Critical temperature of the Potts models on the kagomé lattice

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We investigate the Wu conjecture for the critical temperature of the Potts model on the kagomé lattice. Previous testing of this conjecture has been for small values of q. Our emphasis is on large values of q where we are able to obtain very accurate estimates of the critical temperature which show the conjecture itself to be very accurate for these q values but not exact.

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I. INTRODUCTION

For the q-state Potts model on the square, triangle, and hexagonal lattices one has simple polynomial expressions in the relevant variables which give the exact critical temperature T_c for these models. This has rigorously been shown to be the case at least for $q \geqslant 4$ and $q=2$. For other q values the expressions giving the critical temperature are thought to be exact but have not been proven to be so. However, in the case of the kagomé lattice except for the case of $q=2$, similar results are not available. For this reason there has been special interest in this system for some time. In 1979, Wu [1] presented a polynomial that he conjectured, and which we will denote as the Wu conjecture, gives the exact critical temperature for these systems. Subsequently, Enting and Wu [2] showed that the conjecture cannot hold in certain regions where antiferromagnetic interactions are present. Very recently, 1998, Chen, Hu, and Wu [3] state that "it still needs to be tested, ..., whether the Wu conjecture holds in the ferromagnetic region." Other authors, e.g., Jensen, Guttmann, and Enting [4] believe testing has shown that the conjecture gives very accurate but not exact results.

In addition to the Wu conjecture Tsallis [5] has proposed a different expression for finding the critical temperature. This has been shown rather definitely not to be the exact expression and not to be as accurate as the Wu conjecture.

All of the testing of either conjecture has thus far consisted of looking at small q values in particular for $q=1,3$, or 4 cases (for the $q=2$ case both conjectures are known to be correct). Our emphasis will be on the case of large q values. In this case our approximation method becomes very accurate and we show that the results given by the Wu conjecture though very accurate are not exact. Furthermore, our estimates of the critical temperature may give workers in the future additional information on which to judge any new conjectures for this system.

Our results are based on a generalization of the Bethe approximation which uses a Cayley tree to approximate the lattice being considered. The Cayley tree is constructed of pairs of spins and the nearest-neighbor, n.n., interaction between them. Hence a pair of spins and the n.n. interaction is the basic building block of the Cayley tree. We replace this basic building block of the tree with a collection of spins and the appropriate interactions between these spins. As a particular example in one of our approximations, we consider a collection of three spins forming one of the triangles of the kagomé lattice and the three n.n. interactions between them as the basic building block. We then build a tree structure by starting with a triangle and attaching new triangles of spins to corners of the original triangle. Continuing with this process we build a larger and larger tree structure. A tree structure of this nature, made up of polygons, is known as an Husimi tree. Just as the Bethe approximation can be analyzed through a dynamical systems approach following the step by step construction of a Cayley tree, the approximation presented here can be analyzed through a dynamical systems approach following the step by step construction of a Husimi tree. However, here something of the essential nature of whatever lattice being approximated becomes part of the basic building block and hence the approximation is better, sometimes not just quantitatively but qualitatively better as in the case of the antiferromagnetic Ising model on the triangle lattice see Ref. [6], than that obtained by the Bethe approximation.

This approach allows for a number of interesting features to be explored [7,8] and can be used to estimate not only the critical temperature but also critical exponents [9] for a variety of models. Here we use only the most elementary approach, but nevertheless, we can make some definite statements regarding the Wu conjecture. This is basically due to two features of the approximation. First, as stated earlier, when q increases the accuracy of our approximation increases. Pearce and Griffiths [10] have in fact proven that in the limit of q becoming infinite the mean-field approximation becomes exact. The Bethe approximation is an improvement on the mean field and our Husimi tree approximations are improvements on the Bethe approximation so that in this limit our results should also become exact. It should be pointed out that we have not proven this in any rigorous sense as was done specifically for the mean-field approximation by Pearce and Griffiths. Second, in our situation the estimate we obtain for the critical temperature is larger than the true critical temperature, and hence acts as an upper bound on it. This is related to the results of Krinsky [11] where it is proven that for the nearest-neighbor Ising model the magnetization, and hence the critical temperature given by the Bethe approximation is an upper bound on the exact results. A series of approximations made by the Husimi tree approach for the two-dimensional Ising model [9] as well as for higher spin Ising models [8,12] illustrate this feature, i.e., that one obtains estimates of the critical temperature which

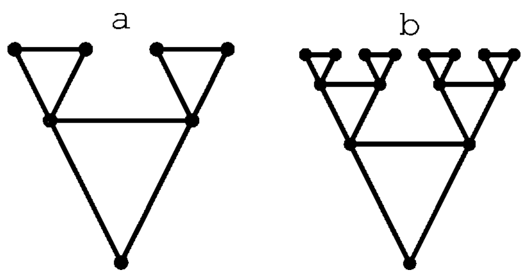

FIG. 1. First and second generation branches for option *A*.

are too high, although again we have no rigorous proof that this is always the case.

The Hamiltonian for the Potts model system under consideration here is

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

where $s=1,2,3,\ldots,q$, the sum is over the nearest-neighbor pairs on the kagomé lattice, and $\delta(x,y)$ is the usual Kronecker delta equal to one if $x=y$ otherwise zero. As stated above we will approximate our lattice spin system by constructing a Husimi tree. Also as mentioned above for our simplest and also least accurate approximation we take as the basic building block of our tree a collection of three spins forming a triangle. A single such building block will be denoted as a zeroth generation branch. To construct the first generation branch we connect two new basic building blocks, one to each of the top sites of the zeroth generation tree, as shown in Fig. 1(a). To construct the second generation branch we make connections at the top 4 sites of the first generation branch. The second generation branch is shown in Fig. 1(b). We can obviously continue this construction *ad infinitum* thereby creating an infinite system which can have a phase transition. This particular Husimi tree we label as option *A*. More detail for this type approach can be found in Ref. [9] where a very similar approach was taken for the lowest level approximation of the Ising model on the square lattice the difference being that a square rather than a triangle was the basic building block. Just as in Ref. [9], a discrete map governing the behavior of this system can be constructed and the fixed point behavior of this discrete map determines the behavior of the system including the critical temperature of the system.

