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Phase Diagrams of Ising Models on Husimi Trees. I. Pure Multisite Interaction Systems

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Lattice spin systems with multisite interactions have rich and interesting phase diagrams. We present some results for such systems involving Ising spins ($\sigma = \pm 1$) using a generalization of the Bethe lattice approximation. First, we show that our approach yields good approximations for the phase diagrams of some recently studied multisite interaction systems. Second, a multisite interaction system with competing interactions is investigated and a strong connection with results from the theory of dynamical systems is made. We exhibit a full bifurcation diagram, chaos, period-3 windows, etc., for the magnetization of the base site of this system.

KEY WORDS: Ising models; Husimi tree; dynamical systems; bifurcation; chaos.

1. INTRODUCTION

Phase transitions for lattice spin systems occurring when the external magnetic field h is zero are the norm. In fact, if one restricts the interactions to ferromagnetic pair interactions, the Lee–Yang circle theorem[1] establishes the fact that only at $h = 0$ can a phase transition occur for the usual spin variable $\sigma = \pm 1$. However, with multisite interactions present, which we will denote simply by MSI and where throughout the paper this will mean interactions involving *three or more sites*, this is not true. For example, in a very recent article by Heringa *et al.*[2] they show evidence through Monte Carlo calculations of phase transitions occurring at $h \neq 0$ for four different lattice spin models with MSIs and for two other systems their results were inconclusive. A partial list of other examples of systems with MSIs where phase transitions are found at $h \neq 0$ includes triangular

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lattice systems with pair and three-site interactions, which have been studied using a variety of approximation schemes,[3–5] as well as exact results such as those of Wu and Wu[6] for a Kagomé lattice with two- and three-site interactions and $h \neq 0$.

We divide examples of the above type into two general sets. All Ising spin systems involving only MSIs, i.e., all interactions involve three or more sites, with the exception of the interaction with the magnetic field, we refer to as pure MSI systems. All six systems of Ref. 2 fall into this category. We denote as mixed interaction systems those systems with both pair interactions and MSIs. References 3–6 involve such mixed interaction systems. The present paper considers only pure MSI systems.

Since exact solutions are generally unavailable, one relies on approximation schemes to gain at least a qualitatively correct picture of the phase diagram. The mean-field approximation is the approximation scheme most commonly used to investigate the phase diagram of a lattice spin system. One basically considers one spin of the system and the effect of the other spins is taken into account by an average molecular field, i.e., a mean field (see Chandler[7] for a detailed presentation). If one has a square lattice with nearest-neighbor pair interactions J_2, four-site interactions J_4 involving the sites on the corners of the elementary squares of the lattice, and an external magnetic field h, then one easily obtains an equation for determining the per-site magnetization m as

$$m = \tanh(4\beta J_2 m + 4\beta J_4 m^3 + \beta h) \tag{1}$$

where $\beta = 1/KT$. The phase diagram resulting from Eq. (1) has been discussed by Thompson.[8] For $J_2 = 0$ and $J_4 > 0$ one has the line of phase transitions in the h–T plane shown in Fig. 1. Yet for $J_2 = 0$ and $J_4 > 0$ this system is self-dual[9] and phase transitions if they occur should be along the line given by

$$\sinh(2\beta J_4)\sinh(2\beta h) = 1 \tag{2}$$

This was one of the systems investigated by Heringa *et al.*[2] The line given by Eq. (2) is shown in Fig. 1 along with the mean-field results. While for ferromagnetic pair interaction systems the mean-field approach presented above gives *qualitatively* correct phase diagrams, one sees that this is *not* the case for multisite interactions. There should occur a phase transition at only $T = 0$ for $h = 0$ according to Eq. (2), yet the mean-field result indicates a phase transition line at $h = 0$ for a substantial interval of the T axis.

