THERMODYNAMIC APPROACH TO
THREE-SITE ANTIFERROMAGNETIC ISING
MODEL IN CHAOTIC REGION

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Abstract

The chaotic properties of the three-site antiferromagnetic Ising model on Husimi
tree are investigated in magnetic field. Macroscopic quantity of three-site antifer-
romagnetic Ising model is generated by one dimensional map. It is shown that in
certain parameter setting strange attractors of this map exhibit multifractal scal-
ing. By applying thermodynamic formalism we find nonanalyticity in free energy
as well as in entropy. We show that the temperature of phase transition depends
on parameter of model and varies from negative to positive value.

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1. INTRODUCTION

One of the formalism to analyze nonlinear physics having complicated fractal objects and strange attractors is the thermodynamic approach\[1, 2\]. The advantage of this formalism is that the number of degrees of freedom is usually enormously large and their properties are described by thermodynamical function which contain most of the relevant information about macroscopic systems. In order to characterize these macroscopic systems order parameter has been sought. One of this order parameters is Lyapunov exponents. The tool with which we can measure Lyapunov exponents and other dynamical quantities is similar to the thermodynamic formalism in equilibrium statistical mechanics. By using thermodynamic formalism many studies have been done on strange attractors and it has been found nonanalities in free energy function and scaling in the distribution of Lyapunov exponents\[3, 4\]. Besides there are many other relationships between Ising-like systems and thermodynamic formalism\[5\].

In this paper we investigate the three-site antiferromagnetic Ising spin model (TSAI) and show how to obtain connection between the TSAI model and thermodynamic formalism. The reason for studying the Ising model with multisite interaction is that it plays an important role for investigations of real physical systems, such as binary alloys\[6\], classical fluids\[7\], solid $^3$He\[8\], lipid bilayers\[9\], and rare gases\[10\]. Recently the multisite interaction Ising model on Husimi tree has been investigated. It is shown, that this approach yields qualitatively good approximation for the ferromagnetic phase diagrams than conventional mean-field calculation\[11\]. In contradiction to ferromagnetic case, when we change the sign of three-site interaction the situation changes drastically. In certain values of temperature and magnetic field the TSAI model has nontrivial thermodynamic limit and as a consequence the magnetization exhibits chaotic behavior\[12, 13\]. In this case the magnetization is not an order parameter. In this paper we introduce Lyapunov exponent as the order parameter in chaotic region using thermodynamic formalism.

With the "thermodynamic formalism" we investigate TSAI model in the chaotic region and describe its chaotic properties via the invariants characterizing fractal sets (e.g. strange attractors). In particular, we obtain the entropy and free energy function and focus on whether the thermodynamical quantities have phase transition\[3\]. It is, in general, hard to determine such behavior unambiguously by numerical methods if one does not have further arguments or exact solutions (as in the case of $x \rightarrow 4x(1-x)$). However, there is a possibility to remedies these deficiencies if one considers the characteristic Lyapunov exponents as an order parameter, which will differ in two phases. In this paper we numerically calculate this order parameter as a function of the "temperature" and show where the phase transition occurs.

The contents of the remainder of this paper is as follows. TSAI system on Husimi tree and recursion relation is presented in Sec. 2. In Sec 3. there is a discussion of the property of TSAI model in thermodynamic limit. In Sec. 4 we present the TSAI model in the case of "fully developed chaos" and obtain the exact connection between this model and chaotic attractors. By using the "thermodynamic formalism", the phase transition in terms of Lyapunov exponents, free energy and entropy function is analyzed. Finally,
in Sec. 6 we summarize our results and comment on their implications for the study of other systems.

2. TSAI MODEL ON HUSIMI TREE AND RECURSION RELATION

The advantage of the Husimi tree is that for models formulated on it, an exact recursion relations can be obtained. The pure Husimi tree [14], shown in Fig.1, is characterized by \( \gamma \), the number of triangles which goes out from each site and \( n \), the number of generation. The 0th-generation is a single site from which come out \( \gamma \) triangles. All subsequent generation comes out by gluing up \( \gamma - 1 \) triangles to each free sites of previous generation.

