Blume-Capel model approximated by a sequence of generalized Husimi trees

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We generalize a systematic approximation method presented by the present author earlier [Monroe, Phys. Rev. E **64**, 016126 (2001)], and which was applied to Ising models with spin one-half. The generalization allows one to consider higher spin systems. In particular we consider the spin-one, Blume-Capel model on a square lattice. We obtain an approximation to the phase diagram of the system that we show is as or more accurate than any presently available. This we are able to do with a rather modest effort thereby illustrating the fact that the method gives one rather accurate results without requiring too extensive computer calculations.

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I. INTRODUCTION

Recently we introduced [1] an approximation method that may be thought of as a generalization of the Bethe lattice approximation. Rather than a Bethe lattice we deal with a generalized Husimi tree, where a collection of sites and the appropriate interactions connecting these sites are the basic building blocks of the graphical structure rather than the two sites and a single nearest neighbor interaction that constitutes the basic building block of the Bethe lattice. By constructing a sequence of these generalized Husimi trees with larger and larger basic building blocks we can obtain better and better approximations to the lattice spin system being studied, achieving, for example, better and better approximations to the phase diagram of the system. Furthermore, in Ref. [1] we used various extrapolation methods to further improve the approximations obtained. For the standard ferromagnetic, nearest neighbor, Ising model on the square lattice our best estimate of the critical temperature was within 0.003% of the exact value. We also found accurate results for the critical line of phase transitions of the antiferromagnetic case of this model in the magnetic field-temperature plane.

As we noted in [1] the method is general enough that it could be applied to a very large variety of lattice spin systems. One avenue of generalization of what was presented in [1] is to higher spin systems where, for example, the spin variable can take on more than two values as is the case with the standard Ising spin models where the spin value is ± 1. One such system is the Blume-Capel model [2,3]. Approximations of this system's phase diagram have been obtained by a large variety of methods. A partial list includes mean-field theory [2,3], renormalization group [4], Monte Carlo renormalization group analysis [5], finite size scaling and the transfer matrix [6], finite size scaling of the partition function zeros [7], mean-field renormalization group [8], and a microcanonical Monte Carlo study [9]. The system has received a lot of attention due to the fact that as a part of the phase diagram one has a tricritical point [10]. We approximate this system with a sequence of only three generalized Husimi tree approximations. We use these three approximations as input into the BST extrapolation method [11] to obtain what we believe is a very accurate overall approximation of this system on the square lattice.

In the following section, Sec. II, we define the Blume-Capel model and present the approximation scheme being used. Section III contains our results along with comparison to a number of results from previous approximations. The final section contains some concluding remarks.

II. BASIC METHOD

The standard Blume-Capel model is a lattice spin system where the spin variable σ is allowed to take on the values ± 1 and 0. The Hamiltonian of the system is

$$\mathcal{H} = -J\sum_{\langle i,j\rangle} \sigma_i\sigma_j - h\sum_i \sigma_i + \Delta\sum_i \sigma_i^2, \tag{1}$$

where the first sum is over all nearest neighbor pairs and the later two sums are over all spin variables comprising the system. Here we will consider only the system on the square lattice and also our results, along with most other results using other approximation methods, will be only for the case where $h=0$. Then the phase diagram in the Δ-T plane, where T is the temperature, consists of a critical line of continuous phase transitions in the region where $-\infty \leqslant \Delta < \Delta_t$ and a connecting line of first order phase transitions for $\Delta_t < \Delta \leqslant 2$. When $\Delta = \Delta_t$ one is at the tricritical point. It is worth noting that for $\Delta \to -\infty$ one has the standard Ising model where the exact critical temperature is known.

As stated in the introduction we approximate such a system with a generalized Husimi tree and we are interested in the behavior of sites deep within the tree just as in the Bethe approximation where one is concerned with the behavior of a central site and not all sites making up the Cayley tree. We can determine the behavior of our central sites by a recursive method. As an example we consider our lowest level approximation. In this case we have a four site basic building block with the sites on the corner of a square and four nearest neighbor interactions connecting the sites. If we consider the four sites as our total system we can take one of our sites to be the base site and can find expressions for Λ_1^+, Λ_1^0, and Λ_1^- that denote respectively the part of the partition function for the four site system where the spin variable on the base site is $+$, 0, and $-$, denoted by the superscript. The subscript 1 denotes the fact that we consider this four site system as our first generation system. To get the second generation system we attach a first generation system at three of the corners

