

Alternative Variational Approach to Cactus Lattices

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In this paper, I will present an alternative approach to the Bethe or cactus lattice approximation, widely employed in the theory of cooperative phenomena. This approach relies on a variational free energy, which is equivalent to the Bethe free energy in that it has the same stationary points, but allows one to simplify analytical calculations, since it is a function of only single-site probability distributions, in the same way as an ordinary mean-field (Bragg-Williams) free energy. As an application, I shall discuss a derivation of closed-form equations for critical points in Ising-like models. Moreover, I will suggest a rule of thumb to choose the cactus lattice connectivity yielding the best approximation for the corresponding model defined on an ordinary lattice.

KEY WORDS: Bethe lattice, Husimi lattice, Bethe approximation, cactus approximation, Ising model

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1. INTRODUCTION

The Bethe (or first-order) approximation is a widely employed tool in the statistical mechanics of lattice systems.^(1,2) It improves the simple mean-field (zeroth-order) approximation by taking into account local correlations between pairs of nearest-neighbor sites, or among sites in suitable clusters. At the pairwise level, it was first proposed by Bethe in 1935, in a self-consistent formulation.⁽³⁾ Almost contemporarily, Guggenheim⁽⁴⁾ gave it a variational formulation, denoted as quasi-chemical approximation, which can be easily generalized to larger clusters.⁽⁵⁾ In the 60s, it was suggested that the Bethe approximation provided the exact solution for models defined on Cayley trees⁽²⁾ (i.e., infinite trees whose leaves are pairs of

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sites), but, in 1974, Eggarter showed that actually the partition function of the simple Ising model on the Cayley tree is analytic at all temperatures, basically due to the fact that the majority of the system is made up of boundary sites.⁽⁶⁾ The Bethe approximation, and the phase transition it predicts for the Ising model, turn out to describe correctly only the behavior of the interior part of the Cayley tree, denoted as Bethe lattice. Such a behavior can be determined by computing the limit of a suitable recursion equation. It is possible to show that even this weaker statement requires some care, in particular when the limit of the recursion equation does not exist, or in the presence of multiple fixed points, i.e., coexistence phenomena.⁽⁷⁾

In the generalized version, sometimes denoted as cactus approximation,⁽⁸⁾ the Cayley tree is replaced by a cactus or Husimi tree, whose leaves are clusters of sites, and the result still describes just the behavior of the interior part of the tree, denoted as cactus or Husimi lattice. In the following, I shall employ the terms *cactus lattice* to denote both Bethe and Husimi lattices, and *cactus approximation* to denote the corresponding approximation schemes. These techniques often provide reliable results for models defined on ordinary lattices, and have been used to investigate a large variety of physical systems: Ising-like models,^(9,10) Potts models,⁽¹¹⁾ complex fluid models,^(12–13) spin liquids,⁽¹⁵⁾ polymers,^(16–20) sandpiles.⁽²¹⁾ More recently, the approximation has also been generalized to treat systems with quenched disorder, such as spin glasses,⁽²²⁾ random heteropolymers,⁽²³⁾ random combinatorial optimization problems,⁽²⁴⁾ random graphs.⁽²⁵⁾ In the context of this generalization, usually denoted as the cavity method, it has also been argued⁽²²⁾ that actually the cactus approximation should provide the exact solution for a regular random graph or hypergraph (i.e., a random graph or hypergraph with fixed connectivity) in the thermodynamic limit. Therefore, the latter turns out to be the most correct definition of a Bethe or Husimi lattice.

As already present in the original formulations by Bethe⁽³⁾ and Guggenheim,⁽⁵⁾ respectively, the cactus approximation allows two different approaches: A recursive one, which exploits the local self-similarity of the cactus lattice, and a variational one, based on a peculiar factorization of the probability distribution of the system. The two approaches have been recently compared and discussed in Ref. 7. The variational approach, in particular, turns out to be equivalent to Kikuchi's cluster variation method^(26–28) with a special choice of basic clusters,⁽⁸⁾ and relies on a variational free energy functional, usually simply denoted as *Bethe free energy*. The Bethe free energy often allows some degree of analytical treatment, mainly in the case of homogeneous systems, or when it is possible to exploit symmetries of the model. Nevertheless, some difficulties may arise, due to the fact that one has to deal with cluster probability distributions, and therefore with a quite large number of variational parameters.⁽¹²⁾ In a previous paper,⁽¹³⁾ devoted to a lattice-fluid model of water, I have employed an alternative method, relying on a simpler variational free energy, which is a function of only single-site probability distributions. In that case, the method allows one to

derive simple equations to determine response functions and their divergence loci (spinodals).⁽¹³⁾

