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Convergence of the cluster-variation method in the thermodynamic limit

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The cluster-variation method (CVM) is discussed in the thermodynamic limit of an infinitely extended lattice. The relationship between the variational principle for the free energy per lattice point as valid in the thermodynamic limit and the CVM formalism is established. It is proved that for suitably chosen hierarchies of CVM approximations the nth approximation to the free energy per lattice point f_n underestimates the exact value f and that $f_n \rightarrow f$ monotonically as $n \rightarrow \infty$. CVM approximations of this kind permit a particularly appealing interpretation of the entropy approximation involved. As a practical consequence, the results of this theoretical investigation suggest how to construct a "best sequence of approximations" that can serve as a basis for extrapolations.

I. INTRODUCTION

The cluster-variation method[1] (CVM) is a method of obtaining approximations to the equilibrium thermodynamic properties of lattice systems. The method has been applied to a variety of systems over a number of years (for examples see Refs. 2—11). However, as pointed out by McCoy *et al.*[12] in a recent paper, there have been very few investigations into the underlying nature of the approximations that are involved in the CVM.[7–10]

This paper reports a theoretical investigation into the CVM specifically addressing the fundamental question whether the CVM approximations converge towards the rigorous solution in the thermodynamic limit of an infinitely extended lattice. In view of the practice of extrapolating CVM results to obtain estimates of the exact values for thermodynamic quantities, this question is of prime importance, also from a practical point of view.

In this paper it is shown rigorously how to construct a sequence of CVM approximations that is guaranteed to converge to the exact result for the free energy per lattice point of the infinite lattice system. This is done by first establishing the relationship between the CVM and the variational principle for the free energy as valid for an infinite lattice system. This extends the analysis of the CVM for a finite system of N lattice points as given by Morita.[13–15] Morita, however, did not consider the influence of taking the thermodynamic limit. This limit procedure is, however, essential to any theoretical analysis of the CVM, since, firstly, mathematical models of physical systems only exhibit thermodynamic behavior in this limit, and secondly, in practice the CVM is applied as if the lattice in question were infinite in extent. This second point is obvious if one considers the way in which the relative occurrence of a specific type of cluster (set of lattice points) is determined and the fact that boundary effects are neglected.

The main results of this work are contained in Theorems 2 and 3. Theorem 2 shows that a suitably chosen hierarchy of CVM approximations underestimates the free energy per lattice point and monotonously converges to some limit; Theorem 3 establishes that this limiting value equals the exact result, under slightly more restricting conditions on the hierarchy of approximations. An interesting implication is that there might be sequences of approximations that do converge, but not towards the exact result. However, this possibility has not been investigated any further.

It will be necessary to make use of some well-established results from rigorous statistical mechanics; in connection with these results the reader is referred to Ref. 16, where references to original papers can be found.

The organization of this paper is as follows. In Sec. II some necessary concepts from statistical mechanics for infinite systems will be reviewed and the relationship between the variational principle for the free energy per lattice point in the thermodynamic limit and the CVM will be established. Section III contains an analysis of the entropy expression used in the CVM. Section IV gives the main theorems and their proofs, and Sec. V contains some final remarks.

II. CVM AS APPROXIMATE VARIATIONAL PRINCIPLE

For simplicity of presentation, this discussion will be restricted to the case of the Ising model on Z^2, the square lattice in two dimensions. (For a discussion of the range of validity of the results, see Sec. V.)

The Ising model can conveniently be described as follows. With each lattice point or site $a \in Z^2$, we associate a variable S_a ("spin"), which can take values in $\Omega_0 = \{-1,1\}$. The configuration space for a finite subset Λ of Z^2 is $\Omega_\Lambda = (\Omega_0)^\Lambda$, and the configuration space for the infinite system on Z^2 is $\Omega = (\Omega_0)^{Z^2}$.

Viewing Ω_0 as a discrete metric space, observables of the system are real-valued elements of $C(\Omega)$, the (continuous) functions on the configuration space Ω. On Ω_0 we have as *a priori* measure the (unnormalized) counting measure μ_0. The product measures on Ω_Λ will be denoted by μ_0 as well. Integration with respect to μ_0 will be denoted by enclosure with a set of angular brackets with a subscript 0.

