

Phase diagram and critical exponent ν for the nearest-neighbor and next-nearest-neighbor interaction Ising model

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We obtain an approximation of the phase diagram of an Ising model with both nearest-neighbor and next-nearest-neighbor interactions on the square lattice. We use the Fisher zeros of the partition functions of a sequence of finite-sized systems along with various extrapolation methods to obtain phase transition points. In addition, we obtain an approximate value of the correlation length critical exponent ν . Our results are compared to previous results for this system using a wide variety of other approaches.

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I. INTRODUCTION

It has been over 60 years since the publication of Onsager's celebrated solution [1] of the Ising model on a square lattice with nearest-neighbor (NN) interactions. Since that time, there have been very few other systems for which exact solutions have been found, even in the case where these other systems are only slight alterations of the original system such as the addition of next-nearest-neighbor (NNN) interactions. Naturally without an exact solution methods of approximating the solution become of major importance and such is the case with the Ising model on the square lattice with NN and NNN interactions. One of the earliest methods used to approximate this system was that of high-temperature series expansions by Dalton and Wood [2]. These series were greatly expanded by later calculations of Oitmaa [3] and Oitmaa and Velgakis [4]. Besides this approach the interface method of Muller-Hartmann and Zittartz has been applied to this model by Burkhardt [5]. Early renormalization calculations by Nauenberg and Nienhuis [6] and Nightingale [7] looked at this model and were followed by the related Monte Carlo renormalization group approach [8]. Nightingale and Blote [9] used finite-size scaling of transfer-matrix results to obtain the most accurate results obtained thus far but for only two points on the phase diagram. Also extensive efforts were applied to this model using standard Monte Carlo methods by Landau [10], Binder and Landau [11,12], and especially Blote, Compagner, and Hoogland [13] whose computations of the transition temperature for various points on the phase diagram were found using runs of as long as 352 h using the Delft Ising System Processor. Berker and Hui [14] have looked at an even more general model that includes the possibility of anisotropic NN and NNN interactions. They obtain some closed-form expressions for phase boundaries using various piecemeal exact information and scaling behavior. More recently the coherent anomaly method of Suzuki has been used to approximate portions of the phase diagram by Minami and Suzuki [15]. Interest continues to exist in determining the specifics of the phase diagram of this model as evidenced by two very recent publications, one containing a closed-form expression for the

critical line of a portion of the phase diagram found by the interface method [16] and the second using a new entropic Monte Carlo scheme [17].

We investigate this model using a method not previously applied to it. Specifically we look at the Fisher zeros of the partition function—i.e., zeros in the complex temperature plane or some related plane—for a sequence of finite-size systems. We will then use various extrapolation techniques to approximate not only the phase diagram for the infinite systems but also the critical exponent of the correlation length, ν . Critical exponents are of special interest because they have been shown to take on nonuniversal values dependent on the ratio of the NN and NNN interactions over a region of the phase diagram. A similar procedure using Lee-Yang zeros [18] has recently been done by one of the present authors [19] to obtain an approximate phase diagram in the magnetic field for the antiferromagnetic, NN, Ising model on the square lattice.

Our basic notation and general methods of approach will be presented in the following section. Section III contains our results, for both the phase diagram and the value of the critical exponents, and in Sec. IV we present some concluding remarks.

II. BASIC METHOD

The Hamiltonian of the model we want to look at is given by

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

where the first sum is over all NN pairs, the second sum is over all NNN pairs, and σ_i is the spin variable on the i th site and can take on values of ± 1 . There are no restrictions on the values of J and J' . The sites are located on a square lattice. The partition function is the standard

$$Z_N = \sum e^{-\beta \mathcal{H}}, \quad (2)$$

where N is the total number of sites and the sum is over all 2^N configurations. The partition function can be written as a

polynomial in b and b' with each defined, respectively, as $e^{\beta J}$ and $e^{\beta J'}$. We will want to express the partition function as a polynomial in only one variable b or b' . We will look only at cases where J and J' are related to each other so that R is a simple fraction or integer where $R \equiv J'/J$ or we will look at cases where either b or b' is given a set value. If R is an integer, then we can write the partition function as a polynomial in b , while if it is a simple fraction, then the partition can be written in terms of b' .