The TSAI model in a magnetic field is defined by the Hamiltonian one

\[
H = -J_3' \sum_\triangle \sigma_i \sigma_j \sigma_k - h' \sum_i \sigma_i, \tag{1}
\]

where \( \sigma_i \) takes values \( \pm 1 \), the first sum goes over all triangular faces of the Husimi tree and the second over all sites. Additionally, we use the notation \( J_3 = \beta J_3' \), \( h = \beta h' \), \( \beta = 1/kT \), where \( h \) is the external magnetic field, \( T \) is the temperature of the system and \( J_3 < 0 \) corresponding to an antiferromagnetic coupling (in all our numerical calculations we put \( J_3' = -1 \)).

The partition function will be written as

\[
Z = \sum_{\{\sigma\}} \exp \left\{ J_3 \sum_\triangle \sigma_i \sigma_j \sigma_k + h \sum_i \sigma_i \right\}, \tag{2}
\]

where the summation goes over all configurations of the system.

When the Husimi tree is cut apart at the base site, it separates into \( \gamma \) identical branches. The partition function can be written as follows:

\[
Z_n = \sum_{\{\sigma_0\}} \exp \{ h \sigma_0 \} \left[ g_n(\sigma_0) \right]^{\gamma - 1}, \tag{3}
\]

where \( \sigma_0 \) are spins of base site, \( n \) is the number of generations (\( n \to \infty \) corresponds to the thermodynamic limit). Each branch, in turn, can be cut along any site of the 1th-generation which is the nearest to the central site. The expression for \( g_n(\sigma_0) \) can therefore be rewritten in the form

\[
g_n(\sigma_0) = \sum_{\{\sigma_1\}} \exp \left\{ J_3 \sum_\triangle \sigma_0 \sigma_1^{(1)} \sigma_1^{(2)} + h \sum_{j=1,2} \sigma_1^{(j)} \right\} \left[ g_{n-1}(\sigma_1^{(1)}) \right]^{\gamma - 1} \left[ g_{n-1}(\sigma_1^{(2)}) \right]^{\gamma - 1}. \tag{4}
\]

From Eq.(4) we easily obtain

\[
g_n(+) = e^{J_3 + 2h} g_{n-1}(+g_{n-1}(+) + 2e^{-J_3} g_{n-1}(+g_{n-1}(-) + e^{J_3 - 2h} g_{n-1}(-) g_{n-1}(+) + e^{-J_3 - 2h} g_{n-1}(-) g_{n-1}(-),
g_n(-) = e^{-J_3 + 2h} g_{n-1}(+g_{n-1}(+) + 2e^{J_3} g_{n-1}(+g_{n-1}(-) + e^{-J_3 - 2h} g_{n-1}(-) g_{n-1}(+) + e^{J_3 - 2h} g_{n-1}(-) g_{n-1}(-).
We introduce the following variable:

\[ x_n = \frac{g_n(+)}{g_n(-)}. \]  

(5)

For \( x_n \) we can then obtain the recursion relation

\[ x_n = f(x_{n-1}), \quad f(x) = \frac{2\mu x^2(\gamma - 1) + 2z\mu x^{\gamma - 1} + z}{\mu x^{2(\gamma - 1)} + 2z\mu x^{\gamma - 1} + 1}, \]  

(6)

where \( z = e^{2h} \), \( \mu = e^{2h} \) and \( 0 \leq x_n \leq 1 \). The function \( f(x) \) is unimodal: it is continuous, continuously differentiable, and has one maximum \( x^* \) in \([0, 1]\). Note that \( f(x^*) = 1 \) for any \( \gamma, h \) and \( T \). This function is nonhyperbolic (hyperbolicity for 1D maps means that \( 1 < |f'| < \infty \) in all points) and maps the interval \([0, 1]\) onto \([z, 1]\).

