Systematic approximation method for the critical properties of lattice spin systems

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We present an extension of past approximations such as the Bethe approximation where we look at generalized Husimi trees. In doing so we obtain a sequence of ever more accurate approximations. The sequence is very systematic, and sequences of as few as three points can be extrapolated to give critical temperature estimates to within 0.1% or better of the exact value for our test cases. In the case of the square lattice, Ising ferromagnet, where five levels of approximation are obtained, estimates within 0.003% are obtained. Critical exponents can also be approximated but with much less accuracy. Much of our attention is devoted to the critical line of the phase diagram of the antiferromagnetic Ising model on the square lattice, where our results compare very favorably with other approximations. The method is general enough to be applicable to any spin lattice system where the spin takes on a discrete set of values.

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I. INTRODUCTION

In recent years we have taken a natural step beyond the Bethe approximation, which we take to mean the approximation based on the behavior of a spin variable at the center of a Cayley tree, to consider Husimi trees. Husimi trees are built up by connecting polygons, e.g., a three-site triangle, rather than the two-site edges as done in the Cayley tree. This was first done by the author [1,2] to study the phase diagrams of Ising model systems with interactions involving more than two sites where clearly the Cayley tree approach could not be applied. In addition this was done to approximate the phase diagram of the antiferromagnetic Ising model on the triangle lattice [3]. This system is the prototypical frustrated system and the Bethe approximation does not even give a qualitatively correct phase diagram much less one with any quantitative accuracy [4]. By building up an Husimi tree composed of three site triangles the frustration arises in a natural way and not only was the qualitatively correct phase diagram obtained but also one with reasonable quantitative accuracy when compared against Monte Carlo approximation or the recently proposed hard-spin, mean-field approximation of Berker [5].

In all the cases studied thus far the connections made in the construction of the tree occur at a single site, either the corners of a square or triangle depending on the system being approximated. Here we go beyond this restriction by making connections at multiple sites. In the manner we more closely approximate the local correlations and naturally get better approximations. More importantly we can develop a very systematic sequence of improving approximations that can then be extrapolated using various methods to obtain estimates of the critical temperature within 0.1% or better of the exact results for our test cases where exact results are known. The sequences are rather brief consisting of only 3 to 5 terms all of which can be obtained using a personal computer. Critical exponents can also be approximated but with less accuracy.

In both the case of the Cayley tree or the Husimi tree approach to determine the behavior of the magnetization of the central sites of the tree one can use a dynamical systems approach [6,7] where a discrete, one dimensional map is found and the phase diagram of the system is determined by the behavior of the fixed points, periodic cycles, etc., associated with the map. We use this approach but by making connections at more than one site we have multidimensional dynamical systems which govern the behavior of the system rather than the one-dimensional maps arising in the study of the previous systems. For completeness one should mention that two site connections are also made in Ref. [8] where a two layer Ising system is studied and connections are therefore made at two sites.

In the following section we present the general method along with some of the extrapolation methods we will use. This is followed by approximating the quintessential test cases two-dimensional, nearest neighbor, ferromagnetic, Ising model systems where exact results for the critical temperature and critical exponents exist. This is followed in Sec. IV by the approximation of the phase diagram of the antiferromagnetic, nearest neighbor, Ising model on the square lattice which has been approximated by a large variety of method over the last 40 years. We compare our results with the most accurate of these previous results. Some concluding remarks appear in the final section.

II. BASIC METHOD

We present the basic method by considering the nearest neighbor, ferromagnetic, Ising model on the square lattice. Five ''levels'' of approximation will be obtained in the following section. Each level of approximation will be based on a tree like structure constructed from basic building blocks. The basic building blocks used in the first three levels are

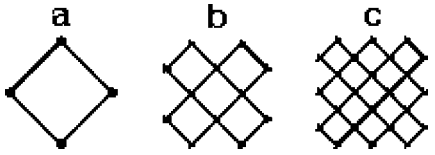

FIG. 1. The basic building blocks for the first three levels of the approximation of the square lattice system.

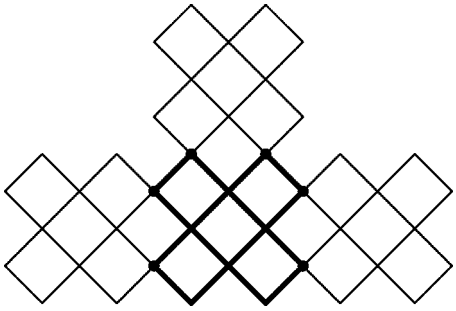

FIG. 2. The first generation branch for the second level approximation of the square lattice system.

shown in Fig. 1. The systematics of these three lowest level building blocks allows one to construct any higher level, basic building block. A single building block will be denoted as a zeroth generation tree, after one series of connections we have a first generation tree, after two series of connections a second generation tree, etc. As an example in Fig. 2 we show the first generation tree of our second level approximation.

