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Pecularities of Bethe-like approximations and long-range-interaction Ising models

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The mean-field approximation and the Bethe approximation are two of the most often used approximations when one wants to obtain approximations of the phase diagrams and the critical temperature of lattice spin systems. Both can and have often been generalized to produce what are known as cluster mean-field and Bethe approximations. Generally, three characteristics are associated with these approximations. First, they give upper bounds to the critical temperature; second, considering larger clusters will result in better approximations; and third, the Bethe approximation is better than the corresponding mean-field approximation. We show what we believe to be a rather surprising result that, for one-dimensional Ising models with algebraically decaying interactions falling off slowly enough, the Bethe cluster approximations violate all three of these characteristics.

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Very few of the many models in the statistical mechanics of phase transitions and critical phenomena have been solved exactly. Hence significant effort has gone into the development of approximation methods. Among the first of these was the Weiss theory of ferromagnetism [1] or the equivalent theory of Bragg and Williams [2] regarding the arrangement of atoms in an alloy. These theories are now generally denoted as mean-field approximations. As an improvement of these approximations—in particular, the Bragg-Williams approximation—Bethe [3] presented an approximation which more correctly took local fluctuations into account. This approximation is now generally known as the Bethe approximation. These approximations fall into a class of approximations known as closed form approximations and have been reviewed by Burley [4] when used to approximate lattice spin systems, which will be considered here.

The particular class of lattice spin systems considered here will consist of Ising model systems with pair interactions. The basic mean-field approximation for such systems can be characterized in the following manner. A site is selected, and the interactions of the Ising spin on this site with other spins in the system are each replaced with the mean-field interactions involving the mean-field magnetization m. Then a self-consistency condition, requiring that the thermal average of the spin being considered equals the mean-field magnetization m, is applied. This condition establishes a critical temperature. To generalize this approximation, one can, rather than fixing attention on a single site, treat a cluster of sites where interactions between a pair of spins inside the cluster are unchanged and only interactions between a spin inside the cluster and the one outside the cluster are replaced with a mean-field interaction. Two characteristics of this type of approximation are the following: (i) the critical temperature obtained is greater than the actual critical temperature and (ii) as the cluster size is increased the accuracy of the estimate of the critical temperature increases. We denote these characteristics as characteristics A and B, respectively. Characteristic A is a rigorously proven characteristic of this approximation. It was first proven by Griffiths [5] for a certain class of lattice spin systems and the mean-field approximation when one uses a single site. This class of systems has been greatly expanded and rather than just the critical temperature, which occurs when the external magnetic field is zero, being an upper bound, the magnetization for all non-negative magnetic fields has been shown to be an upper bound by Pearce [6]. Vigfusson [7] extended the proof of the magnetization being an upper bound to the general cluster mean-field approximation under rather general conditions and for a large class of lattice spin systems. We know of no rigorous proofs of characteristic B, but at the same time know of no exceptions to it, and believe it to be a strongly held belief.

We now focus our attention on the Bethe approximation and its generalizations that we denote as Bethe-type approximations. Since the original paper by Bethe, there have been several alternative ways to present the Bethe approximation besides the approach given in the original paper. One of these involves a Cayley tree and consideration of the behavior of the spins deep inside the tree. If the tree has a branching ratio of $z-1$, then the behavior of these spins is equivalent to that predicted by the original Bethe approximation for a system with z nearest-neighbor spins. See Ref. [8] for details. An even simpler approach, and one that is more like the cluster mean-field approach, consists of considering a central spin and its z nearest neighbors forming a cluster of $z+1$ spins. One replaces the nearest-neighbor interactions that the z spins on the perimeter of the cluster have with spins outside the cluster with mean-field interactions and then requires that the thermal average of the central spin equals that of one of the perimeter spins. In this way, one obtains the results of the Bethe approximation [9]. It is this latter approach that we will use, since it is the most easily generalized and, as previously stated, most like the cluster mean-field approach. When clusters other than a single site and its z nearest neighbors are considered, but the condition that the thermal average of the central spin of the cluster equal the thermal average of one of its nearest neighbors is still required, we will refer to the approximation as a Bethe-type approximation. Bethe-type approximations are generally assumed to have the same two characteristics described above for the mean-field approximations. Indeed, the very recent calculations by Behringer, Pleimling, and Hüller [10] involving systems of clusters for various two-dimensional and three-dimensional Ising and Potts models have these characteristics. For Ising spin systems having only nearest-neighbor pair interactions, Krinsky [11] has proven that the magnetization given by the Bethe approximation, i.e., taking the cluster as a single site and its z nearest neighbors, is an upper bound for the magnetization of the original system again for non-negative external magnetic fields.

