Fisher zeros of the Ising antiferromagnet in an arbitrary nonzero magnetic field

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From the exact partition functions of the Ising model on $L\times L$ square lattices (up to $L=14$) in an arbitrary nonzero external magnetic field H, the precise distributions of the Fisher zeros in the complex temperature ($a=e^{2\beta J}$) plane are obtained. Our results indicate that in the limit $L\to\infty$ the Fisher zeros for $H\neq 0$ do cut the positive real axis at the antiferromagnetic critical point $a_c(H)$; these values are compared with the results of closed-form approximations for the antiferromagnetic critical line. From the Fisher zeros the thermal scaling exponent $y_t=1$ is also obtained along the critical line, indicating the logarithmic singularity of the specific heat for the antiferromagnetic Ising model even in a strong uniform magnetic field.

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I. INTRODUCTION

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

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

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 insight into the problem of the ferromagnetic (FM) Ising model in an arbitrary nonzero external magnetic field at arbitrary temperature by introducing the concept of the zeros of the partition function in the *complex magnetic-field* plane (Yang-Lee zeros).

The partition function zeros in the *complex temperature* plane (Fisher zeros) are also important in understanding the FM and antiferromagnetic (AF) phase transitions [2]. Fisher conjectured [2] that the Fisher zeros in the complex $a=e^{2\beta J}$ plane of the square lattice Ising model for $H=0$ lie on two circles (the FM circle $a_{\mathrm{FM}}=1+\sqrt{2}e^{i\theta}$ and the AF circle $a_{\mathrm{AF}}=-1+\sqrt{2}e^{i\theta}$). Fisher also showed that the logarithmically infinite specific heat singularity of the Ising model for $H=0$ results from the properties of the Fisher zeros. Later, it was concluded that for very special boundary conditions the Fisher zeros of the Ising model for $H=0$ do indeed lie on two circles, while for more general boundary conditions the zeros approach two circles as the size of the lattices increases [3].

It is well known that the FM critical point disappears in the complex a plane for $H\neq 0$ [4]. Matveev and Shrock [5] studied the Fisher zeros of the two-dimensional Ising model for $H\neq 0$ using the high-field, low-temperature series expansion and the partition function on 7×8 square lattice with helical boundary conditions. They found that the density of the Fisher zeros for $H\neq 0$ diverges at a nonphysical critical point, the Fisher edge singularity [5–7], which appears instead of the physical FM critical point ($H=0$). On the other hand, it is generally believed that the physical AF critical point exists in the complex a plane even for $H\neq 0$, that is, the Fisher zeros for $H\neq 0$ cut the positive real axis at the AF critical point. However, the existence of the AF critical point in the complex a plane has never been shown. In this paper we study the AF critical point of the Ising model for $H\neq 0$ using the Fisher zeros evaluated from the exact partition functions on $L\times L$ square lattices up to $L=14$.

II. NUMBER OF STATES

If we define the number of states $\Omega(E,M)$ with a given energy $E=\frac{1}{2}\Sigma_{\langle i,j\rangle}(\sigma_i\sigma_j+1)$ and a given magnetization $M=\frac{1}{2}\Sigma_i(1-\sigma_i)$, where E and M are positive integers $0\leqslant E\leqslant N_b$ and $0\leqslant M\leqslant N_s$, the partition function of the Ising model $Z=\Sigma_{\{\sigma_n\}}e^{-\beta\mathcal{H}}$, a sum over 2^{N_s} possible spin configurations, can be written as

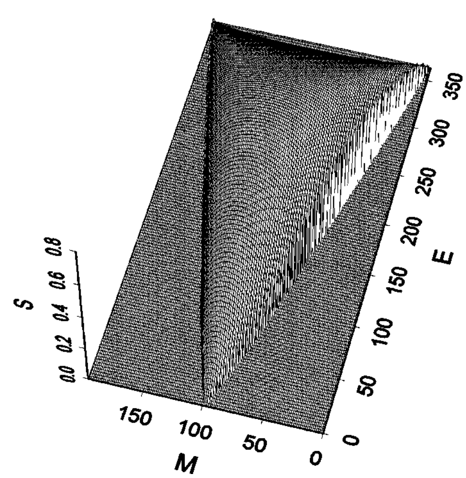

FIG. 1. The entropy $S(E,M)=[\ln\Omega(E,M)]/196$ for the 14×14 Ising model with free boundary conditions.