In this paper, I shall first prove the equivalence of the alternative variational free energy to the original Bethe free energy, since such proof was not reported in the previous paper.⁽¹³⁾ Moreover, I will give another example of application, deriving closed-form equations for the criticality conditions of Ising-like spin models. The latter calculation is based on a Landau expansion of the alternative free energy. Incidentally, I will also discuss a criterion for choosing the cactus lattice connectivity, in order to obtain the best approximation for a given ordinary lattice. Different alternatives are possible in general, but one can observe that, as the limit of infinite connectivity recovers the basic mean-field approximation, low connectivity numbers improve the approximation. The paper is organized as follows. In Sec. 2, I will introduce the cactus approximation in the variational formulation, discussing both the usual approach, and how the alternative approach can be derived. Moreover, I shall explain in which sense the two approaches can be said to be equivalent. In Sec. 3, I will discuss the application to Ising-like models. Sec. 4 is devoted to summary and conclusions.

2. THE CACTUS APPROXIMATION

First of all, let us define a cactus tree via a recursive growth procedure. Let us consider a cluster of sites, for instance a square of 4 sites, as shown in Fig. 1(a), or more generally a cluster of n sites. Let each site be characterized by a configuration variable, which for simplicity is assumed to be a scalar. Let us also assume that a cluster hamiltonian h defines the interactions among sites in the cluster. We can build up a branch of the cactus tree in the following way. Let us define a connectivity constant c , and attach $c - 1$ equivalent clusters to the i -th site of the starting cluster, for $i = 2, \dots, n$. We thus obtain a “second generation” branch, shown in Fig. 1(b), where $c = 2$. Subsequently, we can produce new generations by iterating the procedure, as shown in 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 limit.

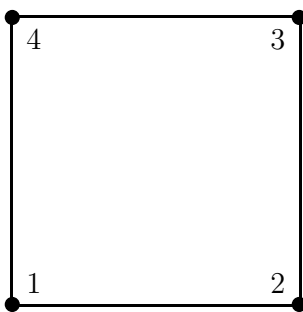
Following Morita,⁽⁸⁾ clusters used as building blocks are denoted as *main clusters*, while intersections of main clusters are denoted as *joint sites*. The total hamiltonian H can be written as a sum over all the main clusters

$$H(X) = \sum_M h(x_M), \quad (1)$$

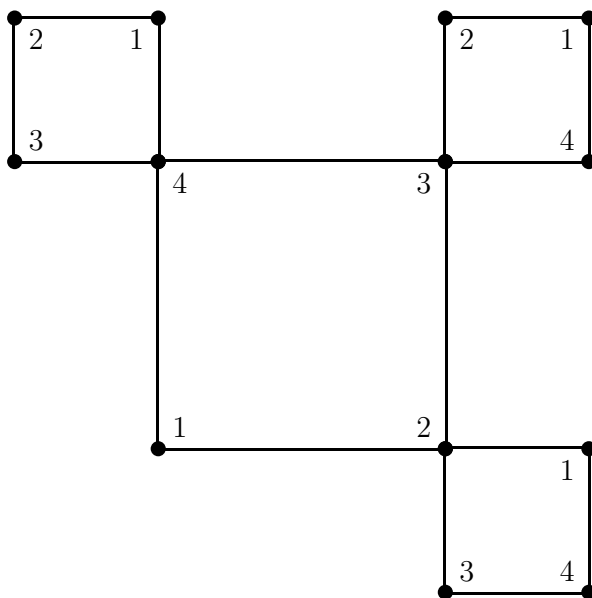
where x_M denotes the set of site configuration variables in the main cluster M , and X denotes the configuration of the whole system. It is possible to show⁽⁷⁾ that the probability distribution of the total configuration $P(X) = Z^{-1} e^{-\beta H(X)}$, where $Z = \sum_X e^{-\beta H(X)}$ is the partition function and β is the inverse temperature, can

be factorized as follows:

$$P(X) = \prod_M \left\{ p_M(x_M) \prod_{J \subset M} [p_J(x_J)]^{-b} \right\}, \quad (2)$$