Of course other choices for the basic building block can be made and an obvious one for approximating the kagomé lattice is shown in Fig. 2. Here, as before we refer to the single basic bulding block as the zeroth generation branch and we construct the first generation branch by connecting at 5 of the 6 outer sites another basic building block. Again this can be done *ad infinitum* thereby producing an infinite system and again a discrete map can be derived based on this construction which governs the behavior of the system. A system constructed with the basic building block of Fig. 2 we label as option *B*.

In Table I we list for a large number of q values the critical temperature as given by the Wu conjecture, as given by a Husimi tree using option *A* and as given by a Husimi tree using option *B*. In addition we calculate the percentage difference between the Wu conjecture critical temperature and that of option *A* or *B* with the percentage difference calculated according to

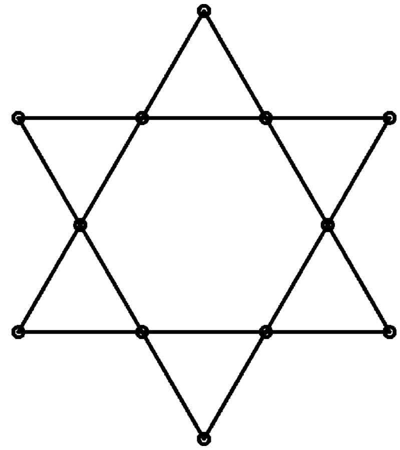

FIG. 2. The basic building block for option *B*.

$$\frac{(\text{option estimate-Wu conjecture})}{(\text{Wu conjecture})}\times 100. \tag{2}$$

We remark that our approximations for the smaller q values, $q\leqslant 4$, do not even begin to approach the accuracy of the results of Jensen *et al.* [4] or Chen *et al.* [3], where their estimates for T_c with $q=3$ are 0.946 06(13) and 0.946 55(18), respectively, where our own is 1.009 5 using option *B*. For these lower values of q the approach given in Ref. [9] where a series of Husimi trees are investigated and a critical temperature obtained using various extrapolation methods can be obtained could be used. For the square lattice Ising model estimates within 0.003% of the exact value were obtained using this approach [9]. However, for large q values it is not feasible due to the extremely large number of configurations one needs to sum over. The more elaborate methods of Ref. [9] are not needed here since as stated earlier as q increases our results become much more accurate because of the fact that our approximations are mean field in nature and as $q\rightarrow\infty$ even the basic mean-field approximation becomes exact [10].

From Table I we see immediately several features, the most important one being that for either option *A* or *B* if one lets the value of q increase sufficiently one reaches a region where the critical temperature given by the Wu conjecture is larger than that given by the Husimi tree approach. Since all evidence supports the fact that the Husimi tree approach gives an upper bound for T_c, this means that the Wu conjecture is not giving us the exact value. One also sees, especially for the largest q values, a very very small difference between our approximate values for T_c and the Wu conjecture values indicating both are very accurate for large q values. The accuracy of the Wu conjecture for small q values has already been well established and in fact as suggested in Ref. [3] may be exact being that the error in some of the

TABLE I. Critical temperatures based on the Wu conjecture, option *A*, and option *B*, along with the percentage differences.

q	T_c(Wu conjecture)	T_c(option A)	% difference	T_c(option B)	% difference
4	0.870129	0.911629	4.769	0.905451	4.059
8	0.719722	0.730843	1.545	0.728723	1.251
16	0.605742	0.608627	0.476	0.607915	0.359
30	0.525255	0.526014	0.145	0.525767	0.098
60	0.455062	0.455185	0.0270	0.455113	0.011
80	0.430429	0.430469	0.00929	0.430426	−0.0008
120	0.399385	0.399375	−0.00250	0.399356	−0.007
160	0.379637	0.379615	−0.00580	0.379604	−0.009
200	0.365469	0.365445	−0.00657	0.365438	−0.0085
440	0.322215	0.322197	−0.00559		
600	0.307659	0.307646	−0.00439		
1000	0.286165	0.286157	−0.00295		

earlier estimates of T_c may have been taken to be too small. Here we do not know the error involved in our approximate values for T_c, but as stated above we believe that these are upper bounds and hence the exact value of the error is not relevant.

We also note that as expected the results using option *B* are more accurate than the results of option A due to the fact that option *B* more correctly approximates locally the structure of the kagomé lattice. Since the option *B* results are more accurate and these values more quickly are below the values given by the Wu conjecture than the option *A* results as q is increased, we believe that with still more accurate approximations this would occur for even lower q values and that actually for $q>2$ the results given by the Wu conjecture are slightly too high.

Estimates for $q>200$ are not given for option *B*. For both options the number of configurations that need to be summed over in constructing the maps governing the behavior of the approximations equals the value of q raised to the number of sites in the basic building block. Even for option *A* with $q>200$, a large number of configurations come into play for option *B* the number is such that the personal computer on which all computations were done was unable to handle the number of configurations with $q>200$.

Based on our results for large q, the results of Ziff and Suding [13] for $q=1$, and the results of Jensen, Guttmann, and Enting [4] for $q=3$ and 4 the Wu conjecture while giving very accurate results for all q values under estimates slightly the critical temperature for $0<q<2$ and over estimates slightly the critical temperature for $2<q<\infty$.

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