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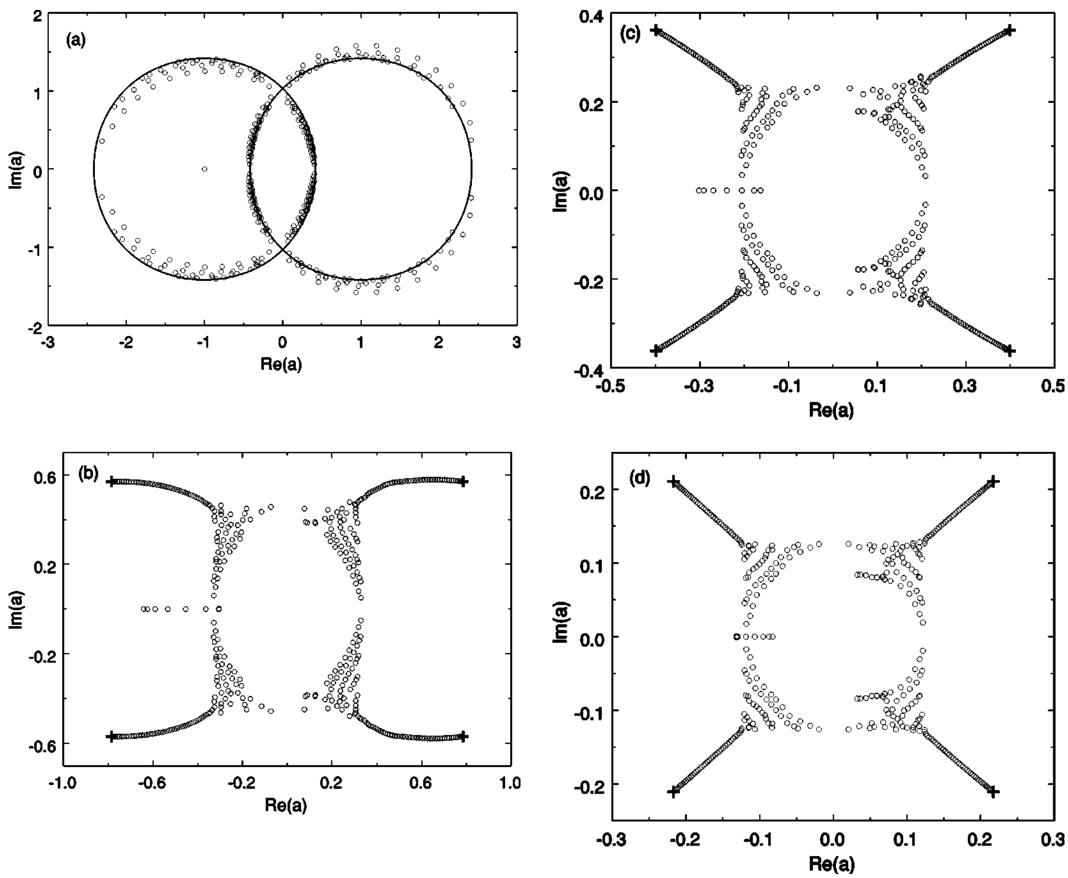

FIG. 2. Fisher zeros in the complex a plane of the 14×14 Ising model with cylindrical boundary conditions for x= (a) 1, (b) 0.1, (c) 0.01, and (d) 0.001. In (a) the two circles are the locus of the Fisher zeros for $x=1$ in the thermodynamic limit. In (b), (c), and (d) the plus symbols show the locations of the Fisher edge singularities a_e estimated from the series analysis.

$$Z(a,x)=\sum_{E=0}^{N_b}\sum_{M=0}^{N_s}\Omega(E,M)a^E x^M, \qquad (2)$$

where $a=e^{2\beta J}$ and $x=e^{-2\beta H}$. For AF interaction $J<0$ the physical interval is $0\leqslant a\leqslant 1$ $(0\leqslant T\leqslant\infty)$, while for FM interaction $J>0$ it is $1\leqslant a\leqslant\infty$ $(\infty\geqslant T\geqslant 0)$.

The microcanonical transfer matrix [6–10] is used to evaluate the *exact* integer values for the number of states $\Omega(E,M)$ of the Ising model on $L\times L$ square lattices with cylindrical and free boundary conditions. Figure 1 shows the entropy $S(E,M)=[\ln\Omega(E,M)]/L^2$ for the 14×14 Ising model with free boundary conditions. The distribution of the entropy is symmetric about $M=98$. There are two AF (FM) ground states with $E=0$ (364) and $M=98$ (0 or 196). The largest number of states is

$$\Omega(181,98)=240\,973\,360\,217\,665\,607\,148\,486\,961\,057\,273\,755\,484\,504\,818\,452\,029\,959\,168, \qquad (3)$$

which is approximately 2.4097×10^{56} and corresponds to $S=0.662\,369$. The distributions of entropy $S(E,M)$ for cylindrical boundary conditions are almost identical to those for

TABLE I. The real and imaginary parts of the first zero $a_1(L)$ at $x=0.01$ for the AF Ising model with cylindrical and free boundary conditions. $y_t(L)$ is the scaling exponent calculated by Eq. (5).

