Journal of Statistical Physics, Vol. 35, Nos. 3/4, 1984

Exact Variational Methods and Cluster-Variation Approximations

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Received August 19, 1983

It is shown that for classical, d-dimensional lattice models with finite-range interactions the translation-invariant equilibrium states have the property that their mean entropy is completely determined by their restriction to a subset of the lattice that is infinite in $(d-1)$ dimensions and has a width equal to the range of the interaction in the dth dimension. This property is used to show proper convergence toward the exact result for a hierarchy of approximations of the cluster-variation method that uses one-dimensionally increasing basis clusters in a two-dimensional lattice.

KEY WORDS: Lattice systems; translation-invariant equilibrium states; variational principle; cluster-variation method.

1. INTRODUCTION

The cluster-variation method[1] (CVM) is a method of obtaining approximations to the equilibrium thermodynamic properties of lattice systems. Although the method has been applied to a variety of systems over a number of years,[2–10] there have been few investigations[11] into the underlying nature of the approximations that are involved in the CVM.[12–15] More specifically, whereas it is the general belief that the CVM can be used to generate a sequence of ever more accurate approximations to thermodynamic quantities, the question of proper convergence of such sequences has received virtually no attention.[15]

This paper originated from an attempt to understand some results of Kikuchi and Brush.[16] They used a sequence of CVM approximations to

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0022-4715/84/0500-0285$03.50/0

the two-dimensional, nearest-neighbor lattice problem in which the basis cluster was increased one dimensionally, in such a way that even in the limiting case the basis cluster only covered a one-dimensionally long double line of lattice points. Notwithstanding the fact that in this way the CVM calculations seemed to refer to a one-dimensional lattice, the results indicated proper convergence toward the exact result for the two-dimensional system. A heuristic explanation has been given by establishing a connection with a transfer-matrix approach under some physically reasonable, but mathematically unproven assumptions.[17] Since, however, the CVM can most conveniently be looked upon as a class of approximations to the variational characterization of translation-invariant equilibrium states provided by the statistical mechanical theory of lattice models,[12–15] it seemed instructive to try and understand the results of Kikuchi and Brush from this point of view.

The organization of this paper is as follows. In Section 2 we review some concepts we will use and introduce the necessary notation. In Section 3 we prove the existence of a variational characterization of restrictions of equilibrium states and prove that translation-invariant equilibrium states have the property that their mean entropy is defined by their restriction to a subset of the lattice which has finite width in one of the directions. This property offers an explanation for the results of Kikuchi and Brush. In Section 4 we describe a sequence of CVM approximations involving one-dimensionally large clusters for which proper convergence can be proven, and in Section 5 we discuss briefly the "C scheme" of CVM approximations introduced by Kikuchi and Brush. Section 6 contains some final remarks.

For simplicity of presentation the arguments will be developed for the case of nearest-neighbor interactions on the square lattice in two dimensions. However the results presented are easily generalized to a much wider class of models (cf. Section 6).

2. PRELIMINARIES

Consider the square lattice in two dimensions, Z^2. The origin $(0,0) \in Z^2$ will be denoted by 0 and δ_1 and δ_2 will be the unit vectors $(1,0)$ and $(0,1)$, respectively. We will identify elements of Z^2 with translations over the corresponding vectors.

Consider the following (Ising) model on Z^2. With each lattice point or site $a \in Z^2$ we associate a variable S_a ("spin"), which can take values in a finite set Ω_0. The configuration space for a finite subset Λ of Z^2 is $\Omega_\Lambda = (\Omega_0)^\Lambda$, and the configuration space for the thermodynamic (infinite) system on the whole of Z^2 is $\Omega = (\Omega_0)^{Z^2}$.

Viewing Ω_0 as a discrete metric space, observables of the system can be identified with real-valued elements of $C(\Omega)$ [respectively, $C(\Omega_\Lambda)$ in the case of a finite subsystem], the continuous functions on the configuration space. On Ω_0 we take as *a priori* measure the (unnormalized) counting measure μ_0. The product measure on Ω_Λ will be denoted by μ_0 as well. Integration with respect to μ_0 will be denoted by the symbol $\langle \cdot \rangle_0$.

The Hamiltonian for the finite nonempty subset Λ of Z^2 is

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

where $\Phi[X]$ is the potential function associated with the cluster (set of lattice points) X. The interaction Φ will be taken to be translation invariant and, as pointed out in the Introduction, for reasons of simplicity of notation and visualization, we will assume that the interaction is nearest neighbor only instead of, more generally, finite range. As a consequence, the energy per site for the thermodynamic system is given by the observable

$$e = \Phi[\{0\}] + \Phi[\{0, \delta_1\}] + \Phi[\{0, \delta_2\}] \tag{2}$$

Notice, that this observable lives on three lattice points only.

In the language of this approach a (macro-) state ρ of the system (a specific configuration can be viewed as a microstate) is a positive linear functional on $C(\Omega)$, normalized in such a way that $\rho(1) = 1$. Restricted to $C(\Omega_\Lambda)$ with Λ finite it defines a density function $\rho[\Lambda]$ such that for all $f \in C(\Omega_\Lambda)$

$$\rho(f) = \langle f \cdot \rho[\Lambda] \rangle_0 \tag{3}$$

The existence of these density functions is guaranteed because of the simple structure of the configuration space.

