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A Note on Cactus Trees: Variational vs. Recursive Approach

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In this article we deal with the variational approach to cactus trees (Husimi trees) and the more common recursive approach, that are in principle equivalent for finite systems. We discuss in detail the conditions under which the two methods are equivalent also in the analysis of infinite (self-similar) cactus trees, usually investigated to the purpose of approximating ordinary lattice systems. Such issue is hardly ever considered in the literature. We show (on significant test models) that the phase diagram and the thermodynamic quantities computed by the variational method, when they deviates from the exact bulk properties of the cactus system, generally provide a better approximation to the behavior of a corresponding ordinary system. Generalizing a property proved by Kikuchi, we also show that the numerical algorithm usually employed to perform the free energy minimization in the variational approach is always convergent.

KEY WORDS: Cactus tree; Husimi tree; cactus approximation; lattice model; Ising model.

1. INTRODUCTION

Cactus trees are lattices with a branched topology,[1,2] and usually also a self-similar structure.[1,3] Model systems on cactus trees are interesting mainly because of two reasons. First they often provide reliable approximations to more realistic models on ordinary lattices,[1,4] and second their statistical mechanics can be generally worked out exactly.[1–4] Because of these facts, a lot of physical systems have been investigated in the framework of tree lattices: a variety of Ising-like models,[5–11] Potts models,[12]

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spin liquids,[13] systems with quenched disorder,[14] polymers,[15–19] abelian sandpiles,[20] electrons in binary alloys[21] and amorphous solids.[22] The simplest class of lattice models, i.e., Ising models, have been most widely investigated also on cactus trees. In order to the approximation of systems on ordinary lattices, it has been shown by Monroe that the cactus approximation turns out to be particularly successful in two relevant cases, namely systems with multi-site interactions[5, 6] and frustrated systems.[8] In both cases the simple mean field theory and the Bethe approximation fail in predicting a qualitatively correct phase diagram.[23, 24] In the special case of the fully frustrated antiferromagnetic Ising model on the triangular lattice, the same holds even for high order *cluster variation method*,[25] while the cactus approximation yields qualitatively correct results.[8] Recently Monroe himself has also shown that a series of cactus approximations with larger and larger building blocks allows not only a more precise determination of phase diagrams[8] but also quite good estimates of critical exponents.[26] As a consequence of such and other positive results, considerable attention has been devoted to the properties of cactus trees[27] and of the methods by which they are studied.[4]

In most papers dealing with cactus trees, calculations are based on the self-similar structure of the system and this feature is exploited to determine its physical properties. In the following we shall refer to such kind of treatments as to the *recursive approach*. Nevertheless it is known that cactus trees can be studied also by means of a *variational approach*, equivalent to the cluster variation method with a special choice of basic clusters.[2] The two methods are in principle equivalent and both give the exact solution for finite cactus trees. Nevertheless, to the purpose of approximating ordinary lattice systems, one is usually interested in the bulk properties of an infinite cactus tree. This can be done exactly only by means of the recursive approach, by evaluating the limit of a recursion relation, or more precisely by investigating the attractor of a dynamical system defined by the recursion relation itself. In order to employ the variational approach as well, one usually assumes some degree of "translational" invariance.[1, 2] Even when such assumption is actually verified in the interior (bulk) of the cactus tree, the variational free energy density evaluated in this way turns out to be only the bulk contribution, not the exact one. The contribution of surface sites, whose number increases exponentially as the tree is expanded,[1] cannot be neglected even in the thermodynamic limit. This has not always been stated so clearly in the literature,[2] and one might expect that a minimization of the bulk free energy density always yields bulk equilibrium properties.

We point out that this is true only under certain conditions, namely when a limit of the recursion relation exists (that is the associated dynamical

system has a fixed point, that is the bulk invariance condition actually holds[1]), and as far as the equation of state is concerned. The latter issue refers to the possibility of multiple stable fixed points, which is related to coexistence phenomena. In this case the two methods generally predict the same solutions but which one is the real attractor of the recursive method depends on boundary conditions. Different criteria have been proposed for the determination, in the presence of multiple fixed points, of the first order transition which best approximates that of an ordinary lattice system, independently of boundary conditions. One, proposed by Gujrati,[4] is based on the bulk free energy density. Another one, proposed by Monroe,[28] is based on the evaluation of the derivatives of the recursion relation at the fixed points. We show analytically that Gujrati's free energy criterion is equivalent to the variational method. By means of actual calculations performed on significant test models we also show numerical evidence that Monroe's criterion may be equivalent as well. When a fixed point does not exist, the presence of boundaries may dramatically affect the bulk behavior of the cactus system, which may be completely different from that predicted by the variational approach. In this case both Gujrati's and Monroe's criteria do not work, but the variational approach seems to provide quite a good approximation to the phase behavior of the corresponding ordinary lattice system, even if it generally does not coincide with the exact bulk behavior of the cactus system. In the last part of the paper we relate such a nice behavior of the variational method, observed for particular cases, to a general property of the algorithm used to perform the free energy minimization, that is the *natural iteration method*.[29] It turns out that the free energy decreases at each step, which implies that, contrary to the recursive approach, the variational approach has always a "fixed point." We actually generalize a proof given by Kikuchi[29] for the Bethe approximation, coinciding with the variational approach to the Cayley tree.[30]

The paper is organized as follows. In Section 2 we introduce the statistical mechanics of cactus trees: the variational approach and the recursive approach. As previously mentioned, we show that, as far as equations of state are concerned, the recursive approach reduces to the variational approach, provided a limit of the recursion relation exists. Moreover we give the analytic proof that, in the same hypothesis, the variational approach is equivalent to Gujrati's criterion for the location of first order transitions. In Section 3 we work out variational calculations for three test models already investigated by the recursive approach, namely the Ising model with pure 4-spin interaction on the square cactus,[5] the antiferromagnetic Ising model on the triangle cactus,[8] and the Ising model with pure 3-spin interaction on the triangle cactus.[5] In the first case the recursive method has always a fixed point. In the second case it shows limit

cycles of period two, and in the third case also higher period limit cycles and chaotic behavior. In Section 4 we prove the property of free energy decreasing and discuss some consequences of such property, concerning results of the previous section. In Section 5 we give some concluding remarks.