In the following we investigate some pure MSI systems by considering a generalization of the Bethe approximation. We begin Section 2 by introducing our method and applying it to the above four-site interaction

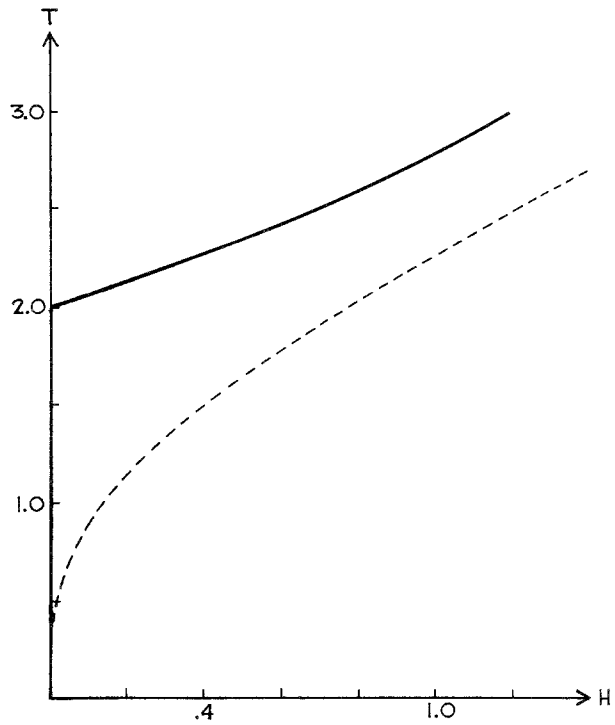


Fig. 1. A comparison of the phase diagram obtained from mean-field results (heavy solid line) and the self-dual line (dashed line) for a square lattice system with four-site interactions on the elementary square of the lattice.

system. As a further test of the method, we consider a self-dual three-site interaction system. We begin by considering the case of ferromagnetic interactions and for both systems we obtain qualitatively correct phase diagrams. In Section 3 we point out similarities between the method presented here and the approach taken by Thompson[10,11] for the Bethe lattice with pair interactions. The emphasis is on the connection that can be made to dynamical systems. This section also contains an introductory study of a multisite interaction system with frustration. Spin models with this characteristic have recently been of great interest. The axial next-nearest-neighbor Ising model, the ANNNI model, where frustration is due to competing pair interactions, has been intensely studied and a connection with dynamical system theory has been pointed out by a number of authors. This is, however, the first time, to our knowledge, that any results regarding multisite interaction models have been presented and here in particular the connection with results from the field of chaos and

dynamical systems is present. We illustrate this connection with magnetization plots showing the full range of period doublings, period-3 windows, etc. We conclude in Section 4 with a brief discussion of some future work.

2. SOME MSI SYSTEMS ON HUSIMI TREES

The Bethe approximation is in general an improvement on the mean-field approximation. For a system with pair interactions the Bethe approximation and the system of Ising spins on a Cayley tree are related, though not completely equivalent.[12] The two are equivalent if one considers only properties of sites deep within the tree and not near the surface. For this situation we will say we are dealing with a Bethe lattice rather than a Cayley tree, following the terminology suggested in Baxter.[13]

For pair interactions we can think of building up the Bethe lattice by taking $q-1$ pair interactions all involving one common site, which we denote as the base site. This structure we call the first-generation branch (see Fig. 2a). If we take $(q-1)$ first-generation branches and connect by a pair interaction each of their base sites to a new base site, we construct a second-generation branch (see Fig. 2b). Continuing this process, we develop higher-generation branches. In our last step to have each site, except the boundary sites, interacting with q neighboring sites we take q nth-generation branches and connect them by pair interactions to a final base site, which we label the 0th site and denote the system as a Bethe lattice and not a branch.

In the above the basic building blocks are the pair interactions. To approximate the four-site interaction system mentioned in the introduction we replace the pair interactions and their two sites with a four-site system

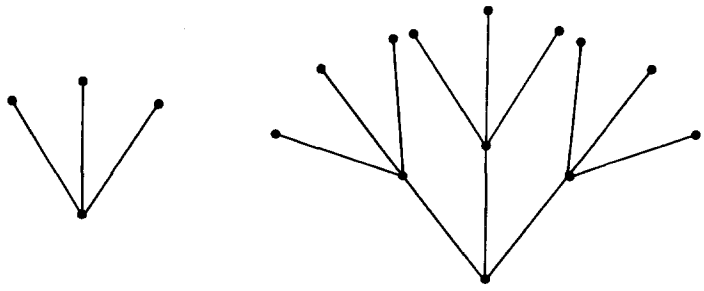


Fig. 2. (a) The first-generation branch and (b) the second-generation branch of the standard Cayley tree with $q=4$.

