Behavior of the critical temperature of Ising thin films with variable surface magnetic moments

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Properties of magnetic thin films are of considerable interest both for applied as well as theoretical reasons. I study the behavior of Ising thin films through the use of layered Bethe lattices and Husimi trees. In particular the behavior of the critical temperature both as a function of the number of layers and as a function of variable magnetic moments of surface spins is presented. The later is motivated by that fact that such variation has been found to occur in physical systems such as Ni and Fe free surfaces and Ni/Co interfaces. The approach used is more accurate than many previously used and most importantly shows a different qualitative behavior of the critical temperature from previous studies.

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I. INTRODUCTION

The magnetic properties of thin films have been of considerable interest for some time due to both the extremely important practical applications (see [1,2], and references therein) and as well as fundamental theoretical questions related to them (see [3,4], and references therein).

On the theoretical side, Ballentine [5], who estimated the critical temperature of a bilayer Ising model, began to study the critical phenomena of layered systems. Since then many extensions and variations of this very simple system have appeared, with many of these of interest because of their relation to specific physical systems. One such extension involves systems where the magnetic moments of the surface spins differ from that of nonsurface spins. It has been shown by Jensen, Dreysse, and Bennemann [6] that several physical systems appear to have layer-dependent magnetic moments. They have studied by mean-field theory some of the effects these variations have on the critical properties of these systems. More recently Ilkovic [7], using a reaction field approximation, has looked at similar systems.

The present paper focuses on the cases studied in [6,7]. The method used here to study such systems is an extension of one used by the present author [8] and, in a slightly less general manner, by Hu, Izmailian, and Oganesyan [9] to approximate the bilayer Ising spin system. The method consists of a dynamical systems approach to obtain the critical temperature of a system of layered Bethe lattices or Husimi trees. One obtains a Bethe-like approximation and such approximations, as pointed out in [10], produce an approximation generally more accurate than that of the mean-field approximation (hereafter MFA). That this is the case is of particular interest here in that our approximation, while giving generally more accurate quantitative results, also differs qualitatively in one important aspect from what has been found previously. This difference and the comparison of our results to previous results is given in Sec. III after presenting in Sec. II notation and details of the models. Conclusions along with possible other avenues of interest are presented in Sec. IV.

II. MODEL & GENERAL METHOD OF STUDY

I consider Ising model systems where the generic Hamiltonian of the system is

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

with s_i the spin variable on the ith site and $s_i = \pm 1$ [for this particular study this will not be the case for surface sites (see below)]. The first sum is over all nearest-neighbor pairs and the second sum is over all sites. For simplicity, J, as well as the Boltzmann constant, k, will be set equal to one. Only ferromagnetic systems will be considered here, in which case a phase transition occurs only for $h=0$.

Ideally I would like to directly consider n layers of a square lattice, Ising model. However, even for the bilayer system, one is forced to use various approximation methods. In the following this will be done primarily by considering an extension of the usual Bethe lattice approach which consists of looking at an Ising model system on a Cayley tree with branching ratio γ. To approximate the thin film system of n layers I take n Bethe lattices and couple them together with interlayer interactions. Previously this has been done only for the case of $n=2$ [6,9]. This is the primary approximation (hereafter denoted BLA) used in this paper to approximate an n-layered system.

As stated earlier using the BLA compared to the MFA, one expects a better approximation. However, a still better approximation can be obtained by using what is known as an Husimi tree approach (hereafter HTA) The simplest Husimi tree for approximating a square lattice system can be constructed in the following manner. Begin with a four-site system with the sites on the corners of a square. Now on each of the corners attach another four-site square system, and then on the new corners attach still other four-site square systems. Continue doing this infinitely many times. This system would then approximate a square lattice Ising model and this HTA is a better approximation than the BLA to the square lattice Ising model [11]. One would expect this improvement could carry over as well to the n-layer systems.

