Critical temperature estimates for higher-spin Ising and Potts models

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We present estimates of the critical temperature of both higher-spin Ising and Potts models on the square and simple cubic lattices based on a Husimi tree, dynamical systems approach. For the square lattice, exact results are available for the Potts model but we can refine and improve some previous estimates based on series expansions for the higher-spin Ising model. For the simple cubic lattice, based on the systematics of this approach, we are able to present accurate estimates for the critical temperature of spin systems with spin values, where estimates by other methods are unavailable or much less accurate. The same is true for the Potts model. All our estimates can be obtained using a personal computer.

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I. INTRODUCTION

Exact results regarding the phase diagram of lattice spin systems are very rare. For this reason and others there has been an immense effort over the last several decades developing and implementing approximation methods for determining the properties of the phase diagram of these systems. One of the approaches where much of this effort has gone is in the production of lengthy high-temperature and low-temperature series expansions, from which estimates of the critical temperature and critical exponents can be made. Since the early papers in the 1960s such as the paper of Domb and Sykes [1] there has been a continual stream of papers, which continues today; see the very recent paper of Butera and Comi [2] which contains in its Introduction an excellent review of some of the work in this area. There have also been a number of closed form approximation methods; see the review by Burley [3]. One of the best known of the closed form methods is the Bethe approximation method, which approximates the lattice system for which an exact result is not obtainable with a Cayley tree where the behavior of the interior sites can be rather easily found.

Recently this author has generalized this approach [4,5]. The generalization can be thought of as having two major aspects. The first centers on replacing the pair of sites and the interaction between them, which is the basic building block of the Cayley tree, with a more extensive basic building block consisting of a larger collection of sites and interactions. One example of this is that when approximating a square lattice one can use a square consisting of four sites as a basic building block in constructing a tree made up of these squares. A tree of this type is known as Husimi tree. Still connections between one basic building block and another occur at a single site. The second major aspect of the generalization is that with still larger basic building blocks than the four-site square, when one is approximating square lattice systems, one may wish to make a connection between two building blocks, which involves more than one site. Basic building blocks with as many as 60 sites and connections involving five sites where considered in Ref. [4].

Our emphasis in this paper is not to look at Husimi tree systems made up of larger and larger basic building blocks, but rather to look at the systematics of the simplest approximation beyond the standard Bethe lattice approximation, as the value of the spin variable is increased when one has either an Ising spin system or a Potts spin system. In the following, we will be able to establish a method that will allow one to rather easily make accurate estimates of the critical temperature for higher-spin values based on the systematics we find regarding our approximation method, and we present critical temperature values beyond what is currently available. We will find approximations for the critical temperature for both square lattice systems and simple cubic lattice systems.

In the following section we outline the method, referring to Ref. [4] for any details. Section III shows the systematics that result from our approach along with the observed results along with some refinements of previous results and for higher-spin Ising systems. Section IV contains similar results for Potts model systems. We finish with some brief concluding remarks.

II. BASIC METHOD AND SYSTEMATICS

As stated above, we wish to approximate the higher-spin Ising model and Potts model systems on the square and simple cubic lattices (other lattice systems could be approximated by this approach as well). The Hamiltonian for the Ising system is

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

where the first sum is over all nearest-neighbor pairs; the second is over all sites; and s_i represents the spin variable on the ith site and can take on the values $s, s-2, s-4, \ldots, -s+2, -s$. Actually by the Lee-Yang circle theorem, one knows that, for these systems with ferromagnetic interactions, there is a phase transition only when $h=0$. For the Potts model system [6] the Hamiltonian is

$$\mathcal{H} = -J\sum_{\langle i,j\rangle} \delta(s_i,s_j) - h\sum_i \delta(s_i,1), \tag{2}$$

where $s=1,2,3,\ldots,q$; the first sum is over nearest-neighbor pairs; the second sum is over all sites; and $\delta(x,y)$ is the

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TABLE I. Critical temperature approximations for Ising spin systems on the simple cubic lattice using the Husimi tree approach (options 3 and 7) and high-temperature series expansions (HTSE) approximation of Ref. [2]. The percentage difference is that between one of the Husimi tree estimates and the HTSE estimates.

