Yang-Lee Zeros of the Antiferromagnetic Ising Model

Seung-Yeon Kim*

School of Computational Sciences, Korea Institute for Advanced Study, Seoul 130-722, Korea

(Received 7 April 2004; published 23 September 2004)

There exists the famous circle theorem on the Yang-Lee zeros of the ferromagnetic Ising model. However, the Yang-Lee zeros of the antiferromagnetic Ising model are much less well understood than those of the ferromagnetic model. The precise distribution of the Yang-Lee zeros of the antiferromagnetic Ising model only with nearest-neighbor interaction J on $L \times L$ square lattices is determined as a function of temperature $a = e^{2\beta J}$ ($J < 0$), and its relation to the phase transitions is investigated. In the thermodynamic limit ($L \to \infty$), the distribution of the Yang-Lee zeros of the antiferromagnetic Ising model cuts the positive real axis in the complex $x = e^{-2\beta H}$ plane, resulting in the critical magnetic field $\pm H_c(a)$, where $H_c > 0$ below the critical temperature $a_c = \sqrt{2} - 1$. The results suggest that the value of the scaling exponent y_h is 1 along the critical line for $a < a_c$.

DOI: 10.1103/PhysRevLett.93.130604 PACS numbers: 05.50.+q, 05.70.–a, 64.60.Cn, 75.10.Hk

The Ising model in an external magnetic field H on a lattice with N_s sites and N_b bonds is defined by the Hamiltonian

$$\mathcal{H} = -J\sum_{\langle i,j\rangle}\sigma_i\sigma_j - H\sum_i \sigma_i, \quad (1)$$

where J is the coupling constant, $\langle i, j\rangle$ indicates a sum over all nearest-neighbor pairs of lattice sites, and $\sigma_i = \pm 1$. The two-dimensional Ising model is the simplest model showing phase transitions at finite temperatures, and consequently it has played a central role in our understanding of phase transitions and critical phenomena. Yang and Lee [1] proposed a mechanism for the occurrence of phase transitions in the thermodynamic limit and yielded an insight into the problem of the ferromagnetic (FM, $J > 0$) Ising model in magnetic field by introducing the concept of the zeros of the grand partition function (GPF) in the *complex* magnetic field plane (Yang-Lee zeros). They [1] also formulated the celebrated circle theorem which states that the Yang-Lee zeros of the FM Ising model lie on the unit circle in the complex $x = e^{-2\beta H}$ plane. Since then, numerous articles have dealt with the various properties of the Yang-Lee zeros of the FM Ising model [2]. However, the properties of the Yang-Lee zeros of the antiferromagnetic (AF, $J < 0$) Ising model [3–6] are much less well understood than those of the FM model. It has been known that all Yang-Lee zeros of the one-dimensional AF Ising model lie on the negative real axis [3]. Suzuki *et al.* [5] studied the Yang-Lee zeros of the AF Ising model on 4×6 square lattice, found the negative real zeros and the complex zeros with $\mathrm{Re}(x) < 0$, and concluded that the precise distribution of the AF Yang-Lee zeros and its relation to the phase transitions remain an open question.

In this Letter, we discuss the Yang-Lee zeros of the AF Ising model by evaluating the exact GPF on $L \times L$ square lattices. Because the Ising model for nonzero magnetic field has the symmetry $x \leftrightarrow 1/x$, Yang-Lee zeros with $|x| > 1$ are obtained from those with $|x| < 1$ by the inversion map $x \to 1/x$. With no loss of generality, we consider only Yang-Lee zeros on the unit disk $|x| \leq 1$.