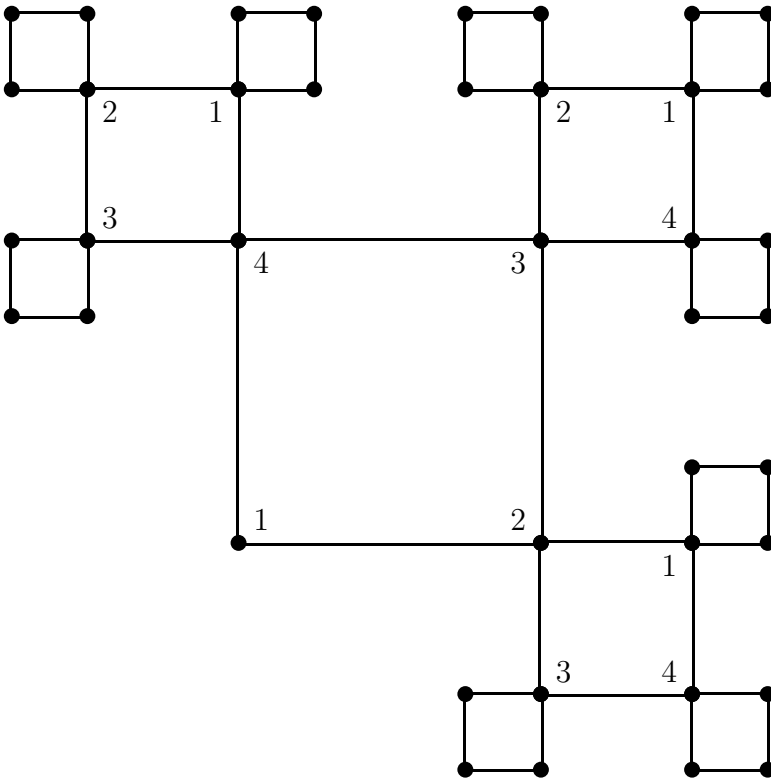


(a)



(b)

Fig. 1. Example of a square cactus tree obtained by a growth procedure: (a) first generation branch; (b) second generation branch; (c) third generation branch. Numerals are meant to denote that the dihedral symmetry of square clusters may be broken.



(c)

Fig. 1. Continued

where $p_M(x_M)$ and $p_J(x_J)$ denote respectively the marginal probability distributions for the configurations x_M (of the main cluster M) and x_J (of the joint site J), and $b \equiv 1 - 1/c$. The outer product runs over all main clusters M , whereas the inner one runs over all joint sites J in the main cluster M .

We can now write the total free energy F as a function of the probability distributions of only main clusters and joint sites. If $\langle \cdot \rangle$ denotes an ensemble average, we have

$$\begin{aligned} \beta F &= \langle \beta H(X) + \log P(X) \rangle \\ &= \sum_M \sum_{x_M} p_M(x_M) \left[\beta h(x_M) + \log p_M(x_M) - b \sum_{J \subset M} \log p_J(x_J) \right]. \end{aligned} \quad (3)$$

Let us notice that this expression coincides with that obtained by the cluster variation method, when the main clusters are chosen as maximal clusters of the cumulant expansion.⁽²⁸⁾ The marginal probability distributions $p_M(x_M)$ and $p_J(x_J)$ can be assumed as variational parameters, and the exact thermodynamic equilibrium state can in principle be determined by minimizing the free energy in Eq. (3), with suitable normalization and compatibility constraints. By compatibility, I mean that joint-site probability distributions $p_J(x_J)$ must be marginal distributions of main-cluster distributions $p_M(x_M)$, i.e.,

$$p_J(x_J) = \sum_{x_{M \setminus J}} p_M(x_M), \quad (4)$$

for all $M \supset J$, where $x_{M \setminus J}$ denotes the configuration of the main cluster M without the joint site J .

Let us notice that this approach would be intractable if one is interested in the properties of the infinite cactus tree, since one would then have to deal with an infinite number of variational parameters and constraints. Nevertheless, the formalism is useful to derive the Bethe free energy (3). It is reasonable that Eq. (3), which is exact for a cactus tree, also tends to be exact for a system which has locally the structure of a cactus tree, but in which every site has the same connectivity, i.e., there is no boundary. As mentioned in the introduction, such a system may be identified with a regular random graph, which is locally tree-like, in the sense that the length of loops diverges as the logarithm of the number of sites (in the thermodynamic limit).⁽²²⁾ For such a system, if the main-cluster hamiltonian h does not depend on M , one can expect that also the thermodynamic state satisfies a “translational” invariance condition, i.e.,

$$p_M(x) \equiv p(x) \quad (5)$$

for all main clusters M . With this condition, one obtains a simpler form of the free energy, which may be quite a good approximation for a corresponding system defined on an ordinary lattice, and is the one which can be denoted as cactus approximation. In the following, as in Eq. (5), $x \equiv \{x_1, \dots, x_n\}$ will denote the total configuration of a generic main cluster, whereas x_i , for $i = 1, \dots, n$, will denote joint-site configurations. If Eq. (5) holds, we shall have to consider only n (in principle) different “types” of joint sites, i.e., n different joint-site probability distributions $p_i(x_i)$.