2. STATISTICAL MECHANICS ON CACTUS TREES

Let us first introduce a recipe to build up a cactus tree. Let us consider a cluster of sites, which may be a triangle of 3 sites, as in Fig. 1(a), or more generally a cluster of n sites. Let each site be characterized by a state variable, which for simplicity is assumed to be a scalar. Let us also assume that a cluster hamiltonian h defines interactions among sites in the cluster. Defining a connectivity constant c, we build a branch of the cactus tree by a "growth" procedure. We attach $c-1$ equivalent clusters to the i-th site of the starting cluster, for $i=2,\ldots,n$ (Fig. 1(b)), and then we produce new generations by iterating the procedure (Fig. 1(c)). Finally we attach c equivalent branches to the base site. Such a system turns out to be self-similar in the infinite generation (thermodynamic) limit.

According to Morita,[2] clusters used as building blocks are denoted as *main clusters*, while intersections of main clusters are denoted as *joint sites*. In the above example all sites in the internal clusters are joint sites, but this is not necessarily the case. The total hamiltonian H can be written as a sum over all the main clusters

$$H(X)=\sum_{M} h(x_M), \tag{1}$$

where x_M denotes the set of site state variables in the main cluster M, and X denotes the state of the whole system. We also have to introduce the *partial partition functions*, which play an important role in the statistical mechanics of cactus trees. Let us consider a branch, whose base site is J and whose first main cluster is M, and a partial hamiltonian obtained by summing over main clusters of the branch. The partial partition function $W_{JM}(x_J)$ of the branch is obtained by summing the Boltzmann weights of the partial hamiltonian over the possible states of the branch minus the base site J. Making use of the partial partition functions, it is possible to write the probability distribution $p_J(x_J)$ of the state x_J of any joint site J as follows

$$p_J(x_J)=Z^{-1}\prod_{M\supset J} W_{JM}(x_J), \tag{2}$$

where $Z=\sum_X e^{-\beta H(X)}$ is the total partition function, the product runs over main clusters M containing J, and $\beta\equiv 1/k_BT$ (being k_B the Boltzmann

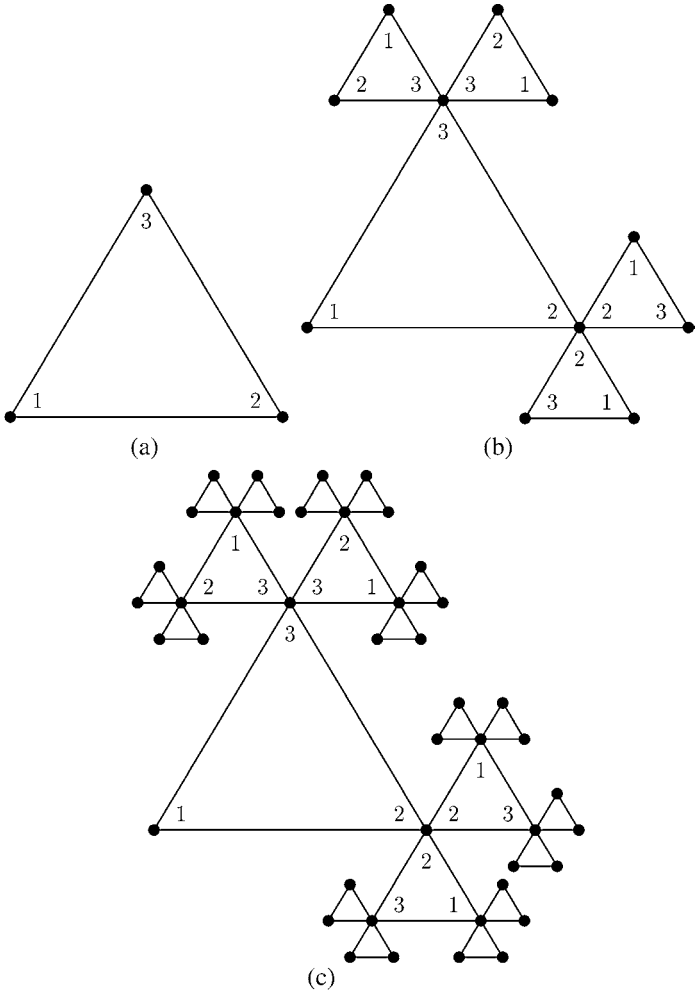

Fig. 1. An example of cactus tree obtained by a growth procedure: (a) first generation branch; (b) second generation branch; (c) third generation branch. Numerals are meant to show that cluster hamiltonians may remove the dihedral symmetry of triangles used to represent clusters.

constant and T the absolute temperature). Moreover, as far as the probability distribution $p_M(x_M)$ of the state x_M of a main cluster M is concerned, it is easy to show that

$$p_M(x_M) = Z^{-1} e^{-\beta h(x_M)} \prod_{J \subset M} \prod_{\substack{M' \supset J \\ M' \neq M}} W_{JM'}(x_J), \tag{3}$$

where the outer product runs over all joint sites J contained in M, and the inner one over all main clusters M' containing J, except M itself. Performing some manipulations, Eqs. (2) and (3) allow to verify that the probability distribution of the whole system $P(X) = Z^{-1}e^{-\beta H(X)}$ takes on the factorized form

$$P(X) = \prod_M \left\{ p_M(x_M) \prod_{J \subset M} [p_J(x_J)]^{-\frac{c-1}{c}} \right\}. \tag{4}$$

The latter is a peculiar property of cactus trees, which can be exploited to work out their statistical mechanics. By now let us only notice that, in order to prove Eq. (4), it is important to take into account the identity

$$\sum_M \left(1 - \sum_{J \subset M} \frac{c-1}{c} \right) = 1, \tag{5}$$

where the outer sum runs over all main clusters M and the inner one over the joint sites J in M. Such "sum rule" can be easily proved by considering the growth procedure described above, where each joint site implies the addition of $c-1$ main clusters. Splitting each contribution from a joint site among main clusters that contain it, one obtains Eq. (5).