As stated in the Introduction we want to use the Fisher zeros of the partition function. To obtain the partition function we use the same basic procedure as originally presented in [20]: see also the earlier works by Binder [21] and Bhanot [22]. Systems of size n sites by $2n$ sites will be used. Periodic boundary conditions will be present in the longitudinal direction, the direction of the $2n$ sites. It is best to use systems of this size rather than what might appear to be the more natural system sizes of n sites by n sites. This is because there is no restriction on the sign of the interactions J and J' —in fact, much of the interest will be for $J' < 0$ —and so antiferromagnetic interactions are a possibility. In that case periodic boundary conditions in a direction with n odd causes frustration and this is reflected in the location of the zeros. This frustration is not part of the infinite system which we are trying to approximate and hence its presence in our finite systems would cause a loss of accuracy in the approximation.

Ideally the zeros of the partition function in the complex temperature plane would fall on a very simple curve such as a circle and all zeros would lie on this circle independent of the size of the system. Then the location of the point where the circle crosses the positive real temperature axis would give a critical temperature. However, as is generally the case the location of the zeros is more complex and in particular the location does depend on system size. In such a case one investigates the location of the leading zero or zeros—i.e., the zero or zeros (the locus of zeros may cross the positive real axis in more than one location and thus there is more than one leading zero) closest to the real positive axis. We will denote such zeros as either $b_{0,n}$ or $b'_{0,n}$ depending on the appropriate variable of the partition function. The behavior of the real part of this leading zero is given by finite-size scaling to be

$$\text{Re}(b_{0,n}) = b_c + an^{-1/\nu}(1 + c_1 n^{-\omega} + c_2 n^{-2\omega} + \dots) \quad (3)$$

and similarly for the imaginary part

$$\text{Im}(b_{0,n}) = dn^{-1/\nu}(1 + e_1 n^{-\omega} + e_2 n^{-2\omega} + \dots), \quad (4)$$

where ω is the correction to scaling exponent, a , d , $\{c_i\}$, and $\{e_i\}$ are constants, ν is the correlation length critical exponent, and finally we have used the symbol b for the variable in which the partition function is given but depending on the value of R it could be b' .

We will primarily be interested in determining b_c and ν in the two above equations. To do so we will use the leading zeros from a sequence of finite-sized systems, determining the value of $b_{0,n}$ or $b'_{0,n}$ for each size system, and then use various extrapolation methods or fitting schemes to deter-

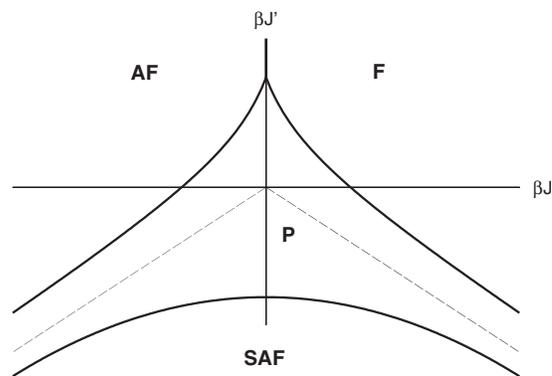


FIG. 1. Phase diagram in the βJ - $\beta J'$ plane with regions having the ferromagnetic (F), paramagnetic (P), antiferromagnetic (AF), and superantiferromagnetic (SAF) phases indicated.

mine these two values. The extrapolation scheme we will use is originally due to Bulirsch and Stoer [23] (BST), used initially in extrapolations in statistical mechanics by Henkel and Patkos [24]. The details of the extrapolation procedure and its major characteristics as they pertain to statistical mechanics are given in [25].