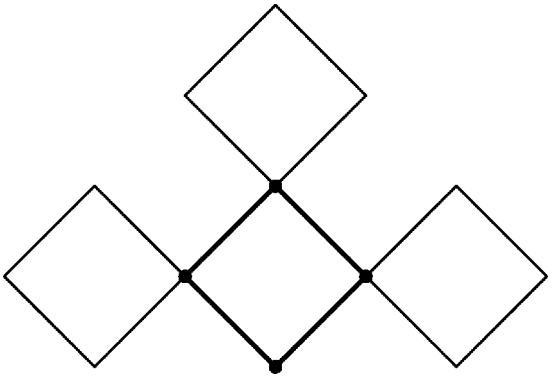

FIG. 1. The second generation branch for the first level approximation of the square lattice system. Circles indicate the connection points.

of a new four site, basic building block as shown in Fig. 1. One can then obtain expressions for Λ_2^+, Λ_2^0, and Λ_2^- where again the superscripts denote the value of the spin variable on the base site. These expressions can be written as functions of Λ_1^+, Λ_1^0, and Λ_1^- as well as $e^{\beta J}$ and $e^{\beta\Delta}$ where $\beta \equiv 1/kT$. One can continue with this building process in an obvious way to produce third generation, fourth generation, etc. graphical structures. For the nth generation tree one can express Λ_n^+, Λ_n^0, and Λ_n^-, the three parts of the partition function for the nth generation tree, in terms of Λ_{n-1}^+, Λ_{n-1}^0, Λ_{n-1}^-, $e^{\beta J}$, and $e^{\beta\Delta}$.

Thus one obtains a three-dimensional, discrete dynamical system and the behavior of the central sites is determined by the fixed points, two cycles, etc. that occur for this system. Attracting fixed points, two cycles, etc., will be of interest since we want to take the thermodynamic limit, i.e., $n\to\infty$. Specifically for an nth generation system the thermal average of the spin variable on the root site, i.e., the magnetization of the root site, is

$$\langle\sigma_i\rangle_n = \frac{\Lambda_n^+ - \Lambda_n^-}{\Lambda_n^+ + \Lambda_n^0 + \Lambda_n^-}, \tag{2}$$

where we have denoted the root site as the ith site. If an attracting fixed point exists, as is often the case, then the magnetization of this root site is in the thermodynamic limit determined by the value of the fixed point the system is attracted to.

Alternatively the magnetization of the root site of the system can be written as

$$\langle\sigma_i\rangle_n = \frac{x_n - y_n}{x_n + 1 + y_n}, \tag{3}$$

where $x_n \equiv \Lambda_n^+/\Lambda_n^0$ and $y_n \equiv \Lambda_n^-/\Lambda_n^0$ thereby reducing the system to a two-dimensional, discrete dynamical system involving

$$x_n = f(e^{\beta J}, e^{\beta\Delta}, x_{n-1}, y_{n-1}), \quad y_n = g(e^{\beta J}, e^{\beta\Delta}, x_{n-1}, y_{n-1}). \tag{4}$$

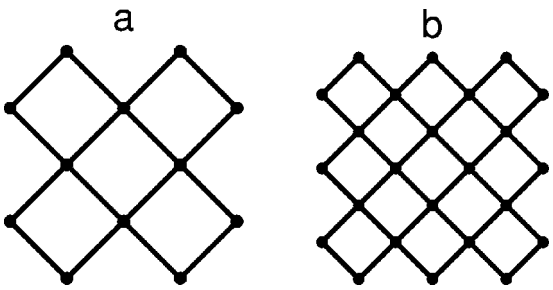

FIG. 2. The basic building blocks or equivalently the first generation branch for the second level approximation (a) and the third level approximation (b) of the square lattice system.

It is this system that is actually used in determining the behavior of the system. We have not written out the explicit expressions for the functions f and g as they are rather lengthy and not particularly illuminating. Nevertheless the expressions can be found rather easily due to the small number of configurations involved in the computation of Λ_1^+, Λ_1^0, and Λ_1^-.

Our higher level approximations involving larger basic building blocks (see Fig. 2) also involve situations where a building block is connected to another at more than one site. If one makes connections in this manner, e.g., involving two sites at a time as done in the second level approximation (see Fig. 3), then for the any spin system where the spins can take on the values ± 1, and zero system one will have an 8, $(3^2 - 1)$, dimensional system. In general if a building block is connected to another through a connection involving p sites then one will have a $3^p - 1$ dimensional system governing the behavior of the generalized Husimi tree. This is to be contrasted with the standard Ising model spin case studied in [1] where the dimension of the discrete dynamical system goes as $2^p - 1$. The larger the number of allowed spin values the more rapid the increase in the dimensionality of the recursive maps governing the behavior of the system and hence in the computational complexity encountered. For this reason we have only gone to three levels of approximation for the Blume-Capel model whereas we had five levels of approximations for the Ising systems of Ref. [1]. Nevertheless as we show in the following section in general the accuracy of our approximations generally matches those obtained by other methods.