s	T_c (option No. 3)	% difference	T_c (option No. 7)	% difference	T_c HTSE [2]
1	2.79950	−37.946	4.83951	7.270	4.51151(4)
2	8.21694	−35.730	13.54628	5.955	12.78496(8)
3	15.86401	−35.018	25.76584	5.542	24.41293(13)
4	25.71291	−34.697	41.48412	5.357	39.3747(3)
5	37.75696	−34.525	60.69860	5.258	57.6659(4)
6	51.99388	−34.421	83.40678	5.199	79.2847(5)

usual Kronecker delta equal to 1 if $x=y$ otherwise zero. To approximate the two lattice systems, we will use the simplest application of the method presented in Refs. [4] and [5]. For the square lattice we take as our basic building block a square consisting of four sites, and for the simple cubic lattice we take as our basic building block a cube consisting of eight sites. We then consider building an Husimi tree with either of these basic building blocks by making connections at the corners of the square or cube. The construction of the tree will be done in a step-by-step manner, emphasizing the recursive method that is used to mathematically analyze the behavior of our final infinite tree, i.e., the systems are analyzed using a dynamical systems approach where a discrete dynamical system of dimension n is produced for each system being approximated. We consider a single basic building block as the zeroth generation of our tree. We then attach at the corners of either the square or the cube additional basic building blocks resulting in a first generation tree. Typically we would make attachments at either three of the corners of the square or seven of the corners of the cube leaving one site, which we denote as the root site, ready to be attached to the corner of a new basic building block when constructing the second generation branch. But one need not make connections at all these corners. In the case of the square lattice approximation, one could make connections at either one, two, or three corners. Making connections at only one corner generates a quasi-one-dimensional system with critical temperature of zero, but for connections at either two or three corners one gets a nonzero critical temperature. As we will see, the square lattice connecting at only two sites results in a critical temperature smaller than the true critical temperature while connecting at three sites results in too large a value.

The discrete maps that determine the behavior of the system can be constructed following the procedure given in Ref. [4]. For the Ising case, with either the square lattice or simple cubic lattice approximation, the dimension of the dynamical system is governed by the allowed values the spin variable can take. For a spin variable having a possibility of p values, the dimension of the dynamical system is $p-1$. Hence for the standard Ising model one has a one-dimensional discrete dynamical system as seen in the level-1 approximation in Ref. [4]. The construction of the exact rational functions involved in the maps becomes more difficult as the allowed values of s increase, but even for $s=8$, the largest value we look at, it can be done in less than 1 h on a typical personal computer using standard software programs such as MATHEMATICA. For the Potts case, because of the nature of the Kronecker delta function, one has a one-dimensional dynamical system regardless of the value of q.

In the Ising model case, what one finds for the behavior of the dynamical system is that for large temperatures there is a single, attracting, physically relevant, fixed point corresponding to zero magnetization; and as the temperature is lowered at some point, this fixed point bifurcates into two new attracting fixed points—one corresponding to positive and one corresponding to negative magnetizations. The temperature at which this bifurcation occurs is naturally the critical temperature.

For the Potts model case the behavior is different. Again at higher temperatures there is a single real valued attracting fixed point corresponding to a disordered state. Then as the temperature is lowered, two new real valued fixed points are created at some temperature—one attracting and one repelling. The system goes to the most stable fixed point. Specifically, as the temperature is lowered, the stability of the fixed point corresponding to the disordered state decreases and the stability of the fixed point corresponding to the ordered state increases. The critical temperature is the temperature at which the stabilities of the two fixed points are equal [7].

We look at two cases for each system. For the square lattice, we make connections at three corner sites as the tree is built (we denote this as option 3 because of the connection at three sites), or at two corner sites (denoted as option 2), and in this case the two sites are diametrically opposite to each other. For the simple cubic lattice approximation we make connections at seven corner sites (option 7) or at three corner sites (option 3). Here in the latter case we make connections at two diametrically opposite sites on one face of the cube and then on the opposite face on one of the sites not a nearest neighbor to the original two sites. The root site is then the diametrically opposite site on this face. Hence, by the time the tree is completed there are four symmetrically placed connections on each cube.