For example, if $a,b \in Z^2$,

$$\langle S_a^2 S_b \rangle_0 = \int_{\Omega_{\{a,b\}}} [S_a(\omega)]^2 S_b(\omega) d\mu_0(\omega) = \sum_{S_a=-1,1} \sum_{S_b=-1,1} S_a^2 S_b \ .$$

In other words, the angular brackets (with subscript 0) denote expectation values without interactions, or, equivalently, at infinite temperature (apart from a normalization factor).

The Hamiltonian for a finite subset Λ of Z^2, $\Lambda \neq \emptyset$, is

$$H[\Lambda] = \sum_{X \subset \Lambda} \Phi[X] \ , \tag{1}$$

where $\Phi[X]$ is the potential function for the cluster (set of lattice points) X.

We shall assume that the interaction Φ has a finite range, i.e.,

$$\Phi[X] \equiv 0 \ \text{ if } \operatorname{diam}(X) > R \tag{2}$$

for some $R > 0$, where

$$\operatorname{diam}(X) = \sup_{a,b \in X} \| a - b \| \ . \tag{3}$$

Moreover, we shall assume that the interaction is translationally invariant. Note that no other kind of symmetry is assumed, such as rotational invariance or isotropy, and that many-body interactions are allowed.

We shall have to make extensive use of the concept of a "state" for the infinite system, which generalizes the concept of "expectation value": a state ρ for the infinite system on Z^2 is a positive linear functional on $C(\Omega)$, normalized in such a way that $\rho(1)=1$. Restricted to $C(\Omega_\Lambda)$, Λ finite, it defines a probability measure $d\rho_\Lambda$ on Ω_Λ, which is absolutely continuous with respect to $d\mu_0$, so we have

$$d\rho_\Lambda = \rho[\Lambda] d\mu_0 \ , \tag{4}$$

where $\rho[\Lambda]$ is the reduced density function associated with the finite subsystem in Λ. This means that for an observable $F \in C(\Omega_\Lambda)$ of the finite system, the expectation value of F in the state ρ is

$$\begin{aligned} \rho(F) &= \int_{\Omega_\Lambda} F(\omega) d\rho_\Lambda(\omega) \\ &= \int_{\Omega_\Lambda} F(\omega) \rho[\Lambda](\omega) d\mu_0(\omega) \\ &= \langle F \rho[\Lambda] \rangle_0 \end{aligned} \tag{5}$$

and

$$\langle \rho[\Lambda] \rangle_0 = 1 \ . \tag{6}$$

Lattice translations induce translations on the set of observables in a natural way; hence a state may be translationally invariant; the set of translation-invariant states will be denoted by I.

We can now formulate the exact variational principle for the free energy per lattice point f as valid for the infinite system in the thermodynamic limit (see, e.g., Ref. 16, p. 48):

$$f = \min_{\rho \in I} [\rho(e) - s(\rho)] \ . \tag{7}$$

Here $\beta = (kT)^{-1}$ has been taken as unity, and

$$\rho(e) = \lim_{\Lambda \leftarrow Z^2} \rho \left[\frac{H[\Lambda]}{|\Lambda|} \right] , \tag{8}$$

$$s(\rho) = \lim_{\Lambda \leftarrow Z^2} \frac{S_\rho(\Lambda)}{|\Lambda|} , \tag{9}$$

and

$$\begin{aligned} S_\rho(\Lambda) &= -\rho(\ln \rho[\Lambda]) \\ &= -\langle \rho[\Lambda] \ln \rho[\Lambda] \rangle_0 \ . \end{aligned} \tag{10}$$

Hence $S_\rho(\Lambda)$ is the entropy for the finite subsystem in Λ in the state ρ, $s(\rho)$ is the mean entropy per site in the thermodynamic limit, and $\rho(e)$ is the mean energy per site in the state ρ in the thermodynamic limit. Note that only $\rho(e)$ has been defined as yet, not e itself.

