

# On the Convergence of Kikuchi's Natural Iteration Method

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In this article we investigate on the convergence of the natural iteration method, a numerical procedure widely employed in the statistical mechanics of lattice systems, to minimize Kikuchi's cluster variational free energies. We discuss a sufficient condition for the convergence, based on the coefficients of the cluster entropy expansion, depending on the lattice geometry. We also show that such a condition is satisfied for many lattices usually studied in applications. Finally, we consider a recently proposed class of methods for the minimization of Kikuchi functionals, showing that the natural iteration method turns out as a particular instance of that class.

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**KEY WORDS:** Cluster variation method; natural iteration method; statistical inference; constrained optimization.

## 1. INTRODUCTION

The cluster variation method (CVM) is a powerful approximate technique for the statistical mechanics of lattice systems, which can improve the simple mean field and Bethe approximations, by taking into account correlations on larger and larger distances. It was first proposed by Kikuchi in 1951<sup>(1)</sup> as an approximate evaluation of the thermodynamic weight, and since then it has been reformulated several times,<sup>(2-4)</sup> mainly to clarify the nature of the approximation and to simplify the way to work it out. Quite a recent formulation<sup>(4)</sup> shows that the CVM consists of a truncation of a cumulant entropy expansion. Each cumulant is associated to a cluster of sites and the truncation is justified by the expected rapid vanishing of

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the cumulants upon increasing cluster size. In this way, the CVM can be viewed as a hierarchy of approximations, each one defined by the set of maximal clusters retained in the cumulant expansion, usually denoted as *basic clusters*. If pairs of nearest-neighbor sites are chosen as basic clusters, the CVM coincides with the Bethe approximation. Generally, using larger basic clusters improves the approximation, even if convergence of the cumulant expansion to the exact entropy has been rigorously proved just in a few cases.<sup>(3,5)</sup>

Due to its relative simplicity and accuracy, the CVM is widely used in every kind of statistical mechanical applications, to determine both thermodynamic properties<sup>(6-8)</sup> and phase diagrams.<sup>(9-12)</sup> CVM results generally compare well with those of Monte Carlo simulations,<sup>(10,11,13)</sup> as well as experimental ones.<sup>(6,8,9,13-15)</sup> Making use of suitable series of CVM approximations, it is also possible to extrapolate quite accurate estimates of critical exponents.<sup>(16-19)</sup> Recently, it has been shown that the belief propagation algorithm, an approximate method for statistical inference, employed for a lot of technologically relevant problems (image<sup>(20)</sup> and signal processing,<sup>(21)</sup> decoding of error-correcting codes,<sup>(21,22)</sup> machine learning<sup>(22)</sup>), is equivalent to the minimization of a Bethe free energy for statistical mechanical models defined on graphs.<sup>(23)</sup> This fact has opened new research areas both to application of the CVM as an improvement of the approximation,<sup>(23)</sup> and to analysis of efficient minimization algorithms,<sup>(24-26)</sup> the latter mainly because belief propagation sometimes fails to converge.

Let us introduce the problem from the CVM point of view. Once the approximate entropy (and hence free energy) for the chosen set of basic clusters has been obtained, one has to face the problem of minimizing a nonconvex functional in the basic cluster probability distributions. An algorithm for minimizing such a functional has been proposed by Kikuchi himself,<sup>(27)</sup> and is known as natural iteration method (NIM). A proof of convergence for this algorithm has been given in the original paper, essentially for the Bethe approximation, which can be easily extended to the Husimi tree.<sup>(28)</sup> Nevertheless, the range of convergent cases seems to be much wider, so that the natural iteration method might be interesting also for the nonconventional applications mentioned above.

In this article we analyze a sufficient condition for the convergence of the NIM. Such a condition is a requirement on the coefficients of the cluster entropy expansion (obtained from the cumulant expansion through a Möbius inversion<sup>(4)</sup>) and is shown to hold for quite a large variety of approximations that are generally used to treat thermodynamic systems. Namely, we consider: a set of “plaquette” approximations on different lattices,<sup>(8,12,27,29)</sup> Kikuchi’s B and C hierarchies for the square<sup>(30)</sup> and

triangular<sup>(31)</sup> lattices, the cube approximation for the simple cubic lattice. As far as the latter case is concerned, we actually analyze a generic hypercube approximation on the hypercubic lattice in  $d$  dimensions, showing that the sufficient condition holds for  $d \leq 3$ . Finally, we take into account a recently proposed algorithm for the minimization of the CVM free energy,<sup>(25)</sup> which allows several alternatives, depending on the possibility of upperbounding the free energy with convex (easy to be minimized) functions. We show that one of the best choices is equivalent to the natural iteration method.