If we define the density of states, $\Omega(E, M)$, with a given energy

$$E = \frac{1}{2}\sum_{\langle i,j\rangle}(1 + \sigma_i\sigma_j) \quad (2)$$

and a given magnetization

$$M = \frac{1}{2}\sum_i (1 - \sigma_i), \quad (3)$$

where E and M are positive integers $0 \leq E \leq N_b$ and $0 \leq M \leq N_s$, the GPF of the Ising model $Z = \sum_{\{\sigma_n\}} e^{-\beta\mathcal{H}}$, a sum over 2^{N_s} possible spin configurations, can be written as

$$\bar{Z}(a, x) = e^{\beta(JN_b - HN_s)}Z(a, x) = \sum_{E=0}^{N_b}\sum_{M=0}^{N_s}\Omega(E, M)a^E x^M, \quad (4)$$

where $a = e^{2\beta J}$ and $x = e^{-2\beta H}$. For AF interaction $J < 0$, the physical interval is $0 \leq a \leq 1$ ($0 \leq T \leq \infty$), while for FM interaction $J > 0$, the physical interval is $1 \leq a \leq \infty$ ($\infty \geq T \geq 0$). The states with $E = 0$ ($E = N_b$) correspond to the AF (FM) ground states.

The microcanonical transfer matrix (μTM) [7–9] is used to evaluate the *exact* integer values for the density of states $\Omega(E, M)$ for $L \leq 14$. For lattices $L > 14$, memory limitations [10] required us to use the restricted canonical transfer matrix (RCTM) which yields, for a fixed value of a, the coefficients

$$\omega(M) = \sum_E \Omega(E, M)a^E \quad (5)$$

as real numbers of finite precision [11].

While we lack the circle theorem to tell us the location of AF Yang-Lee zeros, something can be said about their general behavior as a function of temperature. At zero temperature ($a = 0$) from Eq. (4), the GPF is

$$\bar{Z}(0, x) = \sum_M \Omega(0, M)x^M = 2x^{N_s/2} \ (L = \text{even}). \tag{6}$$

Therefore, the AF Yang-Lee zeros at $T = 0$ lie at $x = 0$. At infinite temperature ($a = 1$), where the AF Yang-Lee zeros and the FM Yang-Lee zeros become identical, the GPF is given by [8]

$$\bar{Z}(1, x) = (1 + x)^{N_s}, \tag{7}$$

and its zeros are N_s-degenerate at $x = -1$.

Figure 1 shows the Yang-Lee zeros in the complex x plane of the 14×14 AF Ising model at several temperatures with a cylindrical boundary condition. At high temperatures (for example, $a = 0.9$), all zeros lie on the negative real axis. They move toward $x = -1$ as the temperature is further increased. As the temperature deceases, complex zeros with $\mathrm{Re}(x) < 0$ begin to appear near $x = -1$. Lieb and Ruelle [6] showed that the locations [7,8] of the FM Yang-Lee edge zeros at a temperature above the critical temperature determine the region free of the AF Yang-Lee zeros at the same temperature. According to the Lieb-Ruelle theorem, at $a = 0.9$, the region free of the AF zeros is the exterior of the circle with center $c = -12.471$ and radius $r = 12.430$, and at $a = 0.5$, it is the interior of the circle with $c = 1.003$ and $r = 0.078$. The results in Fig. 1 are consistent with Lieb-Ruelle theorem. As a approaches the critical temperature $a_c = \sqrt{2} - 1$, the number of complex zeros with $\mathrm{Re}(x) < 0$ increases, but the negative real zeros near $x = 0$ still exist. As shown in Fig. 1(c), at $a = a_c$, two complex zeros with $\mathrm{Re}(x) > 0$ are finally revealed. As the temperature is further lowered, all zeros move toward $x = 0$, and the number of complex zeros with $\mathrm{Re}(x) > 0$ increases. For example, as shown in Fig. 1(d), at $a = 0.1$, the number of complex zeros with $\mathrm{Re}(x) > 0$ is 8. Table I shows the classification of the AF Yang-Lee zeros as a function of temperature for cylindrical and free boundary conditions. The distribution of the AF Yang-Lee zeros for free boundary condition is similar to that for cylindrical boundary condition. However, the number of complex zeros with $\mathrm{Re}(x) > 0$ for free boundary condition is less than or equal to that for cylindrical boundary condition.

