World Academy of Science, Engineering and Technology
International Journal of Physical and Mathematical Sciences
Vol:9, No:2, 2015

Yang-Lee Edge Singularity of the Infinite-Range Ising Model

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Abstract—The Ising ferromagnet, consisting of magnetic spins, is the simplest system showing phase transitions and critical phenomena at finite temperatures. The Ising ferromagnet has played a central role in our understanding of phase transitions and critical phenomena. Also, the Ising ferromagnet explains the gas-liquid phase transitions accurately. In particular, the Ising ferromagnet in a nonzero magnetic field has been one of the most intriguing and outstanding unsolved problems. We study analytically the partition function zeros in the complex magnetic-field plane and the Yang-Lee edge singularity of the infinite-range Ising ferromagnet in an external magnetic field. In addition, we compare the Yang-Lee edge singularity of the infinite-range Ising ferromagnet with that of the square-lattice Ising ferromagnet in an external magnetic field.

Keywords—Ising ferromagnet, Magnetic field, Partition function zeros, Yang-Lee edge singularity.

I. Introduction

PHASE transitions and critical phenomena are the most universal phenomena in nature. The two-dimensional Ising ferromagnet, consisting of magnetic spins, is the simplest system showing phase transitions and critical phenomena at finite temperatures. The Ising ferromagnet has played a central role [1] in our understanding of phase transitions and critical phenomena since the Onsager (Nobel prize winner in 1968) solution [2] of the square-lattice Ising ferromagnet in the absence of an external magnetic field. In addition, the Ising ferromagnet explains the gas-liquid phase transitions exactly. However, the Ising ferromagnet in a nonzero magnetic field has been one of the most intriguing and outstanding unsolved problems except for the trivial one-dimensional Ising ferromagnet [3]−[6].

Phase transitions and critical phenomena can be understood based on the concept of partition function zeros. Yang and Lee (Nobel prize winners in 1957) [7] 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 ferromagnet at arbitrary temperature (T) in a magnetic field (B) by introducing the concept of the zeros of the grand partition function $Z(T, B)$ (for fluid systems, $Z(T, \mu)$ as a function of chemical potential μ) in the *complex* magnetic-field (for fluid systems, chemical potential) plane (the so-called Yang-Lee zeros). They [8] also formulated the celebrated circle theorem, which states that the Yang-Lee zeros of the Ising ferromagnet lie on the unit circle $x_0 = e^{i\theta}$ in the complex fugacity ($x = e^{-2B/k_BT}$) plane.

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At the Curie temperature T_c, Yang-Lee zeros cut the positive real axis at the point $x_c = 1$ ($B_c = 0$) in the thermodynamic limit. The spontaneous magnetization m_0 is determined by the density of Yang-Lee zeros $g(\theta)$ on the positive real axis, i.e., $m_0 = 2\pi g(\theta = 0)$. Above T_c, Yang-Lee zeros do not cut the positive real axis in the thermodynamic limit. There is a gap in the distribution of zeros around the positive real axis; that is, $g(\theta) = 0$ for $|\theta| < \theta_e$. For $T > T_c$, the Yang-Lee zeros at $\theta = \pm\theta_e$ are called the Yang-Lee edge singularities, and their locations depend on temperature. It is well known that $\theta_e = 0$ at T_c and $\theta_e = \pi$ at $T = \infty$ [9]. However, for $T_c < T < \infty$, the location of the Yang-Lee edge singularity $\theta_e(T)$ has never been determined except for the one-dimensional Ising ferromagnet.

The Yang-Lee edge singularity provides key information for finding the unknown equation of state of the square-lattice Ising ferromagnet in a nonzero magnetic field. Therefore, the Yang-Lee edge singularity has been studied extensively for the Ising ferromagnet [10]−[20]. Kortman and Griffiths [10] carried out the first systematic investigation of Yang-Lee zeros for the the square-lattice Ising ferromagnet by using a high field, high-temperature series expansion. They found that the density of Yang-Lee zeros for the square-lattice Ising ferromagnet diverges at the Yang-Lee edge singularity θ_e for high temperatures. Fisher [11] proposed the ideas that the Yang Lee edge singularity could be thought of as a new second-order phase transition with associated critical exponents and that the Yang-Lee edge singularity could be considered as a conventional critical point. The critical point of the Yang-Lee edge singularity is associated with a ϕ^3 theory. The crossover dimension of the Yang-Lee edge singularity is $d_c = 6$. The Yang-Lee edge singularity has also been investigated for the two-dimensional Ising ferromagnet $FeCl_2$ in axial magnetic fields experimentally [17].