III. RESULTS

The general structure of the phase diagram for the model under study can easily be obtained by doing a ground state analysis. One finds there are four phases: a paramagnetic phase, a ferromagnetic phase, an antiferromagnetic phase, and a superantiferromagnetic phase. The later consists of alternating rows or columns of up and down spins. Besides the basic structure one has easily that if $J' = 0$, then the system is just that solved by Onsager and the critical temperature is known. If $J = 0$, then the system decouples into two independent nearest-neighbor models and hence again the critical temperature is known. The basic phase diagram is shown in Fig. 1. There have been various alternative phase diagrams proposed over the years (see Ref. [13] for a discussion of one alternative), but this is the commonly accepted phase diagram at the present and the one supported by our results using Fisher zeros.

We begin with an analysis for the case of $J = J' > 0$. By the symmetry of the phase diagram (see Fig. 1), one also has results for $-J = J' > 0$. Setting $b = b'$ we obtained the Fisher zeros for systems of size $n \times 2n$ sites with periodic boundary conditions along the $2n$ dimension where $n = 3, 4, \dots, 10$. These zeros are shown in the complex- b plane in Fig. 2 for the case of $n = 10$. One sees the zeros tending to cross the real b axis at two locations one with $b > 1$ and the other with $b < 1$. Requiring $J = J' > 0$ we are first interested in the location where the zeros cross with $b > 1$. Taking the real part of the leading zeros for the eight cases $n = 3, 4, \dots, 10$ and using the BST extrapolation method for this eight-element sequence we obtain a value for b_c of 1.209 480(5) where the number in parentheses is an estimate of the error in the last digit presented. Nightingale and Blote [9] obtain a value for b_c of 1.209 482 619 1(3) where again the number in paren-

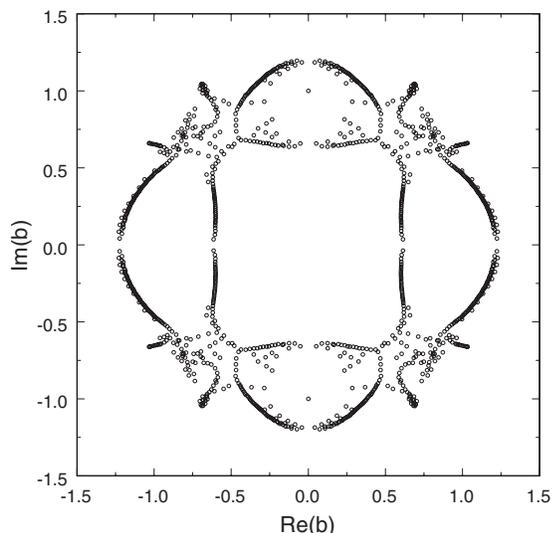


FIG. 2. Fisher zeros for the 10×20 site system with $R=1$.

theses is an estimate of the error in the last digit. Our results agree with those of [9] although clearly not to the same level of accuracy. For completeness we mention that Nightingale and Blote [26] using less extensive calculations had an earlier result of 1.209 482 63(6). Unfortunately it is somewhat difficult to accurately compare the results based on other methods for this case as all other results have been presented graphically and with an accuracy well below the accuracy of the above two results.

It needs to be mentioned that in the use of the BST extrapolation method there is a free parameter whose value is best chosen as $1/\nu$. Here we are finding the transition temperature for the paramagnetic-ferromagnetic phase transition and in this case $\nu=1$, so the choice is a simple one. Also in the use of the BST method the determination of the error in the estimate can be of concern. For all our critical temperature estimates we use error estimates given by Eq. (6) in Ref. [25] where it was shown that this method of estimating errors is generally a very conservative one. That this is the case in the present situation is born out by the fact that using the BST method on the imaginary parts of the leading zeros, where one knows the imaginary part goes to zero for the infinite system, results in $7.1 \times 10^{-7} \pm 1.0 \times 10^{-5}$, clearly covering the known value of zero.