2.1. Usual Approach

Taking into account the homogeneity condition (5), one can study the free-energy density f (per main cluster) and perform only a minimization of f . From

Eq. (3), one can write

$$\beta f = \sum_x p(x) \left[\beta h(x) + \log p(x) - b \sum_{i=1}^n \log p_i(x_i) \right], \quad (6)$$

where the joint-site distributions $p_i(x_i)$ depend on the main-cluster distribution $p(x)$ via the marginalization relation

$$p_i(x_i) \equiv \sum_{x_{\setminus i}} p(x). \quad (7)$$

In this equation, $x_{\setminus i} \equiv \{x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n\}$ denotes the configuration of a main cluster without the i -th joint site, and the sum runs over all possible such configurations. Thus, the free-energy density turns out to be a functional of only the main-cluster distribution $p(x)$. One can work out a minimization of this functional, using the Lagrange multiplier method to impose normalization of $p(x)$. Accordingly, we define the extended functional

$$\beta f_\lambda \equiv \beta f - \lambda \left[\sum_x p(x) - 1 \right], \quad (8)$$

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

$$p(x) = q^{-1} e^{-\beta h(x)} \prod_{i=1}^n [p_i(x_i)]^b, \quad (9)$$

where q is related to λ in an irrelevant way. Taking the sum of both sides of Eq. (9) over all the cluster configurations x , and imposing the normalization condition, one obtains

$$q = \sum_x e^{-\beta h(x)} \prod_{i=1}^n [p_i(x_i)]^b. \quad (10)$$

Equation (9), with q defined by Eq. (10), provides a fixed point equation for $p(x)$, which is usually solved via an iterative procedure, known as natural iteration method.⁽²⁷⁾ Different solutions may be found, starting the procedure from different trial $p(x)$, 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. (9), and plugging the result into Eq. (6), yielding

$$\beta f = -\log q, \quad (11)$$

where q has to be computed at each iteration. From the numerical point of view, it is noticeable that the natural iteration method lowers the free-energy value at each

iteration,^(7,27) so that it does generally converge to minima of the free energy, and not to maxima or saddle points.

2.2. Alternative Approach

Let us now have a look at Eq. (11). Its form suggests that, instead of minimizing f with respect to the main-cluster distribution $p(x)$, one could obtain equivalent equilibrium conditions also by maximizing the functional q , defined by Eq. (10), with respect to the joint-site distributions $p_i(x_i)$. This fact is not obvious, since Eq. (11) holds only at stationary points of f , being derived by taking into account Eq. (9). Hereafter, I will show that the $p_i(x_i)$ obtained as stationary points of q (which I shall denote as *cluster partition function*) coincide with the marginals of the $p(x)$ which stationarizes f . In this sense, $-\beta^{-1} \ln q$, turns out to be a variational free energy equivalent to f .

Let us study the stationary points of the cluster partition function q . We have to take into account the normalization constraint for the joint-site distributions

$$\sum_{x_i} p_i(x_i) = 1 \quad (12)$$

for $i = 1, \dots, n$. Therefore, we define the extended functional

$$q_{\lambda_1, \dots, \lambda_n} \equiv q - \sum_{i=1}^n \lambda_i \left[\sum_{x_i} p_i(x_i) - 1 \right], \quad (13)$$

compute its derivatives with respect to $p_i(x_i)$, and set them at zero. By simple algebra, we obtain the simultaneous equations

$$p_i(x_i) = b \lambda_i^{-1} \sum_{x_{\setminus i}} e^{-\beta h(x)} \prod_{j=1}^n [p_j(x_j)]^b. \quad (14)$$

After the Lagrange multipliers λ_i have been determined by imposing the normalization constraints (12), Eq. (14) turns out to be equivalent to Eq. (9) marginalized to site distributions, as we aimed to prove. As mentioned in the introduction, the advantage of this alternative approach is that the variational parameters of the cluster partition function are only site distributions, whereas the cluster distribution has never to be considered explicitly.

3. EXAMPLES OF APPLICATION: SPIN MODELS

In this section I will present a particular application of the above described approach, showing how it can be exploited to determine closed-form criticality conditions for Ising-like models. Let us first rewrite the cluster partition function,

assuming that the configuration variables are Ising spins:

$$q = \sum_{s_1=\pm 1} \dots \sum_{s_n=\pm 1} e^{-\beta h(s_1, \dots, s_n)} \prod_{i=1}^n [p_i(s_i)]^b. \quad (15)$$