III. ISING MODEL RESULTS

We begin by presenting our results for the simple cubic lattice. These are given in Table I. Along with the critical temperature approximations based on options 3 and 7 using the Husimi tree approach, there is listed the very recent estimate of Butera and Comi [2] of T_c based on using high-

TABLE II. Critical temperature approximations for Ising spin systems on the simple cubic lattice using the Husimi tree approach (options 3 and 7) along with a projected percentage difference and our best estimate of the critical temperature. The values of the percentage differences are set based on the systematic increases and decreases shown in Table I where HTSE estimates are available.

s	T_c (option No. 3)	% difference	T_c (option No. 7)	% difference	Predicted T_c
7	68.42269	−34.353	109.6097	5.161	104.229(1)
8	87.04294	−34.306	139.3068	5.135	132.500(3)

temperature series expansions (HTSE). These are the most accurate estimates we are aware of. In addition, we have calculated the percentage difference between each of our estimates using the Husimi tree approach and the HTSE approach. What one sees is a very systematic progression where the percentage difference decreases as the spin value increases. Based on the very systematic changes in the percentage differences seen in Table I one can then make a rather accurate estimate of the percentage differences for even higher values of spin than have been looked at by Butera and Comi or others. For example, from Table I the percentage difference for $s=5$ and option 7 is 5.258 and this drops to 5.199 for $s=6$, a difference of 0.059. Now when going to $s=7$ we expect a percentage difference less than 5.199 but greater than 5.140 which is $5.199-0.059$. Furthermore the systematics shown in Table I tells us that the percentage difference should be closer to the lower figure 5.140 than the higher 5.199. Hence we have estimated a percentage difference of 5.16 for the case of $s=7$. Similar considerations were made for $s=7$ and option 3 as well as for $s=8$. Hence based on these estimated percentage differences, we estimate the critical temperature for both options and then as our final critical temperature approximation average the two values, one for each option. The error indicated in Table II for these estimates is given as 1/2 the difference between the estimate based on option 3 and option 7 and shows an accuracy similar to the accuracy of the T_c values of Butera and Comi [2] for their somewhat lower-spin values.

In the case of the square lattice system, recently Jensen *et al.* [8] have presented an extensive study of these systems for $s>1$ Ising spins using low-temperature series expansions. They have presented results for cases up to $s=6$. Their results along with our own for both option 2 and option 3, as described above, are given in Table III. Here we see a distinctly different behavior than for the simple cubic lattice case. For spin values of $s=1,2,3$, and 4 there is a systematic percentage difference between the Husimi tree results and the estimates based on the low-temperature expansions. However, when going to $s=5$ and 6 there is a break with this systematics. For this reason we believe the estimates based on the low-temperature expansions for the cases $s=5$ and $s=6$ are too low. Our own estimates, continuing the systematics one sees for the lower value spins, give for $s=5$ a critical temperature value of 31.4261(1) and for $s=6$ a value of 43.315(2). These values were based on estimated percentage differences given in Table IV which are in line with what one has for the lower-spin cases. Both of our critical temperature estimates in Table IV are within the error bars of Ref. [8]. Unfortunately we have no rigorous proof that the percentage difference between the true critical temperature and our estimates either for the simple cubic lattice or for the square lattice should monotonically increase or decrease depending on the lattice and the option being used; however we believe this makes greater intuitive sense than the reversals seen in Table III. Furthermore, the results of the following section involving the Potts model on the square lattice, where an exact value of the critical temperature is known, show a very systematic change in the percentage difference between the exact values and the Husimi tree estimates; therefore supporting our view that the same should occur with the Ising systems.