Lattice translations induce translations on $C(\Omega)$ in a natural way; hence a state may be translation invariant, and the set of translation-invariant states will be denoted by I. It is precisely for states in I that e given by Eq. (2) represents the energy per lattice point.

Translation-invariant equilibrium states (we shall call them simply equilibrium states in this paper) are characterized by the variational principle (cf. Refs. 18 and 19)

$$f = \min_{\rho \in I} \{\rho(e) - s(\rho)\} \tag{4}$$

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

$$s(\rho) = \lim_{\Lambda \to Z^2} \frac{S_\rho(\Lambda)}{|\Lambda|} \tag{5}$$

is the mean entropy of the state ρ; the entropy of the finite subsystem in Λ

in the state ρ, $S_\rho(\Lambda)$, is given by

$$S_\rho(\Lambda) = -\rho(\log \rho[\Lambda]) = -\langle \rho[\Lambda] \log \rho[\Lambda] \rangle_0 \tag{6}$$

f is the free energy per lattice point. Thus, $\bar{\rho} \in I$ is an equilibrum state for the thermodynamic system on Z^2 if and only if

$$f = \bar{\rho}(e) - s(\bar{\rho}) \tag{7}$$

The cluster-variation method (CVM) can be shown to be a method of approximating the variational principle Eq. (4).[15]

3. A RESTRICTED VARIATIONAL PRINCIPLE

In this section we will give our main theorem, which involves a variational characterization of restrictions of equilibrium states.

Let us introduce some notation for subsets of Z^2 which we will use in the sequel:

$$L_n^{\,i} = \{ z = (z_1, z_2) \in Z^2 \mid z_1 \in \{0, \ldots, n-1\}, z_2 = i \} \tag{8}$$

$$D_n^{\,i} = \{ z = (z_1, z_2) \in Z^2 \mid z_1 \in \{0, \ldots, n-1\}, z_2 \in \{i, i+1\} \} \tag{9}$$

$$L^i = \{ z = (z_1, z_2) \in Z^2 \mid z_2 = i \} \tag{10}$$

$$D^i = \{ z = (z_1, z_2) \in Z^2 \mid z_2 \in \{i, i+1\} \} \tag{11}$$

$$R_n^{\,p} = \{ z = (z_1, z_2) \in Z^2 \mid z_1 \in \{0, \ldots, n-1\}, z_2 \in \{-p, p\} \} \tag{12}$$

$$R_n = \{ z = (z_1, z_2) \in Z^2 \mid z_1 \in \{0, \ldots, n-1\} \} \tag{13}$$

(respectively lines, double lines, and rectangles). In those cases where the position of a specific set in the lattice is irrelevant (e.g., because of translational invariance), we will omit the superscript i.

Consider the infinite double line D.

I_D will denote the set of those states on $C(\Omega_D)$ that are invariant for all translations within D; specifically this includes translations over a unit distance in the δ_2 direction as well as all translations in the δ_1 direction. (Of course, within D translations in the δ_2 direction can be applied only to observables that live on either the "lower" or the "upper" line of D only.) Consequently any state $\rho \in I_D$ has the property that if A and B are subsets of D, and A is a translate of B, then the restrictions of ρ to $C(\Omega_A)$ and to $C(\Omega_B)$ are the same (isomorphic). This property is used in the proof of Lemma I below [Eq. (19)].

Definition I. For any state $\rho \in I_D$

$$b(\rho) = \lim_{n \to \infty} \frac{S_\rho(D_n) - S_\rho(L_n)}{n} \tag{14}$$

The existence of this limit follows from the existence of $\lim n^{-1}.S_\rho(L_n)$ and $\lim(2n)^{-1}.S_\rho(D_n)$ (cf. Ref. 18, p. 46). Since for any state $\rho \in I$ the restriction of ρ to $C(\Omega_D)$ belongs to I_D, Definition I can be applied to $\rho \in I$ as well.

For any $\rho \in I$ we have, by a standard argument involving the strong subadditivity of the entropy $S_\rho(\Lambda)$ and translational invariance of ρ (cf. Ref. 18, p. 47),

$$S_\rho(D_n) - S_\rho(L_n) \geqslant n.s(\rho) \tag{15}$$

so

$$b(\rho) \geqslant s(\rho), \qquad \text{for any} \quad \rho \in I \tag{16}$$

It is easy to prove (cf. Ref. 18, p. 44) that $b(\rho)$ is an affine function on I and I_D, meaning that for $\rho, \sigma \in I$ or I_D, and $\alpha \in [0, 1]$,

$$b(\alpha\rho + (1-\alpha)\sigma) = \alpha b(\rho) + (1-\alpha)b(\sigma) \tag{17}$$

Please notice for later reference that the above applies to periodic states on Z^2 or D as well.

We now define the "restricted variational principle":

$$f_D = \min_{\rho \in I_D} \{\rho(e) - b(\rho)\} \tag{18}$$

States that attain the minimum will be called "restricted equilibrium states."

The restricted variational principle differs from the variational principle Eq. (4) in two aspects: the entropy $s(\rho)$ is replaced by $b(\rho)$, which is generally larger by Eq. (16), and the minimum is sought among the states of I_D instead of I. Since the restriction of I to $C(\Omega_D)$ belongs to I_D this includes, but might extend, the range of variation of the "standard" variational principle Eq. (4).