2.1. The Variational Approach

We can now write the total free energy as a function of probability distributions of main clusters and joint sites only. As far as the entropy S is concerned, Eq. (4) allows to write

$$S/k_B = -\langle \log P(X) \rangle = -\sum_M \left\langle \log p_M(x_M) - \sum_{J \subset M} \frac{c-1}{c} \log p_J(x_J) \right\rangle, \tag{6}$$

where $\langle \cdot \rangle$ denotes an ensemble average. For the internal energy U, from Eq. (1) we simply have

$$U = \langle H(X) \rangle = \sum_M \langle h(x_M) \rangle. \tag{7}$$

Expanding ensemble averages, we can express the free energy F by

$$\beta F = \beta U - S/k_B = \sum_M \sum_{x_M} p_M(x_M)\, \varphi_M(x_M), \tag{8}$$

where

$$\varphi_M(x_M) \equiv \beta h(x_M) + \log p_M(x_M) - \sum_{J \subset M} (1 - 1/c) \log p_J(x_J). \tag{9}$$

This expression for the free energy, which is exact, coincides with that of the cluster variation method[31] if main clusters are chosen as maximal clusters. If probability distributions are assumed as variational parameters, the exact thermodynamic equilibrium state can be determined by the minimization of this free energy with suitable compatibility constraints. Namely one has to impose that joint site probability distributions $p_J(x_J)$ are marginal distributions of main cluster distributions $p_M(x_M)$ for all $M \supset J$

$$p_J(x_J) = \sum_{x_{M \setminus J}} p_M(x_M), \tag{10}$$

where $x_{M \setminus J}$ denotes the state of the main cluster M minus the joint site J.

In the limit of an infinite cactus tree, which is relevant to the approximation of ordinary (translationally invariant) lattices, it is not possible to employ the variational approach as previously described, because one would have to deal with an infinity of variational parameters. Therefore one assumes an invariance condition

$$p_M(x) \equiv p(x) \tag{11}$$

for main clusters M in the interior (bulk) of the tree, that is far from the surface. From now on

$$x \equiv \{x_0, x_1, \ldots, x_n\} \tag{12}$$

denotes the total state of a bulk main cluster: joint site states are denoted by x_i, for $i = 1, \ldots, n$, while x_0 denotes the state of sites that are not joint sites. In the hypothesis that Eq. (11) holds, in the bulk we shall have only a number n of (in principle) different "types" of joint sites, i.e., n different joint site probability distributions $p_i(x_i)$, for $i = 1, \ldots, n$. For convenience we denote the state of a bulk main cluster minus the i-th joint site as

$$x_{\setminus i} \equiv \{x_0, x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n\}. \tag{13}$$

Accordingly, joint site distributions can be written as marginal distributions by

$$p_i(x_i) \equiv \sum_{x_{\setminus i}} p(x). \tag{14}$$

As mentioned in the introduction, the variational approach as employed in practice evaluates only the bulk free energy density f (per main cluster) and performs a minimization of f. In this way it may deviate from the exact bulk behavior of the cactus system, but, being independent of boundary conditions, it is expected to approximate that of a corresponding ordinary lattice model. Taking into account Eqs. (8), (9), and the invariance assumption Eq. (11), we can write

$$\beta f = \sum_x p(x)\, \varphi(x), \tag{15}$$

where

$$\varphi(x) \equiv \beta h(x) + \log p(x) - \sum_i (1 - 1/c) \log p_i(x_i), \tag{16}$$

and the sum runs over $i = 1,\ldots, n$. The free energy density f is a functional in $p(x)$ only, being $p_i(x_i)$ dependent on them via Eq. (14). We work out the minimization with respect to $p(x)$, using the Lagrange multiplier method to impose the normalization of $p(x)$. Accordingly, we define the functional

$$\beta f_\lambda = \beta f - \lambda \left[\sum_x p(x) - 1 \right], \tag{17}$$

where λ is the unknown Lagrange multiplier. Taking the derivatives of f_λ with respect to $p(x)$ and setting them to zero, we obtain

$$p(x) = q^{-1} e^{-\beta h(x)} \prod_i [p_i(x_i)]^{1-1/c}, \tag{18}$$

where q is related to λ in an irrelevant way. We take the sum of both sides of Eq. (18) over all the main cluster states x, and impose the normalization, obtaining

$$q = \sum_x e^{-\beta h(x)} \prod_i [p_i(x_i)]^{1-1/c}. \tag{19}$$

Eq. (18), with q defined by Eq. (19), provides a fixed point equation for $p(x)$, which is usually solved via an iterative procedure known as *natural iteration method* (NIM).[29] Different solutions may be found starting the procedure from different guess values $p(x)$, and the stable phase is determined as the solution with the lowest free energy density f. The latter can

be evaluated by taking the logarithm of both sides of Eq. (18), substituting into Eq. (16) and then into Eq. (15), yielding

$$\beta f = -\log q, \tag{20}$$

where q has to be computed at each iteration. In the following we shall verify that such a criterion of stability generally does not predict the actual first order phase transitions for a cactus system in the thermodynamic limit, because it does not take into account surface contributions to the free energy. Nevertheless it seems to be the most reasonable way to approximate the phase behavior of a corresponding ordinary system.[2, 4]

2.2. The Recursive Approach

The recursive approach is based on a simple relationship between the partial partition function of a branch and those of its sub-branches. Substituting Eqs. (2) and (3) into Eq. (10), one can write

$$W_{JM}(x_J) = \sum_{x_{M \setminus J}} e^{-\beta h(x_M)} \prod_{\substack{J' \subset M \\ J' \neq J}} \prod_{\substack{M' \supset J' \\ M' \neq M}} W_{J'M'}(x_{J'}), \tag{21}$$

where the outer product runs over all joint sites J' contained in M except J, and the inner one over all main clusters M' containing J', except M itself. By means of this equation (in a recursive manner, starting from the boundaries) it is possible to determine partial partition functions $W_{JM}(x_J)$ for all branches departing from each joint site J of a finite cactus tree. Then Eqs. (2) and (3) provide respectively joint site and main cluster probability distributions, from which all equilibrium thermodynamic properties can be derived.