Using translational invariance of Φ and ρ, we have

$$\begin{aligned} \rho(e) &= \lim_{\Lambda \leftarrow Z^2} \sum_{X \subset \Lambda} \frac{\rho(\Phi[X])}{|\Lambda|} \\ &= \lim_{\Lambda \leftarrow Z^2} \sum_{X \ni 0} \frac{M_X^-(\Lambda)}{|\Lambda|} \frac{\rho(\Phi[X])}{|X|} \ , \end{aligned}$$

where $M_X^-(\Lambda)$ is the number of translates of X that are contained in Λ, and $0=(0,0)\in Z^2$. For each finite X

$$\lim_{\Lambda\leftarrow Z^2}\frac{M_X^-(\Lambda)}{|\Lambda|}=1$$

and so we have, due to the finite range of the interaction [Eq. (2)],

$$\rho(e)=\sum_{X\ni 0}\frac{\rho(\Phi[X])}{|X|} \quad . \tag{11}$$

Let us now order Z^2 lexicographically and let $\sum_X^*$ denote summation over $X\subset Z^2$ with the property that 0 is the first element of X. Then

$$\rho(e)=\sum_X{}^*\,\rho(\Phi[X]) = \sum_X{}^*\,\langle\rho[X]\Phi[X]\rangle_0 \quad . \tag{12}$$

Equation (12) justifies the definition

$$e=\sum_X{}^*\,\Phi[X] \quad . \tag{13}$$

This way of treating the energy term is standard practice; it provides a way of calculating the energy per site by adding separate contributions from all different types of clusters.

In the cluster-variation formalism the entropy term is treated in an analogous way: Following Morita,[13–15] we introduce the Möbius transform of $\ln\rho$ by

$$\ln\rho[\Lambda]=\sum_{X\subset\Lambda}q[X] \quad , \qquad q[X]=\sum_{Y\subset X}(-1)^{|X\setminus Y|}\ln\rho[Y] \quad , \tag{14}$$

where q is translationally invariant because ρ is.

For the entropy per site we can write

$$-s(\rho)=\lim_{\Lambda\leftarrow Z^2}\sum_X{}^*\frac{M_X^-(\Lambda)}{|\Lambda|}\rho(q[X]) \quad . \tag{15}$$

Note that in contrast to the situation for the energy term, where the number of nonzero terms in the summation is finite for all Λ [Eq. (2)], in this case interchange of limit process and summation is not trivially seen to be valid.

The CVM approximation can now be derived from the variational principle Eq. (7) by making the following three modifications:

(A1) Interchange limit and summation in Eq. (15), thus obtaining for the entropy

$$s(\rho)=-\sum_X{}^*\rho(q[X]) = -\sum_X{}^*\langle\rho[X]q[X]\rangle_0 \quad . \tag{16}$$

(A2) Truncate the series in Eq. (16). Clusters X corresponding to terms retained in the summation will be called "preserved," following Morita's use of this phrase.

(A3) Determine the minimum of the approximate expression for $\rho(e)-s(\rho)$ now obtained:

$$\sum_{\substack{X\\ X\text{ preserved}}}{}^*\;\langle\rho[X](\Phi[X]+q[X])\rangle_0$$

by variation, not of $\rho\in I$, but of those reduced density functions $\rho[X]$ for which X is a preserved cluster, taking into account the necessary consistency relations among them. (The term "consistency relations" is used for relations of the following kind: If $Y\subset X$ then $\rho[X]$ can be "reduced" to $\rho[Y]$ by integrating over the spin variables in $X\setminus Y$.) Thus the CVM is clearly based on three distinct steps of modification. It will be shown that (A1) is fully justified, provided the infinite series in Eq. (16) is interpreted properly. The existence of (A2) has been brought out by Morita in the case of a finite system. An error may be introduced by (A3) because of the fact that, whereas every $\rho\in I$ determines a consistent set $\{\rho[X]\,|\,X\text{ preserved}\}$, the converse may not necessarily be true. The existence of (A3) as a nontrivial modification is entirely due to the fact that we started out from the variational principle for the *infinite* system.

III. THE ENTROPY EXPRESSION

In this section it will be proved that the expression (16), correctly interpreted, actually represents the entropy per lattice point in the thermodynamic limit. In this expression the entropy is calculated as a sum of contributions of all types of clusters, analogous to the representation (12) of the energy term.