What we will show in the sequel is essentially the following: replacing $s(\rho)$ by $b(\rho)$ does no harm because all equilibrium states are found among those states for which equality holds in Eq. (16), and allowing variation among the states of I_D instead of I does no harm because every element of I_D is the restriction of an element of I.

Theorem I. Concerning the relation between the variational principle Eq. (4) and the restricted variational principle Eq. (18) the following holds:

(i) $f_D = f$;

(ii) If $\rho \in I$ is an equilibrium state then the restriction of ρ to $C(\Omega_D)$ is a restricted equilibrium state;

(iii) Any restricted equilibrium state is the restriction to $C(\Omega_D)$ of an equilibrium state.

For the proof of this theorem we will need the following lemma.

Lemma I. For any $\rho \in I_D$ there exists a sequence $(\hat{\rho}_n)$ in I such that

(i) $$\lim_{n\to\infty} s(\hat{\rho}_n) = b(\rho)$$

(ii) $$\lim_{n\to\infty} \hat{\rho}_n(e) = \rho(e)$$

(iii) $$\lim_{n\to\infty} \hat{\rho}_n[A] = \rho[A], \qquad \text{for any finite} \quad A \subset D$$

Proof of Lemma I. Take arbitrarily $\rho \in I_D$ and consider the associated density functions $\rho[D_n]$ and $\rho[L_n]$. Using these functions we define density functions on the rectangular sets $R_n{}^p$ [Eq. (12)] for all $p \in N$ by

$$\tilde{\rho}_n[R_n{}^p] = \frac{\prod_{i=-p}^{p-1} \rho[D_n{}^i]}{\prod_{i=-p+1}^{p-1} \rho[L_n{}^i]} \tag{19}$$

For configurations for which the denominator is zero, the numerator is zero as well and we define the quotient to be zero. Now $\tilde{\rho}_n[R_n{}^p]$ is a well-defined, properly normalized density function and the set of $\{\tilde{\rho}_n[R_n{}^p]\}_{p\in N}$ is compatible, meaning that $\tilde{\rho}_n[R_n{}^{p+1}]$ can be reduced to $\tilde{\rho}_n[R_n{}^p]$ by integration over the spins in $R_n{}^{p+1} \backslash R_n{}^p$. Hence this set of density functions defines a state $\tilde{\rho}_n$ on $C(\Omega_{R_n})$, with R_n given by Eq. (13). The state $\tilde{\rho}_n$ is translation invariant with respect to translations over $z = (0, z_2) \in Z^2$.

Now make $\tilde{\rho}_n$ into a state $\tilde{\rho}_n{}'$ on $C(\Omega)$ (i.e., for the thermodynamic system on Z^2) by covering Z^2 with disjoint copies of R_n and taking the appropriate translate of $\tilde{\rho}_n$ on each of these copies; $\tilde{\rho}_n{}'$ will be the product state of all of these translates. $\tilde{\rho}_n{}'$ is then translation invariant in the δ_2 direction and periodic with period n in the δ_1 direction. From $\tilde{\rho}_n{}'$ we construct a translation-invariant state $\hat{\rho}_n$ by averaging over translations:

$$\hat{\rho}_n = \frac{1}{n} \sum_{z \in L_n{}^0} \tilde{\rho}_n{}' \cdot \tau_z \tag{20}$$

where τ_z denotes translation over z and operates on $C(\Omega)$.[19] In this way we can construct a sequence $(\hat{\rho}_n)$ in I for any state ρ in I_D. We now show that this sequence satisfies the conditions of the lemma.

Since the entropy function $s(\cdot)$ is affine on translation-invariant states as well as on periodic ones,[18,19] we have from Eq. (20)

$$s(\hat{\rho}_n) = s(\tilde{\rho}_n{}') \tag{21}$$

Since $\tilde{\rho}_n{}'$ is a product of states $\tilde{\rho}_n$,

$$s(\tilde{\rho}_n{}') = s(\tilde{\rho}_n) \tag{22}$$

and with Eq. (19) we find

$$\begin{aligned} s(\tilde{\rho}_n) &= \lim_{p\to\infty} \frac{S_{\tilde{\rho}_n}(R_n{}^p)}{n(2p+1)} \\ &= \lim_{p\to\infty} \frac{1}{n(2p+1)} \left[2pS_\rho(D_n) - (2p-1)S_\rho(L_n)\right] \\ &= \frac{S_\rho(D_n) - S_\rho(L_n)}{n} \end{aligned} \tag{23}$$

(Note that this is the entropy of a Markov shift[20]). Combining Eqs. (21), (22), (23), and Definition I we find

$$\lim_{n\to\infty} s(\hat{\rho}_n) = b(\rho)$$

As to the energy term, from Eq. (2) we see that $e \in C(\Omega_{D_2{}^0})$, so

$$\begin{aligned} \rho(e) &= \langle \rho[D_2{}^0].e\rangle_0 \\ &= \langle \rho[D_n{}^0].e\rangle_0, \qquad \text{for all} \quad n \geqslant 2 \end{aligned}$$

By definition [Eq. (20)]

$$\hat{\rho}_n(e) = \frac{1}{n} \sum_{z\in L_n{}^0} \tilde{\rho}_n{}'(\tau_z e)$$