having a four-site interaction. Connecting $q-1$ such systems at a single base site results in a first-generation branch shown in Fig. 3a. Connecting $(q-1)$ first-generation branches to each site of a new four-site system, except the base site of this system, results in the second-generation branch shown in Fig. 3b. We continue this process to develop higher-generation branches. To complete the system, we connect q nth-generation branches at their base site (again the central site of the system we denote as the 0th site). In this manner we construct a pure Husimi tree.[23]

We calculate $\langle \sigma_0 \rangle$ following the method of Eggarter.[14] The calculation involves an iterative process following the steps discussed above to construct the lattice. We start with the 0th-generation branch, which is just a single four-site system. We designate a base site and calculate Λ_0, the partition function for this system. We divided Λ_0 into two parts,

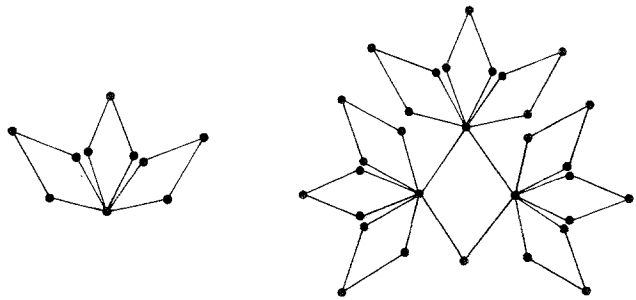
$$\Lambda_0 = \Lambda_0^+ + \Lambda_0^- \tag{3}$$

where Λ_0^+ (Λ_0^-) is the half of the partition function with the base-site spin variable $\sigma = +1$ (-1). Since the base site is the site to which we will be making attachments, the site is special and it is convenient to factor out the term involving this site's interaction with the magnetic field. Hence we write

$$\Lambda_0^+ = e^{\beta h}\lambda_0^+, \qquad \Lambda_0^- = e^{-\beta h}\lambda_0^- \tag{4}$$

thereby defining λ_0^+ and λ_0^-. For the first-generation branch we have $\Lambda_1^+ = e^{\beta h}\lambda_1^+$ and $\Lambda_1^- = e^{-\beta h}\lambda_1^-$, where

$$\begin{aligned}\lambda_1^+ = {} & e^{\beta J_4} e^{3\beta h}(\lambda_0^+)^{3(q-1)} + 3e^{-\beta J_4} e^{2\beta h}(\lambda_0^+)^{2(q-1)}(\lambda_0^-)^{(q-1)} \\ & + 3e^{\beta J_4} e^{-\beta h}(\lambda_0^+)^{(q-1)}(\lambda_0^-)^{2(q-1)} + e^{-\beta J_4} e^{-3\beta h}(\lambda_0^-)^{3(q-1)}\end{aligned} \tag{5}$$



(a) (b)

Fig. 3. (a) The first-generation branch and (b) the second-generation branch of Husimi tree lattice used to approximate the square lattice system with four-site interactions on the elementary squares of the lattice.

λ_1^- is the same except that all $e^{\beta J_4}$ are replaced by $e^{-\beta J_4}$ and vice versa. Hence we see that $\lambda_1^{\pm}$ terms are related to $\lambda_0^{\pm}$ terms by a recursion relation and $\lambda_n^{\pm}$ terms are related to $\lambda_{n-1}^{\pm}$ terms by the same recursion relation.

If one wants to calculate the thermal average of the base site of the nth-generation branch, $\langle \sigma_{\text{base}} \rangle_n$, one has

$$\langle \sigma_{\text{base}} \rangle_n = \frac{e^{\beta h}\lambda_n^+ - e^{-\beta h}\lambda_n^-}{e^{\beta h}\lambda_n^+ + e^{-\beta h}\lambda_n^-} = \frac{e^{2\beta h}Z_n - 1}{e^{2\beta h}Z_n + 1} \tag{6}$$

where $Z_n = \lambda_n^+/\lambda_n^-$ for all $n > 1$. The thermal average of the 0th site, that site where q nth-generation branches are connected, is

$$\langle \sigma_0 \rangle = \frac{e^{\beta h}(\lambda_n^+)^q - e^{-\beta h}(\lambda_n^-)^q}{e^{\beta h}(\lambda_n^+)^q + e^{-\beta h}(\lambda_n^-)^q} = \frac{e^{2\beta h}Z_n^q - 1}{e^{2\beta h}Z_n^q + 1} \tag{7}$$

where

$$Z_n = \frac{a^3 d Z_{n-1}^{3(q-1)} + 3a^2 Z_{n-1}^{2(q-1)} + 3ad Z_{n-1}^{(q-1)} + 1}{a^3 Z_{n-1}^{3(q-1)} + 3a^2 d Z_{n-1}^{2(q-1)} + 3a Z_{n-1}^{(q-1)} + d} \tag{8}$$

and we have defined $a = \exp(2\beta h)$ and $d = \exp(2\beta J_4)$.