Figure 2 shows the Yang-Lee zeros in the complex x plane of the $L \times L$ AF Ising model at $a = 0.2$ with cylindrical boundary condition for (a) $L = 8$, 10, 12, and 14 and (b) $L = 9$, 11, and 13. As shown in the figure, the zeros with the largest value of $\mathrm{Re}(x)$ approach the real axis as L increases. We call these zeros as the first zeros x_1. The first zeros for odd sizes approach the real axis slowly compared to those for even sizes. Table II shows the real and imaginary parts of the first zeros x_1 at $a = 0.2$ for $L = 8$–18 (even sizes) and cylindrical boundary condition [12]. By using the Bulirsch-Stoer (BST) algorithm [13], we extrapolated our results for finite lattices to infinite size and, for $\omega = 1$ (the parameter of the BST algorithm), obtained $x_1 = 0.007\,33(6) - 0.000\,01(4)i$, indicating the phase transition of the AF Ising model in an external magnetic field. The extrapolated result is consistent with values by approximate closed-form expressions [14] for the critical line of the AF Ising model. The BST result from odd sizes is $x_1 = 0.0078(2) + 0.000(2)i$ for $L = 9 \sim 17$ and $0.0075(3) + 0.000(1)i$ for $L = 11 \sim 19$, which is less accurate than that from even sizes. In the rest of the Letter, we consider only even sizes for the BST extrapolation. Itzykson *et al.* [15] showed that the imaginary part $\mathrm{Im}(x_1)$ of the first zero vanishes in the limit

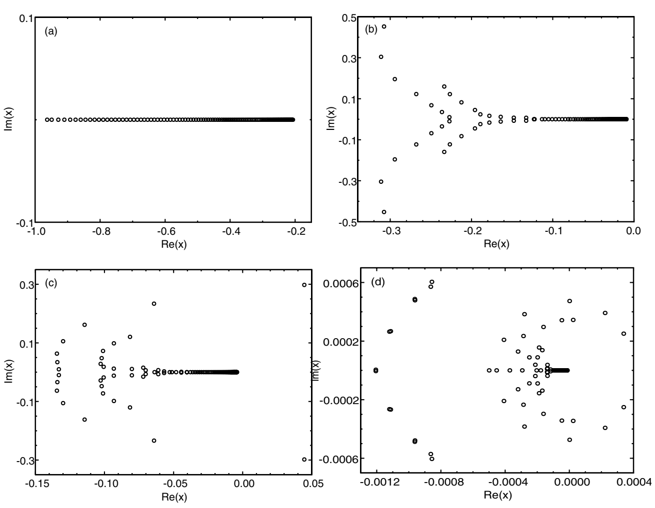

FIG. 1. Yang-Lee zeros in the complex x plane of the 14×14 AF Ising model with cylindrical boundary condition for (a) $a = 0.9$, (b) 0.5, (c) $\sqrt{2} - 1$, and (d) 0.1.

TABLE I. The classification of the Yang-Lee zeros for the 14×14 AF Ising model with cylindrical (free) boundary condition. The total number of the AF Yang-Lee zeros on the unit disk $|x| \leq 1$ is $14^2/2 = 98$. $N(\text{real})$, $N[\mathrm{Re}(x) < 0]$, and $N[\mathrm{Re}(x) > 0]$ denote the number of negative real zeros, the number of complex zeros with $\mathrm{Re}(x) < 0$, and the number of complex zeros with $\mathrm{Re}(x) > 0$, respectively. The numbers in parentheses are those for free boundary condition.

a	$N(\text{real})$	$N[\mathrm{Re}(x) < 0]$	$N[\mathrm{Re}(x) > 0]$
0.9	98 (98)	0 (0)	0 (0)
0.8	94 (94)	4 (4)	0 (0)
0.7	86 (90)	12 (8)	0 (0)
0.6	78 (82)	20 (16)	0 (0)
0.5	66 (70)	32 (28)	0 (0)
$\sqrt{2} - 1$	56 (62)	40 (36)	2 (0)
0.3	50 (52)	44 (42)	4 (4)
0.2	46 (44)	48 (50)	4 (4)
0.1	46 (40)	44 (54)	8 (4)