Of all the n translates $\tau_z e$ of e, only one is not an element of $C(\Omega_{D_n{}^0})$. If $\tau_z e \in C(\Omega_{D_n{}^0})$ then

$$\tilde{\rho}_n{}'(\tau_z e) = \tilde{\rho}_n(\tau_z e) = \langle \rho[D_n{}^0].e\rangle_0 = \rho(e)$$

so $\hat{\rho}_n(e)$ is the average of $(n-1)$ terms $\rho(e)$ and one other (but finite) term. Hence

$$\lim_{n\to\infty} \hat{\rho}_n(e) = \rho(e)$$

In an analogous way one shows that for any finite $A \subset D$

$$\lim_{n\to\infty} \hat{\rho}_n[A] = \rho[A]$$

This concludes the proof of Lemma I. ■

Proof of Theorem I. Let $\bar{\rho} \in I$ be an equilibrium state and let $\bar{\rho}_D$ be its restriction to $C(\Omega_D)$. Then, using Eq. (16),

$$f = \bar{\rho}(e) - s(\bar{\rho}) \geqslant \bar{\rho}(e) - b(\bar{\rho}) = \bar{\rho}_D(e) - b(\bar{\rho}_D) \geqslant f_D$$

so

$$f_D \leqslant f \tag{24}$$

Suppose $f - f_D = \epsilon > 0$ and let $\tilde{\rho} \in I_D$ be such that

$$f_D \leqslant \tilde{\rho}(e) - b(\tilde{\rho}) < f_D + \frac{\epsilon}{2} = f - \frac{\epsilon}{2}$$

According to Lemma I there is a sequence $(\hat{\rho}_n)$ in I such that for n sufficiently large

$$|\hat{\rho}_n(e) - \tilde{\rho}(e)| < \frac{\epsilon}{8}$$

$$\text{and} \quad |s(\hat{\rho}_n) - b(\tilde{\rho})| < \frac{\epsilon}{8}$$

so we have for n sufficiently large

$$f \leqslant \hat{\rho}_n(e) - s(\hat{\rho}_n) \leqslant \tilde{\rho}(e) - b(\tilde{\rho}) + \frac{\epsilon}{4} < f - \frac{\epsilon}{4}$$

which is a contradiction, so it must be that

$$f_D = f$$

This proves the first part of the theorem.

As to the second part, again let $\bar{\rho} \in I$ be an equilibrium state and let $\bar{\rho}_D$ be its restriction to $C(\Omega_D)$. Then

$$f = \bar{\rho}(e) - s(\bar{\rho}) \geqslant \bar{\rho}_D(e) - b(\bar{\rho}_D) \geqslant f_D = f$$

so $\bar{\rho}_D$ is a restricted equilibrium state. Incidentally, this proves also that the minimum in Eq. (18) is indeed attained.

As to the third part, let $\bar{\rho}_D \in I_D$ be a restricted equilibrium state and let $(\hat{\rho}_n)$ be the corresponding sequence of states in I as given by Lemma I. According to Theorem I.4 of Ref. 18 there is a state $\hat{\rho}$ on $C(\Omega)$ such that at least for a subsequence of $(\hat{\rho}_n)$

$$\lim_{n \to \infty} \hat{\rho}_n[K] = \hat{\rho}[K], \qquad \text{for all finite} \quad K \subset Z^2 \tag{25}$$

Obviously, $\hat{\rho}$ is translation invariant. Since

$$s(\hat{\rho}) = \inf_{\Lambda \subset Z^2} \frac{S_{\hat{\rho}}(\Lambda)}{|\Lambda|}$$

there is for any $\epsilon > 0$ a $\Lambda_0 \subset Z^2$ such that

$$s(\hat{\rho}) \leqslant \frac{S_{\hat{\rho}}(\Lambda_0)}{|\Lambda_0|} < s(\hat{\rho}) + \frac{\epsilon}{2}$$

Because of Eq. (25) and the finiteness of the configuration space Ω_0, there is an $N(\epsilon)$ such that for all $n \geqslant N(\epsilon)$

$$\left| \frac{S_{\hat{\rho}_n}(\Lambda_0)}{|\Lambda_0|} - \frac{S_{\hat{\rho}}(\Lambda_0)}{|\Lambda_0|} \right| < \frac{\epsilon}{2} \tag{26}$$

So, for any $\epsilon > 0$ there exist $\Lambda_0 \subset Z^2$ and $N(\epsilon) \in N$ such that for all

$n \geqslant N(\epsilon)$

$$s(\hat{\rho}_n) \leqslant \frac{S_{\hat{\rho}_n}(\Lambda_0)}{|\Lambda_0|} < \frac{S_{\hat{\rho}}(\Lambda_0)}{|\Lambda_0|} + \frac{\epsilon}{2} < s(\hat{\rho}) + \epsilon$$

From this it follows that

$$b(\bar{\rho}_D) = \lim_{n\to\infty} s(\hat{\rho}_n) \leqslant s(\hat{\rho})$$

Since moreover by Eq. (25) $\hat{\rho}_n(e) \to \hat{\rho}(e)$ and by Lemma I $\hat{\rho}_n(e) \to \bar{\rho}_D(e)$, $\hat{\rho}(e) = \bar{\rho}_D(e)$ and we have

$$f = f_D = \bar{\rho}_D(e) - b(\bar{\rho}_D) \geqslant \hat{\rho}(e) - s(\hat{\rho}) \geqslant f$$

Hence $\hat{\rho}$ is an equilibrium state, and combining Eq. (25) and Lemma I (iii) its restriction to $C(\Omega_D)$ is $\bar{\rho}_D$.