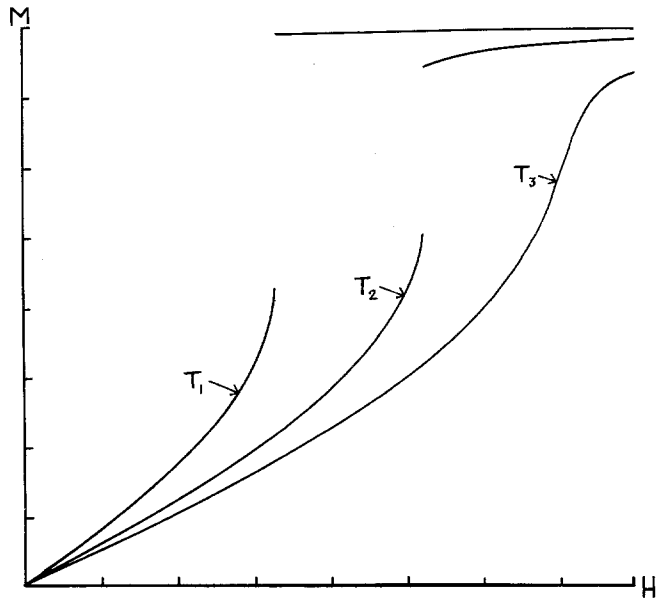


Fig. 4. A plot of the magnetization of the central site $\langle \sigma_0 \rangle$ for the Husimi tree approximation to a square lattice system with four-site interactions on the elementary squares of the lattice. $\langle \sigma_0 \rangle$ is shown for the temperatures indicated with $T_1 < T_2 < T_3$.

In all cases presented in this paper we find $\langle \sigma_0 \rangle_n$ by numerical means. For the square lattice with four-site interactions we numerically iterate Eq. (8) with $q=4$. We then substitute into Eq. (7) to get $\langle \sigma_0 \rangle_n$. A plot of $\langle \sigma_0 \rangle_n$ as a function of h is shown in Fig. 4 for various temperatures. For low enough temperatures one sees the existence of a phase transition at $h \neq 0$. The phase diagram in the h–T plane is shown in Fig. 5 along with the self-dual line given by Eq. (2). We see a qualitatively correct picture of the phase diagram with, for $h=0$, a phase transition only at $T=0$ and hence significant improvement over the mean-field results. Due to the symmetry of the interactions, one knows that $\langle \sigma_0 \rangle_n$ is an odd function of h and hence phase transitions occur for $h<0$ as well as $h>0$; Fig. 5 shows only $h>0$.

We have performed similar calculations for a three-site interaction system as an additional test for the method. The system we wish to approximate is a triangle lattice system with three-site interactions on either all upward-pointing or all downward-pointing triangles, but not

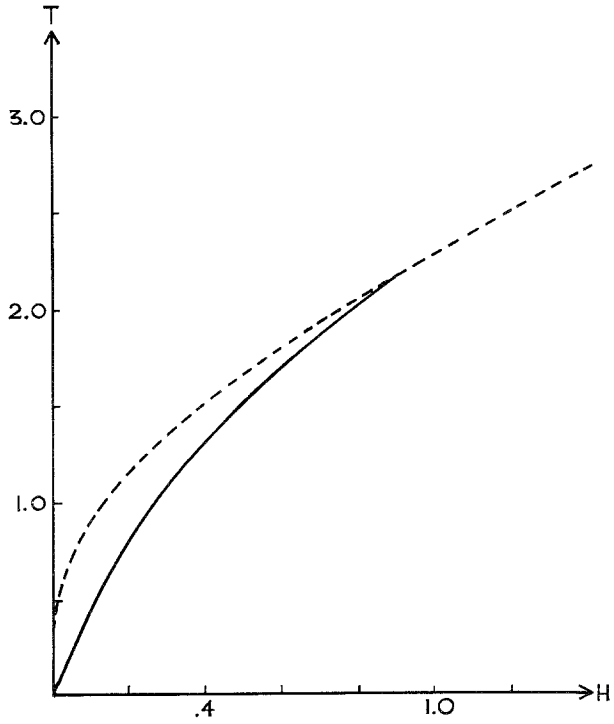


Fig. 5. The phase diagram obtained from our Husimi tree approximation (heavy solid line) and the self-dual line (dashed).

