lattice with periodic boundary conditions. Open circles indicate the partition function zeros obtained from the

ISSN: 2350-0328
International Journal of Advanced Research in Science, Engineering and Technology
Vol. 5, Issue 2 , February 2018

complete partition function with the density of states g(E) from E = 0 to E = 72. Cross (x) symbols indicate the partition function zeros obtained from the partial (that is, the first quarter) partition function with the density of states g(E) from E = 0 to E = 18. As shown in the figure, the number of the partition function zeros for the first-quarter partition function is reduced to quarter. The first partition function zero for the first-quarter partition function is

$$y_1 = 0.4098224 + 0.1455146\, i.$$

Compared with the first partition function zero for the complete partition function, the difference between these two first partition function zeros is not negligible. However, the difference is small, and the first partition function zero for the first-quarter partition function is still a good approximation.

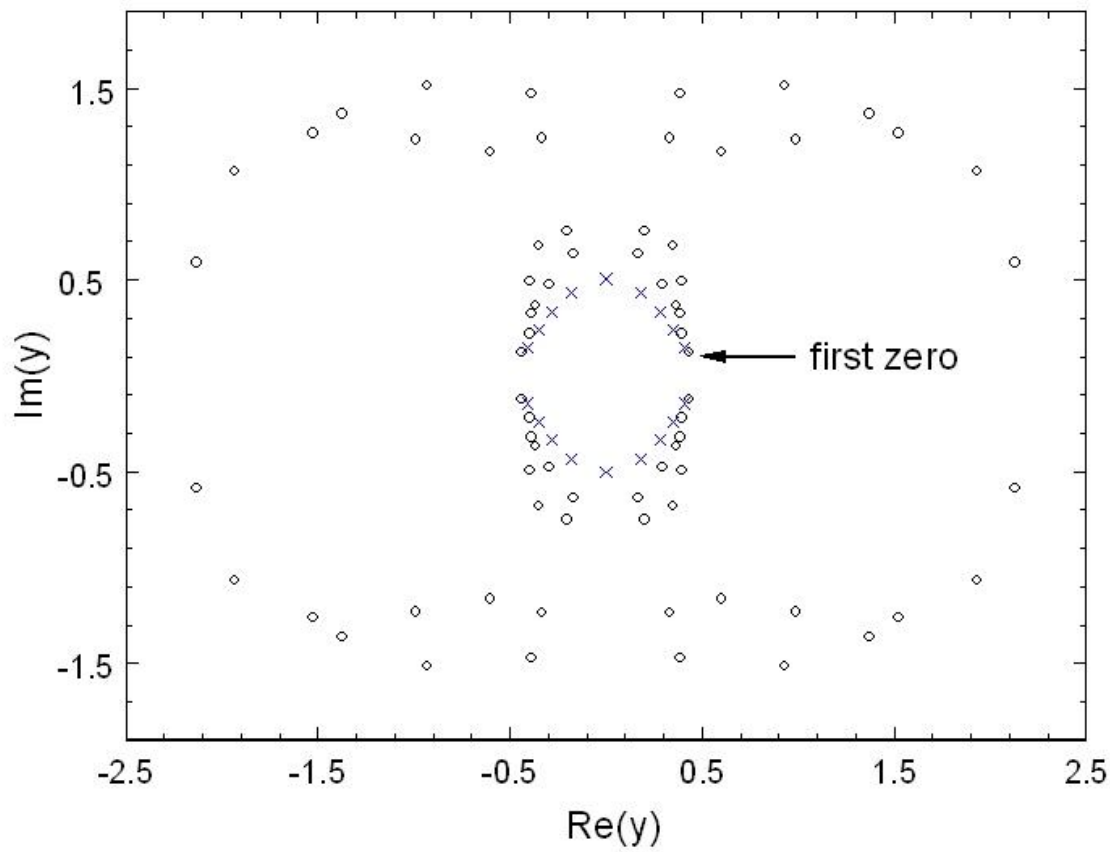

Figure 2. Partition function zeros in the low-temperature variable y of the Ising ferromagnet on 6 x 6 square lattice with periodic boundary conditions. Open circles indicate the partition function zeros obtained from the complete partition function with the density of states g(E) from E = 0 to E = 72. Cross (x) symbols indicate the partition function zeros obtained from the partial partition function with the density of states g(E) from E = 0 to E = 18.