## 2. THE CVM FREE ENERGY

As mentioned in the previous Section, the approximate CVM entropy can be written as a linear combination of cluster entropies<sup>(4)</sup>

$$S = \sum_{\alpha} a_{\alpha} S_{\alpha}, \quad (1)$$

where the sum index  $\alpha$  runs over all basic clusters and their subclusters. We shall always consider clusters in this set only. The cluster entropies are defined as usual

$$S_{\alpha} = - \sum_{x_{\alpha}} p_{\alpha}(x_{\alpha}) \log p_{\alpha}(x_{\alpha}), \quad (2)$$

where  $p_{\alpha}(x_{\alpha})$  denotes the probability of the configuration  $x_{\alpha}$  for the cluster  $\alpha$ , the sum runs over all possible configurations, and the Boltzmann constant  $k$  is set to 1 (entropy is measured in natural units). The coefficients can be determined recursively, starting from basic clusters down to subclusters, making use of the following property<sup>(4)</sup>

$$\sum_{\alpha' \supseteq \alpha} a_{\alpha'} = 1, \quad \forall \alpha. \quad (3)$$

Due to the fact that a basic cluster  $\gamma$  never contains (by definition) another basic cluster, from the above formula we immediately get  $a_{\gamma} = 1 \forall \gamma$ . Here and in the following,  $\gamma$  denotes basic clusters. The other coefficients, namely, those  $a_{\alpha}$  associated to subclusters, depend on the lattice geometry, and in particular they do not have a definite sign. This fact allows the CVM free energy to be nonconvex, and indeed this is the case

for most physically interesting lattices. As far as the hamiltonian is concerned, we assume that it can be written as a sum of contributions  $h_\gamma$  from all basic clusters as

$$\mathcal{H} = \sum_{\gamma} h_{\gamma}(x_{\gamma}), \quad (4)$$

where of course  $x_{\gamma}$  denotes basic cluster configurations. Let us decide to write the whole CVM free energy as a sum over basic clusters, splitting entropy contributions from each subcluster among all basic clusters that contain it (in equal parts). Assuming energies normalized to  $kT$ , we obtain

$$F[p] = \sum_{\gamma} \sum_{x_{\gamma}} p_{\gamma}(x_{\gamma}) \left[ h_{\gamma}(x_{\gamma}) + \log p_{\gamma}(x_{\gamma}) + \sum_{\alpha \subset \gamma} b_{\alpha} \log p_{\gamma}(x_{\alpha}) \right], \quad (5)$$

where

$$p_{\gamma}(x_{\alpha}) \equiv \sum_{x_{\gamma \setminus \alpha}} p_{\gamma}(x_{\gamma}). \quad (6)$$

Let us notice that we have defined new coefficients  $b_{\alpha} \equiv a_{\alpha}/c_{\alpha}$ , where  $c_{\alpha}$  denotes the number of basic clusters that contain  $\alpha$ , and we have expressed subcluster probability distributions as marginals of basic cluster distributions, according to Eq. (6) (the sum runs over configurations  $x_{\gamma \setminus \alpha}$  of the basic cluster  $\gamma$  minus the subcluster  $\alpha$ ).

### 3. THE NATURAL ITERATION METHOD

In the above formulation, basic cluster distributions  $\{p_{\gamma}(x_{\gamma})\}$  are the variational parameters of the free energy (which is denoted in short by  $F[p]$ ), and the thermodynamic equilibrium state can be determined by minimization with respect to these parameters, with suitable normalization and compatibility constraints. By compatibility we mean that marginal distributions  $p_{\gamma}(x_{\alpha})$  must be the same for all basic clusters  $\gamma \supset \alpha$ . Let us notice that, for most thermodynamic applications, one usually makes some homogeneity assumption on the system, and this generally reduces the problem to only one or few different basic cluster distributions. Compatibility constraints may be still necessary to impose the required symmetry.<sup>(31)</sup> We go on with the nonhomogeneous formulation, without loss of generality. The important thing is that, in any case, we deal with constraints that are linear in the probability distributions. According to the

Lagrange method, we transform the constrained minimum problem with respect to  $\{p_\gamma(x_\gamma)\}$  to a free minimum problem for an extended functional which depends on additional parameters (Lagrange multipliers). Due to linearity, the extended functional can be written in the form:

$$\tilde{F}[p, \lambda] = F[p] - \sum_\gamma \sum_{x_\gamma} p_\gamma(x_\gamma) \lambda_\gamma(x_\gamma), \tag{7}$$

where  $\{\lambda_\gamma(x_\gamma)\}$  are the Lagrange multipliers. Of course,  $\{\lambda_\gamma(x_\gamma)\}$  are not all independent variables, but internal relationships are system-dependent, and we do not analyze them. Let us only notice, for future use, that the difference between the new functional and the original one (the last term in Eq. (7)) is independent of the  $\{p_\gamma(x_\gamma)\}$  distributions, provided they satisfy the required constraints.