This completes the proof of Theorem I. ■

Corollary I. If $\bar{\rho} \in I$ is an equilibrium state then

$$s(\bar{\rho}) = b(\bar{\rho})$$

Proof. Since $\bar{\rho}$ is an equilibrium state

$$f = \bar{\rho}(e) - s(\bar{\rho})$$

Since the restriction $\bar{\rho}_D$ of $\bar{\rho}$ to $C(\Omega_D)$ is a restricted equilibrium state (by Theorem I)

$$f = f_D = \bar{\rho}_D(e) - b(\bar{\rho}_D) = \bar{\rho}(e) - b(\bar{\rho})$$

Hence $s(\bar{\rho}) = b(\bar{\rho})$. ■

4. A CONVERGENT MINIMIZING SEQUENCE FOR THE RESTRICTED VARIATIONAL PRINCIPLE

In this section we discuss a specific hierarchy of cluster-variation approximations involving only one-dimensionally long finite clusters and we prove proper convergence for this hierarchy.

Theorem I tells us that it is possible to reduce the number of lattice dimensions involved by one (in the case under consideration from two to one) at the cost of using $b(\rho)$ instead of $s(\rho)$. The CVM in general is based on the idea of approximating $s(\rho)$ by an expression in terms of a finite number of finite clusters. It is a natural idea to try to approximate $b(\rho)$ in a similar fashion. Recalling the definition of $b(\rho)$ we approximate $b(\rho)$ by

$$B_n(\rho) = \frac{S_\rho(D_n) - S_\rho(L_n)}{n} \tag{27}$$

so by Definition I

$$\lim_{n\to\infty} B_n(\rho) = b(\rho) \tag{28}$$

for all $\rho \in I_D$ and all $\rho \in I$.

We now replace the restricted variational principle by the following variational problem:

$$f_n = \min_{\rho_n \text{l.t.}} \{\rho_n(e) - B_n(\rho_n)\} \tag{29}$$

Here the minimum is sought among the "locally translation-invariant" (l.t.) states ρ_n on $C(\Omega_{D_n})$, which means that the state ρ_n should be invariant for translations contained within D_n. In other words, if $\rho_n[D_n]$ is the density function associated with ρ_n, and A and B are subsets of D_n and B is a translate of A, then the density functions $\rho_n[A]$ and $\rho_n[B]$ obtained from $\rho_n[D_n]$ by integrating out the spin variables in $D_n \backslash A$ and $D_n \backslash B$, respectively, should be the same (isomorphic). This notion of local translation invariance (called internal translational invariance in Ref. 15) is what remains of the translation invariance obeyed by the states $\rho \in I_D$ figuring in the restricted variational principle Eq. (18).

By a standard argument (continuous function on a compact set) the minimum in Eq. (29) can be shown to exist.

Lemma II. For any locally translation-invariant state ρ_n on $C(\Omega_{D_n})$ there exists a state $\rho \in I_D$ such that

(i) $b(\rho) = B_n(\rho_n)$

(ii) $|\rho(e) - \rho_n(e)| \leqslant (2/n).\|e\|$

where the norm is the supremum-norm on $C(\Omega)$.

Proof. The proof will be similar to the proof of Lemma I. Cover D with disjunct copies of D_n and take the appropriate translate of ρ_n on each of these copies; denote by $\tilde{\rho}_n$ the product state of all these translates. $\tilde{\rho}_n$ is locally translation invariant for translations in the δ_2 direction and periodic with period n in the δ_1 direction. Define ρ by averaging over translations [cf. Eq. (20)]

$$\rho = \frac{1}{n} \sum_{z \in L_n^0} \tilde{\rho}_n \cdot \tau_z \tag{30}$$

Since $b(\cdot)$ is affine on periodic states

$$\begin{aligned} b(\rho) &= b(\tilde{\rho}_n) \\ &= \lim_{m\to\infty} \frac{S_{\tilde{\rho}_n}(D_m) - S_{\tilde{\rho}_n}(L_m)}{m} \\ &= \frac{S_{\rho_n}(D_n) - S_{\rho_n}(L_n)}{n} = B_n(\rho_n) \end{aligned}$$

Since $e \in C(\Omega_{D_2^0})$ it follows from Eq. (30)

$$\rho(e) = \frac{n-1}{n}\rho_n(e) + \frac{1}{n}\tilde{\rho}_n(\tau_{(0,n-1)}e)$$

so

$$|\rho(e) - \rho_n(e)| \leqslant \frac{2\|e\|}{n}$$

which completes the proof of Lemma II. ■

Theorem II. With f_n defined by Eq. (29) and f by Eq. (4)