IV. POTTS MODEL RESULTS

Here we begin with the square lattice case. An exact value for the critical temperature T_c is given by [6]

$$\exp[J/T_c]=1+\sqrt{q}. \tag{3}$$

TABLE III. Critical temperature approximations for Ising spin systems on the square lattice using the Husimi tree approach (options 2 and 3) and low-temperature series expansions (LTSE) approximation of Ref. [8]. The percentage difference is that between one of the Husimi tree estimates and the LTSE estimates except for the case, where $s=1$, where we have used the exact value.

s	T_c (option No. 2)	% difference	T_c (option No. 3)	% difference	T_c LTSE [8]
1	2.14332	−5.547	2.77078	22.105	2.269185 . . .
2	6.36694	−6.012	7.98894	17.931	6.7442
3	12.34026	−6.158	15.33908	16.647	13.1514
4	20.03668	−6.239	24.80104	16.055	21.3706
5	29.44974	−5.458	36.37012	16.758	31.1522
6	40.57723	−5.414	50.04472	16.654	42.9127

TABLE IV. Critical temperature approximations for Ising spin systems on the square lattice using estimated percentage differences based on the systematics shown in Table III for the cases of $s=1,2,3$, and 4.

s	T_c (option No. 2)	% difference	T_c (option No. 3)	% difference	Predicted T_c
5	29.44974	−6.287	36.37012	15.730	31.426(1)
6	40.57723	−6.319	50.04472	15.530	43.315(2)

Our approximation of T_c using options 2 and 3 are given in Table V along with the exact results and the percentage differences. One sees very clearly the extremely systematic change in the percentage differences as q increases. In particular, using option 3, which is the standard option giving a coordination number of 4 for all sites except those on the boundary, the percentage difference between our approximation and the exact value decreases significantly as q increases, going from $\approx$22.1% to only 2.4% when q is increased from $q=2$ to $q=9$. With option 2 the opposite occurs; the approximation gets poorer as q increases.

When approximating the simple cubic lattice system, we saw in the case of the Ising model that the approximation for this system was more accurate than that of the square lattice approximation. This should be true in the Potts model case as well. This, along with the increase in accuracy as q increases, means that for q values of 8 and 9 we may expect our option 7 results to have less than a 1% error.

No results exist for the Potts model on the simple cubic lattice having near the accuracy as for the corresponding Ising model systems. In fact, as with the Ising model, increasing the value of the spin greatly increases the amount of work necessary to obtain accurate estimates. This is true to some extent with our method as well, but again all our results were obtained on a personal computer with the $q=9$ case, the highest we found, taking several hours to determine T_c. The majority of the results for the simple cubic lattice have been obtained for the $q=3$ case. The largest q values that we are aware of, apart from our results, are those of Chen, Lee, and Kao [9] which go up to $q=7$.

Our results for T_c of the q-state Potts model on the simple cubic lattice for $q=2,3,\ldots,9$ are given in Table VI. For the $q=2$ case the Potts model and Ising model are identical and we have for the simple cubic lattice a percentage difference between our estimate of T_c and the very accurate estimate based on the high-temperature series expansion [2] of 7.270%, while for the square lattice the percentage difference between our estimate and the exact value is 22.105%. Hence the percentage error in going from the two-dimensional to the three-dimensional lattice is reduced by approximately a factor of 3. In the $q=3$ case, we use the value of T_c for the simple cubic lattice system of 1.816 found by Wilson and Vause [10] using a multilattice microcanonical simulation method and also found by Gavai, Karsch, and Peterson [11] using a METROPOLIS Monte Carlo simulation method. We then have a percentage difference of 2.48% with these results, which is less than 1/4 the percentage error we have for the square lattice system. Hence, based on this and the fact that for the square lattice system where the exact values are known, we know for $q\geqslant 6$ that our estimate is within $\approx$4% we expect for these cases where $q\geqslant 6$ that our error is less than 1%. Our results differ from the results of Ref. [9] by less than 1% for both the $q=6$ and $q=7$ cases, the two highest q values which they consider. They obtain 1.347 and 1.274 as their estimates for T_c for the $q=6$ and $q=7$ cases, respectively. Furthermore, as they remark, their estimates are typically too low and ours are too high; so between the two, one has a rather good bound on the actual critical temperature values. Finally if the improvement in our error matches even somewhat the improvement in going from the $q=2$ to the $q=3$ case for the larger q values, our error in the $q\geqslant 6$ range may be considerably less than 1%.