Following Yang and Lee's idea, Fisher [21] introduced the partition function zeros in the complex *temperature* plane (the so-called Fisher zeros) utilizing the Onsager solution of the square-lattice Ising model in the absence of an external magnetic field. 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 in the absence an external magnetic field at the same time. However, there exists no circle theorem for partition function zeros in the complex temperature plane, and studying partition function zeros in the complex temperature plane is a difficult task.

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), phase transitions and critical phenomena can be much more clearly understood. Because the partition function zeros of a given system provide valuable information on its exact solution, earlier studies on partition function zeros were mainly performed in the fields of mathematical physics and rigorous statistical mechanics. Nowadays, the concept of partition function zeros is applied to all fields of physics from particle physics to biophysics, and they are popularly used as one of the most effective methods to determine the critical points and exponents [22]−[58].

In this work, we study analytically the partition function zeros in the complex magnetic-field plane and the Yang-Lee edge singularity of the infinite-range Ising ferromagnet in an external magnetic field. Also, we compare the Yang-Lee edge singularity of the infinite-range Ising ferromagnet with that of the square-lattice Ising ferromagnet in an external magnetic field.

II. Infinite-Range Ising Model

The infinite-range Ising ferromagnet with N (magnetic) spins in an external magnetic field B is defined by the Hamiltonian [58]−[60]

$$\mathcal{H} = -\frac{J}{N}\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\sigma_i\sigma_j - B\sum_{i=1}^{N}\sigma_i, \quad (1)$$

where $\sigma_i = \pm 1$, J is the coupling constant ($J > 0$), and the first term indicates a sum over all possible bonds

$$N_b = \frac{1}{2}N(N-1) \quad (2)$$

between two different spins σ_i and σ_j. If there is a spin configuration with r down ($\sigma_i = -1$) spins and $N-r$ up ($\sigma_i = 1$) spins, the magnetization M is defined by

$$M \equiv \sum_{i=1}^{N}\sigma_i = (N-r) - r = N - 2r. \quad (3)$$

Also, the first sum of the infinite-range Ising ferromagnet is given by

$$\begin{aligned}&\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\sigma_i\sigma_j \\ =\ & \frac{1}{2}r(r-1) + \frac{1}{2}(N-r)(N-r-1) - r(N-r) \\ =\ & \frac{1}{2}(M^2 - N). \quad (4)\end{aligned}$$

Therefore, the Hamiltonian for a spin configuration with r down spins and $N-r$ up spins is simply expressed as

$$\mathcal{H} = -\frac{J}{2N}(M^2 - N) - BM. \quad (5)$$

The partition function (a sum over all 2^N spin states) of the infinite-range Ising ferromagnet

$$Z = \sum_{\{\sigma_n\}} e^{-\beta\mathcal{H}}, \quad (6)$$

where $\beta = 1/k_BT$, k_B is the Boltzmann constant, and T is temperature, can be written as

$$Z = \sum_{r=0}^{N}\binom{N}{r}\exp\left[\frac{\beta J}{2N}(M^2 - N) + \beta BM\right]. \quad (7)$$

And the free energy F is given by

$$F = -k_BT\ln Z. \quad (8)$$

TABLE I
Partition function zeros in the complex magnetic-field ($x = e^{-2\beta B}$) plane of the infinite-range Ising ferromagnet for $N = 20$ at the Curie temperature $T_c = J/k_B$

$-0.991616971016042 - 0.129212161939080i$
$-0.991616971016042 + 0.129212161939080i$
$-0.925154056403051 - 0.379591849123476i$
$-0.925154056403051 + 0.379591849123476i$
$-0.795430982323641 - 0.606044183504509i$
$-0.795430982323641 + 0.606044183504509i$
$-0.608834977858797 - 0.793296898856713i$
$-0.608834977858797 + 0.793296898856713i$
$-0.374912562575763 - 0.927060176268442i$
$-0.374912562575763 + 0.927060176268442i$
$-0.106367073277723 - 0.994326931005256i$
$-0.106367073277723 + 0.994326931005256i$
$0.180851554735243 - 0.983510404189933i$
$0.180851554735243 + 0.983510404189933i$
$0.467185921263300 - 0.884159100486650i$
$0.467185921263300 + 0.884159100486650i$
$0.728276230555473 - 0.685283687247779i$
$0.728276230555473 + 0.685283687247779i$
$0.930316724674649 - 0.366757129161293i$
$0.930316724674649 + 0.366757129161293i$

III. Partition Function Zeros

The partition function is also expressed as

$$Z = \exp\left[\frac{\beta J}{2N}(N^2 - N) + \beta BN\right]\sum_{r=0}^{N}\binom{N}{r}y^{r(N-r)}x^r, \quad (9)$$

where y is the low-temperature variable and x is the fugacity variable, defined by

$$y \equiv \exp\left[-\frac{2\beta J}{N}\right] \quad (10)$$

and

$$x \equiv \exp[-2\beta B]. \quad (11)$$

Then, the reduced partition function

$$\tilde{Z} = \sum_{r=0}^{N}\binom{N}{r}y^{r(N-r)}x^r \quad (12)$$

is a polynomial in variables y and x. That is, equation (12) determines the partition function zeros of the infinite-range Ising ferromagnet.