On each vertex of a graph representing one of our trees we have a spin variable σ which can take on the values ± 1, with σ_i representing the spin variable on the ith site. Each spin variable interacts with a magnetic field h and each edge of the graph represents a pair interaction J between the spins on the two vertexes connected by the edge. The Hamiltonian of the system is

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

where the first sum is over all edges of the graph and the second sum is over all vertexes.

For any nth generation system the thermal average of the spin variable on the ith site, i.e., the magnetization of the ith site is

$$\langle\sigma_i\rangle_n=\frac{\sum\sigma_i e^{-\beta\mathcal{H}}}{\sum e^{-\beta\mathcal{H}}}=\Lambda_n^{-1}\sum\sigma_i e^{-\beta\mathcal{H}}, \tag{2}$$

where the sums are over all configurations, Λ_n is the standard partition function, and $\beta=1/(k_BT)$, k_B being the Boltzmann constant and T the temperature. We will be interested in the behavior of the thermal averages of spins on sites of the central building block of an nth generation tree when $n\to\infty$, i.e., in the thermodynamic limit. Thermal averages in this limit will be denoted by a pair of brackets without any subscript.

As mentioned in the Introduction one can obtain these thermal averages by a dynamical systems approach. For the Cayley tree case see Ref. [6] or [7] and for the Husimi tree case where connections are made at only one site see Ref. [1] or [2]. In these a one-dimensional dynamical system is all that is necessary to describe the system. For more involved systems such as the fully frustrated, Ising, antiferromagnet on the triangle lattice a higher-dimensional dynamical system is necessary [3] to obtain a qualitatively correct phase diagram. But even for the ferromagnetic pair interaction systems if connections are made at more than one site then a higher-dimensional dynamical system is required. In particular if connections are made at n sites then one has a $(2^n\text{-}1)$-dimensional dynamical system.

One can explicitly see this in our second level approximation where connections are made at two sites when connecting to a new building block. Then we obtain a three-dimensional dynamical system. Here in a general way things are similar to the analysis of Hu, Izmalian, and Oganesyan [8]. Since we are first interested in obtaining an approximation of the critical temperature and since, in this section, we are dealing with a system involving only ferromagnetic pair interactions we know by the Lee-Yang circle theorem [9] that this occurs only when the magnetic field is zero. Therefore we set $h=0$. Using Λ_0 to represent the partition function of the zeroth generation branch we have just the 12 site system shown in Fig. 1(b), and one can write

$$\Lambda_0=\Lambda_0^{++}+\Lambda_0^{+-}+\Lambda_0^{-+}+\Lambda_0^{--}, \tag{3}$$

where $\Lambda_0^{\alpha\gamma}$ is the quarter of the partition function with the spin values of the two base sites denoted by the superscripts α and γ. Since all spins can take on the values ± 1 then $\alpha=\pm 1$ and $\gamma=\pm 1$ and there are four possible configurations as indicated in Eq. (3). We do not write out these expressions because they can be quite lengthy. Λ_0 is made up of the 2^{12} configurations of the 12 site system and even each of the Λ_0^{++}, Λ_0^{+-}, Λ_0^{-+}, and Λ_0^{--} consist of 2^{10} configurations. While the expressions are lengthy it takes very little time for a symbolic manipulation program like MATHEMATICA to obtain such expressions.

We use these separate $\Lambda_0^{\alpha\gamma}$ terms when we construct Λ_1, the partition function of the first generation tree shown in Fig. 2. For example as part of Λ_1 we will have a class of configuration of the first generation tree where the spins on the 12 sites of the central or base building block, to which the zeroth generation trees are going to be attached, are all positive. Then we have as the contribution to Λ_1 due to this specification of the spin values of these 12 sites

$$b^{16}(\Lambda_0^{++})^3, \tag{4}$$

where $b\equiv\exp(\beta J)$. The b^{16} factor is due to the 16 nearest neighbor interactions of the basic building block and each of the three Λ_0^{++} factors is due to the fact that we have connected a zeroth generation branch, with their base sites both equal to $+1$, to the left, top, and right of our basic building block. All 2^{12}-1 other configurations specified by setting the spin values on the 12 sites of the new basic building block can be represented by similar expressions where by similar we mean terms involving b to the appropriate power and products of Λ_0^{++}, Λ_0^{+-}, Λ_0^{-+}, and Λ_0^{--}.

From the above it is clear that Λ_1 or more importantly $\Lambda_1^{\alpha\gamma}$ with again $\alpha=\pm 1$ and $\gamma=\pm 1$ can be written in terms of a polynomial involving b, Λ_0^{++}, Λ_0^{+-}, Λ_0^{-+}, and Λ_0^{--}. Of course when we build our second generation tree by connecting first generation trees to the left, top, and right

side of a new basic building block we will need these expressions for Λ_1^{++}, Λ_1^{+-}, Λ_1^{-+}, and Λ_1^{--} and in fact when we begin the construction of Λ_2, the partition function for the second generation tree, we have similar considerations to those involved with Λ_1 but it is clear we can write Λ_2 in terms of b, Λ_1^{++}, Λ_1^{+-}, Λ_1^{-+}, and Λ_1^{--} and in fact in general Λ_n can be written as a polynomial in terms of b, Λ_{n-1}^{++}, Λ_{n-1}^{+-}, Λ_{n-1}^{-+}, and Λ_{n-1}^{--}. Therefore we can develop a set of recursion relations defining a dynamical system.