IV. CONCLUSION

Modern theory of phase transition and critical phenomena, which occur universally in nature, is based on the understanding of the ferromagnet-paramagnet phase transition. Ferromagnet is the most popular magnet in modern science, engineering, and technology. In higher temperature, ferromagnet changes into paramagnet, losing its macroscopic magnetic force. The theory of partition functions zeros is very powerful and efficient method to investigate phase transitions and critical phenomena. To calculate rigorously the partition function zeros, the complete partition function is required. However, it is very difficult to obtain the complete partition function. Therefore, the partition function zeros have been usually calculated from the partial partition functions. The Ising ferromagnet has played a central role in developing modern theory of phase transitions and critical phenomena. We have systematically studied the calculations of the partition function zeros from the complete partition function and from the partial partition functions of the square-lattice Ising ferromagnet with periodic boundary conditions.

We have calculated the partition function zeros of the Ising ferromagnet on 6 x 6 square lattice with periodic boundary conditions by using the complete partition function with the density of states g(E) from E = 0 to E = 72. Also, we have calculated the partition function zeros of the Ising ferromagnet on 6 x 6 square lattice with periodic boundary conditions by using the partial (the first half) partition function with the density of states g(E) from E = 0 to E = 36 and the partial (the first quarter) partition function with the density of states g(E) from E = 0 to E = 18. The locations of the first partition function zeros, the most important zeros, for the complete partition function and the first-half partition function are almost same. The first partition function zero is $y_1 = 0.4361842 + 0.1206869\ i$ for the complete partition function and the first partition function zero is $y_1 = 0.4361895 + 0.1206819\ i$ for the first-half partition function, indicating that the difference between these two first partition function zeros is negligible. The first partition function zero is $y_1 = 0.4098224 + 0.1455146\ i$ for the first-quarter partition function, indicating that the difference from the first partition function zero for the complete partition function is very small but not negligible.

ACKNOWLEDGMENT

This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (grant number NRF-2017R1D1A3B06035840).

REFERENCES

[1]. C. Domb, The Critical Point: A Historical Introduction to the Modern Theory of Critical Phenomena (Taylor and Francis, London, 1996).
[2]. B. D. Cullity and C. D. Graham, Introduction to Magnetic Materials (IEEE Press, New Jersey, 2009).
[3]. I. Bena, M. Dorz, and A. Lipowski, “Statistical Mechanics of Equilibrium and Nonequilibrium Phase Transitions: The Yang-Lee Formalism,” International Journal of Modern Physics B 19 (2005) 4269–4329, and references therein.
[4]. S.-Y. Kim, “Partition Function Zeros of the Q-State Potts Model on the Simple-Cubic Lattice,” Nuclear Physics B 637 (2002) 409-426.
[5]. S.-Y. Kim, “Yang-Lee Zeros of the Antiferromagnetic Ising Model,” Physical Review Letters 93 (2004) 130604: 1-4.
[6]. S.-Y. Kim, “Density of Yang-Lee Zeros for the Ising Ferromagnet,” Physical Review E 74 (2006) 011119: 1-7.
[7]. S.-Y. Kim, “Partition Function Zeros of the Square-Lattice Ising Model with Nearest- and Next-Nearest-Neighbor Interactions,” Physical Review E 81 (2010) 031120: 1-7.
[8]. S.-Y. Kim, “Partition Function Zeros of the Honeycomb-Lattice Ising Antiferromagnet in the Complex Magnetic-Field Plane,” Physical Review E 82 (2010) 041107: 1-7.
[9]. J. Lee, “Exact Partition Function Zeros of the Wako-Saito-Munoz-Eaton Protein Model,” Physical Review Letters 110 (2013) 248101: 1-5.
[10]. J. H. Lee, S-Y. Kim, and J. Lee, “Study on Collapse and Folding Transitions of a Lattice Protein Using Exact Enumeration,” AIP Advances 5 (2015) 127211: 1-10.
[11]. L. Onsager, “Crystal Statistics I: A Two-Dimensional Model with an Order-Disorder Transition,” Physical Review 65 (1944) 117–149.
[12]. B. Kaufman, “Crystal Statistics II: Partition Function Evaluated by Spinor Analysis,” Physical Review 76 (1949) 1232–1243.