Let, for each finite $\Lambda\subset Z^2$, $\Lambda\neq\varnothing$ the first element (in lexicographic order) of Λ be denoted by $p(\Lambda)$. Let

$$Z_+^2=\{z\in Z^2\,|\,0\le z\}$$

Let us now define for any $\rho\in I$ a function D_ρ on the finite subsets of Z^2 as follows:

Definition 1: If $\Lambda\neq\varnothing$,

$$D_\rho(\Lambda)=-\sum_{\substack{X\\ X\subset\Lambda,\,X\ni p(\Lambda)}}\rho(q[X]) = -\sum_{\substack{X\\ X\subset\Lambda,\,X\ni p(\Lambda)}}\langle\rho[X]q[X]\rangle_0 \tag{17}$$

and

$$D_\rho(\varnothing)=0 \quad . \tag{18}$$

Compare this with the expression for $S_\rho(\Lambda)$ from Eqs. (10) and (14):

$$S_\rho(\Lambda) = -\sum_{X\subset\Lambda} \rho(q[X]) = -\sum_{X\subset\Lambda} \langle \rho[X]q[X]\rangle_0 \quad . \tag{19}$$

$D_\rho(\Lambda)$ will act as an approximation to $|\Lambda|^{-1}S_\rho(\Lambda)$. In cases where there is no risk of confusion, the subscripts ρ on $D_\rho(\Lambda)$ and $S_\rho(\Lambda)$ will be omitted, and s will be written for $s(\rho)$.

Lemma 1. For $\rho\in I$ and $\Lambda,\Lambda'\subset Z^2$, finite and nonempty, we state the following:

(i) $D_\rho(\Lambda)=S_\rho(\Lambda)-S_\rho(\Lambda\setminus\{p(\Lambda)\})$.

(ii) $D_\rho(\Lambda)=D_\rho(\Lambda+x)$ for all $x\in Z^2$,

(iii) If $\Lambda\subset\Lambda'$ and $p(\Lambda)=p(\Lambda')$, then

$$D_\rho(\Lambda)\ge D_\rho(\Lambda') \quad .$$

(iv) $D_\rho(\Lambda)\ge s(\rho)\ge 0$.

(v) If (Λ_n), $n\in N$ (where $N\equiv Z_+\setminus\{0\}$) is a sequence of finite subsets of Z^2, where (a) $p(\Lambda_n)=x$ for all n, with x fixed, and (b) $\Lambda_n\subset\Lambda_{n+1}$ for all n, then $\lim_{n\to\infty}D_\rho(\Lambda_n)=L$ exists and $L\ge s(\rho)$. [L may depend on the sequence (Λ_n).]

Proof: Proposition (i) is an immediate consequence of Eqs. (17) and (19).

Proposition (ii) is an immediate consequence of the translational invariance of ρ.

Proposition (iii): With the use of the strong subadditivity property (see, e.g., Ref. 16, p. 45) of the entropy function,

$$S(\Lambda_1\cup\Lambda_2)+S(\Lambda_1\cap\Lambda_2)\le S(\Lambda_1)+S(\Lambda_2) \quad ,$$

with $\Lambda_1=\Lambda'\setminus\{p(\Lambda')\}$ and $\Lambda_2=\Lambda$, we have

$$S(\Lambda')-S(\Lambda'\setminus\{p(\Lambda')\})\le S(\Lambda)-S(\Lambda\setminus\{p(\Lambda)\})$$

or, by (i), $D(\Lambda')\le D(\Lambda)$.

Proposition (iv) can be shown to be a consequence of (iii). For a detailed proof see, e.g., Ref. 17, pp. 40 and 41.

Proposition (v) is an immediate consequence of (iii) and (iv).

Theorem 1. Consider a sequence of finite $\Lambda_n\subset Z^2_+$, $n\in N$, with

(1) $p(\Lambda_n)=0$ for all n,

(2) for any finite $A\subset Z^2_+$ there is an $n_b\in N$ such that for all $n\ge n_b$

$$A\subset\Lambda_n \quad ,$$

then, for any $\rho\in I$,

$$\lim_{n\to\infty} D_\rho(\Lambda_n)=s(\rho) \quad .$$

Proof. Define for $\Lambda\subset Z^2$, Λ finite, sets $\Lambda^{(i)}$ by

$$\Lambda^{(k)}=\Lambda^{(k-1)}\setminus\{p(\Lambda^{(k-1)})\} \quad , \qquad \Lambda^{(0)}=\Lambda \tag{20}$$

(breaking down Λ in lexicographic order). We then have from Lemma 1 (i)

$$S(\Lambda)=\sum_{i=0}^{|\Lambda|-1} D(\Lambda^{(i)}) \quad . \tag{21}$$

Consider a sequence of "mutilated cubes" $C_n\subset Z^2_+$, defined by

$$C_n=\{x=(x_1,x_2)\in Z^2 \mid -n\le x_2\le n-1 \text{ if } x_1\ne 0,\ 0\le x_2\le n-1 \text{ if } x_1=0,\ 0\le x_1\le 2n-1\} \quad .$$

Note $p(C_n)=0$ for all n.