For the determination of the properties of the phase transition we need to obtain an expression for the thermal average of a spin in our basic building block to which the $(n-1)$th generation branches have been attached. If we select as the site of interest the left site of the two base sites of the nth generation tree we can write

$$\langle \sigma_\alpha \rangle = \frac{\Lambda_n^{++} + \Lambda_n^{+-} - \Lambda_n^{-+} - \Lambda_n^{--}}{\Lambda_n^{++} + \Lambda_n^{+-} + \Lambda_n^{-+} + \Lambda_n^{--}}. \tag{5}$$

By defining x_n, y_n, and z_n as

$$x_n = \frac{\Lambda_n^{++}}{\Lambda_n^{--}}, \quad y = \frac{\Lambda_n^{+-}}{\Lambda_n^{--}}, \quad z_n = \frac{\Lambda_n^{-+}}{\Lambda_n^{--}} \tag{6}$$

one has

$$\langle \sigma_\alpha \rangle = \frac{x_n + y_n - z_n - 1}{x_n + y_n + z_n + 1} \tag{7}$$

and one has the three-dimensional mappings

$$x_n = f(b, x_{n-1}, y_{n-1}, z_{n-1}), \quad y_n = g(b, x_{n-1}, y_{n-1}, z_{n-1}),$$

$$z_n = j(b, x_{n-1}, y_{n-1}, z_{n-1}), \tag{8}$$

where $n \geqslant 1$. The functions $x_n = f(b, x_{n-1}, y_{n-1}, z_{n-1})$, $y_n = g(b, x_{n-1}, y_{n-1}, z_{n-1})$, and $z_n = j(b, x_{n-1}, y_{n-1}, z_{n-1})$ are rational functions involving in their numerators and denominators the polynomials mentioned in the previous paragraphs when discussing the partition functions. Again while the above rational functions are lengthy to write down here they can be found easily and quickly, at least for the lower level approximations, using a symbolic manipulation program.

Obviously as one increases the level of approximation the number of configurations which must be summed over increases as well as the number of terms needed to be kept track of due to the increase in the number of connecting sites. The fact that there are three rational functions defining the dynamical system whose properties determine the behavior of the second level, generalized Husimi tree approximation of the square lattice comes about because of the four types of connections to be made, ones involving $(+,+)$, $(+,-)$, $(-,+)$, and $(-,-)$ configurations. When going to the next level approximation with the basic building block shown in Fig. 1(c) connections involving three sites are made and then one must consider the 2^3 values the three spins on a set of these three sites can take. This necessitates using a three variable superscript and eight partition function components $\Lambda_n^{\alpha\gamma\delta}$ where $\alpha = \pm 1$, $\gamma = \pm 1$, and $\delta = \pm 1$. In the computation of the order parameter one has an expression similar to Eq. (5) but with eight terms in the numerator and 8 terms in the denominator. Similar to what was done for the second level approximation one can divide each of these by Λ_n^{---} this results in a $(2^3\text{-}1)$- or seven-dimensional map.

One can continue to develop larger and larger basic building blocks with larger numbers of connections resulting in higher-dimensional maps. As a practical matter the time and computer memory necessary for the explicit construction of the maps grows rapidly as the size of the building blocks increases. Using a typical year 2000 personal computer we have been able to consider five levels of approximation for the square lattice system.

From a statistical mechanics perspective we are interested in the infinite generation tree, i.e., in the thermodynamic limit, which means from the dynamical systems perspective we are interested in the fixed points of the dynamical system. Physically what one expects is that for high temperatures the magnetization of the base sites is zero but as the temperature is lowered the magnetization becomes nonzero. This corresponds to a fixed point behavior where at high temperatures there is a single, real valued, fixed point (there may be numerous complex valued fixed points but they have no physical meaning) corresponding to zero magnetization but as the temperature is lowered one reaches a point below which two new attracting fixed points are created and the original fixed point becomes repelling. The two new fixed points correspond to a positive and negative spontaneous magnetization. This is in fact exactly the behavior one finds.

For each level of approximation one needs to determine the temperature at which this changeover occurs. Strictly speaking the critical temperature is the temperature at which the fixed point corresponding to zero magnetization is neither attracting or repelling but neutral. We find the critical temperature in this manner. That is we find the fixed point corresponding to zero magnetization and determine when it is a neutral fixed point. This occurs when the Jacobian of the dynamical system's maximum eigenvalue is 1. Results for the square lattice approximation as well as a hexagonal lattice approximation are given in the next section.