Through \( x_n \), obtained by Eq.(6), one can express the magnetization of the central base site:

\[ m_n = \langle \sigma_0 \rangle = \frac{e^h g_n^\gamma(+) - e^{-h} g_n^\gamma(-)}{e^h g_n^\gamma(+) + e^{-h} g_n^\gamma(-)} = \frac{e^{2h} x_n^{\gamma} - 1}{e^{2h} x_n + 1}, \]  

(7)

and other thermodynamic parameters, so we can say that the \( x_n \) determines the states of the system. For example, at high values of temperatures (see next subsection) the recursion Eq.(6) tends to a fixed point and therefore the system has an appointed magnetization \( m \). For the free energy function (using Eqs.(3), (4), (5), (6)), we obtain

\[ F_n = -\frac{2\gamma - 3}{3} F_{\text{Cayley}}, \]  

(9)

where \( F_{\text{Cayley}} \) is the free energy function of the triangular Cayley tree. It is easily seen that the expression for magnetization given by Eq.(7), can be obtained by differentiating the free energy function of Eq.(8) with respect to the magnetic field \( h \). It is interesting to mention that Eq.(9) is the generalization of the results obtained in Ref.\[15, 16\].

3.THERMODYNAMIC LIMIT

Let us consider the magnetization of the central base site. In order to achieve thermodynamic limit we tend the number of generation to infinity \((n \to \infty)\). If we set \( \gamma = 4 \) in Eqs.(5), (6) and vary the temperature and magnetic field, then for sufficiently large \( T \) we see that function \( f(x) \) has a stable fixed point at every value of \( h \) and therefore map \( x_n = f(x_{n-1}) \) attracts every point to \( x^* = f(x^*) \) in the thermodynamic limit \((n \to \infty)\). At such temperature the magnetization \( m \), is a well defined function of \( h \) (see Fig.2a) in thermodynamic limit. Then we lower \( T \), at some values of \( h \) the point \( x^* = f(x^*) \) becomes unstable, but now two new stable points \( x_1, x_2 \) arise in function \( f(f(x)) \), which is an
attracting periodic orbit of period 2 for map $x_n = f(x_{n-1})$ and we find that there is a single bubble in the plot of $m$ versus $h$ (Fig. 2b). As we continue to lower $T$, new bubbles are formed as parts of the old bubbles (Fig. 2c, attracting periodic orbits of period $2^N$), and for still lower $T$ we reach a region where for intermediate values of $h$ we have chaos, period-three windows, etc. (see Fig. 2d).

One can say that the reason for this is that we have the presence of frustration effects and taking into account antiferromagnetic nature of the three-site interaction identifies two different magnetization in fixed field and temperature with magnetization of sublattice, as in antiferromagnetic phase and chaotic region with spin glass phase [17]. But as one can note from our calculation different magnetization corresponds to different sample with different number of generation. Therefore the appearance of a bubble due to fact that our system does not have trivial thermodynamic limit and in that limit different samples with different number of generation are not macroscopically equivalent systems.

Obviously magnetization can’t be an order parameter in chaotic region. How can we identify the appearance of chaotic region? From the theory of dynamical system we know that Lyapunov exponents are good order parameter and become positive when attractors of the system become chaotic or strange [5]. A statistical-thermodynamic method for the description of fluctuation of the Lyapunov exponents has been introduced, using a partition function [1, 2]. Later on we use thermodynamic formalism in order to characterize TSAI system in chaotic region.

It is interesting to note that similar chaotic behavior has been found in other frustrated hierarchical lattices [17, 18]. The Husimi tree like other hierarchical lattices are effectively infinite dimensional. But in Husimi or Bethe like lattices the number of neighborhood remain constant in contradiction to other hierarchical lattices for which in thermodynamic limit surface sites interacts with infinitely many neighborhood. Another difference is in nonequivalence of the lattice sites. In Husimi or Bethe like lattices the sites lying deep inside lattices are equivalent [19].

4. TSAI SYSTEM AND ”THERMODYNAMIC FORMALISM”

How to apply the ”thermodynamic formalism” to the TSAI system? For this we need a natural partition and that is provided by the cylinders (we follow here Ref. [3]).