both. This model is again self-dual[9,2] and if a phase transition occurs, it will be along the line given by Eq. (2). We construct a pure Husimi tree as before, where now, however, a three-site triangle is our basic building block. Husimi trees of this type are known as cacti.[23] We attach $q-1$ triangles to each site except the base site to construct a first-generation branch and continue as before, eventually finishing by connecting q nth-generation branches at the 0th site. We look at the case $q=3$ and find again a phase transition for $h=0$ with $h>0$. Note that we do not have the symmetry we had with the four-site interactions and thus $\langle\sigma_0\rangle$ is not an odd function of h. We will return to this model in Section 3 for $h<0$.

We have considered the above model rather than the Baxter–Wu model,[24] which is a model having three-site interactions on all triangles, because the above model is most similar to the four-site interaction model we began with. The critical feature is that each of the systems studied here has a single translationally invariant MSI. The Baxter–Wu model has two translationally invariant MSIs, one on the upward-pointing triangles, the other on the downward-pointing triangles. Another way of seeing the similarity is that for both of our models the thermodynamics in zero-field is trivial,[25,26] whereas in the Baxter–Wu model it is not.

In cases involving the mean-field approach, one can improve on the usual approximation by applying what is known as the cluster mean-field approximation. Then, rather than focusing on only one site, one considers a cluster of sites, taking into account the interactions among the spins of the cluster in an exact manner and interactions between spins in the cluster with spins outside the cluster accounted for by the mean field. A somewhat similar approach can be used here. Rather than a three-site triangle as the basic building block, we can use a six-site triangle. This six-site triangle is made up of four elementary triangles, three of which point in the same direction and hence have three-site interactions; the central triangle points in the opposite direction and no interaction is present involving its sites. We connect these new building blocks only at the corners, as done with the smaller triangles in the previous case. Calculation of $\langle\sigma_0\rangle_n$ is similar to the previous calculations and again results in phase transitions for $h\neq 0$. The results for this system are presented in Fig. 6 along with those of the previous triangular system involving only three-site triangles. As in the cluster mean-field approximation, by increasing the size of the cluster one achieves an improvement in the results of the approximation.

The above results indicate that by going from the mean-field approximation to our Bethe-like approximation we have obtained a significant improvement which we would characterize as going from a qualitatively incorrect phase diagram of the mean-field approach to a qualitatively correct one using the Bethe-like approach. We plan to

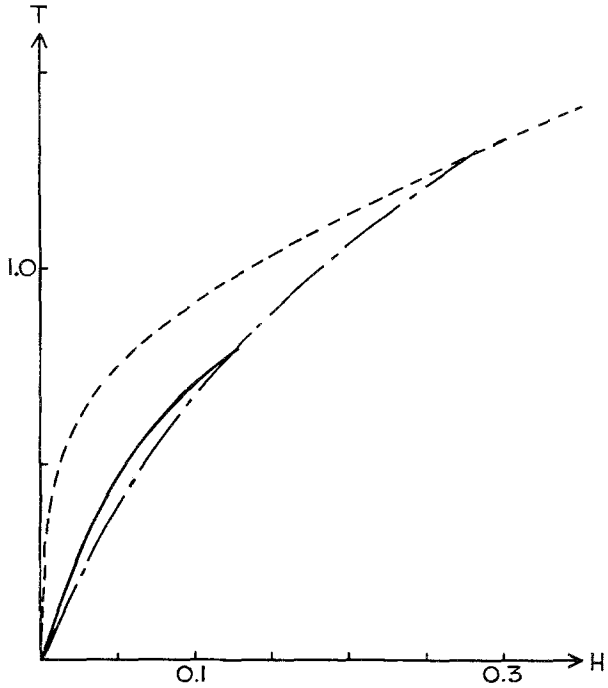


Fig. 6. A comparison of the phase diagrams obtained from our two Husimi tree approximations and the self-dual line for the three-site interaction system of the text. The dot-dashed line (solid line) is the result using a single triangle (a six-site large triangle) as the basic building block. The dashed line is the self-dual line.

continue this study by looking at a variety of other MSI systems. In particular, a system with both pair and multisite interactions present needs to be used as a test and here a prime test case would be the Kagomé lattice with two- and three-site interactions and an external magnetic field where one has the exact results in the full J_2, J_3, and h space[6] to compare with.