Having a sequence of ever improving approximations of the critical temperature such as the above allows one to use various extrapolation methods to obtain an improved final approximation to the critical temperature. Using a finite size scaling like approach one can write

$$T_c(L) = T_c^* + aL^{-\omega_1} + bL^{-\omega_2} + cL^{-\omega_3} + \cdots, \tag{9}$$

where T_c^* is the critical temperature for the lattice being approximated, $T_c(L)$ is the critical temperature for the Lth level approximation and where $0 < \omega_1 < \omega_2 < \omega_3 < \cdots$. Given the critical temperature for five (three) levels of approximation one can truncate the right hand side to include three (two) terms and get an approximation for T_c^*. Since we have five (three) levels of approximation for the square (hexagonal) lattice we do this in Sec. III where our results for the ferromagnetic case are reported.

Furthermore assuming a relationship such as Eq. (9) various authors have developed extrapolation schemes that can be used to get T_c^*. One of these is that of Vanden Broeck and Schwartz (VBS) [10] introduced into statistical mechanics by Hamer and Barber [11]. The algorithm takes the critical temperature estimates of the various cluster sizes as input and reduces this set of data to a single more accurate value through a series of steps.

Using the notation of Hamer and Barber [11] one has given a sequence of values $T_c(L)$ which converge to a limiting value T_c^* one forms a table of approximants to T_c^* denoted by $[L,N]$ where $[L,0]=T_c(L)$ and the $(N+1)$th column of approximants is generated from the Nth and $(N-1)$th columns via the formula

$$\frac{1}{[L,N+1]-[L,N]}+\frac{\alpha_N}{[L,N-1]-[L,N]} =\frac{1}{[L+1,N]-[L,N]}+\frac{1}{[L-1,N]-[L,N]} \tag{10}$$

with $[L,-1]\equiv\infty$.

The above defines a broad class of transformations based on the definition of α_N. For the case where the sequence converges as in Eq. (9) Barber and Hamer [12] show that a good choice for the value of α_N to be

$$\alpha_N=-\frac{[1-(-1)^N]}{2} \tag{11}$$

for $N=0,1,2,\ldots$. This is what will be used in the following section.

In addition to the VBS extrapolation method we use a method of Bulirsch and Stoer (BST) [13]. Again we start with a sequence of values $T_c(L)$. The algorithm allows one to construct a table of extrapolants much like the VBS method. For $L=1,2,3,4,5$ we have

$$\begin{array}{ccccccccc} T_{c,0}^1 & & & & & & & & \\ & T_{c,1}^1 & & & & & & & \\ T_{c,0}^2 & & T_{c,2}^1 & & & & & & \\ & T_{c,1}^2 & & T_{c,3}^1 & & & & & \\ T_{c,0}^3 & & T_{c,2}^2 & & T_{c,4}^1 & & & & \\ & T_{c,1}^3 & & T_{c,3}^2 & & & & & \\ T_{c,0}^4 & & T_{c,2}^3 & & & & & & \\ & T_{c,1}^4 & & & & & & & \\ T_{c,0}^5 & & & & & & & & \end{array} \tag{12}$$

and the $T_{c,q}^n$ are computed from

$$T_{c,-1}^n=0, \tag{13}$$

$$T_{c,0}^n=T_c(n), \tag{14}$$

$$T_{c,m}^n=T_{c,m-1}^{n+1}+(T_{c,m-1}^{n+1}-T_{c,m-1}^n) \times\left[\left(\frac{n}{n+m}\right)\left(1-\frac{T_{c,m-1}^{n+1}-T_{c,m-1}^n}{T_{c,m-1}^{n+1}-T_{c,m-2}^{n+1}}\right)-1\right]^{-1}, \tag{15}$$

where $m\geqslant 1$ and where ω is a free parameter. Henkel and Patkos [14] were the first to use the algorithm in the area of critical phenomena. Later Henkel and Schutz [15] examined the characteristics of this algorithm in a number of settings. The choice of ω in any particular application can be problematic and this was one of the aspects of the algorithm discussed in Ref. [15]. There it is suggested that one define

$$\epsilon_m^{(i)}=2|T_{c,m}^{i+1}-T_{c,m}^i|, \tag{16}$$

($\epsilon_m^{(i)}$ was defined without the absolute value signs but they are needed to minimize $\epsilon_m^{(i)}$) to get some idea of the reliability of the approximation. Henkel and Schutz [15] also state that in the limit $i\to\infty$ one should expect

$$|T_{c,m}^i-T_c|\leqslant|\epsilon_m^{(i)}|, \tag{17}$$

where T_c is the exact value. Most importantly Henkel and Schutz suggest that ''minimizing $\epsilon_m^{(i)}$ gives an intrinsic criterion for choosing ω'' [16]. However, we find that this procedure cannot be used in most cases, because in most cases including this one, one can find values of ω where $\epsilon_m^{(i)}$ equals zero thereby producing a result with apparently no error. Also in cases where one knows the exact value of the quantity being approximated it is seen these values of ω do not give particularly good results. We will further address the issue of ω when we present our results for the ferromagnetic case in the next section.