The derivatives of  $\tilde{F}$  with respect to  $p_\gamma(x_\gamma)$  turn out to be

$$\frac{\partial \tilde{F}[p, \lambda]}{\partial p_\gamma(x_\gamma)} = h_\gamma(x_\gamma) + \log p_\gamma(x_\gamma) + \sum_{\alpha \subset \gamma} b_\alpha \log p_\gamma(x_\alpha) - \lambda_\gamma(x_\gamma) + \text{const.}, \tag{8}$$

where the additive constant is irrelevant and we can absorb it into the Lagrange multipliers. Setting the above derivatives to zero resolves stationarization with respect to probability distributions. The natural iteration method consists in rewriting such equations in a fixed point form, that is

$$\hat{p}_\gamma(x_\gamma) = e^{\lambda_\gamma(x_\gamma) - h_\gamma(x_\gamma)} \prod_{\alpha \subset \gamma} [p_\gamma(x_\alpha)]^{-b_\alpha} \tag{9}$$

and then solving them by simple iteration. A new estimate of the basic cluster probability distribution  $\hat{p}_\gamma(x_\gamma)$  is obtained from the previous one  $p_\gamma(x_\gamma)$  through its marginals  $p_\gamma(x_\alpha)$ . The Lagrange multipliers must be determined at each iteration, so that also  $\hat{p}_\gamma(x_\gamma)$  satisfies the required constraints. This job can be done in different ways by a nested procedure (inner loop), for instance a Newton–Raphson method or a suitable fixed point method.<sup>(31,32)</sup> In this paper we do not deal with the determination of Lagrange multipliers, but we focus only on the convergence of the main loop.

#### 4. SUFFICIENT CONDITION FOR THE CONVERGENCE

As usual for iterative algorithms designed to minimize functionals that are bounded from below, a proof of convergence can be given by the decreasing of the functional value at each iteration. This is actually the case for the natural iteration method. Nevertheless, let us notice that convergence does not prove that a fixed point is a global minimum, and not even a minimum, but only a stationary point. Free energy decreasing is only suggestive of the fact that the method “goes in the right direction”. From experience, one observes that local minima are generally stable fixed points, and this fact may be sometimes exploited to investigate metastable states, whereas maxima and saddles are usually unstable. These facts are likely to be related to the particular form of the NIM equations (9), but they are not in the scope of the present paper.

Let us consider the free energy difference  $F[\hat{p}] - F[p]$  for two subsequent iterations  $p, \hat{p}$ , where  $F[p]$  is defined by Eqs. (5) and (6). Taking the logarithm of both sides of Eq. (9), we can rewrite the NIM equations in two different ways, that are

$$\log \hat{p}_\gamma(x_\gamma) = \lambda_\gamma(x_\gamma) - h_\gamma(x_\gamma) - \sum_{\alpha \subset \gamma} b_\alpha \log p_\gamma(x_\alpha), \quad (10)$$

$$\sum_{\alpha \subset \gamma} b_\alpha \log p_\gamma(x_\alpha) = \lambda_\gamma(x_\gamma) - h_\gamma(x_\gamma) - \log \hat{p}_\gamma(x_\gamma). \quad (11)$$

Let us replace the former into  $F[\hat{p}]$  and the latter into  $F[p]$ . Remembering that probability distributions satisfy the constraints, whence the latter term on the right-hand side of Eq. (7) depends on Lagrange multipliers only, we obtain

$$F[\hat{p}] - F[p] = \sum_\gamma \sum_{x_\gamma} \left\{ p_\gamma(x_\gamma) \log \frac{\hat{p}_\gamma(x_\gamma)}{p_\gamma(x_\gamma)} - \hat{p}_\gamma(x_\gamma) \sum_{\alpha \subset \gamma} b_\alpha \log \frac{p_\gamma(x_\alpha)}{\hat{p}_\gamma(x_\alpha)} \right\}. \quad (12)$$