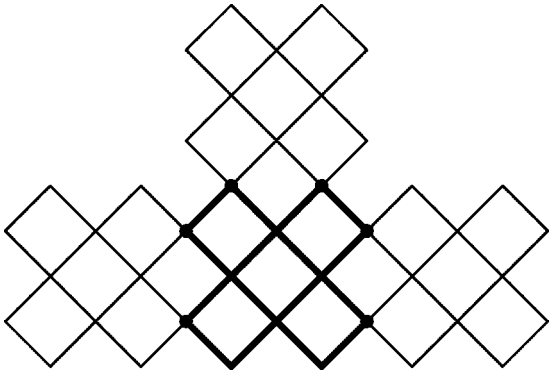

FIG. 3. The second generation branch for the second level approximation of the square lattice system.

TABLE I. Critical temperatures for each of the three levels of approximation used.

Δ	$T_c(1)$	$T_c(2)$	$T_c(3)$
−4.0	2.551 100	2.388 530	2.320 361
−2.0	2.360 477	2.216 211	2.155 746
0.0	1.997 236	1.875 236	1.824 143
0.2	1.943 525	1.824 058	1.774 016
0.4	1.884 739	1.767 896	1.718 942
0.6	1.819 919	1.705 815	1.657 986
0.8	1.747 725	1.636 518	1.589 871
1.0	1.666 213	1.558 118	1.512 731
1.2	1.572 302	1.467 665	1.423 663
1.4	1.460 585	1.360 030	1.317 644
1.6	1.319 560	1.224 563	1.184 362
1.7	1.229 384	1.138 670	1.100 157
1.8	1.112 097	1.029 125	0.993 653
1.9	0.901 329	0.856 306	0.832 459
1.96	0.688 039	0.654 504	0.643 483
1.98	0.625 302	0.584 099	0.570 376
1.99	0.585 940	0.535 213	0.521 051

To obtain our most accurate results we use, for a given Δ, the critical temperature found from each of our three levels of approximation as input into an extrapolation procedure developed by Bulirsch and Stoer [11] and used in various statistical mechanical applications by Henkel and co-workers [12,13]. We have selected this method over various other approaches used in [1] as it gave the best results for the Ising spin systems looked at there. As in [1] having a sequence of ever improving approximations of the critical temperature such as described above allows one to use various extrapolation methods to obtain an improved final approximation to the critical temperature. Using a finite size scalinglike approach one can write

$$T_c(L)=T_c^*+aL^{-\omega_1}+bL^{-\omega_2}+cL^{-\omega_3}+\cdots, \tag{5}$$

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 $0<\omega_1<\omega_2<\omega_3<\cdots$. The BST method allows one to construct a table of extrapolants. For $L=1$, 2, 3 we have

$$\begin{array}{ccccc} T_{c,0}^1 & & & & \\ & T_{c,1}^1 & & & \\ T_{c,0}^2 & & T_{c,2}^1 & & \\ & T_{c,1}^2 & & & \\ T_{c,0}^3 & & & & \end{array} \tag{6}$$

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

$$T_{c,-1}^n=0, \tag{7}$$

$$T_{c,0}^n=T_c(n), \tag{8}$$

TABLE II. Critical temperatures using the BST extrapolation method and comparison with results based on alternate approaches.

Δ	T_c with $\omega=0.9405$	T_c with $\omega=0.9496$	T_c from Ref. [9]	T_c from Ref. [6]
−4.0	2.1445	2.1459		
−2.0	1.9998	2.0011		
0.0	1.6925	1.6936	1.7151	1.695
0.2	1.6450	1.6461	1.6648	
0.4	1.5927	1.5938	1.612 381	
0.6	1.5346	1.5356	1.5579	
0.8	1.4695	1.4705	1.4935	
1.0	1.3954	1.3964	1.4137	1.398
1.2	1.3098	1.3107	1.3194	
1.4	1.2077	1.2086	1.2098	
1.6	1.0796	1.0804	1.0759	
1.7	0.9994	1.0003		
1.8	0.9002	0.9052	0.8806	
1.9	0.7495	0.7504		
1.96	0.6206	0.6208	0.6324	
1.98	0.5417	0.5418		
1.99	0.4947	0.4949		0.550