The recursion function Eq. (3) with $\gamma = 4$ has the following form

$$f(x) = \frac{z\mu^2 x^6 + 2\mu x^3 + z}{\mu^2 x^6 + 2z\mu x^3 + 1}. \quad (10)$$

Simultaneously considering the following system of equation,

$$\begin{cases} f(x_0) = x_0 \\ f(1) = x_0 \end{cases}, \quad (11)$$

we obtain

$$z = \frac{\mu^{-2/3} + \mu^{-8/3} - 2\mu^{-1}}{1 + \mu^{-2} - 2\mu^{-5/3}}, \quad x_0 = \mu^{-2/3}. \quad (12)$$
For a crisis map (Eqs. (10), (12)) we want to describe the scaling properties of the attracting set which in this case is the entire interval \( I = [x_0, 1] \) (Fig. 3). For an index \( n \), \( I \) is partitioned into \( 2^n \) intervals or n-cylinders, these being the segments with identical symbolic-dynamics sequences of length \( n \) taken with respect to the maximum point \( x^* = c \). The inverse function of Eq. (10), \( h = f^{-1} \), has two branches, \( h_{-1} \) and \( h_1 \) as shown in (Fig. 3) and the n-cylinders are all the nth-order preimages of \( I \). The length of the cylinders is denoted by \( l_{\epsilon_1, \epsilon_2, \ldots, \epsilon_n} = h_{\epsilon_1} \circ h_{\epsilon_2} \circ \ldots \circ h_{\epsilon_n}(I) \) where \( \epsilon \in \{-1, 1\} \).

The partition function \( Z(\beta) \) is defined [3] as

\[
Z_n(\beta) = \sum_{\epsilon_1, \epsilon_2, \ldots, \epsilon_n} l^\beta_{\epsilon_1, \epsilon_2, \ldots, \epsilon_n} \prod_{\epsilon_1, \epsilon_2, \ldots, \epsilon_n} e^{-\beta \ln l_{\epsilon_1, \epsilon_2, \ldots, \epsilon_n}} \tag{13}
\]

where \( \beta \in (-\infty, \infty) \) is a free parameter, the inverse "temperature". In the limit \( n \to \infty \) the sum behaves as

\[
Z_n(\beta) = e^{-n\beta F(\beta)}, \tag{14}
\]

which defines the free energy, \( F(\beta) \). The entropy \( S(\lambda) \) is the Legendre transform

\[
S(\lambda) = -\beta F(\beta) + \lambda \beta, \tag{15}
\]

where the relation between \( \lambda \) and \( \beta \) is found from

\[
\lambda = \frac{d}{d\beta}(\beta F(\beta)), \quad \beta(\lambda) = S'(\lambda), \tag{16}
\]

and these have the following meaning: In the limit \( n \to \infty \), \( e^{nS(\lambda)} \) is the number of cylinders with length \( l = e^{-n\lambda} \) or, equivalently, with Lyapunov exponent \( \lambda \), which we consider as an order parameter for TSAI model. The Hausdorff dimension of the set of points in \( I \) having Lyapunov exponent \( \lambda \) is \( S(\lambda)/\lambda \) [3].

By using the Eqs. (10), (12), (13), (14) we can numerically calculate the free energy at different value \( \mu \) which is shown in Fig. 4. One can see from Fig. 4a that the free energy have a singularity around \( \beta_c = -1 \) at low values of \( \mu \) while at high values of \( \mu \) the free energy have a singularity around \( \beta_c = 1 \) (Fig 4b), which shows the existence of the phase transition of first order in this regions of \( \beta \).

How can the transition be determined accurately?