Let us consider the inequality  $\log \xi \leq \xi - 1$ , where equality holds if and only if  $\xi = 1$ . By applying this inequality to the first logarithm (the one involving basic cluster probability distributions) in Eq. (12), and taking into account that distributions are normalized, we obtain

$$F[\hat{p}] - F[p] \leq - \sum_\gamma \sum_{x_\gamma} \hat{p}_\gamma(x_\gamma) \sum_{\alpha \subset \gamma} b_\alpha \log \frac{p_\gamma(x_\alpha)}{\hat{p}_\gamma(x_\alpha)}, \quad (13)$$

where equality holds if and only if  $\hat{p}_\gamma(x_\gamma) = p_\gamma(x_\gamma) \forall \gamma, x_\gamma$ . The same result could be obtained by observing that actually the upperbounded terms coincide with (minus) the Kullback–Liebler distances between the probability distributions  $p_\gamma(x_\gamma)$  and  $\hat{p}_\gamma(x_\gamma)$ . If all subcluster coefficients  $b_\alpha$  were negative, we could apply the same argument to all terms, and the upperbound would be zero. Such a situation occurs for instance in the Bethe<sup>(27)</sup> and Husimi tree<sup>(28)</sup> approximations, and the proof of convergence would be complete. In a general case, we have to require a condition on the  $b_\alpha$  coefficients. The basic idea is to “couple” smaller cluster terms with a positive coefficient to larger cluster terms with a negative coefficient, yielding a sum of Kullback–Liebler distances (some between conditional probability distributions) with negative coefficients, which can then be upperbounded by zero. The details are given in the following.

**Theorem (sufficient condition for the convergence).** Let  $\{b_{\alpha^-|\alpha^+}\}$  be a set of nonnegative coefficients (allocation coefficients), defined for each pair of subclusters  $\alpha^-, \alpha^+$ , such that  $b_{\alpha^-} < 0, b_{\alpha^+} > 0$ , and  $\alpha^- \supset \alpha^+$ . If the following properties hold for all basic clusters  $\gamma$ :

$$b_{\alpha^+} = \sum_{\alpha^+ \subset \alpha^- \subset \gamma} b_{\alpha^-|\alpha^+}, \quad \forall \alpha^+ \subset \gamma, \tag{14}$$

$$-b_{\alpha^-} \geq \sum_{\alpha^+ \subset \alpha^-} b_{\alpha^-|\alpha^+}, \quad \forall \alpha^- \subset \gamma, \tag{15}$$

then

$$F[\hat{p}] - F[p] \leq 0, \tag{16}$$

$$F[\hat{p}] - F[p] = 0 \iff \hat{p} = p. \tag{17}$$

Equation (16) means that the free energy can be decreasing or constant during the procedure, while Eq. (17) ensures that it is constant only if the procedure has already reached convergence (i.e., the free energy can only decrease during the procedure). A relevant consequence of Eq. (17) is that it prevents the dynamical system defined by the NIM equations from having limit cycles at constant free energy, which could occur in principle.

*Proof.* Let us consider the right-hand side of Eq. (13) and split the sum over subclusters  $\alpha \subset \gamma$  in two sums over subclusters  $\alpha^+, \alpha^-$  with positive or negative coefficients, respectively. Positive coefficients  $b_{\alpha^+}$  can be

replaced by Eq. (14), while, according to Eq. (15), negative coefficients can be replaced by

$$b_{\alpha^-} = - \sum_{\alpha^+ \subset \alpha^-} b_{\alpha^-|\alpha^+} - d_{\alpha^-} \tag{18}$$

for certain  $d_{\alpha^-} \geq 0$ . Defining, for each  $\alpha^- \supset \alpha^+$ , the conditional probability distributions

$$p_{\gamma}(x_{\alpha^-}|x_{\alpha^+}) \equiv \frac{p_{\gamma}(x_{\alpha^-})}{p_{\gamma}(x_{\alpha^+})}, \tag{19}$$

after some simple manipulations we obtain

$$\begin{aligned}
 - \sum_{\alpha \subset \gamma} b_{\alpha} \log \frac{p_{\gamma}(x_{\alpha})}{\hat{p}_{\gamma}(x_{\alpha})} &= \sum_{\alpha^- \subset \gamma} \left[ d_{\alpha^-} \log \frac{p_{\gamma}(x_{\alpha^-})}{\hat{p}_{\gamma}(x_{\alpha^-})} \right. \\
 &\quad \left. + \sum_{\alpha^+ \subset \alpha^-} b_{\alpha^-|\alpha^+} \log \frac{p_{\gamma}(x_{\alpha^-}|x_{\alpha^+})}{\hat{p}_{\gamma}(x_{\alpha^-}|x_{\alpha^+})} \right]. \tag{20}
 \end{aligned}$$

The logarithm inequality  $\log \xi \leq \xi - 1$  can now be applied to all terms in the previous equation, because all coefficients are positive (or equivalently we get a sum of Kullback–Liebler terms), and the zero upper-bound of Eq. (16) is obtained. As previously mentioned, Eq. (17) is proved by the fact that the logarithm inequality holds if and only if  $\xi = 1$ , i.e., the Kullback–Liebler distance between two probability distributions is zero if and only if the two distributions are equal. ■

### 5. SOME PARTICULAR CASES

In this section we consider some particular choices of basic clusters, that is, some particular CVM approximations for regular lattices on which several model systems are defined.