	Cylindrical			Free		
L	$\mathrm{Re}[a_1(L)]$	$\mathrm{Im}[a_1(L)]$	$y_t(L)$	$\mathrm{Re}[a_1(L)]$	$\mathrm{Im}[a_1(L)]$	$y_t(L)$
6	0.195240	0.0772936	1.036353	0.155101	0.0894437	0.901943
8	0.202102	0.0573671	1.019655	0.174446	0.0690021	0.946469
10	0.205402	0.0456928	1.011293	0.184192	0.0558650	0.959265
12	0.207336	0.0379990	1.006665	0.190076	0.0469012	0.965282
14	0.208602	0.0325371		0.194027	0.0404168	

TABLE II. The critical points $a_c(x)$ and the thermal scaling exponents $y_t(x)$, in the limit $L\to\infty$, for the AF Ising model with cylindrical and free boundary conditions, estimated from the Fisher zeros $a_1(L)$ on finite lattices $L=6\sim14$ (even sizes only).

	Cylindrical		Free	
x	$a_c(x)$	$y_t(x)$	$a_c(x)$	$y_t(x)$
0.9	$0.41403(8)+0.00001(7)i$	1.000(8)	$0.4140(3)+0.0000(3)i$	1.003(2)
0.5	$0.40584(7)+0.00001(8)i$	1.000(8)	$0.4058(3)+0.0001(4)i$	1.006(9)
0.1	$0.33770(2)+0.0001(2)i$	1.019(5)	$0.3374(4)+0.000(1)i$	0.993(8)
0.01	$0.2140(2)+0.0000(2)i$	1.010(9)	$0.2133(8)+0.000(4)i$	0.9816(8)
0.001	$0.1240(1)+0.0001(6)i$	0.992(7)	$0.125(1)+0.003(2)i$	0.93(9)
0.0001	$0.0713(3)+0.0000(3)i$	0.99(1)	$0.0710(9)+0.00(2)i$	0.97(1)
0.00001	$0.0402(24)+0.00002(7)i$	0.99(1)	$0.0402(97)+0.000(1)i$	0.98(3)

free boundary conditions. The additional discussions on entropy $S(E,M)$ are given in Ref. [10].

III. FISHER ZEROS IN A MAGNETIC FIELD

The precise distributions of the Fisher zeros of the Ising model for $x\neq1$ are obtained from the exact partition functions on finite lattices. Because the Ising model has the symmetry $x\leftrightarrow 1/x$, with no loss of generality, we consider only Fisher zeros for $x\leqslant1$ ($H\geqslant0$). Figure 2 shows the Fisher zeros in the complex a plane of the 14×14 Ising model for cylindrical boundary conditions. The Fisher zeros for $x=1$ [Fig. 2(a)] lie close to the FM and AF circles, and cut the positive real axis at the FM critical point ($a=1+\sqrt{2}$) and at the AF critical point ($-1+\sqrt{2}$) in the limit $L\to\infty$ [3,9]. As x decreases, the Fisher zeros approach the origin. In the limit $x\to0$ ($H\to\infty$) the partition function of the Ising model becomes $Z(a,0)=\Sigma_E\Omega(E,0)a^E=a^{N_b}$, and all Fisher zeros lie on $a=0$. More discussions on the Fisher zeros of the square-lattice Ising model in a magnetic field are given in Ref. [5].

For $x\neq1$ [Figs. 2(b)–2(d)], the FM critical point disappears but the Fisher edge singularities a_e appear. For small values of x, the Fisher edge singularities and the zeros near them lie close to the lines $\mathrm{Re}(a)/\mathrm{Im}(a)=\pm1$, as shown in Fig. 2(d). Figure 2 also shows accumulation of the Fisher zeros near a_e. The density of zeros near a_e is given by [5–7]

$$g(a)\sim(a-a_e)^{1-\alpha_e}. \tag{4}$$

The high-field, low-temperature series expansion for the square-lattice Ising model [11] has been used to estimate the values of a_e and α_e. The estimated values by Dlog Padé approximants [12] are $\alpha_e=1.19(1)$ ($x=0.1$), 1.20(5) ($x=0.01$), 1.19(12) ($x=0.001$), 1.17(16) ($x=0.0001$), and 1.17(18) ($x=0.000\,01$). They are in good agreement with the values for $x>0.1$, reported in [5]. The value of α_e may be independent of x [5–7], and a conjectured value is $\alpha_e=\frac{7}{6}$ [7].