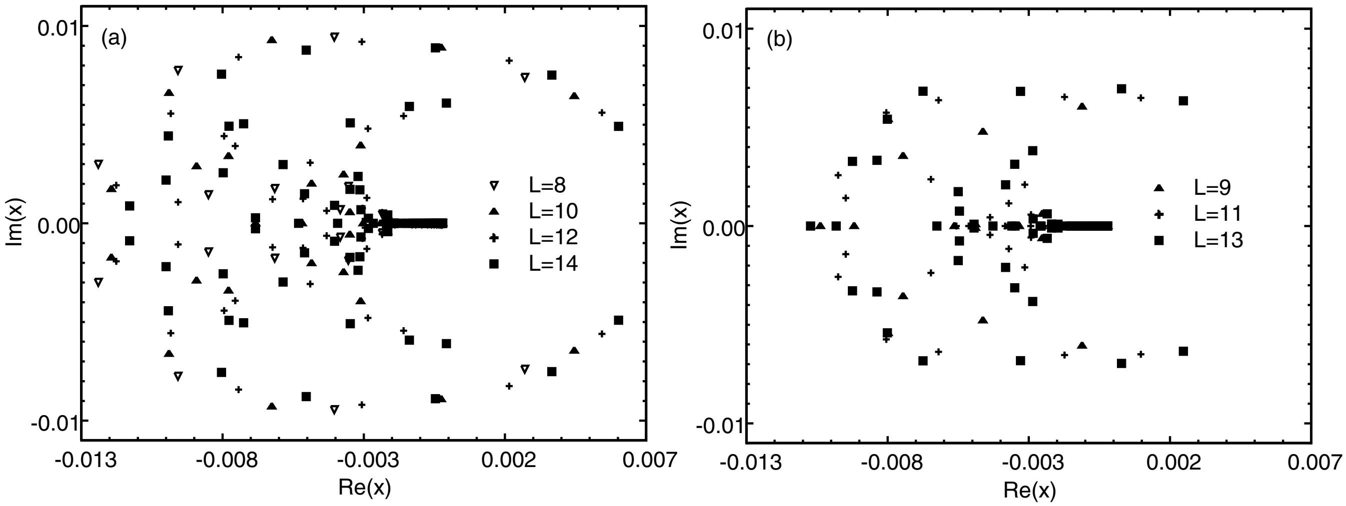

FIG. 2. Yang-Lee zeros of the $L \times L$ AF Ising model at $a = 0.2$ with cylindrical boundary condition for (a) $L = 8$, 10, 12, and 14 and (b) $L = 9$, 11, and 13. In (b), the zeros on the negative real axis between -1 and -0.04 are omitted. The numbers of the omitted zeros are 5, 6, and 7 for $L = 9$, 11, and 13, respectively.

$L \to \infty$ following the finite-size scaling

$$\mathrm{Im}(x_1) \sim L^{-y_h}. \tag{8}$$

From this scaling law we obtain the scaling exponent [9]

$$y_h(L) = -\frac{\ln\{\mathrm{Im}[x_1(L+2)]/\mathrm{Im}[x_1(L)]\}}{\ln[(L+2)/L]} \tag{9}$$

for finite lattices. The fourth column of Table II shows the values of the scaling exponent $y_h(L)$. The extrapolated value ($\omega = 1$) is $y_h = 1.00(3)$, indicating that the exact value of the scaling exponent y_h may be 1.

Similarly, with $\omega = 1$, we have obtained $x_1 = 0.000\,396\,29(4) + 0.000\,000(3)i$ and $y_h = 0.99(3)$ for $a = 0.1$, and $x_1 = 0.0505(2) - 0.0002(7)i$ and $y_h = 0.98(8)$ for $a = 0.3$. The extrapolated values for x_1 are in excellent agreement with those by closed-form approximations [14]. The extrapolated values for y_h are consistent with $y_h = 1$. For free boundary condition, the extrapolated values ($\omega = 1$) are $x_1 = 0.000\,40(7) + 0.000\,00(1)i$ and $y_h = 0.99(8)$ for $a = 0.1$, $x_1 = 0.00725(3) - 0.0001(3)i$ and $y_h = 1.0(1)$ for $a = 0.2$, and $x_1 = 0.050(5) - 0.001(4)i$ and $y_h = 0.8(2)$ for $a = 0.3$. These values are less accurate than those for cylindrical boundary condition. Figure 3 shows that the extrapolated values of x_1 are in agreement with the results of closed-form approximations. In the figure, the Wu-Wu approximation [14] and the Wang-Kim approximation [14] are not distinguishable, but their results are slightly different. For example, the Wang-Kim approximation results in $x_1 = 0.007\,03\ldots$ for $a = 0.2$ whereas the Wu-Wu approxima-