There is a third characteristic which we believe to be widely held and it is that the Bethe-type approximation is an improvement of the corresponding mean-field approximation; by "corresponding" we mean when considering equal size clusters and only the consistency reqirements being the difference between the two approximations. Hereafter, we refer to this characteristic as characteristic C. Discussions of this can be found in the paper of Gujrati [12] and is stressed in Ref. [10] as well. To our knowledge, no exceptions have been shown to exist regarding characteristic C.

Besides the innate desire to be able to have an understanding of the characteristics that one has when dealing with an approximation as fundamental as the Bethe-type approximation, we point out that the behavior of these series approximations is critical when dealing with methods such as the coherent anomaly method of Suzuki [13] or the molecular field finite-size scaling recently presented by Behringer, Pleimling, and Hüller [10] where one hopes to extract very accurate estimates of the critical temperature and critical exponents of the systems by using a sequence of cluster approximations and various extrapolation methods. This is particularly stressed in Ref. [13].

We show in the following that all three characteristics presented above are not met by the Bethe-like approximations when dealing with a system that has been studied in great detail over the past three decades, namely, the one-dimensional Ising model with algebraically decaying interactions if the strength of the interaction falls off sufficiently slowly. In particular, we consider a one-dimensional lattice of sites, where on the ith site we have a spin variable $s_i = \pm 1$. The Hamiltonian of the system is

$$\mathcal{H} = -\sum_{\langle i,j\rangle} \frac{J}{|i-j|^{1+\sigma}} s_i s_j, \tag{1}$$

where $|i-j|$ represents the distance between sites i and j with the distance between adjacent sites set equal to 1. For a thorough review of what has been established for this set of Ising systems, see Refs. [14,15]. One of the main proven results for this system is that when $0 < \sigma \leqslant 1$ the system has been shown to have a phase transition. In particular, one has a line of phase transitions at $h=0$ for all $T < T_c$, where T_c (the Curie point) is a critical end point. Much effort has gone into determining the value of T_c using a large variety of techniques, see Ref. [14].

Here, we use the mean-field and the Bethe-type cluster approximations described above to determine T_c, and our interest is in determining characteristics of the Bethe-type approximations as described above. We will present approximations for T_c based on the use of various clusters, the smallest having only 3 sites and the largest 25 sites. As a specific example of the calculations performed, we consider the smallest cluster, i.e., the three-site cluster. As described above, the interactions between spins in the cluster are retained and only interactions between a spin inside the cluster with a spin outside the cluster are replaced. Hence, the Hamiltonian for the three-site cluster is

$$\mathcal{H} = -J[s_1 s_2 + s_2 s_3] - \frac{J}{2^{1+\sigma}} s_1 s_3 - \sum_{d=1}^{\infty} \left[\frac{J}{d^{1+\sigma}} + \frac{J}{(d+2)^{1+\sigma}} \right] [s_1 + s_3] m - 2\sum_{d=1}^{\infty} \frac{J}{(d+1)^{1+\sigma}} s_2 m, \tag{2}$$

where s_1, s_2, and s_3 are the three Ising spins of the cluster; the first term in the Hamiltonian has the nearest-neighbor interactions present, the second term has the one next-nearest-neighbor interaction, the third term contains all the mean-field interactions replacing interactions which s_1 and s_3 have with spins outside the cluster, and the fourth and final term contains all mean-field interactions replacing interactions which s_2 has with spins outside the cluster. Finally, m is the mean magnetization of a site outside the cluster. Using the above one can calculate the thermal average of s_1, s_2, or s_3. Then in the mean-field approximation one requires the thermal average of s_2 to be equal to m and in the Bethe-type approximation one requires the thermal average of s_2 to be equal to the thermal average of one of its nearest neighbors in this case, either s_1 or s_3, the two are by symmetry equivalent. For larger clusters one could in the Bethe-type approximation choose to take the central site and require its thermal average to equal the thermal average of some site other than one of the nearest-neighbor sites of the central site, but we have not done so in this paper.