According to Lemma 1 (v)

$$\lim D(C_n)=L\ge s \tag{22}$$

for some L. Now choose $\epsilon>0$. From Eq. (22), there exist some $n_b\in N$ such that

$$|D(C_n)-L| < \frac{\epsilon}{2}, \quad \forall n\ge n_b \quad . \tag{23}$$

Consider C_n for $n>n_b$. From Eq. (21),

$$S(C_n)=\sum_{i=0}^{4n^2-n-1} D(C_n^{(i)}) \quad . \tag{24}$$

For every $C_n^{(i)}$ with the property that

$$C_{n_b}\subset[C_n^{(i)}-p(C_n^{(i)})] \tag{25}$$

(meaning that C_{n_b} is contained in the translate of $C_n^{(i)}$ with 0 as its first element) we have, combining Lemma 1 (ii)–(v) and Eq. (23),

$$L\le D(C_{2n})\le D(C_n^{(i)})\le D(C_{n_b})<L+\frac{\epsilon}{2} \quad .$$

Hence

$$|D(C_n^{(i)})-L| < \frac{\epsilon}{2} \quad . \tag{26}$$

The number of sets $C_n^{(i)}$ with this property (25) is readily seen to be

$$A(n)=4(n-n_b)^2+3(n-n_b) \quad . \tag{27}$$

For $C_n^{(i)}$ without property (25) we shall use

$$0\le D(C_n^{(i)})\le D(\{0\})=S(\{0\}) \ ,$$

where use was made of Lemma 1 (iv), (iii), and (i). The number of sets $C_n^{(i)}$ without property (25) is

$$B(n)=|C_n|-A(n)$$
$$=-4n+8nn_b-4n_b^2+3n_b=O(n) \ . \qquad (28)$$

We now have

$$\left|\frac{S(C_n)}{|C_n|}-L\right|=\left||C_n|^{-1}\sum_{\substack{i\\ \text{without}(25)}}D(C_n^{(i)})+|C_n|^{-1}\sum_{\substack{i\\ \text{with}(25)}}D(C_n^{(i)})-L\right|$$
$$\le\frac{B(n)}{|C_n|}S(\{0\})+\left||C_n|^{-1}\sum_{\substack{i\\ \text{with}(25)}}[D(C_n^{(i)})-L]\right|+\left|\left[|C_n|^{-1}\sum_{\substack{i\\ \text{with}(25)}}L\right]-L\right|$$
$$\le\frac{B(n)}{|C_n|}S(\{0\})+\frac{A(n)}{|C_n|}\frac{\epsilon}{2}+\frac{B(n)}{|C_n|}L<\epsilon$$

for n sufficiently large. Hence

$$|C_n|^{-1}S(C_n)\to L \ .$$

However, $|C_n|^{-1}S(C_n)\to s$, and so

$$\lim_{n\to\infty} D(C_n)=s \ . \qquad (29)$$

Now consider the sequence (Λ_n) of the theorem. From Eq. (29) and Lemma 1 (iv)

$$s\le D(C_p)<s+\epsilon$$

for any $\epsilon>0$ and p sufficiently large. For n sufficiently large $C_p\subset\Lambda_n$, hence by Lemma 1 (iii) and (iv)

$$s\le D(\Lambda_n)\le D(C_p)<s+\epsilon \ ,$$

and hence

$$\lim_{n\to\infty} D(\Lambda_n)=s \ .$$

Since we have established

$$s=\lim_n D(\Lambda_n)=\lim_n -\sum_{\substack{X\\ X\subset\Lambda_n}}^{*}\rho(q[X]) \ ,$$

the above theorem provides us with the correct interpretation of the infinite series

$$-\sum_X^{*}\rho(q[X])$$

for the entropy $s(\rho)$ [cf. Eq. (16)].