TABLE II. The real and imaginary parts of the first zeros x_1 at $a = 0.2$ for $L = 8$–18 (even sizes only) and cylindrical boundary condition. $y_h(L)$ is the scaling exponent calculated by Eq. (9). The last row is the BST extrapolation to infinite size.

L	$\mathrm{Re}(x_1)$	$\mathrm{Im}(x_1)$	$y_h(L)$
8	0.002 698 29	0.007 395 14	0.613 694
10	0.004 451 78	0.006 448 71	0.770 260
12	0.005 432 77	0.005 603 80	0.855 450
14	0.006 024 46	0.004 911 49	0.906 055
16	0.006 402 87	0.004 351 80	0.938 070
18	0.006 656 37	0.003 896 59	
∞	0.007 33(6)	−0.000 01(4)	1.00(3)

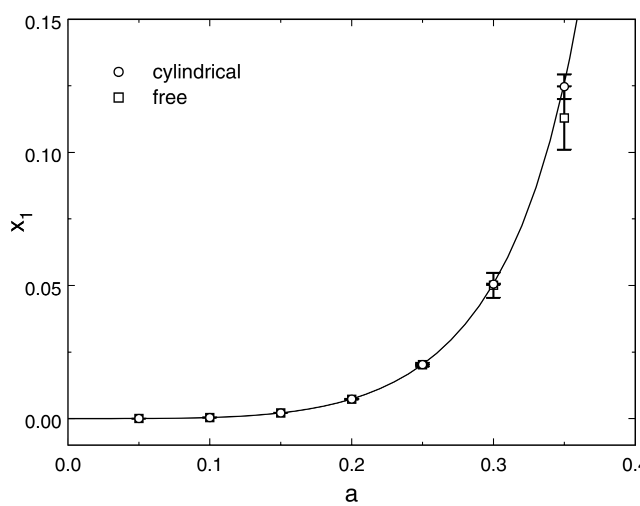

FIG. 3. The extrapolated values of x_1 as a function of a for cylindrical (circles) and free (squares) boundary conditions. The extrapolated values are obtained from $L = 8 \sim 18$ for $a \leq 0.3$ and from $L = 8 \sim 20$ at $a = 0.35$. The solid line represents the results of closed-form approximations.

tion gives $x_1 = 0.007\,33\ldots$ in better agreement with the extrapolated value 0.007 33(6).

The value of $y_h = 1$ may imply $\gamma = (2y_h - d)/y_t = 0$ and the logarithmic divergence of the magnetic susceptibility along the critical line. It is known that the leading contribution to the susceptibility of the square-lattice Ising antiferromagnet in a weak uniform magnetic field near the critical temperature $T_c = 2J/k_B \ln a_c = 2J/k_B \ln(\sqrt{2} - 1)$, and $H = 0$ is given by [16]

$$\chi = C_1 H^2 \ln(1/|t|) + C_2 t \ln(1/|t|), \tag{10}$$

where C_1 and C_2 are constants and $t = (T - T_c)/T_c$. The results obtained by the AF Yang-Lee zeros suggest that the logarithmic divergence of the susceptibility of the AF Ising model can occur even in a strong uniform magnetic field $\pm H_c(a)$ well below the critical temperature a_c. It is also possible that the value of $\gamma = 0$ results from the nonsingular part of the free energy where the hyperscaling relation $\gamma = (2y_h - d)/y_t$ is not applicable and $y_h = 1$ could be accidental.