For the BLA there are a number of techniques that allow one to obtain the critical temperature, T_c. One such technique involves a dynamical system approach. This was presented for a single-layer Bethe lattice system by Eggarter [12] and has been extended and used in connection with single-layer Husimi trees by the present author to look at multisite inter-

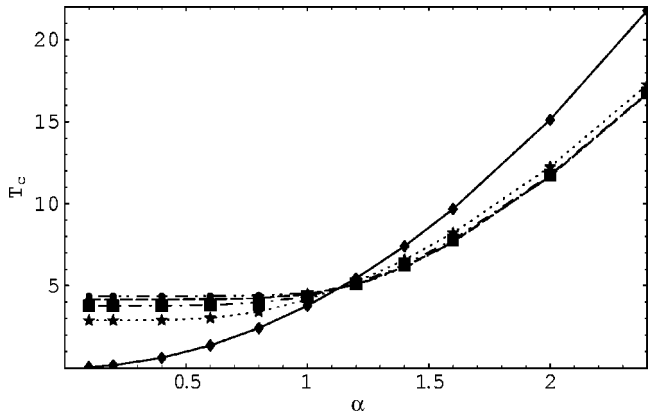

FIG. 1. T_c vs α for $n=2$-, 3-, 4-, 5-, and 6-layer systems with the spins on both surfaces taking on values $\pm\alpha$. For small α, T_c increases significantly as n increases so one can easily distinguish the $n=2$, 3, 4, 5, and 6 cases.

action systems [15], frustrated systems [16], and higher spin systems [17,18], etc. Just as a single-layer system, whether using a Bethe lattice or Husimi tree, can be thought of as being built up in a step-by-step fashion resulting in a discrete dynamical system, so can an n-layer system. Since the basic method is presented in numerous previous papers, see e.g., [13–15], it has not been presented here. Here I look at n, $n \geqslant 2$, layers of Bethe lattices or Husimi trees.

The mathematical mechanism present in this approach, which corresponds to the occurrence of a phase transition for the layered systems, is the same as it is for other ferromagnetic systems studied in the past, see Sec. II of Ref. [13]. At high temperatures there is a single, attracting, real-valued, fixed point that corresponds to the disordered state. As the temperature is lowered, one reaches a point where this fixed point becomes repelling and two new, attracting, fixed points are created, one corresponding to a positive and one to a negative spontaneous magnetization. The temperature at which this changeover occurs is T_c, and can be found to arbitrary numerical precision using a program such as MATHEMATICA. Here MATHEMATICA not only constructs the dynamical system but finds the fixed points and determines if they are repelling or attracting by constructing the Jacobian of the dynamical system.

III. VARIATION OF BOTH SURFACE MAGNETIC MOMENTS

In this section results are presented where following Jensen, Dreysse, and Bennemann [7], the magnetic moments of the spins on both surfaces of an n-layer system take on the values $\pm\alpha$ as opposed to all other spins which take on the values ± 1.

In Fig. 1 are plotted the T_c values as a function of α for systems consisting of n-layered Bethe lattices with $\gamma=3$ and $2 \leqslant n \leqslant 6$. This figure should be compared to Fig. 8 of [7], which shows results using the reaction field approximation (hereafter RFA) for n-layered systems with $n=3$, 5, and 10. Their variable r is equivalent to my variable α. The results in [7] are for a layered face-centered cubic lattice rather than the layered simple cubic lattice studied here; nevertheless qualitatively the two figures look identical. Specifically one sees, if α is less than some value, what I will temporarily denote as α_c, that T_c increases as n increases, while for $\alpha > \alpha_c$, the opposite occurs. They are not, however, qualitatively the same. The difference will be presented after discussion of the more obvious similarities.

To gain some perspective on the accuracy of the results one can begin by looking at the value of T_c at α_c. This value of T_c is the approximation's equivalent to the critical temperature of the bulk system since at α_c increases in the number of layers have no effect on T_c. As stated the system studied in [8] is a slice of the fcc lattice. Here for nonsurface sites there are 12 nearest-neighbor sites and for the bulk system the MFA gives $T_c=12$. As Ilkovic points out in [8] the RFA is an improvement over the MFA. The MFA of the T_c can be shown rigorously to be an upper bound on the true critical temperature [17]. The reaction field approximation at α_c gives $T_c=10.898$ [8] while series expansion result for T_c for the bulk are $T_c \cong 9.796$ [18] with an 11.2% difference. In the case of a simple cubic lattice the MFA gives $T_c=6$. A crude reading of Fig. 1 gives $T_c \cong 4.79$ and the series expansion estimates for this system gives $T_c \cong 4.511$ [18] the latter two differing by only 6.2%.