#### 5.1. “Plaquette” Approximations

By “plaquette” approximations we mean a class of approximations in which basic clusters are of a unique type (which we denote as plaquette, for example, a square on a square lattice), while subclusters with nonzero coefficients are only single sites and nearest neighbor pairs. Let us denote



such clusters by 1 and 2, respectively, and, according to the notation introduced in Section 2, let us denote by  $a_1$  and  $a_2$  the coefficients of the cluster entropy expansion, by  $c_1$  and  $c_2$  the numbers of plaquettes sharing a given subcluster, and by  $b_i = a_i/c_i$  the normalized coefficients. In this class of approximations, it is possible to show that all the coefficients can be obtained as a function of  $c_1, c_2$  and of the lattice coordination number  $q$ . Making use of Eq. (3), and remembering that basic clusters (plaquettes) have unit  $a$ -coefficient, we can write

$$a_2 + c_2 = 1, \quad (21)$$

$$a_1 + qa_2 + c_1 = 1, \quad (22)$$

from which  $b_i = a_i/c_i$  are easily obtained:

$$b_2 = -\frac{c_2 - 1}{c_2}, \quad (23)$$

$$b_1 = \frac{q(c_2 - 1) - (c_1 - 1)}{c_1}. \quad (24)$$

Then, we have to impose the sufficient conditions on the coefficients, Eqs. (14) and (15). From Eq. (23) we easily see that  $b_2 \leq 0$ , which is ok for upperbounding, but usually  $b_1 \geq 0$ . We then have to couple each site to pairs that contain it and are contained in a given plaquette. Let us adopt the strategy of splitting the site coefficient among such pairs in equal parts, so that, being  $b_{2|1}$  the only allocation coefficient and  $r$  the number of pairs, Eqs. (14) and (15) read

$$b_1 = rb_{2|1}, \quad (25)$$

$$-b_2 \geq 2b_{2|1}. \quad (26)$$

The allocation coefficient may be easily eliminated, yielding the single condition

$$\frac{b_1}{r} + \frac{b_2}{2} \leq 0. \quad (27)$$

It is possible to show that also the  $r$  parameter depends on  $c_1, c_2, q$  only. Let us imagine to multiply the number  $q$  of nearest-neighbor pairs sharing a site times the number  $c_2$  of plaquettes sharing a pair. It is easy to realize

**Table I. Coefficients for Plaquette Approximations**

Lattice	Plaquette	$q$	$c_2$	$c_1$	$q(c_2 - 1)$	$2(c_1 - 1)$
Square	Square	4	2	4	4	6
Triangular	Triangle	6	2	6	6	10
Honeycomb	Hexagon	3	2	3	3	4
sc	Square	6	4	12	18	22
fcc	Triangle	12	4	24	36	46
fcc	Tetrahedron	12	2	8	12	14

The first two columns report, respectively, the lattice and plaquette (basic cluster) type. The following three columns display the independent coefficients:  $q$  (coordination number),  $c_2, c_1$  (number of plaquettes sharing a given pair, site). The last two columns verify the sufficient condition  $q(c_2 - 1) < 2(c_1 - 1)$ .

that in this way we have *overcounted*  $r$  times the number  $c_1$  of plaquettes sharing the given site, i.e.,

$$rc_1 = qc_2. \quad (28)$$

With the above manipulation, the condition (27) can be rewritten as

$$q(c_2 - 1) \leq 2(c_1 - 1). \quad (29)$$

In this form, we can easily verify its validity, which is done in Table I for a set of typical plaquette approximations. We have considered: the 2d square, triangular, and honeycomb lattices with a 4-site square,<sup>(12,29)</sup> a 3-site triangle,<sup>(29)</sup> and an elementary hexagon as basic cluster, respectively, the simple cubic (sc) lattice with a 4-site square<sup>(29)</sup> as basic cluster, and the face-centered cubic (fcc) lattice with a 3-site triangle<sup>(29)</sup> or a 4-site tetrahedron<sup>(8,27)</sup> as basic cluster.