IV. CONVERGENCE OF THE CVM

Consider a sequence of finite subsets of Z^2, (Λ_n), with the properties that, for all $n\in N$,

(1) $p(\Lambda_n)=0$,
(2) $\cup\{X\subset Z^2\,|\,p(X)=0 \text{ and } \Phi[X]\neq 0\}\subset\Lambda_n$,
(3) $\Lambda_n\subset\Lambda_{n+1}$.

Consider the sequence (or hierarchy) of CVM approximations defined by

$$f_n=\min_{\rho[\Lambda_n]\text{IT}}\left\{\left\langle\rho[\Lambda_n]\sum_{\substack{X\\ X\subset\Lambda_n}}^{*}\{\Phi[X]+q[X]\}\right\rangle_0\right\} \ . \qquad (30)$$

In view of the specific way of truncating the series for the entropy, the entire approximate expression for $[\rho(e)-s(\rho)]$ can be and has been written in a form with only the density function $\rho[\Lambda_n]$ for the largest preserved cluster appearing explicitly. The abbreviation IT stands for "internally translationally-invariant," meaning that the state on $C(\Omega_{\Lambda_n})$ defined by $\rho[\Lambda_n]$ is translationally invariant under translations within Λ_n. This is the consequence of the consistency relations to be obeyed by the set of $\rho(X),X$ preserved cluster. Condition (2) on the sequence (Λ_n) ensures that the energy term is not affected by the approximations and is just technically convenient but unessential. The minimum defined in (30) can be shown to exist using a compactness argument.

Theorem 2. Let Λ_n and f_n be as above and let f be the true free energy per lattice point in the thermodynamic limit. Then

(i) $f_n\le f$ for all n ,

(ii) $f_n\le f_{n+1}$ for all n ,

(iii) $\lim_{n\to\infty} f_n=f_\infty$ exists , and $f_\infty \le f$.

Proof. Consider for $\rho \in I$ the expression

$$\rho(e) - D_\rho(\Lambda_n) = \left\langle \rho[\Lambda_n] \sum_{\substack{X \\ X\subset\Lambda_n}}^{*} \{\Phi[X]+q[X]\} \right\rangle_0 .$$

By Lemma 1 (iv)

$$\min_{\rho\in I}\{\rho(e)-D_\rho(\Lambda_n)\} \le \min_{\rho\in I}\{\rho(e)-s(\rho)\} = f .$$

Since each $\rho \in I$ determines an internally translationally-invariant reduced density function $\rho[\Lambda_n]$, while the converse may not be true, we have

$$f_n = \min_{\rho[\Lambda_n]\mathrm{IT}} \left\{ \left\langle \rho[\Lambda_n] \sum_{\substack{X \\ X\subset\Lambda_n}}^{*} \{\Phi[X]+q[X]\} \right\rangle_0 \right\}$$

$$\le \min_{\rho\in I}\{\rho(e)-D_\rho(\Lambda_n)\} \le f .$$

This proves (i). To prove (ii), note that

$$f_{n+1} \ge \min_{\rho[\Lambda_{n+1}]\mathrm{i.t.}} \left\langle \rho[\Lambda_{n+1}] \sum_{\substack{X \\ X\subset\Lambda_n}}^{*} \{\Phi[X]+q[X]\} \right\rangle_0 + \min_{\rho[\Lambda_{n+1}]\mathrm{IT}} \left\langle \rho[\Lambda_{n+1}] \sum_{\substack{X \\ X\subset\Lambda_{n+1}, X\not\subset\Lambda_n}}^{*} q[X] \right\rangle_0 .$$

In the first term we can reduce the density function $\rho[\Lambda_{n+1}]$ to $\rho[\Lambda_n]$ and in minimizing with respect to $\rho[\Lambda_n]$ instead of $\rho[\Lambda_{n+1}]$, we only drop the condition that $\rho[\Lambda_n]$ is derived from an i.t. $\rho[\Lambda_{n+1}]$, so the first term is greater than or equal to

$$\min_{\rho[\Lambda_n]\mathrm{i.t.}} \left\langle \rho[\Lambda_n] \sum_{\substack{X \\ X\subset\Lambda_n}}^{*} \{\Phi[X]+q[X]\} \right\rangle_0 = f_n .$$