It is worth noting here that Lin, Che, and Xia [19] attribute to Allan [20] a Bethe approximation for the n-layer system of square lattices restricted to the case of $\alpha=1$. However, this is not the approximation used here. Allan modifies the usual nonlayer Bethe approximation where the critical temperature is given by

$$\tanh[J/kT_c] = 1/(q-1), \tag{2}$$

and where q is the coordination number of the system being approximated, $q=6$ in our case, by substituting for $q=6$ the value of the mean coordination number for the n-layered system which for n-layered square lattices is

$$q_{ave} = (6n-2)/n. \tag{3}$$

This gives easy approximations for any n. However, the approximations are less accurate than those found using my layer BLA, giving, for example, for $n=3$, $T_c \cong 4.255$ while the approximation method presented here gives $T_c \cong 4.159$. This should be compared to the series expansion results [21], which give $T_c \cong 3.647 \pm 0.005$.

In addition to the T_c values, mention needs to be made of the values of α_c. A straight-forward MFA for the both the simple cubic lattice or the face-centered cubic lattice gives $\alpha_c = 6/5$. For the MFA to these layered systems one obtains a set of simultaneous equations which must be solved. These are a simple generalization of Eq. (2) of [22]. Consideration of what has been presented thus far might cause one to wonder why there is even such a thing as an α_c. The author knows of no *a priori* reason for such behavior. Furthermore, seeing that for both the sc and fcc lattice the α_c value given by the MFA takes on the same numerical value, it raises the possibility that the MFA may be unable to distinguish certain differences much as it predicts the same T_c value for both the simple cubic lattice and the triangle lattice. When one goes to the RFA, one sees the value of α_c decrease in value, Ilk-

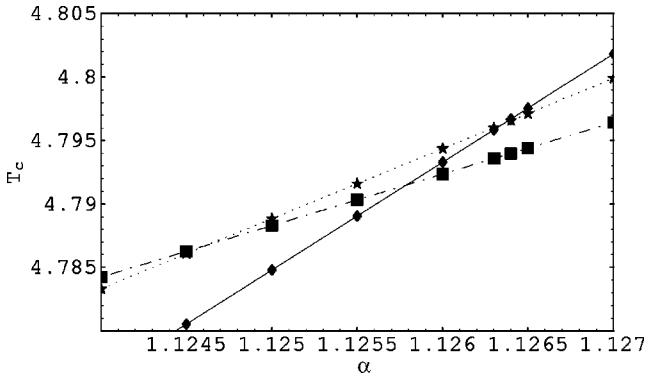

FIG. 2. Magnified view of Fig. 1 in the vicinity of crossover values of T_c but showing only the T_c values for $n=2$ (solid line), 3 (dotted line), and 4 (dot-dashed line). Lines are drawn to guide the eye.

ovic in [8] gives $\alpha_c=1.177$, but nevertheless an α_c. What is found using the layered BLA is quite different. The appearance of an α_c value occurs only because of the scale of Fig. 1. Qualitative results of this approach are seen in Fig. 2 where a magnified view of the situation around the area that appears to be α_c of Fig. 1 is presented. There is, in fact, no α_c where T_c is independent of the thickness of the layer. Rather there is a region around $\alpha=1.125$ where one layer system's T_c may equal that of another layer. Specifically the T_c line for the $n=2$ case crosses the T_c line for the $n=3$ case at a point I will denote as α_{2-3} and similarly there is an α_{3-4}, etc. One has that T_c decreases at the $\alpha_{k-(k+1)}$ crossover points as k increases, thereby moving closer to the bulk T_c. Numerical estimates of T_c in the crossover region are given in Table I for the BLA.