## 5.2. B and C Hierarchies

The B and C hierarchies, originally proposed by Kikuchi and Brush,<sup>(30)</sup> are series of approximations with increasing cluster size, suitable for 2d square<sup>(30)</sup> and triangular<sup>(31)</sup> lattices. They are interesting mainly because they converge towards the exact free energy, in spite of the fact that the cluster size increases only in one direction. This result has been proved rigorously only for the C hierarchy,<sup>(3)</sup> but there are numerical evidences for

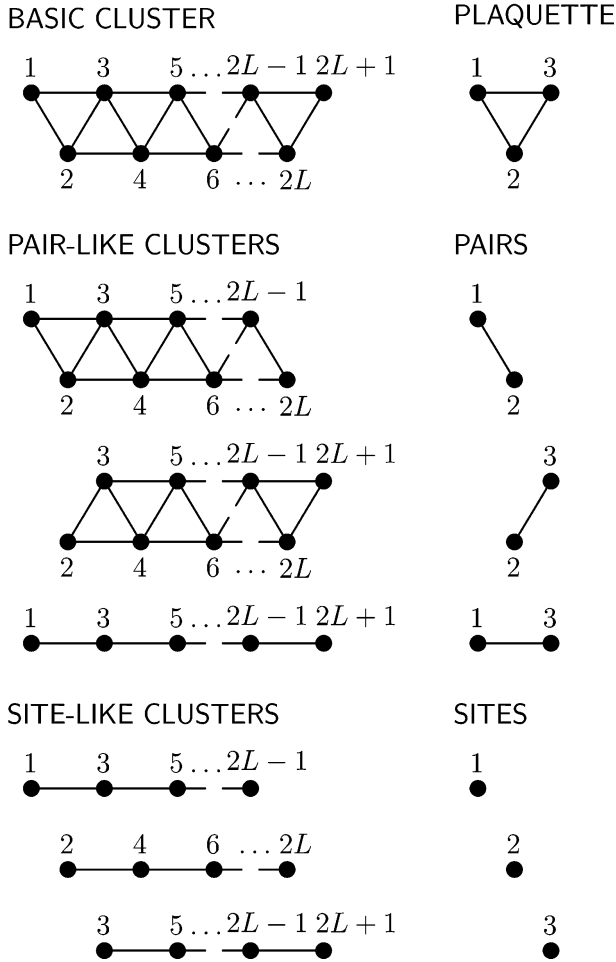


Fig. 1. Basic cluster and subclusters for the B hierarchy (left side) and for the corresponding (triangle) plaquette approximation.

both.<sup>(30,31)</sup> Such results<sup>(3)</sup> are related to the transfer matrix concept: As the Bethe approximation solves exactly an Ising-like chain, the CVM, with infinitely long 1d stripes as basic clusters (to which the B and C hierarchies tend), solves exactly a 2d lattice. Here we are interested in showing that these approximations verify the sufficient condition for the convergence discussed above. Let us consider for instance the B hierarchy on the triangular lattice (a completely analogous treatment holds for the C hierarchy and/or for the square lattice). The basic clusters, shown in Fig. 1 (top row, left column), are made up of a sequence of  $L - 1$  up- and  $L$  down-pointing triangles, where

$L$  is an adjustable parameter. Of course, also corresponding clusters with  $L$  up- and  $L - 1$  down-pointing triangles are allowed, but all basic clusters always extend only in one direction. This choice can be viewed as a generalization of the triangle plaquette approximation (see Fig. 1, top row, right column), where of course also up-pointing triangles are included in the set of basic clusters. In the following rows of Fig. 1, also the subclusters of the given basic cluster, having nonzero coefficients in the cluster entropy expansion ( $a$ -coefficients), are displayed. They are divided in pair-like and site-like subclusters, in that they can be put in one-to-one correspondence with pair and site subclusters for the triangle plaquette approximations. Such analogy is not only a pictorial one. In fact, it is possible to show (for instance making use of Eq. (3), but see also ref. 30) that the  $a$ -coefficients are  $a_2 = -1$  for pair-like clusters and  $a_1 = 1$  for site-like clusters, like for the triangle plaquette approximation. The same holds for  $c$ -coefficients, i.e., the numbers of basic clusters sharing a given subclusters, which turn out to be  $c_2 = 2$  and  $c_1 = 6$ , respectively, whence  $b_2 = -1/2$  and  $b_1 = 1/6$ . Finally, from Fig. 1 one easily sees that also the same “allocation” technique as for the plaquette approximation can be used. Inside a given basic cluster, each site-like subcluster is shared by  $r = 2$  pair-like clusters, and each pair-like cluster contains 2 site-like subclusters, whence inequality (27) is satisfied.