The location of the zeros shown in Fig. 2 indicates one advantage of the Fisher-zeros approach compared to other past methods. With this approach one obtains two transition points, not just one, due to the fact, already mentioned, that the zeros tend to cross the real axis at two locations. Hence the same partition function calculations give not only results for the case of $J=J' > 0$ (and trivially by symmetry $-J=J' > 0$), but they also lead to results for the case of $J=-J' > 0$ —i.e., $R=-1$ (and again trivially based on the symmetry of the phase diagram for $-J=-J' > 0$). Now in this case one is looking at the paramagnetic-superantiferromagnetic transition. As stated in the Introduction one of the reasons for the consistent interest in this model is that for this transition indications based on several methods are that the critical exponents are nonuniversal. As

stated above in order to properly use the BST extrapolation procedure to obtain a critical temperature estimate one needs the value of the critical exponent ν . Hence we begin by determining an approximate value for ν . Using Eq. (4) one can produce a sequence of estimates of ν by considering two different-sized systems and disregarding the correction to scaling terms. Doing so one has

$$\nu(n) = \frac{\ln[(n+1)/n]}{\ln[\text{Im}(b_{0,n+1})/\text{Im}(b_{0,n})]}. \quad (5)$$

Knowing the appropriate dominant zero values for eight different-sized systems as we do, one can generate a sequence of seven increasingly accurate estimates of ν as larger systems are considered. Furthermore, it is logical to assume that this sequence itself can be extrapolated using the BST approach. Doing so, for the $R=-1$ case, results in $\nu = 0.8481(2)$, clearly indicating the nonuniversal behavior found by others for this transition. As a check on the accuracy of this approach one can go back to the dominant zeros involved in the paramagnetic-ferromagnetic transition and obtain a value for ν . Doing so one obtains $\nu=1.001(1)$ which is obviously close to the exact known value of 1. In this case unlike the case of the scaling behavior of the zeros which has been rigorously established by Itzykson, Pearson, and Zuber [27] one assumes a behavior along the lines of Eq. (3) and (4). In doing so it is not known what the appropriate analog to $1/\nu$ is and also, since the original estimates of ν used in the BST extrapolation method are the result of using Eq. (5) which involves two system sizes, it is not certain what value of n should be used. We have therefore increased by a factor of 2 the error bounds to be on the conservative side. Our results match the recently obtained results of Malakis, Kalozoumis, and Tyraskis [17] who obtained $\nu=0.833(30)$. Other accurate comparisons with previous results are again somewhat difficult due to previous presentations being graphical. From Fig. 2 of [8] one has $\nu=0.870(15)$ which is slightly above our estimates.

Having obtained a value for ν we now can estimate the critical temperature. Using the leading zeros from the same eight partition functions but in the $b < 1$ region we obtain $b_c=0.618\,85(7)$. Berker and Hui [14] give a very simple closed-form expression for the phase boundary between the paramagnetic and superantiferromagnetic transitions. They consider the case of anisotropic NNN interactions but we have specialized the equation to the case we are considering: that of isotropic interactions. Their equation is

$$|\sinh[2\beta J']| = \cosh[\beta J]. \quad (6)$$

Solving for the case of $J=-J' > 0$ one obtains $b_c = 0.618\,034\dots$, lying slightly outside our results. For low J/J' Monte Carlo renormalization group calculations [8] have given the expression

$$\beta_c J' = -0.440687 - C_2(J/J')^2 - C_4(J/J')^4, \quad (7)$$

with $C_2=0.0312 \pm 0.000\,10$ and $C_4=0.0084 \pm 0.0010$. For the present case, which technically is beyond the region of low J/J' , one obtains $b_c=0.6186(12)$ which gives an interval for b_c that overlaps our own estimates. Using a coherent

TABLE I. Critical temperature estimates via b'_c along with estimates of ν using the Fisher zeros. Comparisons with estimates using other methods of approximation are also given as the appropriate reference.

	$R=2$	$R=1/2$	$R=1/4$	$R=-1/4$	$R=-2$
Our results for b'_c	1.282493(4)	1.140432(2)	1.0206924(1)	0.840045(10)	0.6381(7)
Comparison of results		1.140428 [3]		0.84004049(4) [9]	
Our results for ν					0.938(1) [13]
Comparison of results					0.975(15) [8]

anomaly approach Minami and Suzuki [15] obtain $b_c = 0.61784$. The most accurate previously obtained results for $R=-1$ are the recent results of Malakis, Kalozoumis, and Tyraskis [17] who focusing only on this case and using a new entropic Monte Carlo scheme to generate estimates of T_c obtain $b_c = 0.61863(24)$, clearly agreeing with our own results. Finally for completeness it should be noted that our extrapolation of the imaginary part of the dominant zeros for this case gives 0.000024 ± 0.000026 using $\nu = 0.848$.