Let us now turn to the infinite cactus tree and to the evaluation of its bulk properties. In the framework of the recursive approach one can compute the i-th (bulk) joint site probability distribution $p_i(x_i)$ by (i) connecting c k-th generation branches of the i-th type, (ii) evaluating the central site distribution $p_{i,k}(x_i)$, and (iii) investigating the asymptotic behavior for $k \to \infty$. The existence of a limit is equivalent to the bulk invariance condition Eq. (11). Let us notice that actually one considers the central site of n (in principle) different trees of increasing dimensions. This does not evaluate correctly the properties of sites close to the surface of the real tree, but should become exact for bulk sites. Let us denote the partial partition function of a k-th generation branch attached to an i-th type site as $W_{i,k}(x_i)$, for $i = 1,\ldots, n$. According to Eq. (21), one can write

$$W_{i,k}(x_i) = \sum_{x \setminus i} e^{-\beta h(x)} \prod_{i' \neq i} [W_{i',k-1}(x_{i'})]^{c-1}. \tag{22}$$

Starting from the boundary conditions $k = 0$, such equation could determine in principle the partial partition function of any k-th generation branch, until the thermodynamic limit $\lim_{k\to\infty} W_{i,k}(x_i)$, necessary to obtain bulk properties. In practice this is not possible, because such limit equals infinity. Performing a normalization at each step, one can obtain a feasible recursion relation in the following form

$$w_{i,k}(x_i) = g_{i,k}^{-1} \sum_{x\setminus i} e^{-\beta h(x)} \prod_{i'\neq i} [w_{i',k-1}(x_{i'})]^{c-1}, \tag{23}$$

where $w_{i,k}(x_i)$ denote normalized partial partition functions, and

$$g_{i,k} \equiv \sum_{x} e^{-\beta h(x)} \prod_{i'\neq i} [w_{i',k-1}(x_{i'})]^{c-1} \tag{24}$$

is the normalization constant. Specializing Eq. (2) we can write

$$p_{i,k}(x_i) = z_{i,k}^{-1} [w_{i,k}(x_i)]^c, \tag{25}$$

where

$$z_{i,k} \equiv \sum_{x_i} [w_{i,k}(x_i)]^c. \tag{26}$$

Finally, if the limit exists,

$$p_i(x_i) = \lim_{k\to\infty} p_{i,k}(x_i). \tag{27}$$

Let us now show explicitly that the recursion relation Eq. (23), with $g_{i,k}$ defined by Eq. (24), is equivalent to the NIM equations (18) and (19) in the thermodynamic limit $k \to \infty$, still in the hypothesis that the limit exists.[1] Substituting Eq. (25) into Eq. (23), and multiplying both sides by $[p_{i,k}(x_i)]^{1-1/c}$, we obtain

$$p_{i,k}(x_i) = q_{i,k}^{-1} \sum_{x\setminus i} e^{-\beta h(x)} [p_{i,k}(x_i)]^{1-1/c} \prod_{i'\neq i} [p_{i',k-1}(x_{i'})]^{1-1/c}, \tag{28}$$

where

$$q_{i,k} \equiv g_{i,k}\, z_{i,k}^{1/c} \prod_{i'\neq i} z_{i',k-1}^{1/c-1}. \tag{29}$$

Using Eq. (25), the fact that $\sum_x \equiv \sum_{x_i} \sum_{x\setminus i}$, Eq. (23), and Eq. (26), it is possible to verify that Eq. (29) ensures normalization of $p_{i,k}(x_i)$. As a consequence, remembering Eq. (14), we see that, if the limit Eq. (27) exists, for

$k \to \infty$ Eq. (28) becomes equivalent to Eq. (18) "marginalized" to joint site probability distributions (i.e., after a summation of both sides over $x_{\setminus i}$), which proves the equivalence with the variational method. Moreover it is evident that

$$\lim_{k \to \infty} q_{i,k} = q \tag{30}$$

(independently of i), where q is defined by Eq. (19). The latter equation, together with Eqs. (20) and (29), allows us to write

$$\beta f = -\lim_{k \to \infty} \left\{ \log g_{i,k} + \frac{1}{c} \left[\log z_{i,k} - (c-1) \sum_{i' \neq i} \log z_{i',k-1} \right] \right\}. \tag{31}$$

Let us notice that, in the special case of a Cayley tree, Eq. (31) reduces to the formula proposed by Gujrati (Eq. (3) in ref. 4) to evaluate the bulk free energy density in the framework of the recursive approach. A minor difference consists in the presence of the term $\log g_{i,k}$, which disappears when unnormalized partial partition functions are considered, but is essential to numerical evaluation. The same bulk free energy density comes in a more natural way from the variational approach.

3. TEST MODELS

In this section we investigate three test models, which we find very significant and have been previously investigated by the recursive approach.[5,8] We perform variational calculations and compare the results with those of the recursive approach. This is meant, on the one hand, to clarify the discussion of the previous section about the case in which the limit $k \to \infty$ exists and, on the other hand, to give suggestions about what happens when recursion relations have no fixed point.

3.1. Pure 4-Spin Ising Model

Let us consider first an Ising model with pure 4-spin interaction and uniform magnetic field[5] on the square cactus. Main clusters are squares of four sites, and each site is a joint site, characterized by a spin state variable $(s_1, s_2, s_3, s_4 = \pm 1)$. The main cluster hamiltonian is

$$h(s_1, s_2, s_3, s_4) = -J s_1 s_2 s_3 s_4 - H \frac{s_1 + s_2 + s_3 + s_4}{c}, \tag{32}$$

where $J > 0$ is the 4-spin coupling constant and H is the magnetic field.