As for estimates of the critical exponents since one can numerically find, knowing the fixed point values, the spontaneous magnetization as a function of $(T-T_c)/T_c$ for $T<T_c$ or the magnetization as a function of the magnetic field at $T=T_c$ then one can use the coherent anomaly method (hereafter CAM) of Suzuki [16] to approximate the critical exponents α, β, and δ. Specifically one has for the spontaneous magnetization of the Lth approximation $m_s(L)$

$$m_s(L)=\overline{m}_s(L)|\varepsilon|^{1/2}, \quad \text{where} \quad \epsilon=\frac{T-T_c(L)}{T_c(L)}. \tag{18}$$

The quantity ϵ is to the power 1/2, which is the classical value of the critical exponent β. Quantities similar to $\overline{m}_s(L)$ can be defined for the magnetization at the critical temperature as a function of the magnetic field $m_c(L)$ and for the zero field susceptibility $\chi(L)$. Suzuki [16] defines these as the coherent anomalies and shows these coefficients are related to the nonclassical critical exponents by

$$\overline{m}_s(L)\approx[T_c(L)-T_c^*]^{\beta-1/2}, \quad \overline{\chi}(L)\approx[T_c(L)-T_c^*]^{1-\gamma},$$

$$\overline{m}_c(L)\approx[T_c(L)-T_c^*]\delta^{-\gamma(\delta-3)/[3(\delta-1)]}. \tag{19}$$

TABLE I. Critical temperatures and coherent anomalies for the five levels of approximation of the ferromagnetic system on the square lattice.

Level approximation	T_c	$\overline{m}_s(L)$	$\overline{m}_c(L)$
1	2.770783	2.540892	1.557678
2	2.566925	3.071698	2.024774
3	2.482781	3.464550	2.391354
4	2.436614	3.783494	2.700819
5	2.407311	4.056260	2.973345

To determine $\overline{m}_s(L)$ and $\overline{m}_c(L)$ we numerically determine the magnetization at $h=0$ and $T<T_c(L)$ and then at $h\neq 0$ and $T=T_c(L)$, respectively. For $\overline{\chi}(L)$ we use (see Suzuki [16])

$$\overline{\chi}(L)=\frac{\overline{m}_c(L)^3}{\overline{m}_s(L)^2}. \tag{20}$$

Prior to presenting our results we need to mention a final technical item that concerns the final step in the construction of the tree. Rather than have two base sites that interact with only two nearest neighbor sites we complete our tree in the most symmetric manner possible and consider a central building block where nth generation branches are connected to all four sides of the central building block. For the case on the square lattice approximation this then gives a structure where all sites except the boundary sites have four nearest neighbor interactions. It is in this manner that the magnetizations leading to the coherent anomalies are calculated.

III. RESULTS FOR THE FERROMAGNETIC CASES

In Table I we present the results of our five levels of approximation of the square lattice system. In particular, for each of the five levels of approximation used we have listed the critical temperatures $T_c(L)$ and the coherent anomalies $\overline{m}_s(L)$ and $\overline{m}_c(L)$. There is some choice in determining the $\overline{m}_s(L)$ and $\overline{m}_c(L)$ values. While we complete the construction of our system in the most symmetric manner possible, so that in the completed system all sites except boundary sites have a coordination number of four, nevertheless we do not have translational symmetry and hence the value of $\overline{m}_s(L)$ and $\overline{m}_c(L)$ depend on which site or sites of our basic building block we use in the calculation of the magnetization. In all our basic building blocks there is a central, four site square (see Fig. 1 for the first three levels) and by the symmetry of the system the magnetization of any of these four sites is the same. Since these sites are at the very center of our generalized Husimi tree it is the magnetization of one of these sites which we have used to calculate $\overline{m}_s(L)$ and $\overline{m}_c(L)$.

TABLE II. Critical temperatures and coherent anomalies for the three levels of approximation of the ferromagnetic system on the hexagonal lattice.

Level approximation	T_c	$\overline{m}_s(L)$	$\overline{m}_c(L)$
1	1.728218	3.113132	2.350285
2	1.640906	3.784388	3.088127
3	1.605865	4.278950	3.663006

Using the values reported in Table I as data for our extrapolation procedures we find the following results. First, if we truncate the right hand side of Eq. (9) after the third term we have five unknowns to solve for, one being T_c. Since we have five levels of approximations we can find these five unknowns and in particular we find for T_c the value of $2.269127\cdots$ which differs from Onsager's exact result by less than 0.003%. Because in the case of the hexagonal lattice we have only three levels of approximation we consider this situation for the square lattice to see the level of accuracy obtained. Using data from $L=1$, 2, and 3 levels and the first two terms on the right hand side of Eq. (9) we have $T_c=2.19126$, while using data from levels 2, 3, and 4 we have $T_c=2.24096$, and finally using data from levels 3, 4, and 5 gives $T_c=2.25360$. As expected using the higher level approximations results in more accurate estimates of T_c with the last estimate within 0.7% of the exact value.