Defining magnetizations as thermal averages of spin variables

$$m_i \equiv \langle s_i \rangle = p_i(+)-p_i(-), \quad (16)$$

we can use them to parametrize joint-site distributions as

$$p_i(s_i) = \frac{1 + s_i m_i}{2}, \quad (17)$$

for $s_i = \pm 1$. In this way, the maximization of q can be carried out with respect to the magnetizations m_i , with no constraint, except that $-1 \leq m_i \leq 1$. To simplify the notation, let us also define the linear functional

$$\mathcal{W}\{\xi\} \equiv \sum_{s_1=\pm 1} \dots \sum_{s_n=\pm 1} e^{-\beta h(s_1, \dots, s_n)} \xi(s_1, \dots, s_n), \quad (18)$$

where $\xi \equiv \xi(s_1, \dots, s_n)$ denotes any function of joint-site spins in a main cluster. From Eqs. (15) and (17), we can then write

$$q = \frac{1}{2^{nb}} \mathcal{W} \left\{ \prod_{i=1}^n (1 + s_i m_i)^b \right\}. \quad (19)$$

Being interested in critical conditions, we work out a Landau expansion of Eq. (19) in the hypothesis $m_i \rightarrow 0$. From the binomial expansion

$$(1 + s_i m_i)^b = 1 + b s_i m_i + \binom{b}{2} m_i^2 + o(m_i^2), \quad (20)$$

where we have taken into account that $s_i^2 = 1$, we can easily derive

$$\begin{aligned} \prod_{i=1}^n (1 + s_i m_i)^b &= 1 + \sum_{i=1}^n \left[b s_i m_i + \binom{b}{2} m_i^2 + b^2 \sum_{j=i+i}^n s_i s_j m_i m_j \right] \\ &\quad + o(m_i m_j), \end{aligned} \quad (21)$$

where of course $o(m_i m_j)$ denotes an infinitesimal of higher order than any product $m_i m_j$. Substituting into Eq. (19) and taking into account the linearity of \mathcal{W} , we obtain the desired Landau expansion

$$q = q^\circ + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n q''_{ij} m_i m_j + o(m_i m_j), \quad (22)$$

where the elements of the hessian matrix turn out to be

$$q''_{ii} = -\frac{b(1-b)}{2^{nb}} \mathcal{W}\{1\}, \quad (23)$$

$$q''_{ij} = \frac{b^2}{2^{nb}} \mathcal{W}\{s_i s_j\} \quad \text{for } i \neq j, \quad (24)$$

and

$$q^\circ = \frac{1}{2^{nb}} \mathcal{W}\{1\}. \quad (25)$$

Note that the first-order terms disappear, in the hypothesis that the cluster hamiltonian is invariant under spin inversion, i.e.,

$$h(-s_1, \dots, -s_n) = h(s_1, \dots, s_n). \quad (26)$$

This implies $\mathcal{W}\{\xi\} = 0$, if ξ changes sign under spin inversion, as is the case for a single spin. Once the model (i.e., the main-cluster hamiltonian h) is defined, it is easy to determine $\mathcal{W}\{1\}$ and $\mathcal{W}\{s_i s_j\}$ (i.e., the hessian matrix elements q''_{ij}), as a function of the model parameters. Subsequently, one can determine the eigenvalues and eigenvectors of the hessian matrix, for example with the help of a symbolic manipulator like Mathematica. The equations, obtained by setting each eigenvalue at zero, define the criticality conditions, while the correspondent eigenvectors determine the types of symmetry breaking.

3.1. Example I: Ising Model

As a first test model, let us consider the simple Ising model on the square lattice. In order to work out the cactus approximation, let us also consider a cactus lattice, whose building blocks are square plaquettes of 4 sites. In principle, $c = 2$ or $c = 4$ are both reasonable choices for the connectivity. In the former case, there is no overcounting of the energy, whereas, in the latter case, pair interactions turn out to be doubly-counted, so that, in general, the main-cluster hamiltonian can be written as

$$h(s_1, s_2, s_3, s_4) = -\frac{2}{c} J (s_1 s_2 + s_2 s_3 + s_3 s_4 + s_4 s_1). \quad (27)$$

We can now perform the previously described calculation, and determine the (4×4) hessian matrix of the cluster partition function. As mentioned above, the matrix can be diagonalized symbolically by Mathematica, and its eigenvectors turn out to be

$$\begin{aligned} \underline{v}_1 &= (+1, 0, -1, 0) \\ \underline{v}_2 &= (0, +1, 0, -1) \\ \underline{v}_3 &= (+1, -1, +1, -1) \\ \underline{v}_4 &= (+1, +1, +1, +1), \end{aligned} \quad (28)$$

while the corresponding eigenvalues are

$$\begin{aligned}
 \lambda_1 &= -16 + 4c - 2c e^{8\beta J/c} - 2c e^{-8\beta J/c} \\
 \lambda_2 &= \lambda_1 \\
 \lambda_3 &= -8 - 4c - 2c e^{8\beta J/c} + (6c - 8)e^{-8\beta J/c} \\
 \lambda_4 &= -8 - 4c + (6c - 8)e^{8\beta J/c} - 2c e^{-8\beta J/c}.
 \end{aligned}
 \tag{29}$$