More accurate results are obtained through the use of the Husimi tree approach. The results for these systems are qualitatively the same as in the layered Bethe lattice case; in particular there exists no single α_c but rather a series of $\alpha_{k-(k+1)}$ values. T_c values are shifted lower closer to accurate series expansion values when available. Numerical estimates of T_c, using n-layered Husimi trees, for the crossover region are given in Table II.

While I know of no rigorous proof that a single α_c value cannot exist, the fact that the HTA is more accurate than the BLA, which is more accurate than the MFA, which has been

TABLE I. T_c estimates as a function of α with spins on both surfaces taking on the value $\pm\alpha$ for the region of α values where crossover occurs. Estimates are based on n-layer Bethe lattices.

	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$
$\alpha=1.1264$	4.7967	4.7966			
$\alpha=1.1263$	4.7959	4.7960			
$\alpha=1.1247$		4.7872	4.7871		
$\alpha=1.1246$		4.7866	4.7867		
$\alpha=1.1242$			4.7850	4.7850	
$\alpha=1.1241$			4.7846	4.7847	4.7847
$\alpha=1.1240$				4.7844	4.7844

TABLE II. T_c estimates as a function of α with spins on both surfaces taking on the value $\pm\alpha$ for the region of α values where crossover occurs. Estimates are based on n-layer Husimi lattices.

	$n=2$	$n=3$	$n=4$	$n=5$
$\alpha=1.1344$	4.73227	4.73218		
$\alpha=1.1343$	4.73144	4.73164		
$\alpha=1.1323$		4.72076	4.72070	
$\alpha=1.1322$		4.72021	4.72030	
$\alpha=1.1316$			4.71789	4.71781
$\alpha=1.1315$			4.71749	4.71749

demonstrated in [10,11,13–16] for a large variety of two-dimensional models supports the fact that the same is likely to be the case here for n-layer systems.

While the focus of this paper is when $\alpha\neq 1$, I conclude with some further comparisons for the $\alpha=1$ case, which is the most studied. In this case there exists a lengthy high temperature series and therefore rather accurate estimates of T_c. To gain some appreciation of the level of accuracy one finds for the $n=3$ case, in increasing order of accuracy, that the MFA gives $T_c\cong 5.414$, Alan's Bethe approximation gives $T_c\cong 4.255$, the layered BLA gives $T_c\cong 4.1591$, and the layered HTA using the simplest Husimi tree gives $T_c\cong 4.0641$. High temperature series expansion gives $T_c\cong 3.647\pm 0.005$. For larger values of n, similar results occur. As n increases, the layered system approaches presented here increase in accuracy when compared to the T_c values based on series expansion methods. This makes sense in that the layered systems used here are true layered systems and the approximation is really only the approximation of the individual layers.

Adjusting the values of the magnetic moments for both surfaces in some cases may not be appropriate, e.g., one surface of the film may be a free surface and the other may be attached to some substrate causing the magnetic moment on only one surface to differ from the bulk value. If α is small then there should be no qualitative change from what

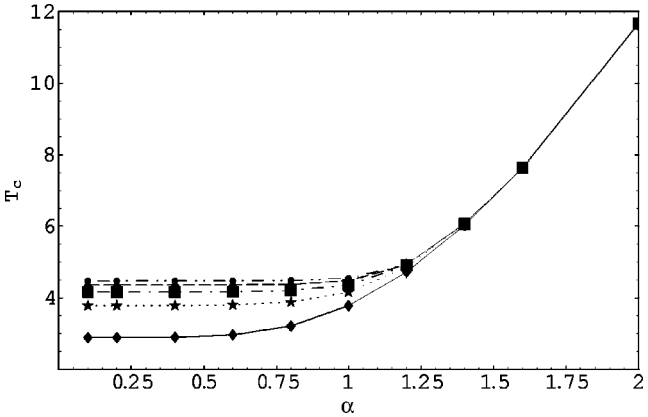

FIG. 3. T_c vs α for $n=2$-, 3-, 4-, 5-, and 6-layer systems with the spins on only one surface taking on values $\pm\alpha$. For small α, T_c increases significantly as n increases so one can easily distinguish the $n=2$, 3, 4, 5, and 6 cases.