Our second and third set of results makes use of the VBS and BST approaches. All five levels of approximation are used in both cases. With the VBS approach we obtain a critical estimate of $T_c=2.26373$. This gives a value approximately 0.2% from the exact value. The BST result shows one of the problems with this approach. As mentioned earlier with this approach we have a free parameter ω. If Eq. (9) consisted of only the first two terms then the choice of ω should be the value ω_1 as shown in Ref. [15] however for more complex and realistic situations its choice is unclear. In our use of the five levels of data and the truncation of Eq. (9) to include the first three terms we find $\omega_1=0.93895$. Using this as our value for ω we obtain for the critical temperature estimate 2.27040 off by approximately 0.05% from the exact value. Thus given the five levels of approximation from our systematic series we obtain estimates of T_c within 0.2% or less of the exact value.

We now use the CAM which has the advantage of not only giving us an estimate of the critical temperature but also the critical exponents. Critical exponents are generally more difficult to approximate and our results confirm this. To obtain estimates for the critical exponents β, γ, and δ we use the three CAM relationships given in Eq. (19) along with Eq. (18). Only three levels can be used in each determination so we have results using $L=1,2,3$, $L=2,3,4$, and $L=3,4,5$. These results are presented in Table III. Here the worst approximation for the critical temperature of the nine values is 2.2664 which differs from the exact value by only 0.2%. For the critical exponents unfortunately the estimates are not nearly so accurate with percent errors ranging from approximately 1.6% for γ to 11.2% for β.

We now consider the hexagonal lattice. Our basic building blocks for the first two levels are shown in Fig. 3 and results for three levels of approximation are given in Table II. Note in the case of the hexagonal lattice that our approxi-

TABLE III. CAM results for the critical temperature and critical exponents for the ferromagnetic system on the square lattice.

		T_c	β	δ	γ
Using $T_c(L)$	levels 1, 2, 3	2.2664	0.134		
and	levels 2, 3, 4	2.2676	0.135		
$\overline{m}_s(L)$	levels 3, 4, 5	2.2696	0.139		
Using $T_c(L)$	levels 1, 2, 3	2.2665		14.38	
and	levels 2, 3, 4	2.2672		14.18	
$\overline{m}_c(L)$	levels 3, 4, 5	2.2690		13.78	
Using $T_c(L)$	levels 1, 2, 3	2.2666			1.786
and	levels 2, 3, 4	2.2668			1.786
$\overline{\chi}(L)$	levels 3, 4, 5	2.2684			1.779

mation scheme consists of building blocks whose connections are quite different from those used in the square lattice example. In particular, connections are made along edges, hence rather than a site being shared by two building blocks the interaction is also. This results in even the simplest connection involving two sites and every increasingly higher level of approximation having a connection involving two more sites not one more site as in the square lattice case. This results in the dimension of the dynamic system increasing more rapidly. For this reason and to a lesser extent the fact that the number of sites involved (6, 18, and 36 sites for the first three levels) increases more rapidly in the hexagonal lattice series than in the square lattice series we have only three levels of approximation. At the third level approximation for the hexagon lattice we have a 63 (2^6-1) dimensional dynamical system. It should be noted that various symmetries exist which allows one to significantly reduce the dimensions of the mapping. These symmetries were used for both lattice systems studied to reduce the amount of computer memory and computation time necessary to obtain our results (see further comments in Sec. V).

Results using the first two terms of Eq. (9), the VBS approach, and the BST approach (again taking $\omega=0.93895$) give critical temperature estimates of 1.494, 1.58237, and 1.51929, respectively. As in the case of the square lattice the BST results are the most accurate of these three approaches with only a 0.05% error from the exact value of $1.518651\cdots$. The method better handles short sequences of input as mentioned in Henkel and Schutz [15]. In the case of Eq. (9) we have used $L=1$, 2, and 3 to obtain the estimate of 1.494 following what was done for the square lattice. However L should reflect the size of the system and it does for these values in the case of the square building block but with the building blocks used for the hexagonal approximation (the first two levels of which are shown in Fig. 3) it might be more appropriate to use the square root of the number of lattice sites in a building block. With this for our values of L we obtain the much better estimate of 1.5206 differing from the exact result by just over 0.1%. Results found using the CAM on the data involving the hexagonal lattice are given in Tables III and IV. The result for T_c are very good with the worst estimate being off by 0.15% of the exact result and the average of all six estimates differing from the exact value by only 0.04%. Again the errors in the estimates of the critical exponent values are much greater than for the critical temperature and range from 3 to 12 %.