Results for $R=2, 1/2, 1/4, -1/4$, and -2 are given in Table I.

Besides setting the value of R in one very thorough and extensive investigation of this system by Blote, Compagner, and Hoogland [13] the value of b was set and then the value of b' at which the paramagnetic-ferromagnetic phase transition occurs was determined. In that work very long runs using Monte Carlo simulations on the Delft Ising System Processor (DISP), a special purpose computer for the simulation of Ising models, were used along with renormalization group methods to obtain accurate values of the phase transition point for the paramagnetic to ferromagnetic transition. We can set the value of b and then investigate the behavior of the Fisher zeros of the partition function as a function of b' . We do this for two cases $b=e$ and $b=e^2$. When the value of b is set we can go to systems one step larger than for our above results, leaving b and b' as variables; i.e., we can go to $n=11$.

For the case of $b=e$ taking the real part of the leading zeros for the eight cases, $n=4, 5, \dots, 11$, and using the BST extrapolation method for this eight-element sequence we obtain a value for $K'_c = \ln b'_c = \beta J'$ of $-0.3675(4)$. This matches the result from [13] where K'_c was found to be equal to $-0.3674(5)$. Going to the case where $b=e^2$ we obtain $K'_c = -0.9450(46)$ using a sequence of seven data points from $n=5, 6, \dots, 11$. This is to be compared to the results of [13] for this case which are $K'_c = -0.9482(8)$. We have found that as the value at which b is set increases the smaller-sized systems behave in an increasingly spurious manner due to their small size. Hence in the $b=e$ case we have not used the $n=3$ results and in the $b=e^2$ case we have not used the $n=3$ and 4 results.

The results for $b=e$ and $b=e^2$ given in the previous paragraph are for the paramagnetic-ferromagnetic transition

which is the only transition type for which numerical results are given in [13]. However, we also obtain results for the paramagnetic-superantiferromagnetic transition. For this transition the effect of the size of the system is even more apparent than what is seen for the material presented in the previous paragraph. Specifically for the case of $b=e^2$ the real parts of the leading zeros for the cases of $n=3-8$ increase but from $n=8$ on they decrease. Because of this, our results are much less accurate than what was found for the various values of R studied. For $b=e^2$ we obtain $K'_c = -1.033(6)$ using a four-data-point sequence with $n=8, 9, 10$, and 11 and for $b=e$ we have $K'_c = -0.6085(5)$ using a six-data-point sequence with $n=6, \dots, 11$.

IV. CONCLUSIONS

In the above we have shown that one can obtain accurate estimates of not only phase transition points in the overall phase diagram but also values for the critical exponent ν using the Fisher zeros of a sequence of finite-sized systems. Our estimates in many cases are as accurate or more accurate than previous estimates, the main exception being the results for the case of $R=1$ of Nightingale and Blote [9], which are significantly more accurate.

One of the advantages of the method presented here is that the method has embedded in it not only information about a single phase transition but rather two phase transitions, possibly two paramagnetic-ferromagnetic transitions or a paramagnetic-ferromagnetic transition and a paramagnetic-superantiferromagnetic transition depending on the value of R . As with any approximation method the value is generally dependent on not only the accuracy but the amount of work and often the computer resources necessary to obtain the results. Therefore it should be mentioned that all calculations of the partition function, which timewise is the dominate part of the calculations, were done on a personal computer and for the largest system size investigated—i.e., the (10×20) -site system—took 88 h for $R=1$ while for $R=2$ it took 148 h. Computer runs on the DISP ran for 47 h for the $b=e$ case to 352 h for the $b=e^2$ case [13].

Overall we believe we have shown that it is worth investigating the Fisher zeros, as one approach, if one wants to get reasonably accurate approximations of phase transition values for complex systems.

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