The NIM equations (18) take the form

$$p(s_1, s_2, s_3, s_4) = q^{-1} e^{-\beta h(s_1, s_2, s_3, s_4)} [p_1(s_1)\, p_2(s_2)\, p_3(s_3)\, p_4(s_4)]^{1-1/c}, \tag{33}$$

where $p(s_1, s_2, s_3, s_4)$ denotes the main cluster probability distribution, and q is determined by normalization. In principle we can distinguish four different site distributions $p_i(s_i)$ and four different magnetizations

$$m_i = \langle s_i \rangle = p_i(+) - p_i(-), \tag{34}$$

for $i = 1, 2, 3, 4$, but from the calculation we obtain only homogeneous phases with magnetization $m_i \equiv m$ independent of i.

As far as the recursive method is concerned, on the Ising square cactus Eq. (23) reads

$$w_{1,k}(s_1) = g_{1,k}^{-1} \sum_{s_2, s_3, s_4 = \pm 1} e^{-\beta h(s_1, s_2, s_3, s_4)} [w_{2,k-1}(s_2)\, w_{3,k-1}(s_3)\, w_{4,k-1}(s_4)]^{c-1} \tag{35}$$

for site 1, and similarly (by a circular permutation of subscripts) for sites 2, 3, 4. Eqs. (25) and (26) as a whole read, for $s = \pm 1$,

$$p_{i,k}(s) = \frac{[w_{i,k}(s)]^c}{[w_{i,k}(+)]^c + [w_{i,k}(-)]^c}. \tag{36}$$

In order to simplify the recursion relations, we can define the ratio

$$r_k \equiv \frac{w_{i,k}(+)}{w_{i,k}(-)}. \tag{37}$$

Notice that it is independent of i, due to the fact that we assume homogeneous boundary conditions and the main cluster hamiltonian possesses a dihedral symmetry. Using Eqs. (34), (36), and (37), we can compute the magnetization as

$$m = \lim_{k \to \infty} \frac{r_k^c - 1}{r_k^c + 1}, \tag{38}$$

where, due to Eq. (35), r_k obey the equation

$$r_k = a \frac{a^3 d r_{k-1}^{3(c-1)} + 3a^2 r_{k-1}^{2(c-1)} + 3a d r_{k-1}^{(c-1)} + 1}{a^3 r_{k-1}^{3(c-1)} + 3a^2 d r_{k-1}^{2(c-1)} + 3a r_{k-1}^{(c-1)} + d}, \tag{39}$$

with $a \equiv e^{2\beta H/c}$ and $d \equiv e^{2\beta J}$. Eq. (39) is solved recursively with the free boundary condition $r_0 = a$, corresponding to a magnetic field equal to H on all boundary sites.

In Fig. 2 we report the phase diagrams obtained by both methods for $H > 0$ (field inversion $H \to -H$ implies $m \to -m$). We set $c = 4$ to approximate the model on the ordinary square lattice. The phase diagrams turn out to be qualitatively correct, unlike that obtained by the mean field theory (see ref. 5 for a discussion). We obtain a first order transition line at $H \neq 0$, which separates a phase with lower magnetization from a phase with higher magnetization. The line ends at a critical point. According to the previous section, the equation of state is the same for both methods, due to the fact that the recursion relation Eq. (39) has always a fixed point. On the contrary the phase diagrams are only qualitatively equivalent but quantitatively different. This is due to the fact that in the variational approach a first order transition is determined by a crossover of the bulk free energy densities of two different phases, i.e., two solutions of the NIM equations obtained by different guess values. On the contrary, the standard recursive method has a fixed starting point, corresponding to the boundary conditions, and detects a first order transition as an abrupt change in the attractor of the dynamical system defined by the recursion relation. The transition observed in this way is the actual transition for the system on the cactus tree with the given boundary conditions. As it could be expected, when two competing phases degenerate into one (i.e., at the critical point)

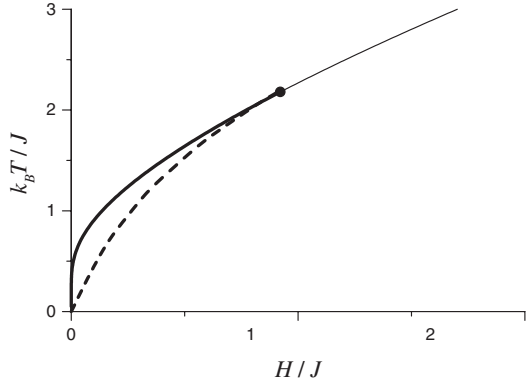

Fig. 2. Phase diagram of the 4-spin Ising model on the square cactus (temperature vs. magnetic field). A dashed line denotes the first order transition, computed by the standard recursive method with free boundary conditions. A circle denotes the critical point. A thick solid line denotes the same transition evaluated by the variational method. A thin solid line represents the self-dual line.

the two methods give the same result, which agrees with the analytic proof that they are equivalent as far as the equation of state is concerned, when a fixed point exists.

Let us notice that the Ising model with pure 4-spin interaction on the ordinary square lattice is self-dual,[32] and phase transitions should occur (if they do) along the line given by

$$\sinh(2\beta J)\sinh(2\beta H) = 1. \tag{40}$$

We can observe that the transition line obtained by the variational approach coincides (within numerical precision) with the self-dual line. This is a nice evidence of the fact that the variational approach is suitable to approximate ordinary lattice systems, even if it is not exact in predicting the phase behavior of cactus trees. Nevertheless, when a fixed point of the recursion relation always exists, like in this model, one can obtain good results also by modifying the standard recursive approach with criteria that have been mentioned in the introduction. In the previous section we have shown analytically that Gujrati's criterion[4] turns out to be equivalent to the variational approach, because both rely on the minimization of the bulk free energy density. Moreover ref. 28 shows that for this model the transition line obtained by Monroe's criterion coincides with the self-dual line as well, and that equivalence to the variational method is found also for the Potts model. We then have numerical evidence that also Monroe's criterion may be equivalent in general, still assuming that a fixed point exists.