Let us consider the characteristic Lyapunov exponent as an order parameter which will differ in the two phases. Fig 5 shows this order parameter for different \( \mu \) and sizes of the system, corresponding to \( n = 7, 9, 11, 13 \). The curves converge towards a line and the result is the first order transition, whereas in a class of maps close to \( x \to 4x(1-x) \) a phase transitions of the first order occur only with negative \( \beta_c \). We would like to mention that it is hard to determine the critical "temperature" of phase transition by numerical methods with high precision. Consequently, the obtained value of critical "temperature" is approximate. In connection with this it is important to note, that there is a literature on phase transition in fully developed chaotic maps with neutral points leading to intermittent dynamics [4], that claims the existence of a phase transition in a free energy at "temperature" \( = 1 \).
Large deviations of fluctuations of a Lyapunov exponents can be described by the entropy. To consider the above results in terms of the entropy function $S(\lambda)$, let us first discuss the general appearance of the entropy function. First of all, it should be positive on some interval $[\lambda_{\text{min}}, \lambda_{\text{max}}]$. The value $\lambda = \ln 2$ must belong to that interval, which follows from the fact that the sum of the lengths of all cylinders on a given level is 1. Secondly it is often found that the values of $\lambda_{\text{min}}$ and $\lambda_{\text{max}}$ are given by the logarithms of the slopes at the origin.

The precise form of the entropy function is, as mentioned in the introduction, not easy to obtain with great accuracy. The existence of a first order phase transition implies that there should be a straight line segment in $S(\lambda)$ and the slope of the line equal to $\beta_c$. This scenario is seen in Fig. 6. The curve in the figure corresponds to $n = 13$. Of course, with the finite-size data, it is impossible to determine the straight line segment in $S(\lambda)$ and with increasing $n$, the straight line will be increased.

6. CONCLUSION

In this paper we have investigated the TSAI model by approximating it with a Husimi tree structures in an external magnetic field, and a strong connection with results from the theory of dynamical systems including chaos has been pointed out.

An exact connection between that statistical system and fully developed chaotic attractors is obtained. Is is shown that in the chaotic region the magnetization, which are the order parameter for ferromagnetic phase, must be replaced by Lyapunov exponent in order to characterize TSAI model in chaotic region. The chaotic properties of the anti-ferromagnetic multisite system is described via the invariants characterizing a fractal set (e.g. a strange attractor). It is shown that this system in the chaotic region displays a phase transition. It is, in general, hard to determine such behavior unambiguously by numerical methods if one does not have further arguments or exact solutions. In this paper we have considered the characteristic Lyapunov exponents as an order parameter, which will differ in two phases. We’ve managed to calculate this order parameter as a function of the ”temperature” and approximately showed where the phase transition will occur, since it describes transitions in the distribution of the characteristic Lyapunov exponents. This phase transition in terms of free energy and entropy function is also analyzed.

It is interesting to note that for $\gamma = 3$ the above situation changes dramatically and it will be very difficult to study numerically the chaotic region of TSAI system in terms of the ”thermodynamic formalism” [12].

On other hand, the study of chaotic statistical physical system has opened new challenges for theories of stochastic processes, especially in the direction of stochasticity of the vacuum in QCD [20, 21]. In this direction interesting results for the $Z(Q)$ gauge model with a double plaquette representation of action on the flat and generalized Bethe lattices were obtained [22, 23]. Note that it is possible to get a chaotic region in the $Z(Q)$ gauge model with a three plaquette representation of the action. The detailed investigations of these questions will be published elsewhere.
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Fig.1. Husimi tree with $\gamma = 4$. 
Fig. 2. Plots of $m$ versus $h'$ for different temperatures $T$ ($\gamma = 4$). a - $T = 3$, b - $T = 1.3$, c - $T = 1.15$, d - $T = 0.7$. 
Fig. 3. The function of Eq. (10) for values of $\mu = 105$ and $z$ given by Eq. (12).
Fig. 4. The free energy $F(\beta)$, for different values of $\mu$. a - $\mu = 5$, b - $\mu = 105$. 
Fig. 5. The order parameter $\lambda(\beta)$ calculated for different sizes of the system, corresponding to $n = 9, 11, 13$ and different $\mu$. a - $\mu = 5$, b - $\mu = 105$. 
Fig.6. The entropy function corresponding to \( n = 13 \) for different \( \mu \). a- \( \mu = 5 \), b - \( \mu = 105 \).