### 5.3. Hypercube Approximation in $d$ Dimensions

Finally, let us consider the case of a hypercubic lattice in  $d$  dimensions, and let us choose a  $d$ -dimensional hypercube ( $d$ -cube) as basic cluster. Of course, the relevant cases are  $d = 2, 3$ , the former of which coincides with the square plaquette approximation, mentioned above, but the interest of a general treatment will be clearer later. It is possible to show, by repeated use of Eq. (3), that clusters with nonzero coefficients are only  $i$ -cubes, for  $i = 1, \dots, d$ , and the  $i$ -cube coefficient in  $d$  dimensions is  $a_i^{(d)} = (-1)^{d-i}$ . Moreover, the number of  $d$ -cubes sharing a given  $i$ -cube (in  $d$  dimensions) is  $c_i^{(d)} = 2^{d-i}$ . As a consequence, the normalized coefficients turn out to be

$$b_i^{(d)} = \left(-\frac{1}{2}\right)^{d-i}. \quad (30)$$

Let us now impose the sufficient conditions, Eqs. (14) and (15). Let us notice that the positive coefficients, those who give problems for upper-bounding, have the  $i$  index with the same parity as  $d$ , that is  $i = d - 2, d - 4, \dots$ . Then we can couple each  $i$ -cube with  $(i + 1)$ -cubes that contain it and are contained in a given  $d$ -cube. As for plaquette approximations, let

us split the  $i$ -cube coefficient in equal parts, so that we have a single  $b_{i+1|i}^{(d)}$  allocation coefficient. We still have to observe that each  $i$ -cube is shared by  $d-i$   $(i+1)$ -cubes contained in the same  $d$ -cube (the equivalent of the  $r$  parameter for plaquette approximations), and that each  $(i+1)$ -cube contains  $2(i+1)$  different  $i$ -cubes (the equivalent of 2 sites in a pair). We can then rewrite Eqs. (14) and (15) as

$$b_i^{(d)} = (d-i)b_{i+1|i}^{(d)}, \quad (31)$$

$$-b_{i+1}^{(d)} \geq 2(i+1)b_{i+1|i}^{(d)}. \quad (32)$$

By eliminating the allocation coefficient, we obtain

$$\frac{b_i^{(d)}}{d-i} + \frac{b_{i+1}^{(d)}}{2(i+1)} \leq 0, \quad (33)$$

which, replacing Eq. (30) and taking into account that  $d-i$  is always even (as previously mentioned), becomes

$$2i \leq d-1. \quad (34)$$

Such inequality becomes more and more difficult to be satisfied as the sub-cluster index  $i$  increases. Therefore, we have to consider the worst case, that is  $i=d-2$ , leading to

$$d \leq 3. \quad (35)$$

This results essentially proves the convergence for  $d=3$ , because the  $d=2$  case coincides with the square plaquette approximation. Nevertheless, it is mainly interesting in that it gives us the opportunity to experiment the natural iteration method in a case in which the sufficient condition is not verified. We have implemented the procedure for the simple Ising model on the  $d=4$  hypercubic lattice, easily finding cases in which the behavior is nonconvergent (oscillating). This fact lead us to conjecture that actually the sufficient condition might be also a necessary one.

## 6. AN EQUIVALENT FORMULATION

In a recent paper,<sup>(25)</sup> a general method for the minimization of non-convex functionals, relying on the existence of suitable upperbounds to the functional to be minimized, is proposed and applied to the case of the

CVM free energy. Different possible choices for the upperbounding functional are investigated. Hereafter, we show that one choice proposed there, which by the way turns out to be quite convenient in terms of computation time, is equivalent to the natural iteration method. First, let us briefly recall the general method, which is based on the following.

**Theorem.** Let  $F[p]$  be a differentiable functional in the set of variables  $p$ , defined in some domain  $\Omega$ , and  $\bar{F}[p, p']$  an auxiliary differentiable functional in a pair of variable sets  $p, p'$ , defined in the domain  $\Omega^2$ , as

$$\bar{F}[p, p'] \equiv F[p'] + D[p, p'], \quad (36)$$

where  $D[p, p']$  is some kind of distance functional, i.e., satisfying the following requirements:

$$D[p, p'] \geq 0, \quad (37)$$

$$D[p, p'] = 0 \iff p' = p. \quad (38)$$

In other words, the auxiliary functional is an upperbound to the original functional, and equality holds if and only if the two arguments of the former are equal. Moreover, let the auxiliary functional have a unique minimum with respect to  $p'$  for each fixed  $p$ . Then the application  $\varphi: p \mapsto \hat{p}$  defined by

$$\hat{p} = \arg \min_{p' \in \Omega} \bar{F}[p, p'] \quad (39)$$

enjoys the properties

$$F[\hat{p}] \leq F[p], \quad (40)$$

$$F[\hat{p}] = F[p] \iff \hat{p} = p, \quad (41)$$

$$\hat{p} = p \implies \nabla F[p] = 0. \quad (42)$$

*Proof.* It is easy to obtain the following inequality chain

$$F[\hat{p}] \leq \bar{F}[p, \hat{p}] \leq \bar{F}[p, p] = F[p], \quad (43)$$

where both inequalities hold as equalities if and only if  $\hat{p} = p$ . The former is a direct consequence of the properties of the distance functional, Eqs. (37) and (38); the latter is a consequence of the definition of  $\varphi$ ,