The methods presented in this Letter can be applied to the studies of the Yang-Lee zeros and the phase transitions of the AF Ising model on triangular and hexagonal lattices and of the AF Q-state Potts models with $Q \neq 2$.

This work was supported by Grant No. R01-2003-000-11595-0 from the Basic Research Program of the Korea Science & Engineering Foundation.

---

*Electronic address: sykim@kias.re.kr

[1] C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404 (1952); T. D. Lee and C. N. Yang, *ibid.* **87**, 410 (1952).
[2] C. Binek, *Ising-Type Antiferromagnets* (Springer, Berlin, 2003), and references therein.
[3] C. N. Yang, *Special Problems of Statistical Mechanics* (University of Washington, Seattle, 1952).
[4] S. Katsura, Phys. Rev. **127**, 1508 (1962);Adv. Phys. **12**, 391 (1963); D. B. Abraham and J. De Coninck, Commun. Math. Phys. **108**, 13 (1987).
[5] M. Suzuki, C. Kawabata, S. Ono, Y. Karaki, and M. Ikeda, J. Phys. Soc. Jpn. **29**, 837 (1970).
[6] E. H. Lieb and D. Ruelle, J. Math. Phys. (N.Y.) **13**, 781 (1972).
[7] B. Stošić, S. Milošević, and H. E. Stanley, Phys. Rev. B **41**, 11466 (1990); G. Bhanot, M. Creutz, and J. Lacki, Phys. Rev. Lett. **69**, 1841 (1992); R. J. Creswick, Phys. Rev. E **52**, 5735 (1995); R. J. Creswick and S.-Y. Kim, *ibid.* **56**, 2418 (1997); S.-Y. Kim, Nucl. Phys. B **637**, 409 (2002), and references therein.
[8] S.-Y. Kim and R. J. Creswick, Phys. Rev. Lett. **81**, 2000 (1998).
[9] G. Bhanot, J. Stat. Phys. **60**, 55 (1990).
[10] The memory requirement during μTM calculation is $2 \times 4 \times (N_s/2 + 1) \times (N_b + 1) \times P_m \times 2^L$ byte for the Ising model, where P_m is the maximum size for storing very long integer numbers. For $L = 14$ and cylindrical boundary condition, the memory requirement is already 3.44×10^{10} byte. Here, cylindrical boundary condition means the boundary condition that is periodic in the horizontal direction and free in the vertical direction.
[11] When we use double precision, the memory requirement during RCTM calculation is $2 \times 8 \times (N_s/2 + 1) \times 2^L$ byte for the Ising model. It is 6.84×10^8 byte for $L = 18$ and 3.37×10^9 byte for $L = 20$.
[12] For $L = 12$, the exact value of x_1 obtained from $\Omega(E, M)$ is $0.005\,432\,772\,596\,453\,68\ldots + 0.005\,603\,803\,864\,606\,91\ldots i$ whereas the approximate value obtained from $\omega(M)$ is $0.005\,432\,772\,596\,453\,57 + 0.005\,603\,803\,864\,606\,88i$. For $L = 14$, the exact value is $0.006\,024\,462\,054\,678\,59\ldots + 0.004\,911\,490\,297\,167\,50\ldots i$ whereas the approximate value is $0.006\,024\,462\,054\,678\,79 + 0.004\,911\,490\,297\,167\,52i$. Their differences are so small that the values of x_1 obtained from $\omega(M)$ for $L > 14$ are good approximations.
[13] M. Henkel and G. Schütz, J. Phys. A **21**, 2617 (1988).
[14] X. N. Wu and F. Y. Wu, Phys. Lett. A **144**, 123 (1990); X.-Z. Wang and J. S. Kim, Phys. Rev. Lett. **78**, 413 (1997); J. L. Monroe, Phys. Rev. E **64**, 016126 (2001), and references therein.
[15] C. Itzykson, R. B. Pearson, and J. B. Zuber, Nucl. Phys. B **220**, 415 (1983).
[16] M. E. Fisher, Proc. R. Soc. London A **254**, 66 (1960); *ibid.* **256**, 502 (1960); M. Kaufman, Phys. Rev. B **36**, 3697 (1987), and references therein.