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

Proof. Let $\bar{\rho} \in I_D$ be a restricted equilibrium state; hence by Theorem I

$$f = \bar{\rho}(e) - b(\bar{\rho}) \tag{31}$$

Then, for all n

$$f_n \leqslant \bar{\rho}(e) - B_n(\bar{\rho}) \tag{32}$$

Let, for each n, $\hat{\rho}_n$ be a l.t. state on $C(\Omega_{D_n})$ for which

$$f_n = \hat{\rho}_n(e) - B_n(\hat{\rho}_n) \tag{33}$$

By Lemma II states $\tilde{\rho}_n \in I_D$ exist such that

$$\begin{aligned} f &\leqslant \tilde{\rho}_n(e) - b(\tilde{\rho}_n) \leqslant \hat{\rho}_n(e) + \frac{2\|e\|}{n} - B_n(\hat{\rho}_n) \\ &= f_n + \frac{2\|e\|}{n} \end{aligned} \tag{34}$$

Combining Eqs. (32) and (34) we find

$$f - \frac{2\|e\|}{n} \leqslant f_n \leqslant \bar{\rho}(e) - B_n(\bar{\rho}) \tag{35}$$

Taking $n \to \infty$, we find

$$f \leqslant \lim_n f_n \leqslant \bar{\rho}(e) - b(\bar{\rho}) = f$$

Hence $\lim_{n\to\infty} f_n = f$ and the proof of Theorem II is complete. ■

Our next theorem will show in what sense solutions of the variational problem Eq. (29) approximate true equilibrium states. First we formulate another lemma.

Lemma III. For any locally translation-invariant state ρ_n on $C(\Omega_{D_n})$ there exists a state $\bar{\rho}_n \in I$ with

(i) $$s(\bar{\rho}_n) = B_n(\rho_n)$$

(ii) $$|\bar{\rho}_n(e) - \rho_n(e)| \leqslant \frac{2.\|e\|}{n}$$

Proof. The proof of this lemma is contained in the proof of Lemma I. Alternatively, one can combine Lemma I and II. ■

With regard to the subsequent theorems, it is of interest to notice that the proof of Lemma III is constructive in nature: given ρ_n, $\bar{\rho}_n$ can be constructed by the procedure outlined in the proof of Lemma I.

Theorem III. Let, for each n, $\hat{\rho}_n$ be a l.t. state on $C(\Omega_{D_n})$ such that

$$f_n = \min_{\rho_n \text{l.t.}} \{\rho_n(e) - B_n(\rho_n)\} = \hat{\rho}_n(e) - B_n(\hat{\rho}_n)$$

Let, for each n, $\bar{\rho}_n \in I$ be the state on $C(\Omega)$ corresponding to $\hat{\rho}_n$ according to Lemma III. Then any w^*-limit point of $(\bar{\rho}_n)$ is an equilibrium state.

Proof. Let $\bar{\rho} \in I$ be a w^*-limit point of $(\bar{\rho}_n)$. This means there is a subsequence which we will denote by $(\bar{\rho}_n)$ as well such that $\bar{\rho}_n[A] \to \bar{\rho}[A]$ for all finite A in Z^2. Choose arbitrarily $\epsilon > 0$. Now write

$$\begin{aligned}\bar{\rho}(e) - s(\bar{\rho}) = &\left[\bar{\rho}(e) - \bar{\rho}_n(e)\right] + \left[\bar{\rho}_n(e) - \hat{\rho}_n(e)\right] + \left[\hat{\rho}_n(e) - B_n(\hat{\rho}_n)\right] \\ &+ \left[B_n(\hat{\rho}_n) - s(\bar{\rho}_n)\right] + \left[s(\bar{\rho}_n) - s(\bar{\rho})\right] \end{aligned} \tag{36}$$

For n sufficiently large we now have

$$|\bar{\rho}(e) - \bar{\rho}_n(e)| < \frac{\epsilon}{4} \tag{37}$$

because $\bar{\rho}_n \xrightarrow{w^*} \bar{\rho}$;

$$|\bar{\rho}_n(e) - \hat{\rho}_n(e)| < \frac{\epsilon}{4} \tag{38}$$

by Lemma III;

$$\hat{\rho}_n(e) - B_n(\hat{\rho}_n) = f_n < f + \frac{\epsilon}{4} \tag{39}$$

by Theorem II;

$$B_n(\hat{\rho}_n) - s(\bar{\rho}_n) = 0 \tag{40}$$

by Lemma III; and

$$s(\bar{\rho}_n) - s(\bar{\rho}) < \frac{\epsilon}{4} \tag{41}$$

by the upper semicontinuity of s.[18,19] Hence

$$f \leqslant \bar{\rho}(e) - s(\bar{\rho}) < f + \epsilon$$

Thus $f = \bar{\rho}(e) - s(\bar{\rho})$, which means that $\bar{\rho}$ is a translation-invariant equilibrium state.

This completes the proof of Theorem III. ■

5. THE "C-SCHEME" OF THE CVM

In the paper[16] which introduced the idea of using the CVM with one-dimensionally increasing basis clusters to obtain a sequence of approximations to the variational problem for two-dimensional lattice systems, Kikuchi and Brush proposed a hierarchy of CVM approximations they called the C scheme. In this scheme the following expression was used as the nth approximation to the entropy per site $s(\rho)$:

$$C_n(\rho) = \left[S_\rho(D_n) - S_\rho(L_n) \right] - \left[S_\rho(D_{n-1}) - S_\rho(L_{n-1}) \right] \tag{42}$$

The variational problem corresponding to this approximation is

$$f_n^{\,c} = \min_{\rho_n \text{l.t.}} \{ \rho_n(e) - C_n(\rho_n) \} \tag{43}$$

where the minimum is sought among the locally translation-invariant states ρ_n on $C(\Omega_{D_n})$.