In all the cases, we have used MATHEMATICA to generate the appropriate expressions for the magnetizations of the appropriate sites and numerically determined the critical temperature as described above. All calculations have been done on a personal computer. Using MATHEMATICA one can obtain the critical temperature approximation based on a specific cluster to arbitrary accuracy. For the case of $\sigma = 0.1$ one has for a three-site cluster, using the mean-field approach, a value of $21.078\,195\,05\ldots$ for T_c. We use the three-site cluster because we want to compare this value with the corresponding Bethe-like approximation, and the smallest cluster for this is a three-site cluster. Using the Bethe-type approximation one obtains $19.697\,564\,42\ldots.$ Luijten and Blöte [14], using a sophisticated Monte Carlo approach along with finite-size scaling, obtained for T_c a value of $21.000\,99 \pm 0.000\,26$. The present author [16] obtained the almost identical result, specifically $T_c = 21.000\,97$, using a combination of cluster mean-field approximations and the Vanden Broeck and Schwartz extrapolation procedure. Hence, one can see immediately that for this case, i.e., $\sigma = 0.1$, characteristics A and C do not apply to the Bethe approximation. Here, the Bethe approximation is below the actual T_c and the Bethe approximation gives a poorer and not a better estimate of T_c. Of course, this holds for a range

TABLE I. Critical temperature estimates. The first estimates being the three-site Bethe approximation values, the second Monte Carlo and finite-size scaling from Refs. [14,17,18], and the third estimates using the coherent anomaly method (CAM) results given in Ref. [19].

	$\sigma=0.1$	$\sigma=0.2$	$\sigma=0.3$	$\sigma=0.4$	$\sigma=0.5$
Bethe	19.6975 . . .	9.7369 . . .	6.4395 . . .	4.8054 . . .	3.8349 . . .
Monte Carlo	21.00099	10.84229	7.3470	5.5203	4.3638
	± 0.00026	± 0.00026	± 0.0001	± 0.0001	± 0.0001
CAM results [19]	10.791	10.791	7.298	5.492	4.363
	$\sigma=0.6$	$\sigma=0.7$	$\sigma=0.8$	$\sigma=0.9$	$\sigma=1$
Bethe	3.1949 . . .	2.7428 . . .	2.4073 . . .	2.1490 . . .	1.9443 . . .
Monte Carlo	3.540	2.926	2.431	2.002	1.5257
	± 0.006	± 0.006	± 0.004	± 0.002	
CAM results [19]	3.577	2.987	2.517	2.116	1.750

of σ values not just $\sigma=0.1$. However for $\sigma=1.0$, the Bethe approximation gives as an estimate of 1.944 379 . . . for T_c, while the corresponding mean-field approximation gives 2.797 843 . . . . Both are greater than the actual value of T_c, which has been estimated using a wide variety of methods with a rather large spread of values, but most recently has been estimated to be 1.5256 ± 0.001 [17]. Thus, here both characteristics *A* and *C* hold.

Since for low values of σ in the interval (0,1] for the three-site cluster, the Bethe-type approximation gives estimates below the actual value and at the upper end of the interval it gives estimates which are too large; at some point in the interval it must be exact. Unfortunately, we have been unable to analytically determine that point. Numerically, one can by comparing the Bethe approximation with estimates by other means, as done in Table I, see that this occurs in the interval $0.8<\sigma<0.9$.