3. HUSIMI TREE SOLUTION AS DYNAMICAL SYSTEMS AND $J_3 < 0$

Thompson[10] in an early paper stressed the connection between solutions of the Bethe-lattice and dynamical systems. In particular, for the usual pair interaction on the Bethe lattice he develops an iterative scheme for computing the magnetization in the ith shell from the surface, in terms of the magnetization of the $(i-1)$th shell from the surface. For ferromagnetic interactions the values of the m_i converge monotonically to

the usual Bethe approximation expression for the magnetization. For set values of h and T this is just the fixed point of the recursion relation. Physically, as one goes into the interior of the lattice, one expects the magnetization per site to converge to a fixed value and it does. In our scheme we have a similar process, but rather than going from one shell to the next, we are building up larger and larger branches and looking at the magnetization of the base site at each step. Again, physically, we would expect that the magnetization of the base site converges to a fixed value as the branch size increases. This is exactly what happens in all of the cases presented above. The fixed point is discontinuous as a function of h, thereby indicating a phase transition.

When Thompson[10] looks at the case of antiferromagnetic pair interactions he finds for certain h and T a 2-cycle rather than a fixed point, i.e., there is a bifurcation. Again the 2-cycle result matches what one would expect from physical considerations. It was pointed out, however, that with

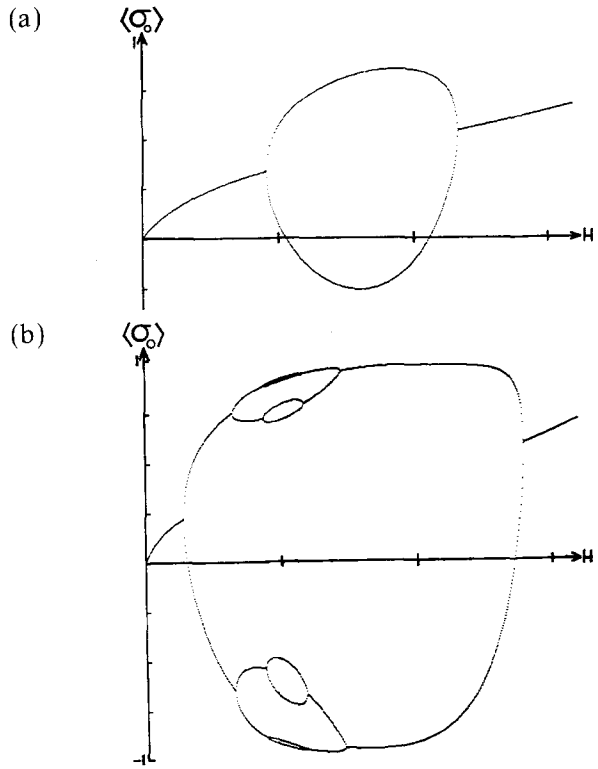


Fig. 7. Plots of $\langle \sigma_0 \rangle_n$ for our three-site interaction system with $J_3 = -1.0$. (a) $T = 1.2$; (b) $T = 0.6$.

competing interactions it may be possible for more complicated and interesting patterns to appear. That this occurs has now been shown, with a number of authors presenting results.[11,15–18] Here the emphasis has been on approximation schemes for the ANNNI model as mentioned in the introduction, that is, a model with ferromagnetic n.n. interactions and some antiferromagnetic interactions involving various n.n.n. pairs of sites. There have also been results for spin-one models[19] as well as cases where the presence of third-nearest-neighbor interactions have been include,[20] all on Bethe lattices.