It is easy to see that $\lambda_1 = \lambda_2$ never change sign, so that the corresponding eigenvectors $\underline{v}_1, \underline{v}_2$ do not correspond to any real symmetry breaking. Conversely, by solving the equations $\lambda_3 = 0$ and $\lambda_4 = 0$, we obtain

$$e^{\pm 8\beta J/c} = 1 - \frac{2}{c} + 2\left(\sqrt{1 + \frac{1}{c^2}} - 1\right)
 \tag{30}$$

(+, - signs descend respectively from $\lambda_3 = 0, \lambda_4 = 0$), which determine two different critical values of βJ of equal magnitude and opposite sign. The \underline{v}_3 and \underline{v}_4 eigenvectors indicate that the symmetry breakings are respectively of antiferro- or ferro-magnetic type. Of course, since $J = -|J|$ and $J = |J|$ respectively for the two cases, the critical temperature turns out to be the same.

In Fig. 2, I report the scaled critical temperature $1/4\beta_c|J|$ for $c = 2$ and $c = 4$, together with the exact value for the Ising model on the ordinary square

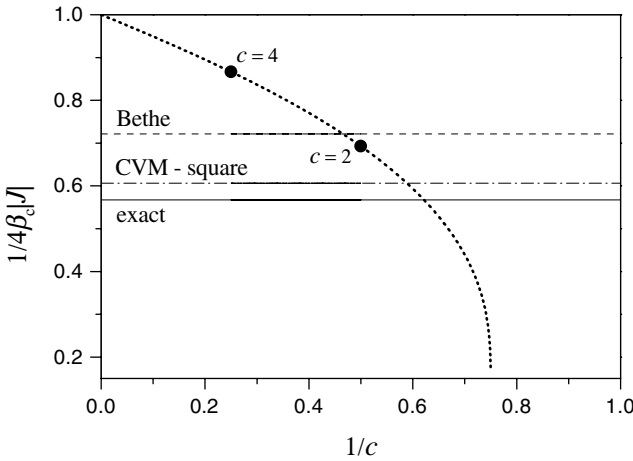


Fig. 2. Scaled critical temperature $1/4\beta_c|J|$ for the Ising model in the square cactus approximation for $c = 2$ and $c = 4$ (circles) and its analytical continuation, as a function of $1/c$ (dotted line). Thin lines denote the exact critical temperature of the Ising model on the square lattice, and the approximate temperatures obtained by the ordinary Bethe lattice approximation and by the square approximation of the cluster variation method.

lattice^(1,29)

$$2\beta_c|J| = \sinh^{-1} 1 \tag{31}$$

and the values obtained by the cluster variation method in the square approximation⁽³⁰⁾ (equivalent to the Kramers-Wannier approximation⁽³¹⁾)

$$2\beta_c|J| = \ln \frac{5 + \sqrt{17}}{4} \tag{32}$$

and by the basic (pair) Bethe approximation⁽¹⁾

$$2\beta_c|J| = \ln 2. \tag{33}$$

One can observe that the square cactus approximation yields quite a poor result for $c = 4$, whereas it slightly improves the Bethe approximation for $c = 2$, although it is not so good as the cluster variation method (Kramers-Wannier) result. It is also interesting to investigate the analytical continuation of the critical temperature value, Eq. (30), for any value of c . The result is also reported in Fig. 2, as a function of $1/c$. In particular, let us consider what happens for large c . Equation (30) can be expanded in powers of $1/c$, yielding

$$1 \pm \frac{8\beta J}{c} + o\left(\frac{1}{c}\right) = 1 - \frac{2}{c} + o\left(\frac{1}{c}\right), \tag{34}$$

so that, in the limit $c \rightarrow \infty$, Eq. (34) leads to

$$\mp 4\beta J = 1, \tag{35}$$

which is exactly the mean-field value.⁽¹⁾ This result could be expected, since, according to Eq. (27), $h(x)$ contains c in its denominator, so that, for $c \rightarrow \infty$, the stationary point Eq. (9) gives

$$p(x) = \prod_{i=1}^n p_i(x_i), \tag{36}$$

which actually coincides with the mean-field (Bragg-Williams) hypothesis.⁽¹⁾

According to these results, I suggest that, as a rule of thumb, the connectivity constant of the cactus lattice, used to work out the approximation of the ordinary lattice model, is to be chosen as small as possible. High connectivity values approach the mean-field approximation, whereas low connectivity values seem to improve the approximation, and one can expect that such a behavior should be quite general. Of course, one also expects that in general there will be a price to pay, namely, that choosing smaller connectivities implies choosing larger main clusters. For example, this is actually what happens in our case, while passing from the basic Bethe approximation ($c = 4$, with a 2-site main cluster: $n = 2$) to the more effective square cactus approximation ($c = 2$, with a 4-site main-cluster:

$n = 4$). Let us notice that, for the simple Ising model, the improvement obtained is just quantitatively relevant. Nevertheless, it may become even qualitatively important, for models in which correlations between more than two sites play a significant role, as is the case, for instance, in the previously cited lattice models of water.^(12–13)

3.2. Example II: Ising Model with 1st and 2nd Neighbor Interactions

Let us now consider another interesting example, namely, the Ising model with nearest-neighbor (J) and next-nearest-neighbor (K) interactions on the two-dimensional Kagomé lattice. This is quite a well-suited test model, since it exhibits a rich phase diagram (with 4 different ordered phases, some of which are frustrated, and reentrance phenomena), and it has been solved exactly.⁽³²⁾ Moreover, the model has also been investigated by a cactus approximation, showing good qualitative agreement with the exact results.⁽⁹⁾ The cactus lattice structure of Ref. 9 is reported in Fig. 3(a), where the main clusters have 5 sites, 4 of which (those on the vertices of each square) are joint sites. Interactions on horizontal bonds are equal to those between a joint site and a central site, and correspond to nearest-neighbor interactions (J) for the original Kagomé lattice. Interactions on vertical bonds are (in principle) different, and correspond to next-nearest neighbor interactions (K) on the Kagomé lattice. The main-cluster hamiltonian reads

$$h(s_0, s_1, s_2, s_3, s_4) = -J[s_1s_2 + s_3s_4 + s_0(s_1 + s_2 + s_3 + s_4)] - K(s_2s_3 + s_4s_1), \tag{37}$$

where $s_0 = \pm 1$ denotes the spin of a central site and $s_1, s_2, s_3, s_4 = \pm 1$ denote the spins of joint sites. Let us note that here, in order to reduce the problem to the previously described framework, we have actually to work on an effective 4-site hamiltonian $\tilde{h}(s_1, s_2, s_3, s_4)$, obtained by summing over the central spin configurations, i.e.,

$$e^{-\beta\tilde{h}(s_1, s_2, s_3, s_4)} \equiv \sum_{s_0=\pm 1} e^{-\beta h(s_0, s_1, s_2, s_3, s_4)}. \tag{38}$$

As in the previous case, we can then compute a 4×4 hessian matrix, whose eigenvectors turn out to be

$$\begin{aligned} \underline{v}_1 &= (+1, -1, -1, +1) \\ \underline{v}_2 &= (+1, -1, +1, -1) \\ \underline{v}_3 &= (+1, +1, -1, -1) \\ \underline{v}_4 &= (+1, +1, +1, +1). \end{aligned} \tag{39}$$

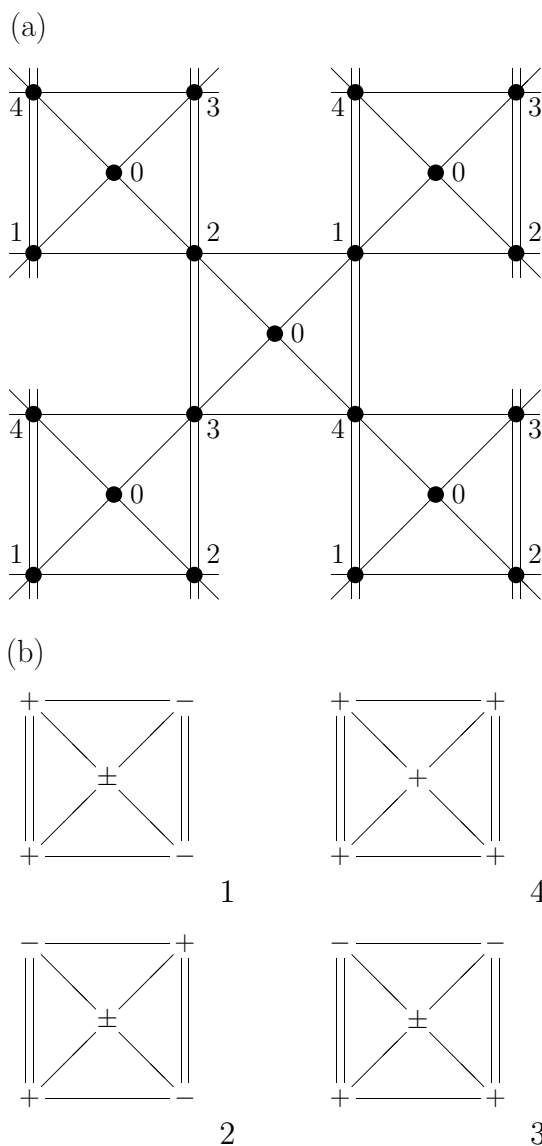


Fig. 3. (a) Sketch of the cactus lattice employed for the approximation of the Kagomé lattice model: single segments denote J (nearest-neighbor) interactions, double segments K (next-nearest-neighbor) interactions; 0 denote central sites, 1, 2, 3, 4 joint sites with (in principle) different magnetizations m_1, m_2, m_3, m_4 . (b) Different types of ordering displayed by the model: + and - denote the sign of site magnetizations, \pm denotes equally probable spin values ($m_0 = 0$).