TABLE II
YANG-LEE EDGE SINGULARITY x_e OF THE INFINITE-RANGE ISING FERROMAGNET AT THE CURIE TEMPERATURE $T_c = J/k_B$ FOR $N = 20 \sim 160$

N	x_e
20	$0.930316724674649 + 0.366757129161293i$
30	$0.961275775929932 + 0.275588248316772i$
40	$0.974554786275155 + 0.224149433521897i$
50	$0.981653381379761 + 0.190674169267056i$
60	$0.985966142256138 + 0.166945399231453i$
70	$0.988816229521337 + 0.149139076821627i$
80	$0.990815402977553 + 0.135221437732441i$
90	$0.992281546821177 + 0.124005370198921i$
100	$0.993394561919970 + 0.114748613707665i$
110	$0.994263131699981 + 0.106961791973334i$
120	$0.994956396771223 + 0.100308367168573i$
130	$0.995520225970465 + 0.094548821693947i$
140	$0.995986125280646 + 0.089507755241911i$
150	$0.996376378112817 + 0.085053589805401i$
160	$0.996707144074488 + 0.081085565613602i$

Table I shows the the partition function zeros in the complex magnetic-field ($x = e^{-2\beta B}$) plane of the infinite-range Ising ferromagnet for $N = 20$ at the Curie temperature $T_c = J/k_B$, obtained from (12). As shown in the table, the partition function zeros always have their complex conjugates to make the real partition function and the number of the partition function zeros is equal to N. The partition function zero $x_e = 0.930316724674649 + 0.366757129161293i$ (its complex conjugate $0.930316724674649 - 0.366757129161293i$) lies closest to the positive real axis, and it is the Yang-Lee edge singularity. Table II shows the Yang-Lee edge singularity x_e of the infinite-range Ising ferromagnet at the Curie temperature $T_c = J/k_B$ for $N = 20 \sim 160$.

IV. EQUATION OF STATE

The density of state $\Omega(M)$ for the infinite-range Ising ferromagnet is given by

$$\begin{aligned}\Omega(M) &= \binom{N}{r} = \frac{N!}{(N-r)!r!} \\ &= \frac{N!}{[\frac{1}{2}(N+M)]![\frac{1}{2}(N-M)]!}.\end{aligned} \tag{13}$$

And the unitless entropy $S(M)$ is written as

$$S(M) = \ln\Omega = \ln N! - \ln\left[\frac{1}{2}(N+M)\right]! - \ln\left[\frac{1}{2}(N-M)\right]!. \tag{14}$$

For large N, using Stirling's formula for the factorial

$$\ln N! = N\ln N - N, \tag{15}$$

we obtain

$$\frac{d}{dM}\ln\left[\frac{1}{2}(N\pm M)\right]! = \pm\frac{1}{2}\ln\left[\frac{1}{2}(N\pm M)\right]. \tag{16}$$

TABLE III
EXACT VALUES FOR THE YANG-LEE EDGE SINGULARITY $x_e(T)$ AND ITS ARGUMENT $\theta_e(T)$ OF THE INFINITE-RANGE ISING FERROMAGNET IN THE THERMODYNAMIC LIMIT

T/Tc	x_e	θ_e
1.5	$0.95877114 + 0.28417935i$	0.288150
2	$0.84147098 + 0.54030231i$	0.570796
2.5	$0.70216810 + 0.71201121i$	0.792358
3	$0.56709298 + 0.82365378i$	0.967824
3.5	$0.44448284 + 0.89578736i$	1.110199
4	$0.33577382 + 0.94194264i$	1.228370
5	$0.15586085 + 0.98777902i$	1.414297
10	$-0.32148301 + 0.94691535i$	1.898092
20	$-0.63180497 + 0.77512739i$	2.254676

Thus, the derivative of the entropy is simply given by

$$\frac{d}{dM}S(M) = \frac{1}{2}\ln\frac{N-M}{N+M}. \tag{17}$$

The restricted partition function $z(M)$ is defined by

$$z(M) \equiv \binom{N}{r}\exp\left[\frac{\beta J}{2N}(M^2 - N) + \beta BM\right]. \tag{18}$$

Then, the derivative of $\ln Z(M)$ is written as

$$\begin{aligned}\frac{d}{dM}z(M) &= \frac{1}{2}\ln\frac{N-M}{N+M} + \frac{\beta JM}{N} + \beta B \\ &= \frac{1}{2}\ln\frac{1-m}{1+m} + \beta Jm + \beta B,\end{aligned} \tag{19}$$

where $m \equiv \frac{M}{N}$ is the magnetization per volume. The optimal condition

$$\frac{d}{dM}z(M) = 0 \tag{20}$$

yields

$$\ln\frac{1-m}{1+m} = -2\beta(Jm + B). \tag{21}$$

Finally, we reach the equation of state

$$m = \tanh\beta(Jm + B) \tag{22}$$

for the infinite-range Ising ferromagnet in the thermodynamic limit [58]−[60].