V. CONCLUSION

Estimates of the critical temperature of lattice spin systems have been of interest for several decades. Vast amounts of time and energy have gone into their calculation. One of the methods resulting in some of the most accurate estimates has been the series expansion method. Here computation of an additional term in the series may take more time than the computation of the entire preceding series. The most recent

TABLE V. Critical temperature approximations for Potts spin systems on the square lattice using the Husimi tree approach (options 2 and 3) and exact T_c values from Eq. (3).

q	T_c (option No. 2)	% difference	T_c (option No. 3)	% difference	Exact T_c
2	1.07166	−5.543	1.38539	22.105	1.1345926 . . .
3	0.87829	−11.718	1.10652	11.222	0.9948728 . . .
4	0.78447	−13.817	0.97657	7.287	0.9102392 . . .
5	0.72544	−14.807	0.89666	5.300	0.8515283 . . .
6	0.68357	−15.358	0.84083	4.126	0.8076068 . . .
7	0.65172	−15.696	0.79883	3.333	0.7730589 . . .
8	0.62633	−15.918	0.76564	2.784	0.7449044 . . .
9	0.60543	−16.069	0.73851	2.379	0.7213475 . . .

TABLE VI. Critical temperature approximations for Potts spin systems on the simple cubic lattice using the Husimi tree approach and option 7.

T_c for $q=2$	T_c for $q=3$	T_c for $q=4$	T_c for $q=5$
2.419753	1.861418	1.612691	1.463613
T_c for $q=6$	T_c for $q=7$	T_c for $q=8$	T_c for $q=9$
1.361277	1.285278	1.225857	1.177676

extension for higher-spin Ising models on the simple cubic lattice [2] emphasizes this point by noting that in one specific case it took only minutes to get the first 21 terms but to get the next four terms took several days of computer time.

We have used an Husimi tree approach; a generalization of the Bethe lattice approach, which as used here by itself cannot give results comparable to those obtained by the series expansion method. However because of the systematics, in particular the increasing accuracy of the estimates as the spin value increases and the availability of accurate estimates for several lower-spin values ($S \leqslant 6$), we have for the simple cubic lattice case been able to obtain accurate estimates for higher-spin values. Furthermore, the method has allowed us, in the case of the square lattice Ising model, to reduce for several larger values of the spin the amount of error associated with the estimates obtained only recently for this system [8]. For the square lattice Potts model exact results are known, and show for our approximation of these systems that one has an increase in the accuracy of our T_c approximations as q increases. Based on this we have argued that our estimates for the simple cubic lattice Potts model are within 1% of the exact value for $q \geqslant 6$.

It should be pointed out that what has been done here uses only a part of the power of the dynamical systems, Husimi tree approach. As was done for the standard Ising model in Ref. [4] and for the Blume-Capel model in Ref. [5], one could generate a series of increasingly accurate approximations for the critical temperature for a given value of q or s, which could then be extrapolated for a final estimate of the critical temperature. In the case of the standard Ising spin variable on the square lattice, we obtained a series of five estimates that led to an extrapolated value within 0.003% of the exact Onsager value. Here we run into the same problem as with the series expansions, in that each new term in the general series of approximations takes significantly more time and effort to calculate, as well as increasing the values allowed to be taken by the spin value results in a larger dynamical system.

Note added. Recently the author came to know about a preprint by Butera and Comi [12] where recently extended high-temperature series expansions are combined with low-temperature expansions of Ref. [8] and have been used to improve various critical point estimates. One such improvement involves the estimation of the critical temperature of the higher-spin Ising model on the square lattice. In particular, Butera and Comi [12] obtain for $s=5$ an estimate of $T_c=31.430(1)$ and for $s=6$ an estimate of $T_c=43.318(5)$. Hence for $s=6$ this corresponds almost exactly to our own estimate and for $s=5$ there is a difference in only the third decimal place or a difference of less than 0.01%.

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