3.2. "Antiferromagnetic Triangle" Ising Model

The second test model we consider is the antiferromagnetic Ising model with uniform magnetic field[8] on the triangle cactus (see Fig. 1). Each site is a joint site, characterized by a spin state variable $(s_1, s_2, s_3 = \pm 1)$, and the connectivity constant is $c = 3$. The main cluster hamiltonian reads

$$h(s_1, s_2, s_3) = -J(s_1 s_2 + s_2 s_3 + s_3 s_1) - H\frac{s_1 + s_2 + s_3}{c}, \tag{41}$$

where $J < 0$ is the antiferromagnetic coupling constant and H is the magnetic field.

The NIM equations are similar to Eq. (33)

$$p(s_1, s_2, s_3) = q^{-1} e^{-\beta h(s_1, s_2, s_3)} [p_1(s_1)\, p_2(s_2)\, p_3(s_3)]^{1-1/c}, \tag{42}$$

(with obvious meaning of symbols), while magnetizations can be obtained by Eq. (34) for $i = 1, 2, 3$. From the calculation we obtain a homogeneous phase and a symmetry-broken phase, where on every triangle we have (for $H > 0$) two sites with equal positive magnetization and one site with negative magnetization. The situation is inverted for $H < 0$. The phase diagram is displayed in Fig. 3 and is symmetric with respect to $H = 0$. The transition line is always first order. This model turns out to be interesting as an approximation of the antiferromagnetic Ising model on the ordinary triangular lattice, for which, due to frustration, ordinary mean field like approximations,[24] included the cluster variation method,[25] fail in predicting the (qualitatively) correct phase diagram, and exhibit a phase transition at zero field.

As far as the recursive method is concerned, Eq. (23) reads

$$w_{1,k}(s_1) = g_{1,k}^{-1} \sum_{s_2, s_3 = \pm 1} e^{-\beta h(s_1, s_2, s_3)} [w_{2,k-1}(s_2)\, w_{3,k-1}(s_3)]^{c-1} \tag{43}$$

for site 1, and similarly (by a circular permutation of subscripts) for sites 2, 3. The procedure is analogous to the previous case, except that we preserve the dependence on i, to be able to consider inhomogeneous boundary

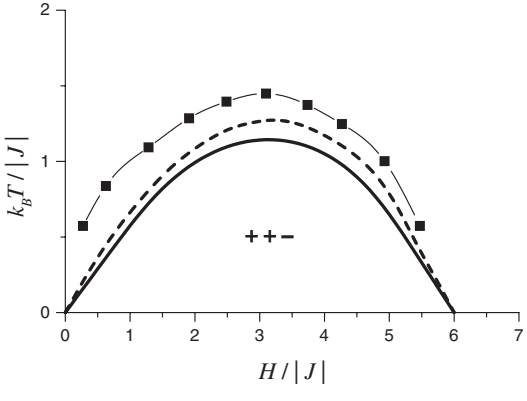

Fig. 3. Phase transitions of the antiferromagnetic Ising model on the triangle cactus (temperature vs. magnetic field). The symmetry-broken phase is denoted by $++-$. A thick solid line denotes the first order transition to the uniform phase, as predicted by the variational method. A dashed line denotes the same transition obtained by the "sequential" recursive method (see the text). Squares denote results from Monte Carlo simulations of the model on the ordinary triangular lattice (the thin solid line is an eyeguide).

conditions (if homogeneous boundary conditions are imposed the dependence on i disappears because of the dihedral symmetry of the main cluster hamiltonian). Being

$$r_{i,k} \equiv \frac{w_{i,k}(+)}{w_{i,k}(-)}, \tag{44}$$

we obtain the following recursion relation

$$r_{1,k} = a \frac{a^2 d^2 r_{2,k-1}^{c-1} r_{3,k-1}^{c-1} + a(r_{2,k-1}^{c-1} + r_{3,k-1}^{c-1}) + 1}{a^2 r_{2,k-1}^{c-1} r_{3,k-1}^{c-1} + a(r_{2,k-1}^{c-1} + r_{3,k-1}^{c-1}) + d^2}, \tag{45}$$

for site 1, and similar ones for sites 2, 3 (circular permutation). Magnetizations are computed by

$$m_i = \lim_{k \to \infty} \frac{r_{i,k}^c - 1}{r_{i,k}^c + 1}. \tag{46}$$

The results of the recursive approach turns out to be dramatically affected by boundary conditions for the present model. Let us work at fixed temperature $k_B T/|J| = 1$ and vary the field H, considering the following cases. For uniform free boundary condition $r_{1,0} = r_{2,0} = r_{3,0} = a$ (magnetic field equal to H on all boundary sites) we obtain the results displayed in Fig. 4(a). The dependence on i is removed but, in a region $0 < H < H_c$, the recursion relation has no fixed point and displays a limit cycle of period 2. The magnetization of the central site oscillates between two values shown in the figure, the positive value for even k and the negative one for odd k. In both cases triangles in consecutive generations alternatively display two sites with positive magnetization and one site with negative magnetization, or vice-versa. On the contrary, for $H = 0$ and $H \geqslant H_c$, a fixed point exists and a paramagnetic phase with uniform magnetization is obtained. The latter is equivalent to that predicted by the variational approach. We also consider the case of inhomogeneous boundary conditions $r_{1,0} = r_{2,0} = a$ and $r_{3,0} = a^{-2}$ (magnetic field equal to H on 2/3 of boundary sites and $-H$ on the remaining ones). We obtain the results displayed in Fig. 4(b). The behavior is equivalent to the previous one, except in a subinterval of $(0, H_c)$, where a fixed point exists, and the dependence on i is preserved. More precisely we obtain the same symmetry-broken phase predicted by the variational method, with the same numerical values of magnetizations. This is in agreement with the discussion performed in the previous section. We finally compare the above results with those obtained by Monroe[8] by solving the recursion relation Eq. (45) in a