$$T_{c,m}^n=T_{c,m-1}^{n+1}+(T_{c,m-1}^{n+1}-T_{c,m-1}^n)\times\left[\left(\frac{n}{n+m}\right)^{\omega}\left(1-\frac{T_{cm-1}^{n+1}-T_{c,m-1}^n}{T_{c,m-1}^{n+1}-T_{c,m-2}^{n+1}}\right)-1\right]^{-1}, \tag{9}$$

where $m\geqslant 1$ and ω is a free parameter. (The superscript ω is unfortunately missing in Eq. (15) of Ref. [1]). Henkel and Patkos [12] were the first to use the algorithm in the area of critical phenomena. Later Henkel and Schutz [13] examined the characteristics of this algorithm in a number of settings. The choice of ω in any particular application can be both problematic and beneficial. This was one of the aspects of the algorithm discussed in [1,13]. We will describe our choices for ω in the following section.

III. RESULTS

In Table I we present the results of our three levels of approximation. In particular, for each of the three levels of approximation used we have listed the critical temperatures, $T_c(L)$, for a large set of values of Δ. In Table II we list our critical temperature estimates after using the BST method. As stated in the preceding section ω is a free parameter. We have listed our results for two different values of ω. The values of ω used were chosen based on the following. First, for $\Delta\rightarrow-\infty$ we know we have the standard Ising model and for the square lattice one knows the exact critical temperature. Hence we can use this as a reference point. We vary ω when using the critical temperature values, $T_c(L)$ for $L=1$, 2, and 3, for the Ising case and choose ω such that it gives Onsager's exact critical temperature value. One then finds, to four figure accuracy, $\omega=0.9405$. As a second reference point one has the special case where $\Delta=0$. The $\Delta=0$ case is just the standard spin-one Ising model and has been studied by an

extremely thorough and intensive finite size scaling approach [14] as well as an equally intensive low temperature series expansion approach [15,16] resulting in estimates of the critical temperature of $1.693\,557 \pm 0.000\,020$ and $1.693\,558\,3 \pm 0.000\,002\,5$, respectively. Using this as a second reference point and our three estimates of the critical temperature we find we want to set $\omega = 0.9496$ to get a match between our BST extrapolation result and the best estimates from finite size scaling and series expansions. We report BST extrapolation values for both these values of ω in Table II as well as estimates of T_c found by Beale [6] and Care [9]. Note that while the results using $\omega = 0.9496$ are always larger than those found using $\omega = 0.9405$ the difference between the two results is typically very small and increases as $\Delta \to -\infty$. For $\Delta = -4$, where the difference is greatest, the difference is 0.065% while for $\Delta = -4$, it is 0.018%.

In Table II along with our results we have presented the results of Care [9] and Beale [6] that we believe are the most accurate available except for special cases such as in the $\Delta = 0$ case mentioned above. Comparisons seen in Table II indicate the accuracy of our results appears to match or better that of the other two methods presented there except perhaps in the area around $\Delta = 2$. For $\Delta = 0$ using the value of ω, $\omega = 0.9405$, chosen because it gives a correct BST extrapolation when $\Delta \to -\infty$, we have $T_c = 1.6925$ while from Ref. [9] one has 1.7151 and for Ref. [6] one has 1.695. Our result differs from the extremely accurate results for this special case of references [14–16] by approximately 0.062% while that of reference differs by 1.27% and that of Ref. [6] by 0.085%. Additionally the more recent result of Xavier *et al.* [18] based on conformal invariance and finite size scaling for the special case of $\Delta = 0$ is $T_c = 1.681(5)$ that is also less accurate than our result. (Only two T_c are reported in [18] for the spin-one case and, therefore, we have not included their results in Table II.) Based on the above with $\omega = 0.9405$ in the region of Δ from $-\infty$ to 0 our results have an accuracy of 0.06% or better.

For the case where $\omega = 0.9496$ our results for $\Delta = 0$ match those of [14–16] and using this value of ω for $\Delta \to -\infty$ our results differ from the exact Onsager result by 0.08%. Based on this for Δ around $\Delta = 0$ our results should have an accuracy significantly greater than 0.08%. Overall our results for both values of ω used in the BST extrapolation method are very close to those of Refs. [6,9] indicating overall good quantitative agreement regarding the phase diagram based on all three approaches. The only place where this is not true is in the region where Δ approaches the value of 2 and the value of T_c approaches 0. Our results in this region differ from those of Refs. [6,9] by approximately 20.0% at, for example, $\Delta = 1.99$.