Notice that, quite apart from the reasoning employed by Kikuchi c.s. to obtain the approximation Eq. (42), the kind of expression as given in Eq. (42) can be expected to approximate $s(\rho)$ if one adopts the intuitive reasoning that for any large set Λ of lattice points $S_\rho(\Lambda)$ should be more or less equal to $|\Lambda|.s(\rho)$. The fact, however, that these C approximations do not contain nor utilize information about the lattice system apart from that contained in the subsystem D, even for $n \to \infty$, remains a bit puzzling from this point of view. The picture is clarified, of course, by the contents of the previous sections of this paper, since obviously $C_n(\rho)$ should be regarded as an approximation to $b(\rho)$ rather than $s(\rho)$, and the corresponding variational problems Eq. (43) are in first instance approximations to the restricted variational principle Eq. (18) rather than to the variational principle Eq. (4). In this respect the C scheme is analogous to the sequence of approximations utilizing $B_n(\rho)$ introduced in Section 4 and in fact the relation between the approximations $B_n(\rho)$ introduced in Eq. (27) and the approximations $C_n(\rho)$ is a close one: the sequence $B_n(\rho)$ is just the first Cesàro mean of the sequence $C_n(\rho)$:

$$B_n(\rho) = \frac{1}{n} \sum_{i=1}^{n} C_i(\rho) \tag{44a}$$

$$C_n(\rho) = nB_n(\rho) - (n-1)B_{n-1}(\rho) \tag{44b}$$

First, let us show that $C_n(\rho) \to b(\rho)$, as expected.

Lemma IV. For any $\rho \in I_D$

$$\lim_{n \to \infty} C_n(\rho) = b(\rho)$$

Proof. Write

$$C_n(\rho) = \left[S_\rho(D_n{}^0) - S_\rho(D_n{}^0 \backslash \{0\}) \right] + \left[S_\rho(D_n{}^0 \backslash \{0\}) - S_\rho(D_{n-1}^0) \right] - \left[S_\rho(L_n^0) - S_\rho(L_{n-1}^0) \right] \tag{45}$$

Using translational invariance of ρ and the strong subadditivity of the entropy $S_\rho(\cdot)$ it can be shown (Ref. 18, p. 47) that each of the three terms in angular brackets in Eq. (45) is a decreasing function of n and bounded from below by zero, so $\lim_n C_n(\rho)$ exists and it is equal to $b(\rho)$ by Eqs. (44). ■

Our next theorem deals with the convergence of the C scheme. Unfortunately, in this case we have not been able to prove unconditional convergence. The basic difficulty may be illustrated by the following example.

Consider the function $f: [0, 1] \to R$ defined by $f(x) = (x - \frac{1}{2})^2$. Then

$$M = \min_{x \in [0,1]} f(x) = 0$$

and the minimum is attained in the point $X = \frac{1}{2}$. We will now construct a sequence of approximations f_n to f such that $f_n(x) \to f(x)$ for all $x \in [0, 1]$, but with $M_n \nrightarrow M$ and $X_n \nrightarrow X$, where

$$M_n = f_n(X_n) = \min_{x \in [0,1]} f_n(x)$$

Consider the well-known C^∞ function $\phi: R \to R$ defined by

$$\phi(x) = \exp\left(\frac{-1}{1 - x^2} \right), \qquad \text{if} \quad x \in (-1, 1)$$

$$\phi(x) = 0, \qquad \text{if} \quad x \in R \backslash (-1, 1)$$

Now take

$$f_n(x) = f(x) - \tfrac{5}{4} \, .e.\phi(2nx - 2)$$

It is easily shown that for all $x \in [0, 1]$ $f_n(x) \to f(x)$, and that $M_n \to -1$ and $X_n \to 0$.

In the case of the approximations $B_n(\rho)$ to $b(\rho)$ discussed in Section 4 the "extension theorems" Lemmas II and III served to exclude this kind of "pathological" behavior.

In the case of the C scheme we can offer the following theorem, which proves convergence subject to a (in practical cases verifiable) condition [Eq. (46)].

Theorem IV. Let, for each n, $\hat{\rho}_n$ be a l.t. state on $C(\Omega_{D_n})$ such that

$$f_n{}^c = \min_{\rho_n \text{l.t.}} \{ \rho_n(e) - C_n(\rho_n) \} = \hat{\rho}_n(e) - C_n(\hat{\rho}_n)$$

Let, for each n, $\bar{\rho}_n \in I$ be the state corresponding to $\hat{\rho}_n$ as given by Lemma III. Let $\bar{\rho} \in I$ be a w^*-limit point of the sequence $(\bar{\rho}_n)$. Suppose the following condition holds:

$$\lim_{n\to\infty} \left[C_n(\hat{\rho}_n) - B_n(\hat{\rho}_n) \right] = 0 \tag{46}$$

Then (i) $\lim_{n\to\infty} f_n^c = f$ and (ii) $\bar{\rho}$ is an equilibrium state.