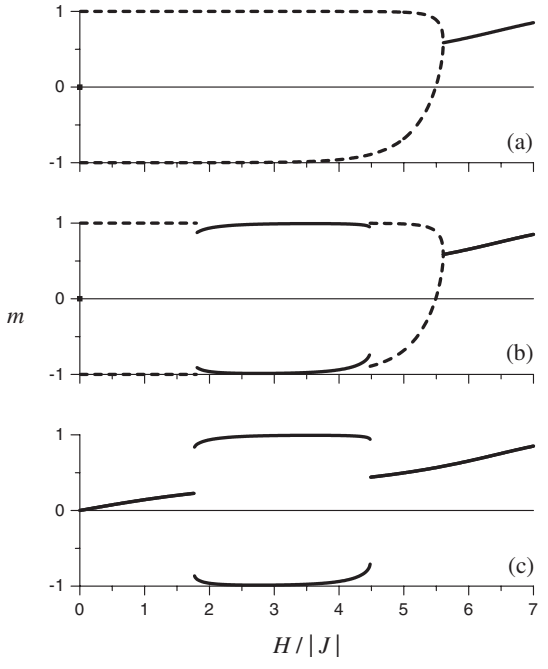

Fig. 4. Magnetizations of the antiferromagnetic Ising model on the triangle cactus at fixed temperature $k_B T/|J| = 1$ as a function of the magnetic field. Results obtained by the recursive method with: (a) free boundary conditions; (b) reversed field on $1/3$ of boundary sites; (c) free "ragged" boundary conditions ("sequential" method). Solid lines refer to fixed point magnetizations, dashed lines to limit cycles (period 2).

"sequential" way. Even if this actually correspond to a different system (a tree with a "ragged" surface), it turns out that a fixed point always exists, and the behavior of magnetizations, displayed in Fig. 4(c), is quantitatively equivalent to that predicted by the variational approach (except the positions of first order transitions).

After these results, we are led to suggest that, when recursion relations have no fixed point, the bulk behavior of cactus systems may provide unreliable information about the behavior of the corresponding ordinary lattice system, and the recursive approach must be employed with some caution. Actually in such cases one should expect a symmetry breaking in the ordinary system, but it is not possible to solve the problem simply by means of criteria for the location of transitions, as in the previous model. One can at most perform some trick to obtain recursion relations with a fixed point, such as Monroe's sequential recursive procedure. Remarkably the latter gives, with respect to the variational method, a transition line

which is closer to the Monte Carlo result[33] for the ordinary triangular lattice, but this seems to be a peculiarity of the model.

3.3. Pure 3-Spin Ising Model

The third test model we investigate is an Ising model with pure 3-spin interaction and uniform magnetic field on the triangle cactus. This model has been previously investigated by the recursive method,[5] with the aim of approximating a model with 3-spin interaction on upward pointing (or downward pointing) triangles of an ordinary triangular lattice. The main cluster hamiltonian reads

$$h(s_1, s_2, s_3) = -Js_1s_2s_3 - H\frac{s_1+s_2+s_3}{c}, \tag{47}$$

where $J > 0$ is the triangle interaction, H is the magnetic field, and $c = 3$. All calculations are analogous to the previous model. The recursion relation turns out to be

$$r_{1,k} = a\frac{a^2 d r_{2,k-1}^{c-1} r_{3,k-1}^{c-1} + a(r_{2,k-1}^{c-1} + r_{3,k-1}^{c-1}) + d}{a^2 r_{2,k-1}^{c-1} r_{3,k-1}^{c-1} + ad(r_{2,k-1}^{c-1} + r_{3,k-1}^{c-1}) + 1} \tag{48}$$

for site 1, and similar ones can be derived (by the usual circular permutation) for sites 2, 3.

We obtain the phase diagram shown in Fig. 5. For $H > 0$ only homogeneous phases are obtained, with a first order transition line, which separates a lower magnetization phase from a higher magnetization phase, and eventually ends at a critical point. In this region the phase behavior is qualitatively similar to the square cactus model described previously. The standard recursive method with free boundary conditions predicts, with respect to the variational method, a different transition line but the same critical point. The recursive method with Monroe's criterion gives a transition line identical to the variational method. For $H < 0$ a symmetry-broken phase appears. According to the variational method, each triangle has two sites with equal negative magnetization and a site with positive magnetization. This phase is separated from the paramagnetic phase by a first order transition. In almost the same region of the phase diagram the recursive method displays a complex behavior, involving limit cycles of high period and chaos.[5] In Fig. 5 we report the boundaries of such region, drawn from data published in ref. 5. In analogy with the previous model, we conjecture that in this case the correct phase diagram of the ordinary lattice system is predicted by the variational approach, while the anomalous behavior

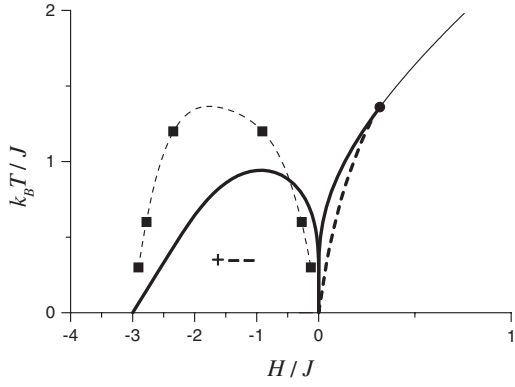

Fig. 5. Phase transitions of the 3-spin Ising model on the triangle cactus (temperature vs. magnetic field). Thick solid lines denote first order transitions computed by the variational method. A circle denotes the critical point. A thin solid line represents the self-dual line. A thick dashed line denotes the first order transition between homogeneous phases obtained by the standard recursive method with free boundary conditions. The symmetry-broken phase region is denoted by $+--$. Squares mark the boundary of the region in which the recursive method displays limit cycles and chaos (the thin dashed line is an eyeguide).

observed in ref. 5 (and also ref. 10 for a similar model) is a peculiarity of the cactus tree. Our conjecture is supported by the fact that, applying Monroe's sequential procedure,[8] we have obtained results that agree with the variational approach.