As to the second term,

$$\left\langle \rho[\Lambda_{n+1}] \sum_{\substack{X \\ X\subset\Lambda_{n+1}, X\not\subset\Lambda_n}}^{*} q[X] \right\rangle_0 = \left\langle \rho[\Lambda_{n+1}] \left[\sum_{X\subset\Lambda_{n+1}} - \sum_{X\subset\Lambda_{n+1}\setminus\{0\}} - \sum_{X\subset\Lambda_n} + \sum_{X\subset\Lambda_n\setminus\{0\}} \right] q[X] \right\rangle_0$$

$$= \left\langle \rho[\Lambda_{n+1}] \ln \left\{ \frac{\rho[\Lambda_{n+1}]\rho[\Lambda_n\setminus\{0\}]}{\rho[\Lambda_{n+1}\setminus\{0\}]\rho[\Lambda_n]} \right\} \right\rangle_0$$

$$\ge 1 - \left\langle \frac{\rho[\Lambda_n]\rho[\Lambda_{n+1}\setminus\{0\}]}{\rho[\Lambda_n\setminus\{0\}]} \right\rangle_0 ,$$

where we have used the inequality

$$\ln t \ge 1 - \frac{1}{t} .$$

Integrating out the spin variable at 0, this last expression is seen to be equal to zero, so the second term is greater than or equal to 0 and hence

$$f_{n+1} \ge f_n ,$$

proving (ii). (iii) now follows from (i) and (ii).

Theorem 3. Let Λ_n, f_n, f_∞, and f be as above, and let the sequence (Λ_n) obey the following additional condition:

(4) For any finite $A \subset Z_+^2$, there is an $n_b \in N$ such that, for all $n > n_b$, $A \subset \Lambda_n$. Then

$$\lim_{n\to\infty} f_n = f .$$

To motivate the proof, the following should be noted. Theorem 1 shows that for any translationally invariant state of the infinite system the entropy expression used in the CVM approximations defined by Eq. (30) is "almost correct" for large n. This gives us control over approximation steps (A1) and (A2) (see Sec. II). However, (A3) might introduce a lowering of the free energy that does not vanish as $n\to\infty$. It will be shown that such an assumption leads to a contradiction.

Proof. From Theorem 2, we have

$$\lim_n f_n = f_\infty \le f .$$

Assume $f_\infty < f$. By Theorem 2, this implies there is an $\epsilon > 0$, so that for all n

$$f_n \le f - \epsilon . \tag{31}$$

Let for each n the density function $\hat{\rho}_n[\Lambda_n]$ minimize the expression in Eq. (30) and let $\hat{\rho}_n$ be the state on $C(\Omega_{\Lambda_n})$ associated with this density function. So

$$f_n=\left\langle \hat{\rho}_n[\Lambda_n] \sum_{\substack{X \\ X\subset\Lambda_n}}^{*} \{\Phi[X]+\hat{q}_n[X]\} \right\rangle_0 , \qquad (32)$$

where $\hat{q}_n$ is the Möbius transform of $\ln\hat{\rho}_n$. Let us write, for $\Lambda\subset\Lambda_n$,

$$D_{\hat{\rho}_n}(\Lambda)=-\sum_{\substack{X \\ X\subset\Lambda, X\ni p(\Lambda)}} \langle\hat{\rho}_n[\Lambda_n]\hat{q}_n[X]\rangle_0$$

$$=-\sum_{\substack{X \\ X\subset\Lambda, X\ni p(\Lambda)}} \langle\hat{\rho}_n[X]\hat{q}_n[X]\rangle_0 . \qquad (33)$$

Compare this with Eq. (17). Although $\hat{\rho}_n$ is an internally translationally-invariant state for the finite system in Λ_n and not a translationally-invariant state for the infinite system, statement (iii) of Lemma 1 is valid for Λ and Λ' contained in Λ_n, by the same proof. So

$$D_{\hat{\rho}_n}(\Lambda)\geq D_{\hat{\rho}_n}(\Lambda') \qquad (34)$$

for $\Lambda\subset\Lambda'\subset\Lambda_n$ with $p(\Lambda)=p(\Lambda')$. Equation (32) can now be written as

$$f_n=\hat{\rho}_n(e)-D_{\hat{\rho}_n}(\Lambda_n) . \qquad (35)$$

According to Theorem 1.4 of Ref. 16, the sequence $(\hat{\rho}_n)$ has a subsequence $(\hat{\rho}_k)$ that tends to a thermodynamic limit state $\hat{\rho}$ on $C(\Omega_{Z_+^2})$, which means that for each finite set $A\subset Z_+^2$

$$\hat{\rho}_k[A]\rightarrow\hat{\rho}[A]\text{(pointwise) as } k\rightarrow\infty . \qquad (36)$$

Using translational invariance, $\hat{\rho}$ can be extended to a translationally-invariant state $\hat{\rho}$ on $C(\Omega)$ with the same mean energy $\hat{\rho}(e)$ and mean entropy $s(\hat{\rho})$.