We now discuss characteristic *B*. In doing so, we investigate the behavior of the estimates of the critical temperature as the size of the clusters is varied. We know of no previously discussed situation where using the mean-field cluster approximation, considering larger clusters, does not improve the estimate. The same is true of the cluster Bethe-like approximations. In particular, the results of Behringer, Pleimling, Hüller [10], as well as Suzuki [20] show that for nearest-neighbor models and Bethe-type approximations, as the cluster increases in size, the estimates increase in accuracy. This is true as well for many values of σ in the interval (0,1], but by no means for all values. If it were true, we could have determined σ for which the Bethe-like approximation is exact, and that approximation would have to be independent of the size of the system being exact for all clusters.

One finds, for the lower values of σ in the interval (0,1], the estimates of T_c increase as the cluster size increases, hence converging monotonically toward the exact value. Actually, we have no general proof of this, but see it to be the case for the cluster sizes which we are able to investigate. These involve clusters involving as many as 25 sites. The estimates for various cluster sizes for $\sigma=0.1$ are presented in Table II. For σ values at the high end of the interval (0,1], one finds that with increasing cluster sizes the estimates for T_c increase in accuracy, although now converging monotonically from above rather than below which occurs for small σ values. As an example of this, the estimates for various cluster sizes for $\sigma=0.9$ are presented in Table II.

TABLE II. Critical temperature approximations for clusters from 3 to 25 sites for a variety of σ values, all based on the Bethe-type approximation scheme.

Number of cluster sites	$\sigma=0.1$	$\sigma=0.7$	$\sigma=0.77$	$\sigma=0.8$	$\sigma=0.9$
3	19.6975 . . .	2.74280 . . .	2.49847 . . .	2.40733 . . .	2.14906 . . .
5	20.1954 . . .	2.77287 . . .	2.50382 . . .	2.40308 . . .	2.11650 . . .
7	20.4056 . . .	2.78749 . . .	2.50369 . . .	2.39710 . . .	2.09285 . . .
9	20.5244 . . .	2.79792 . . .	2.50402 . . .	2.39333 . . .	2.07647 . . .
11	20.6016 . . .	2.80620 . . .	2.50483 . . .	2.39107 . . .	2.06456 . . .
13	20.6561 . . .	2.81307 . . .	2.50592 . . .	2.38974 . . .	2.05552 . . .
15	20.6968 . . .	2.81893 . . .	2.50714 . . .	2.38900 . . .	2.04841 . . .
17	20.7284 . . .	2.82401 . . .	2.50841 . . .	2.38864 . . .	2.04267 . . .
19	20.7536 . . .	2.82848 . . .	2.50968 . . .	2.38852 . . .	2.03793 . . .
21	20.7744 . . .	2.83246 . . .	2.51092 . . .	2.38857 . . .	2.03396 . . .
23	20.7917 . . .	2.83602 . . .	2.51213 . . .	2.38874 . . .	2.03057 . . .
25	20.8065 . . .	2.83924 . . .	2.51329 . . .	2.38898 . . .	2.02765 . . .

It is, in general, the region of $\sigma = 0.7$ to $\sigma = 0.85$ where increasing cluster sizes does not result in necessarily more accurate estimates for T_c. Results for $\sigma = 0.7$, $\sigma = 0.77$, and $\sigma = 0.8$ are given in Table II where one finds the estimates for T_c increasing and decreasing as the cluster size is increased. In particular, we examine the case where $\sigma = 0.77$ and observe what happens when one goes from the five-site cluster estimate of $T_c = 2.503\,82\ldots$ to the seven-site cluster estimate where the estimate drops to $T_c = 2.503\,69\ldots$; then if the actual T_c is greater than the average of the estimates based on the five- and seven-site clusters, i.e., $T_c = 2.503\,75\ldots$, then when one goes from the five- to the seven-site estimate one decreases the accuracy of the estimate. However, when one goes from the seven- to the nine-site estimate of $T_c = 2.504\,02\ldots$, an increase in the value, if T_c is less than the average of the two estimates, i.e., less than $2.503\,85\ldots$, then one has a less accurate estimate given by the nine-site cluster than the seven-site cluster. Since T_c must be greater than $2.503\,75\ldots$ or less than $2.503\,85\ldots$, one of the transitions from the five- to the seven-site estimates or from the seven- to the nine-site estimates is such that we go from a better to a poorer approximation despite increasing the size of the system, and the generally correct characteristic B is not correct in this case.