was found in the previous situation involving both surfaces, i.e., the more layers the system has, the higher T_c. Here even if α is allowed to take on large values, the fact that only one surface, rather than two, has the enhanced magnetic spins means this may not be enough to produce the cross-over point where, if α is greater than this value, the system with the smaller number of layers actually has the higher critical temperature. This is, in fact, what the layered BLA has as a result. For all values of α the critical temperature is a monotonically increasing function of n. T_c as a function of α and with $n=2$, 3, 4, 5, and 6 is plotted in Fig. 3.

IV. CONCLUSION

In the above sections, systems of layered Bethe lattices or Husimi trees have been used to approximate T_c of n-layered, square-lattice, Ising models. Overall the method is one more example of many systems, examples and references given above, which can be approximated rather successfully by this approach. For the n-layered Ising systems investigated here the method gives a qualitatively different scenario for the behavior of T_c than that presented by other authors. I have tried to show that based on other successful approximations by these general methods one must at the very least consider that the special property of an α_c, at which T_c is independent of the number of layers, may be an artifact of previous methods and not a property of the real systems.

The method is rather robust and for the above systems a further increase in the accuracy of the approximations could be made by considering ever bigger basic building blocks for the layered Husimi tree case, which is something beyond the four-site square used above. In addition since one can generate a series of ever increasingly accurate approximations based on ever bigger basic building blocks for the tree one can use various extrapolation techniques on this series to gain even greater accuracy. For the $n=2$ case this has already been done and the estimates of the critical temperature are amongst the most accurate available [10] compared to five other methods used to approximate the bilayer system.

[1] M. T. Johnson, P. J. H. Bloemen, F. J. A. den Broeder, and J. J. de Vries, Rep. Prog. Phys. **59**, 1409 (1996).
[2] P. Poulopoulos and K. Baberschke, J. Phys.: Condens. Matter **11**, 9495 (1999).
[3] K. Binder, *Phase Transitions and Critical Phenomena* edited by C. Domb and M. S. Green (Academic, New York, 1983), Vol. 8.
[4] J. T. Ou, F. Wang, and D. L. Lin, Phys. Rev. E **56**, 2805 (1997).
[5] L. E. Ballantine, Physica (Amsterdam) **30**, 1231 (1964).
[6] P. J. Jensen, H. Dreysse, and K. H. Bennemann, Europhys. Lett. **18**, 463 (1992).
[7] V. Ilkovic, Thin Solid Films **312**, 280 (1999).
[8] J. L. Monroe, Physica A **335**, 563 (2004).
[9] C. K. Hu, N. Sh. Izmailian, and K. B. Oganesyan, Phys. Rev. E **59** 6489 (1999).
[10] P. D. Gujrati, Phys. Rev. Lett. **74**, 809 (1995).
[11] J. L. Monroe, Phys. Rev. E **64**, 016126 (2001).
[12] T. P. Eggarter, Phys. Rev. B **9**, 2989 (1974).
[13] J. L. Monroe, J. Stat. Phys. **65**, 255 (1991); **67**, 1185 (1992).
[14] J. L. Monroe, Physica A **256**, 217 (1998).
[15] J. L. Monroe, Phys. Rev. E **65**, 026109 (2002).
[16] J. L. Monroe, Phys. Rev. E **66**, 066129 (2002).
[17] J. O. Vigfusson, Lett. Math. Phys. **10**, 71 (1985).
[18] M. F. Sykes, D. S. Gaunt, P. D. Roberts, and J. A. Wyles, J. Phys. A **5**, 640 (1972).
[19] D. L. Lin, H. Che, and Y. Xia, Phys. Rev. A **46**, 1805 (1992).
[20] G. A. T. Allan, Phys. Rev. B **1**, 352 (1970).
[21] T. W. Capehart and M. E. Fisher, Phys. Rev. B **13**, 5021 (1976).
[22] X.-G. Wang, S.-H. Pan, and G.-Z. Yang, Solid State Commun. **113**, 59 (2000).