V. YANG-LEE EDGE SINGULARITY

From the equation of state, the critical temperature T_c (the so-called Curie temperature) for $B = 0$ is given by

$$\beta_c J = 1, \tag{23}$$

equivalently,

$$T_c = \frac{J}{k_B}. \tag{24}$$

Differentiating the equation of state with respect to m, we obtain the useful relation

$$1 = \beta J[1 - \tanh^2\beta(Jm + B)] = \beta J(1 - m^2), \tag{25}$$

TABLE IV
ARGUMENT OF THE YANG-LEE EDGE SINGULARITY FOR THE SQUARE-LATTICE ISING FERROMAGNET IN THE THERMODYNAMIC LIMIT, ACCURATELY ESTIMATED FROM THE EXACT PARTITION FUNCTION ZEROS FOR FINITE LATICES

T/Tc	θ_e
1.5	0.18544 ± 0.00009
2	0.42578 ± 0.00004
2.5	0.63180 ± 0.00003
3	0.80234 ± 0.00002
3.5	0.94444 ± 0.00002
4	1.06449 ± 0.00002
5	1.25667 ± 0.00001
10	1.771000 ± 0.000008
20	2.159285 ± 0.000005

from which the spontaneous magnetization (per volume)

$$m_0(T) = \pm\sqrt{1 - \frac{k_B T}{J}} = \pm\sqrt{1 - \frac{T}{T_c}} \qquad (26)$$

is derived.

In the thermodynamic limit, the equation of state determines the Yang-Lee edge singularity x_e of the infinite-range Ising ferromagnet according to the following equation

$$x_e(T) = \exp[-2\beta B_e] = \exp[2(\beta J m_0 - \tanh^{-1} m_0)] \qquad (27)$$

for $T > T_c$. Hence, the argument of the Yang-Lee edge singularity is given by

$$\theta_e(T) = -i \ln x_e(T). \qquad (28)$$

Table III shows the exact values for the Yang-Lee edge singularity and its argument of the infinite-range Ising ferromagnet in the thermodynamic limit. As shown in the table, the Yang-Lee edge singularity is not far from the point $x = 1$ ($\theta = 0$) in low temperature. As temperature increases, it moves away and approaches $x = -1$ ($\theta = \pi$).

For comparison, we also show the argument of the Yang-Lee edge singularity for the square-lattice Ising ferromagnet in the thermodynamic limit, accurately estimated from the exact partition function zeros for finite latices [20], as shown in Table IV. The error estimates are twice the difference between the $(n-1,1)$ and $(n-1,2)$ approximants of the Bulirsch-Stoer extrapolation method [61]. Until now, the exact values for the Yang-Lee edge singularity and its argument of the square-lattice Ising ferromagnet have never been known. Clearly, we notice that the argument of the Yang-Lee edge singularity of the infinite-range Ising ferromagnet is larger than that of the square-lattice Ising ferromagnet, as shown in the table.

VI. CONCLUSION

The Ising ferromagnet, consisting of magnetic spins, is the simplest system showing phase transitions and critical phenomena at finite temperatures. The Ising ferromagnet in a nonzero magnetic field has been one of the most intriguing and outstanding unsolved problems. The partition function zeros in the complex magnetic-field plane (shortly, the Yang-Lee zeros) of the Ising ferromagnet has played a central role in understanding its properties in a nonzero magnetic field. Above the Curie temperature, the Yang-Lee zero at the edge of the zero distribution of the Ising ferromagnet is called the Yang-Lee edge singularity. The Yang-Lee edge singularity has been indispensable in investigating the unknown properties of the Ising ferromagnet in a nonzero magnetic field. We have studied analytically the partition function zeros in the complex magnetic-field plane and the Yang-Lee edge singularity of the infinite-range Ising ferromagnet in an external magnetic field. In addition, we have compared the Yang-Lee edge singularity of the infinite-range Ising ferromagnet with that of the square-lattice Ising ferromagnet in an external magnetic field.

ACKNOWLEDGMENT

The author is grateful to Prof. R. J. Creswick for very useful discussions. 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-2014R1A1A2056127).

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