They define the four different ordered phases depicted in Fig. 3(b). In phases 1 to 3, spins + and - in the central site are equally probable, as observed in Ref. 9, although this fact is not evident by the present treatment. The corresponding eigenvalues are

$$\begin{aligned}
 \lambda_1 &= -\cosh(2\beta J) - e^{-2\beta K} \cosh(2\beta J) - \frac{1}{4}e^{2\beta K}(e^{6\beta J} - e^{-2\beta J}) \\
 \lambda_2 &= -\cosh(2\beta J) - e^{-2\beta K} \sinh(2\beta J) - \frac{1}{4}e^{2\beta K}(e^{6\beta J} + 3e^{-2\beta J}) \quad (40) \\
 \lambda_3 &= -\cosh(2\beta J) + e^{-2\beta K} \sinh(2\beta J) - \frac{1}{4}e^{2\beta K}(e^{6\beta J} + 3e^{-2\beta J}) \\
 \lambda_4 &= -\cosh(2\beta J) - e^{-2\beta K} \cosh(2\beta J) + \frac{1}{4}e^{2\beta K}(e^{6\beta J} - e^{-2\beta J}).
 \end{aligned}$$

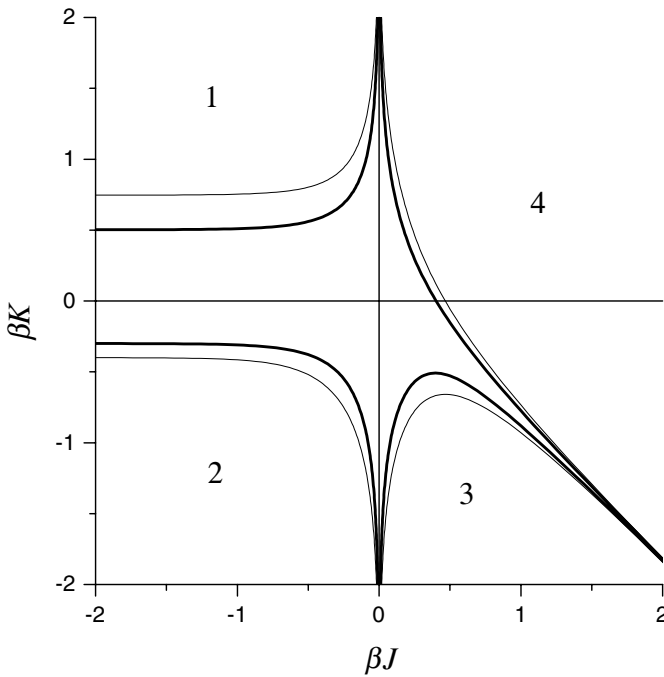


Fig. 4. Phase diagram of the Ising model with nearest- and next-nearest-neighbor interactions on the Kagomé lattice (thin lines), compared to the results from the cactus approximation (thick lines). All transitions are second order (critical). Numerals denote the ordered phases corresponding to those shown in Fig. 3(b). The central region is the paramagnetic phase.

Setting each eigenvalue at zero yields the critical lines, which we report in Fig. 4. These lines have been already computed numerically in Ref. 9, whereas the present method allows one to derive closed-form equations for them. As shown in Fig. 4, they provide quite a good approximation of the exact critical lines.⁽³²⁾

4. SUMMARY

In this paper, I have proposed an alternative variational formulation of the Bethe and cactus approximations. This approach is based on a variational free energy, which is defined in the subspace of single-site probability distributions, but is equivalent to the Bethe free energy in the sense that it yields the same marginals as stationary points. This approach may be useful to deal analytically with the cactus approximation of different model systems. Analytical treatments become useful to investigate certain loci of a phase diagram, such as spinodals or critical points, where some response functions diverge, so that numerical calculations become difficult. I had previously employed this approach to investigate spinodals in the phase diagram of a lattice model of water, without giving details about the proof of equivalence. Here, I have presented such a proof in full detail and I have also described an application of the method, to determine closed-form criticality conditions, for spin models with inversion symmetry. Moreover, I have observed that a good criterion for the connectivity constant of the cactus lattice, used to build up the approximation scheme, may be to choose the lowest possible one. This fact could be expected since, conversely, large connectivities tend to make the approximation similar to an ordinary mean-field theory.

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