Besides determining the critical temperature one is interested in the type of phase transition that occurs. For each level of approximation there is, beginning with $\Delta = -\infty$, a range of Δ values where one obtains a continuous transition but as expected for a large enough value of Δ one obtains a first order phase transition. The point at which this crossover occurs is the tricritical point denoted by (Δ_t, T_t). In each successive level of approximation we obtain a more accurate approximation to this point. The tricritical point for the first, second, and third level of approximation are (1.906 75, 0.8684), (1.923 95, 0.7758), and (1.932 79, 0.734 78), respectively. Here again we use the BST extrapolation method to obtain our best approximation but this time we use it on both the Δ sequence and T sequence for our two ω values to obtain the location of the tricritical point for $\omega = 0.9405$ to be (1.9622, 0.6233) and for $\omega = 0.9496$ to be (1.9619, 0.6233). This is to be compared with the values of $(1.9696 \pm 0.01, 0.5969 \pm 0.0008)$, $(1.965 \pm 0.001, 0.610 \pm 0.005)$, $(1.9655 \pm 0.015, 0.6091 \pm .003)$, and (1.967, 0.604) from, respectively, Refs. [9,6,5,7].

It is worth contrasting the behavior of the fixed points that result in the continuous phase transition region with the first order phase transition region. In the region where one has a continuous transition there is for high temperatures a single, positive, real-valued fixed point that is attracting and that corresponds to the case of zero magnetization. As the temperature is lowered the stability of this fixed point, i.e., based on standard dynamical systems theory the maximum eigenvalue of the Jacobian of the map evaluated at the fixed point value, increases to a point where the maximum eigenvalue is 1. This is then a neutral fixed point. Lowering the temperature still further causes a bifurcation of the original fixed point resulting in the creation of two new positive, real-valued, fixed points. These two new fixed points are attracting and correspond to positive and negative values for the magnetization given by Eq. (3) if dealing with the first level approximation or similar equations for higher level approximations. Since the value of the magnetization depends on the fixed point values the system is attracted to, as illustrated by Eq. (3) for the first level approximation, and the value of the fixed point the system is attracted to varies continuously as the temperature is lowered the phase transition is continuous.

This is in contrast to the situation where a first order phase transition occurs. Here as before at high temperatures there is a single, positive, real-valued fixed point that is stable (attracting) and corresponds to zero magnetization. As the temperature is lowered again the stability of this fixed point decreases, however, before becoming a neutral fixed point two new, positive, real-valued fixed points are created (corresponding to positive and negative magnetizations) and these fixed points are also stable or attracting. At this point there are then three attracting fixed points and which fixed point the system is attracted to depends on ones approach. One can take a strict dynamical system's approach and allow the boundary condition, which are the values assigned to x_0 and y_0 in Eq. (4) if one is dealing with the first level approximation, to determine which attracting fixed point the system is attracted to. However, as we have shown [17] the better criteria, a criteria that for other systems has been shown to agree with results based on selecting the phase corresponding to the minimum free energy the more standard statistical mechanics approach, is to simply have the system go to the more stable fixed point. That is to the fixed point having the smallest value for the maximum eigenvalue of the Jacobian of the map evaluated at the fixed point value. In this case the system jumps from the fixed point value corresponding to zero magnetization to a very different fixed point corresponding to nonzero magnetization as the temperature is

lowered. Since the value of the one fixed point does not move continuously into the value of the other as the temperature is decreased this results in the discontinuity of the magnetization and a first order phase transition.

IV. CONCLUSIONS

In the above we have shown the systematic approximation presented in [1] and applied to spin one-half, Ising model systems there can be generalized to higher spin systems. In the case of higher spin systems the dimension of the dynamical system increases more rapidly and, therefore, one may not be able to go to as high a level of approximation as with the spin one-half case. Nevertheless using the Blume-Capel model as an example we have shown that even with only three levels of approximation and the BST extrapolation method one can obtain accurate numerical results. Since the method depends only on the spin taking on discrete values one could besides investigating even higher spin systems such as the spin-3/2 case that was the main system under consideration in [18] one could add addition interactions such as next nearest neighbor, biquadratic interactions that are generally included in the generalization of the Blume-Capel model known as the Blume-Emery-Griffiths model, or multisite interactions.

ACKNOWLEDGMENT

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