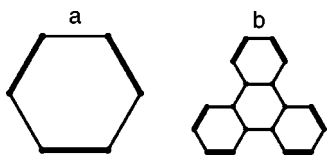

FIG. 3. The basic building blocks for the first two levels of the approximation of the hexagonal lattice system.

TABLE IV. CAM results for the critical temperature and critical exponents for the ferromagnetic system on the hexagonal lattice.

	T_c	β	δ	γ
Using $T_c(L)$ and $\overline{m}_s(L)$	1.5197	0.140		
Using $T_c(L)$ and $\overline{m}_c(L)$	1.5180		16.6	
Using $T_c(L)$ and $\overline{\chi}(L)$	1.5164			1.81

IV. RESULTS FOR THE ANTIFERROMAGNETIC CASE

In this section we present the results for the antiferromagnetic, Ising model, on the square lattice. For this system there is a critical line in the h-T plane and it is this critical line we wish to approximate. Unlike the two earlier systems investigated there are no exact results for this system. However, there have been twenty or more approximations over the last 40 years. We compare our results to five of the most accurate of these approximations.

We have for eight different temperature values running from 0.10 to 2.00 found the value of the critical magnetic field. Actually the critical line is symmetric about the h axis and we need only look at $h>0$. This has been done for five levels of approximation just as was done for the square lattice, ferromagnetic case. These results are presented in Table V. The square lattice is a bipartite lattice and we have an A and B sublattice. When we build up our trees we must distinguish between connections at B sublattice sites from connections at A sublattice sites. This results in the doubling of the dimensions of the dynamical systems generated at the various levels. This is similar to what occurred in our approximation [3] of the triangle lattice, Ising, antiferromagnet only there because of having A, B, and C sublattice sites there is a tripling of the dimensions of the dynamical system.

Here we look at the staggered magnetization as the order parameter for a given temperature there is an attracting fixed point corresponding to zero staggered magnetization for sufficiently large magnetic field but as the magnetic field value is decreased this fixed point becomes repelling and two new fixed points appear corresponding to nonzero staggered magnetization. It is the value of the magnetic field where this change from an attracting to a repelling fixed point is made that is recorded in Table V.

Based on the results presented in Table V we use both the VBS and BST approaches to find our best estimates for the

TABLE V. Critical magnetic field values for various temperatures for the five levels of approximation of the antiferromagnetic system on the square lattice.

Temperature	First level approx.	Second level approx.	Third level approx.	Fourth level approx.	Fifth level approx.
0.1000$\cdots$	3.9658737	3.9535046	3.9482128	3.9451893	3.9432202
0.2500$\cdots$	3.9146842	3.8837614	3.8705319	3.8629732	3.8580506
0.5000$\cdots$	3.8291128	3.7672380	3.7407626	3.7256352	3.7157833
0.854449635	3.6965658	3.5895826	3.5436203	3.5173337	3.5002049
1.0000$\cdots$	3.6298789	3.5027626	3.4479148	3.4165128	3.3690378
1.5000$\cdots$	3.3054913	3.0953012	3.0019620	2.9580392	2.9126861
1.924363127	2.8554956	2.5360157	2.3866082	2.2982119	2.2393348
2.0000$\cdots$	2.7512629	2.4040987	2.2392320	2.1408287	2.0748739

critical magnetic field. These values are presented in Table VI along with the results from five other approximation methods which we briefly describe. The first of these approximations is due to Muller-Hartmann and Zittartz [17] (denoted MHZ in Table VI) and is based on their interface method. This gives an analytic expression for the critical line which was initially conjectured to be exact since it was known to be exact for $h=0$. This has subsequently been shown not to be the case. Nevertheless the results are quite accurate.

Following the results of Muller-Hartmann and Zittartz in Table VI are the results of Wu and Wu [18] and the closely associated results of Blote and Wu [19]. These are results that take as their starting point some estimates of critical points along the h-T line by Blote and den Nijs [20] who used finite size scaling and a large scale computer calculation involving the calculation of the eigenvalues of the transfer matrix for strips of widths up to 16 sites to obtain the critical temperature for four different values of the magnetic field. These results were used by Wu and Wu [18] to obtain a closed form expression for the critical line. Blote and Wu [19] go back to the finite-size scaling approach of Blote and den Nijs [20] but look at more points along the h-T critical line curve and use widths up to 20 sites across. Based on these results they rule out the polynomial expression of Ref. [18] and produce one of their own. Results based on these polynomials or the direct finite size scaling results are presented in columns 6 and 7 of Table VI.