In all the above references only pair interactions are present. Here we present results where multisite interactions are present. We will see that many of the results are somewhat similar to those found for competing pair interaction systems like the ANNNI model. By going to n.n.n. interactions the recursion relations become rather complex, while for our system by

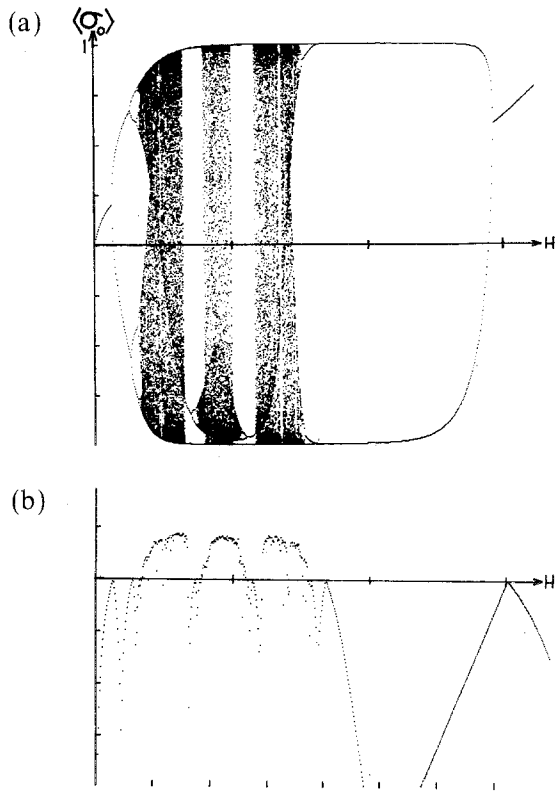


Fig. 8. (a) A plot of $\langle\sigma_0\rangle_n$ for our three-site interaction system with $J_3 = -1.0$ and $T = 0.3$. (b) A plot of the Liapunov exponent for the system of part (a).

looking at a single multisite interaction they remain no more complicated than what appeared in Section 2. Specifically, the system we look at is our three-site inhteraction system of Section 2, but now with $h>0$ and $J_3<0$. By symmetry this is equivalent to looking at $h<0$ and $J_3>0$. Here we have the same type of competition one has with Thompson's antiferromagnetic model. With $h>0$ the external field wants all spins to point upward, while the interaction $J_3<0$ wants one or three spins pointing down. For high temperatures a single fixed point exists, but as with Thompson's[10] antiferromagnetic n.n. pair interaction, as the temperature, is lowered a bifurcation occurs. Here, however, the 2-cycle region is centered around some $h\neq 0$ rather than $h=0$ as in the pair interaction case (see Fig. 7a). The real distinguishing feature between this and the results from ref. 10 occurs as we continue to lower the temperature. An entire period-doubling sequence or what has been called a complete period-doubling cascade occurs just as one finds for the prototype example of a dynamical system, the quadratic or logistic map. At an intermediate temperature as in Fig. 7b we have an incomplete period-doubling cascade, which has been studied by Bier and Bountis.[21] Finally, in Fig. 8a, following further lowering of the temperature, we obtain the full picture of the transition from cyclic to chaotic behavior, with period-3 windows, etc., seen so frequently for the quadratic or logistic map. Figure 8a is accompanied by Fig. 8b, where a plot of the Liapunov exponent is presented.

4. CONCLUSIONS

In this paper we have studied pure MSI systems by approximating them with Husimi tree structures. Besides the standard Bethe lattice with n.n. pair interactions and Ising spin variables, previous papers have investigated a number of generalizations of this system, e.g., systems with interactions beyond n.n. interactions, Potts model spin variables, etc. Bethe-like lattices similar to ours and denoted as "cacti" have been studied with pair interactions present[22]; however, this is the first time that results for MSI systems on such structures have been presented. For the case of $J_3>0$ and $J_4>0$, with $h>0$, in the systems presented we have found phase diagrams in qualitative agreement with results reported previously for these systems. Furthermore, we illustrated how systematic improvements can be obtained. We feel that these initial results are promising and we plan to continue to investigate this line of approach for several other systems. In particular, we will look at some of the mixed interaction systems mentioned in the introduction.

We have also seen, since the method of solution involves an iterative process, that there are interesting connections to be made with the area of

dynamical systems. In particular, when $J_3 < 0$ and $h > 0$ for the three-site interaction system presented, we found that a full bifurcation diagram results as well as chaotic regions with positive Liapunov exponent values, and period-three, -five, etc., windows. Hence we see many of the very intensely studied and by now familiar properties of dynamical systems theory arising in a new context and in a very simple manner. The ANNNI model, which involves competing pair interactions and which, as we referenced earlier, has been approximated by a number of authors on the Bethe lattice, is the closest material presented which is similar to the above. We can approximate a system of competing n.n. interactions and n.n.n. interactions by looking at our four-site square basic building block as we did in Section 2, but where we replace J_4 with n.n. and n.n.n. pair interactions. We plan to present such results in the future.

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