As shown in Fig. 2, some Fisher zeros lie close to the positive real axis between 0 and $-1+\sqrt{2}$ for $H\neq0$. The zero closest to the positive real axis is called the first zero $a_1(L)$. Itzykson *et al.* [4] showed that the imaginary part $\mathrm{Im}[a_1(L)]$ of the first zero vanishes in the limit $L\to\infty$, following the finite-size scaling $\mathrm{Im}[a_1(L)]\sim L^{-y_t}$. From this scaling law we obtain the thermal scaling exponent

$$y_t(L)=-\frac{\ln\{\mathrm{Im}[a_1(L+2)]/\mathrm{Im}[a_1(L)]\}}{\ln[(L+2)/L]} \tag{5}$$

for finite lattices. Table I shows the values of the first zero $a_1(L)$ and the scaling exponent $y_t(L)$ of the AF Ising model for $x=0.01$. By using the Bulirsch-Stoer (BST) algorithm [13], we extrapolated our results for finite lattices to infinite size. Table II shows the BST estimations with $w=1$ (the parameter of the BST algorithm) of the AF critical points $a_c(x)$

TABLE III. The results of the Wu-Wu approximation [14] and the Wang-Kim approximation [15] for the AF critical line $a_c(x)$.

x	Wu-Wu	Wang-Kim
0.9	0.41401	0.41402
0.5	0.40581	0.40578
0.1	0.33768	0.33802
0.01	0.21440	0.21625
0.001	0.12516	0.12677
0.0001	0.07125	0.07215
0.00001	0.04022	0.04068

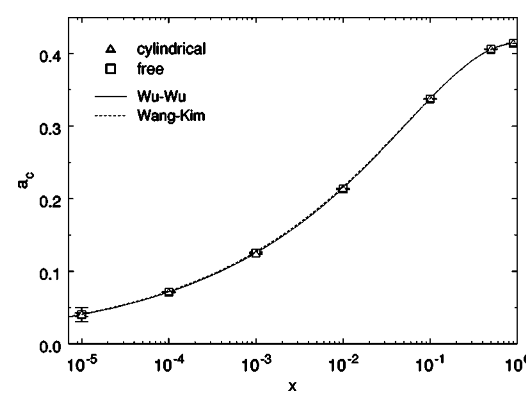

FIG. 3. The critical points $a_c(x)$ for the AF Ising model with cylindrical (triangles) and free (squares) boundary conditions, obtained from the Fisher zeros. The solid and dashed lines represent the results of the Wu-Wu and Wang-Kim approximations, respectively. These approximations are not clearly distinguishable within the figure.

and the thermal scaling exponents $y_t(x)$ for different values of x. The values of the imaginary parts in Table II are estimated from the Fisher zeros in the *complex* temperature plane for finite lattices that have the imaginary parts (for example, Table I). The extrapolated results indicate that the Fisher zeros for $x \neq 1$ do cut the positive real axis at the AF critical points $a_c(x)$.

We do not know the *exact* expression of the critical line, as a function of the external magnetic field, of the square-lattice Ising antiferromagnet. Instead, we have the different *approximations* [14,15] to the antiferromagnetic critical line in a magnetic field. Table III shows the results of the Wu-Wu approximation [14] and the Wang-Kim approximation [15] for the AF critical line $a_c(x)$. Usually, the results of Wu-Wu approximation are closer to those estimated from the Fisher zeros. Figure 3 shows the critical points $a_c(x)$ obtained from the Fisher zeros and the results of the closed-form approximations.

The results for the thermal exponent $y_t(x)$ (Table II) imply $y_t(x)=1$ and $\alpha=2-d/y_t=0$ (the critical exponent related to the specific heat). Because the Fisher zeros in the complex *temperature* plane cut the positive real axis in the thermodynamic limit, $\alpha=0$ means the logarithmic singularity of the specific heat. The logarithmic singularity of the specific heat for $H\neq 0$ has been reported in the study of a two-dimensional superexchange antiferromagnet [16] whose exact solution is known, because this simple model is transformed into the Onsager solution of the square-lattice Ising model in the *absence* of a magnetic field. However, it is not clear whether this kind of behavior results from the special character of the superexchange model, or whether it is a general property that is also present in the AF Ising model and other AF models. Our results clearly show that the specific heat of the AF Ising model retains the logarithmic singularity even in a strong uniform magnetic field.

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