The general behavior of the approximations in the region of $\sigma = 0.7$ to $\sigma = 0.85$ is quite varied. In the case of $\sigma = 0.77$, as one increases the cluster size, the T_c estimates increase in value from the three- to the five-site cluster, then decrease from the five- to the seven-site cluster, increase from the seven- to the nine-site cluster, and thereafter increase for all clusters up to the largest cluster of 25 sites investigated here. However for the case of $\sigma = 0.8$, the estimates decrease in value as the cluster size is increased until one reaches the 19-site cluster and then beyond that the estimates increase in value again at least for clusters having as many as 25 sites.

The above shows that the three commonly held characteristics discussed above and denoted as characteristics A, B, and C are found not to hold for Bethe-type approximations of various algebraically decaying, long-range, ferromagnetic, pair interaction Ising models. This is, to the best of our knowledge, the first time this has been shown, to be the case, and is of interest not only because of the fact that Bethe-like approximations are used so often and one would wish to fully understand their characteristics but also because the cluster type generalizations can and have been used in various extrapolation methods to get accurate estimates of the critical temperature and critical exponents.

Ideally, we would like to be able to present some very specific criteria for when the characteristics generally met by Bethe-type approximations are valid and when they are not. Unfortunately, at present, we are unable to do so. Generally, both the mean-field and Bethe-type approximations neglect flucuations which work against having a phase transition, and because of this give estimates for the critical temperature which are too high. Ordinarily considering larger clusters means that these fluctuations are more properly treated and a lower and hence better estimate for T_c is obtained. In the case of very long-range interactions being present, these fluctuations are not as dominant, due specifically to the long-range nature of the interaction, and the above shows that the Bethe-type approximation overestimates rather than underestimates the effect of the fluctuations, thereby producing too low an estimate of T_c.

[1] P.R. Weiss, J. Phys. Radium **6**, 661 (1907).

[2] W.L. Bragg and E.J. Williams, Proc. R. Soc. London, Ser. A **145**, 699 (1934).

[3] H.A. Bethe, Proc. R. Soc. London, Ser. A **150**, 552 (1935).

[4] D.M. Burley, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M.S. Green (Academic, New York, 1972), Vol. 2.

[5] R.B. Griffiths, Commun. Math. Phys. **6**, 121 (1967).

[6] P.A. Pearce, J. Stat. Phys. **25**, 309 (1981).

[7] J.O. Vigfusson, Lett. Math. Phys. **10**, 71 (1985).

[8] R.J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic, New York, 1982).

[9] M. Suzuki, J. Phys. Soc. Jpn. **55**, 4205 (1986).

[10] H. Behringer, M. Pleimling, and A. Hüller, Eur. Phys. J. B **31**, 81 (2003).

[11] S. Krinsky, Phys. Rev. B **11**, 1970 (1975).

[12] P.D. Gujrati, Phys. Rev. Lett. **74**, 809 (1995).

[13] M. Suzuki, *Coherent Anomaly Method* (World Scientific, Singapore, 1995), p. 17.

[14] E. Luijten and H.W.J. Blöte, Phys. Rev. B **56**, 8945 (1997).

[15] M. Aizenman, J.T. Chayes, L. Chayes, and C.M. Newman, J. Stat. Phys. **50**, 1 (1988).

[16] J.L. Monroe, J. Phys. A: Math. Gen. **31**, 9809 (1998).

[17] E. Luijten and H. Meßingfeld, Phys. Rev. Lett. **86**, 5305 (2001).

[18] K. Uzelac, Z. Glumac, and A. Aničić, Phys. Rev. E **63**, 037101 (2001).

[19] J.L. Monroe, R. Lucente, and J. Hourlland, J. Phys. A **23**, 2555 (1990).

[20] M. Suzuki, M. Katori, and X. Hu, J. Phys. Soc. Jpn. **56**, 3092 (1987).