Eq. (39), and of the fact that  $\bar{F}[p, p']$  has a unique minimum with respect to  $p'$ ; the equality descends from Eq. (38). This proves Eqs. (40) and (41). Eq. (42) is proved by differentiability, together with the properties of the distance functional, Eqs. (37) and (38). ■

Let us spend a few words to discuss the (weak) sense in which the above theorem provides a method to minimize the original functional. We have shown that (i) the mapping  $\varphi$  lowers the functional value at each step, and (ii) its fixed points are stationary points of the original functional. Therefore, we are “reasonably allowed to expect” that the method converges to local minima, even if, as already mentioned for the natural iteration method, we cannot a priori exclude convergence to other kinds of stationary points.

Let us now consider the distance functional defined by

$$D[p, p'] \equiv \sum_{\gamma} \sum_{x_{\gamma}} p'_{\gamma}(x_{\gamma}) \sum_{\alpha \subset \gamma} b_{\alpha} \log \frac{p_{\gamma}(x_{\alpha})}{p'_{\gamma}(x_{\alpha})}. \tag{44}$$

It turns out that this is a suitable distance functional, satisfying Eqs. (37) and (38), in that it coincides with (minus) the right-hand side of Eq. (13), which we have proved to be upperbounded by zero, as a sufficient condition for the convergence of the NIM. According to Eq. (36), where  $F[p']$  is taken to be the CVM free energy (5), we obtain the following auxiliary functional:

$$\bar{F}[p, p'] = \sum_{\gamma} \sum_{x_{\gamma}} p'_{\gamma}(x_{\gamma}) \left[ h_{\gamma}(x_{\gamma}) + \log p'_{\gamma}(x_{\gamma}) + \sum_{\alpha \subset \gamma} b_{\alpha} \log p_{\gamma}(x_{\alpha}) \right]. \tag{45}$$

Let us observe that basic cluster probability distributions now appear as  $p'$ , whereas subcluster probability distributions as  $p$ . In this way,  $F[p, p']$  turns out to be convex with respect to  $p'$ , therefore, if it has a stationary point, it is also unique, and is a minimum. Performing stationarization of this functional with respect to  $p'$ , with the usual linear constraints, in complete analogy to the calculation shown in Section 3, one exactly recovers the NIM equations (9), which in this way can be used to define the application  $\varphi$ .

## 7. CONCLUSIONS

Let us finally summarize our results. We have investigated on the convergence of the natural iteration method, proposed by Kikuchi as a

minimization procedure for cluster variational free energies and widely employed in a lot of applications of the CVM. We have discussed a condition on the coefficients of the cluster entropy expansion, which is sufficient to prove that the free energy decreases at each iteration, ensuring convergence of the method. Such a condition is based on the idea of pairing subcluster entropies with a positive coefficient to larger subcluster terms with a negative coefficient, yielding a set of conditional entropy terms with negative coefficients. It had already been proved by Kikuchi in the original paper<sup>(27)</sup> that negative coefficient terms give decreasing contributions to the free energy. We have also taken into account a set of common CVM approximations defined on various regular lattices, frequently encountered in applications, showing that the sufficient condition is always satisfied. In particular, we have devoted some attention to the class of hypercube approximations on the generic ( $d$ -dimensional) hypercubic lattice, showing that the sufficient condition is verified for  $d \leq 3$ . We have also implemented the natural iteration method for  $d=4$  on the simple Ising model, and found that several (random as well as uniform) initial conditions give rise to nonconvergent (oscillating) behavior. This fact has led us to conjecture that the sufficient condition might be also a necessary one. Finally, we have established a connection with a general method for the minimization of nonconvex functionals, which has been recently applied to the CVM free energy.<sup>(25)</sup> Such a method is based on the existence of suitable upperbounding functionals to the functional to be minimized. In ref. 25, several choices of upperbounding functionals are proposed and applied to simple inhomogeneous systems. We have shown that one of the upperbounding choices proposed there (indeed quite a good choice in terms of computation time) is equivalent to Kikuchi's natural iteration method. It turns out explicitly that the upperbounding condition implies free energy decreasing, whence convergence.

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