4. CONVERGENCE OF THE VARIATIONAL METHOD

The last two examples suggest that, as far as the approximation of ordinary lattice systems is concerned, the most relevant problems of the recursive method occur when a fixed point does not exist. On the contrary, the variational approach seems to overcome such problems. In this section we try to give a more rigorous argument, showing a property of the NIM equations (18). As previously mentioned, the NIM is a numerical iterative procedure for the minimization of the variational free energy density. By a generalization of Kikuchi's proof for the Bethe lattice,[29] it turns out that the free energy decreases at each iteration, and the algorithm is always convergent. Let us first give the proof and then discuss some consequences.

Starting from Eq. (15), we write the difference between the free energies of two consecutive steps of the iterative procedure as

$$\beta(\hat{f}-f)=\sum_{x}\left[\hat{p}(x)\hat{\varphi}(x)-p(x)\,\varphi(x)\right], \tag{49}$$

where a hat denotes the latter step, and accordingly

$$\hat{\varphi}(x) = \beta h(x) + \log \hat{p}(x) - \sum_i (1 - 1/c) \log \hat{p}_i(x_i), \tag{50}$$

while $\varphi(x)$ is defined by Eq. (16). Taking the logarithm of both sides of Eq. (18) (where the left hand side is now denoted by a hat), we can write the NIM equations in two different ways, that are

$$\log \hat{p}(x) = -\log q - \beta h(x) + \sum_i (1 - 1/c) \log p_i(x_i) \tag{51}$$

and

$$\sum_i (1 - 1/c) \log p_i(x_i) = \log q + \beta h(x) + \log \hat{p}(x). \tag{52}$$

We substitute the former into $\hat{\varphi}(x)$, the latter into $\varphi(x)$, and finally both into Eq. (49), yielding

$$\beta(\hat{f} - f) = \sum_x p(x) \log \frac{\hat{p}(x)}{p(x)} + \sum_i (1 - 1/c) \sum_{x_i} \hat{p}_i(x_i) \log \frac{p_i(x_i)}{\hat{p}_i(x_i)}. \tag{53}$$

We then consider the inequality $\log \xi \leqslant \xi - 1$, that holds for all real numbers ξ (the equality holds only if $\xi = 1$). By applying the inequality to all logarithms in Eq. (53), taking into account that $c > 1$, and that probability distributions are normalized at each step, we can finally write

$$\hat{f} - f \leqslant 0 \tag{54}$$

$$\hat{f} - f = 0 \Leftrightarrow \hat{p}(x) = p(x) \quad \forall x. \tag{55}$$

Eq. (54) means that the free energy can be decreasing or constant during the procedure, while Eq. (55) assures that it is constant only if the procedure has already reached convergence (i.e., the free energy can only decrease during the procedure).

The above property, generally desirable for a numerical method that aims to minimize a function, has some relevant consequences and makes a significant difference between the NIM and the recursive method. Eqs. (54) and (55) prevent the dynamical system defined by the NIM equations from

having limit cycles. In this way the variational approach always determines the best solution compatible with the invariance condition Eq. (11), and this is the reason why it works for the examples given in the previous section. As a drawback, we have to remark that the variational method cannot detect whether the invariance hypothesis is too restrictive or not. In the form presented here, it can describe correctly a symmetry breaking with a period less than or equal to the width of a main cluster, but would not be able to indicate the existence of phases with higher period (or even incommensurate phases, as observed for instance in the ANNNI model[34]). We then conclude that also the variational approach must be used with some caution in the approximation of ordinary lattice systems, if there are reasons to suspect that a violation of Eq. (11) occurs, not only in the cactus system.[11] In such cases the recursive approach is important because, like in the second example of the previous section, it gives information about the nature of the symmetry breaking.

5. CONCLUSIONS

In this paper we have discussed several properties of the variational approach to cactus trees, compared to the more usually employed recursive approach. First of all we have put in evidence that the variational approach is based on an exact factorization of the equilibrium probability distribution, and can in principle solve exactly finite cactus trees, as well as the recursive method. Moreover we have considered different issues, concerning the bulk behavior of infinite (self-similar) cactus trees and the approximation of ordinary lattice systems (cactus approximation).

We have shown that the variational method allows a simple evaluation of the bulk free energy density. The minimization of bulk free energy yields the correct equation of state for the interior of an infinite cactus tree. In the presence of multiple solutions, i.e., coexistence phenomena, first order transitions determined by the variational method are not the exact ones for the cactus tree, but turn out to be independent of boundary conditions, and provide reliable approximations to phase transitions of a corresponding ordinary system. On the contrary the standard recursive method determines exact phase transitions for the infinite cactus tree, on the basis of changes in the attractor of a dynamical system, defined by recursion relations. If the dynamical system has fixed points, the method predicts the same equation of state as the variational one, but the location of first order transitions depends on boundary conditions, and usually provides poorer approximations to ordinary systems. We have then considered alternative criteria for the determination of first order transitions, that have been proposed in the literature to overcome this problem. We have shown analytically that

Gujrati's free energy criterion[4] is equivalent to the variational approach, and we have obtained numerical evidence that also Monroe's criterion, based on recursion relation derivatives,[28] may be equivalent as well.

We have finally investigated what may happen if recursion relations have no fixed points. On the basis of results obtained for test models, we have suggested that in such case the recursive method may lead to incorrect conclusions about the physics of the ordinary lattice model, if no other information is available. In this case alternative criteria cannot be applied, while the variational method seems to provide reliable results all the same. We have given a rigorous explanation of such a nice behavior, by proving that the convergence of the free energy minimization algorithm is guaranteed by a general property.

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