Now

$$\hat{\rho}(e)-s(\hat{\rho})=\{\hat{\rho}_k(e)-D_{\hat{\rho}_k}(\Lambda_k)\}+\{\hat{\rho}(e)-\hat{\rho}_k(e)\}$$
$$+\{D_{\hat{\rho}_k}(\Lambda_k)-D_{\hat{\rho}_k}(\Lambda_m)\}$$
$$+\{D_{\hat{\rho}_k}(\Lambda_m)-D_{\hat{\rho}}(\Lambda_m)\}$$
$$+\{D_{\hat{\rho}}(\Lambda_m)-s(\hat{\rho})\} . \qquad (37)$$

As $e\in C(\Omega_{\Lambda_1})$ [see Eq. (13)], we have for the second term in curly brackets in (37), from Eq. (36),

$$|\hat{\rho}(e)-\hat{\rho}_k(e)|<\frac{\epsilon}{6}$$

for k sufficiently large. For the third term in curly brackets in (37) we have from Eq. (34)

$$D_{\hat{\rho}_k}(\Lambda_k)-D_{\hat{\rho}_k}(\Lambda_m)\leq 0 \quad \text{for } k\geq m .$$

For the fourth term in curly brackets in (37) we have from Eq. (36)

$$|D_{\hat{\rho}_k}(\Lambda_m)-D_{\hat{\rho}}(\Lambda_m)|<\frac{\epsilon}{6}$$

for k sufficiently large. For the fifth term in curly brackets in (37) we have from Theorem 1

$$|D_{\hat{\rho}}(\Lambda_m)-s(\hat{\rho})|<\frac{\epsilon}{6}$$

for m sufficiently large. So, first choosing m and then k, we arrive at the contradictory

$$f=\min_{\rho\in I}\{\rho(e)-s(\rho)\}$$
$$\leq\hat{\rho}(e)-s(\hat{\rho})$$
$$\leq f_k+\frac{\epsilon}{6}+0+\frac{\epsilon}{6}+\frac{\epsilon}{6}$$
$$\leq f-\frac{\epsilon}{2}$$

[the latter two inequalities being by Eqs. (35) and (37) and Eq. (31), respectively.] Hence we must have that $f_\infty=f$.

V. DISCUSSION AND CONCLUSIONS

Convergence towards the exact result has been shown for a specific class of hierarchies of CVM approximations [see Eq. (30)]. These specific hierarchies emerge in a natural way from an analysis of the entropy expression Eq. (16) that is basic to the CVM. Correct limiting behavior of a hierarchy of CVM approximations is ensured only in the event of the entropy approximations involved converging correctly. Entropy approximations are always partial sums of the infinite sum in Eq. (16). The particular type of partial sum $D_\rho(\Lambda_n)$ [see, e.g., Eq. (17)] that has been used throughout this paper is, again, natural in the sense that it permits an intuitively satisfying physical interpretation of the corresponding entropy approximation: The entropy per site in the thermodynamic limit is approximated by the increase in entropy when one lattice point is added to a large but finite system. This, in fact, is Lemma 1 (i). On the basis of the results presented in this paper, it would seem advisable to use hierarchies as defined in Eq. (30) as a basis for extrapolations.

The presentation in this paper has been limited to the case of the Ising model on Z^2, but the results are readily seen to be valid for any system with a finite configuration space per lattice point Ω_0 on any lattice that permits a total ordering invariant under lattice translations. The interaction Φ must obey the condition of translational invariance and of finite norm:

$$||\Phi||=\sum_X^{*}||\Phi[X]||_\infty<\infty ,$$

where $||\Phi[X]||_\infty$ is the supremum-norm on $C(\Omega_X)$.

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