Two very recent approaches to approximating the critical line for this model have been given by Wang and Kim [21,22] and Tarasenko, Jastrabik, Nieto, and Uebing [23]. The first of these uses the zeros of a pseudopartition function, their relation to the free energy, and Griffith's smoothness postulate to obtain the following equation for the critical line:

$$e^{4\beta|J|}=e^{4\beta_c|J|}\cosh^2[f(|h|)]+\sinh^2[f(|h|)], \tag{21}$$

where β_c is the critical value for $h=0$. The function $f(|h|)$ must be determined. Wand and Kim [22] give two approximations for $f(|h|)$. We present only the most accurate

$$f(|h|)\approx 0.542578|h|+0.0034874|h|^2-0.00353295|h|^3. \tag{22}$$

Wang and Kim use two numerical results as input in order to determine the numerical coefficients of the above polynomial. First they use the numerical value for the slope of the critical line at $T=0$ and $h=4$ determined by Baxter *et al.* [24]. The authors were apparently unaware of the more accurate results of Kamieniarz and Blote [25]. Second they used the value of α found by Rapaport and Domb [26] in the following equation which describes the behavior of the critical line near $h=0$

$$T_c(h)=T_c(0)[1-\alpha h^2]+O(h^4). \tag{23}$$

TABLE VI. A comparison of results for the antiferromagnetic system on the square lattice.

T	BST ($\omega=0.92484$)	BST ($\omega=0.93895$)	VBS	MHZ [17]	Wu and Wu [18]	Blote and Wu [19]	Wang and Kim [22]	T,J,N, and U [23]
0.100	3.93307	3.93318	3.93467	3.93069	3.93329	3.93330	3.93372	3.96483
0.250	3.83269	3.83297	3.83668	3.82671	3.83324	3.83334	3.83582	3.88802
0.500	3.66506	3.66561	3.67280	3.65309	3.66611	3.66614	3.67589	3.72636
0.853449635	3.41418	3.41491	3.42529	3.39233	3.41346	3.41380	3.43583	3.43914
1.000	3.29303	3.29391	3.30570	3.26843	3.29200	3.29261	3.31764	3.29923
1.500	2.73243	2.73396	2.74868	2.70401	2.73094	2.73176	2.75099	2.70149
1.924363127	1.92565	1.92788	1.94166	1.90214	1.92436	1.92436	1.92695	1.93176
2.000	1.71629	1.71872	1.73093	1.69490	1.71492	1.71499	1.71512	1.73878

Again the authors were apparently unaware of the value for α found by Kaufman [27] which is accurate to an additional five figures. Using these more accurate values we obtain for $f(|h|)$

$$f(|h|)\approx 0.5426784|h|+0.00343704|h|^2-0.00352666|h|^3 \tag{24}$$

which improves the results of Wang and Kim [22] particularly in the region near $h=0$. We present these modified results column 8 of Table V.

Finally the results of Tarasenko, Jastrabik, Nieto, and Uebing [23] who use real-space renormalization group techniques with two types of majority rules are presented in the last column of Table VI.

For the full range of temperature values our results shown in the second and third columns are among the most accurate available. These results are based on the five levels of approximation along with the BST extrapolation method. We have used two values of ω: one, $\omega=0.93895$, is the value mentioned in the previous section, and the other, $\omega=0.92484$, is the value of ω (to five figure accuracy) which when used with the five levels for the ferromagnetic system and the BST method gives the correct T_c, that found by Onsager, for the ferromagnetic system. Of course this is also the correct T_c value for the antiferromagnetic case when $h=0$. We also present the results after using the VBS approach which again shows the BST approach to be the superior method.

For the best comparison of the approximations we look at $T=1.924363127$ where Blote and Wu [19] through extensive finite size scaling calculations obtain $h=1.924363127$ so that $T=h$ in this case. In this case using either value of our two ω values our results are the closest to the Blote and Wu value of all approximations. We also point out the $T=0.853449635$ case which is another value investigated by Blote and Wu using finite size scaling but is not a temperature value considered directly by Wu and Wu [18]. Thus the h value given in column 6 is from Wu and Wu's polynomial expression and one sees the discrepancy with the finite size scaling value. The difference between the two values being approximately the same size as the difference between the Husimi tree results and the Blote and Wu result.

V. CONCLUSIONS

In the preceding two sections we have established the accuracy of our methods beginning with comparisons with exact results for the ferromagnetic case and then with comparisons with a number of other approximations for the antiferromagnetic case. But any approximation needs to be judged not only on its accuracy but also the amount of time and facilities required to get the approximations and also on its ability to handle more than a select set of systems. In these regards we mention first, that all calculations were performed on a personal computer (400 MHz, 256 Mbyte RAM) with the most lengthy calculations, those involving $\overline{m}_c(L)$ taking approximately 10 h for the $L=5$ case. Second, the method is in theory applicable to any discrete spin system on a lattice as then the methods outlined in Sec. II can be applied to construct the appropriate map. However, the larger the number of allowed spin values the more rapidly the dimensions of the dynamical system increase, thereby limiting the number of levels one may be able to effectively handle. Nevertheless as mentioned earlier even a single level where connections are made at a single site may be enough to model rather complex phase diagrams as in the case of frustrated systems [3]. We have here fixed our attention on rather simple systems where we investigated the accuracy achievable by this systematic approach.

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