Proof. Choose $\epsilon > 0$. Now

$$\bar{\rho}_n(e) - s(\bar{\rho}_n) = \bar{\rho}_n(e) - \hat{\rho}_n(e) + \hat{\rho}_n(e) - C_n(\hat{\rho}_n) + C_n(\hat{\rho}_n) - B_n(\hat{\rho}_n) + B_n(\hat{\rho}_n) - s(\bar{\rho}_n) \leqslant \frac{\epsilon}{2} + f_n^c + \frac{\epsilon}{2} + 0$$

for n sufficiently large, so on one hand we have for n sufficiently large

$$f \leqslant \bar{\rho}_n(e) - s(\bar{\rho}_n) \leqslant f_n^c + \epsilon \tag{47}$$

On the other hand, with $\rho_e \in I$ an equilibrium state, so

$$f = \rho_e(e) - s(\rho_e) = \rho_e(e) - b(\rho_e) \tag{48}$$

we have for n sufficiently large

$$f_n^c \leqslant \rho_e(e) - C_n(\rho_e) \leqslant \rho_e(e) - b(\rho_e) + \epsilon = f + \epsilon \tag{49}$$

Combining Eqs. (47) and (49) we find

$$f - \epsilon \leqslant f_n^c \leqslant f + \epsilon$$

for n sufficiently large; hence $f_n^c \to f$. This proves the first part of the theorem.

As to the second part, consider a subsequence of $(\bar{\rho}_n)$ which converges to $\bar{\rho}$. Now

$$\bar{\rho}(e) - s(\bar{\rho}) = \bar{\rho}(e) - \bar{\rho}_n(e) + \bar{\rho}_n(e) - \hat{\rho}_n(e) + \hat{\rho}_n(e) - C_n(\hat{\rho}_n) + C_n(\hat{\rho}_n) - B_n(\hat{\rho}_n) + B_n(\hat{\rho}_n) - s(\bar{\rho}_n) + s(\bar{\rho}_n) - s(\bar{\rho})$$

$$\leqslant \frac{\epsilon}{5} + \frac{\epsilon}{5} + \left(f + \frac{\epsilon}{5} \right) + \frac{\epsilon}{5} + 0 + \frac{\epsilon}{5}$$

for n sufficiently large. Thus

$$f \leqslant \bar{\rho}(e) - s(\bar{\rho}) \leqslant f + \epsilon$$

so $\bar{\rho}$ is an equilibrium state. This completes the proof of Theorem IV. ■

Notice that in actual computations utilizing the C scheme it is easy to compute $C_n(\hat{\rho}_n) - B_n(\hat{\rho}_n)$ after the nth CVM-approximation to the equilibrium state has been obtained. Consequently it is possible in practice to get at least an indication whether condition (46) is fulfilled.

6. FINAL COMMENTS

Although the discussion in this paper has been limited to the case of nearest-neighbor interactions on Z^2 for reasons of simplicity of notation and visualization, the results can be generalized immediately to general finite-range interactions on any d-dimensional lattice that can be mapped one-to-one onto Z^d. For instance, if the lattice is Z^d and the interaction has range r, the role of the sets D_n will be taken over by sets

$$U_n = \{z = (z_1, \ldots, z_d) \in Z^d \mid 0 \leqslant z_i \leqslant n-1 \text{ for } i = 1, \ldots, d-1;\ 0 \leqslant z_d \leqslant r-1\}$$

and the sets L_n should be replaced by

$$V_n = \{z = (z_1, \ldots, z_d) \in Z^d \mid 0 \leqslant z_i \leqslant n-1 \text{ for } i = 1, \ldots, d-1;\ 0 \leqslant z_d \leqslant r-2\}$$

Instead of $b(\rho)$ the following quantity is of interest;

$$t(\rho) = \lim_{n\to\infty} \frac{S_\rho(U_n) - S_\rho(V_n)}{n^{d-1}}$$

All the results presented in this paper hold, with appropriate changes, for this more general situation.

Instead of restricting one's attention to translation-invariant equilibrium states one can deal with periodic states in exactly the same way. This corresponds to the admission of a sublattice structure.

As illustrated by the example of a sequence of smooth functions on [0, 1] in Section 5, simple pointwise approximation of $s(\rho)$ by an expression in terms of a finite number of finite clusters, as is the nature of the CVM, is generally speaking insufficient to guarantee that the CVM approximations to the free energy and to the equilibrium state converge toward the exact results. This observation might serve as a stimulus to investigate the question of convergence of hierarchies of CVM approximations in more detail.

On an altogether different level, the investigation reported on in this paper may be regarded as an attempt to extend the treatment of the one-dimensional lattice gas on the basis of the variational principle as given by Brascamp[21] to more dimensions. Brascamp points out the connection between his exact calculation and the Bethe approximation, which is known to be exact in one dimension. Since it is also well known that the CVM can be regarded as an extension of the Bethe approximation, it is not surprising that extensions of Brascamps procedure supply information about the CVM.

ACKNOWLEDGMENTS

The author is indebted to the Management of Shell Research B.V. for permission to publish this paper. He also wishes to thank Professor M. Winnink of the Mathematical Physics Group of the University of Groningen for stimulating discussions and for critical reading of the manuscript.

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