Analyticity of a Hard-Core Multicomponent Lattice Gas

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A multicomponent "anti-Widom–Rowlinson" lattice gas is introduced. An arbitrary number M of particle types is permitted, all having the same activity. The only interactions are nearest-neighbor exclusions of *like* particles (analogous to map-coloring problems). For any lattice it is shown that there is a finite number M_0 (depending only on the coordination number of the lattice) such that for all $M \geq M_0$ the infinite volume correlation functions exist and are analytic functions of the activity, for all positive values of the common activity.

KEY WORDS: Lattice gas; map colorings; Möbius functions; phase transition.

1. INTRODUCTION

We discuss here a lattice statistics model related to but distinct from several well-known models. A model introduced by Widom and Rowlinson[1] postulated a binary system of particles for which like particles were non-interacting and unlike particles interacted through a hard-core repulsion. In two or more dimensions the model has been proved to have a phase transition,[2] as have lattice versions[3] and the extension of the lattice version to an arbitrary number of particle types with equal activities[4]—still with hard-core repulsion between any unlike particles (we call this the WR model of

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M components). These models are essentially ferromagnetic models and the proofs of the phase transitions have been the Peierls-type argument about the effect of boundary conditions, such as used with the ferromagnetic Ising model (see, e.g., Ref. 5).

We introduce here an "anti-Widom–Rowlinson" model (AWR) partaking of antiferromagnetic character: Unlike particles are noninteracting, while like particles interact through a hard-core repulsion. We allow an arbitrary number M of particle types, but restrict attention to a lattice gas version where the hard-core exclusion extends only to nearest-neighbor sites.

The $M = 1$ case is simply the hard square lattice gas, known to exhibit a phase transition[6] and thought to be isomorphic to the WR model as its number of components becomes infinitely large.[4] It is easy to show that the $M = 2$ AWR and the $M = 2$ WR models are in fact isomorphic to an open lattice; in two or more dimensions this model is known to have a phase transition, again assuming the two particle types have the same activity.[3] If all types have the same activity it appears plausible to expect the AWR model to become effectively noninteracting as $M \to \infty$ and become isomorphic to the $M = 1$ WR model (ideal lattice gas). We shall not actually prove this statement, but we will show that there exists a finite M_0 such that there is no phase transition for the AWR model for $M \geqslant M_0$.

The AWR model can also be viewed as a map-coloring problem, inasmuch as the exclusion of like neighboring types (or colors) is the essence of such coloring problems. A particularly interesting case is $M = 3$ on the square lattice at high activity, so that all sites are occupied. Computing the number of allowed configurations of this model is equivalent to calculating the entropy of square ice.[7]

For another reason the case $M = 3$ is worthy of note. For $M = 1$ or 2, the cases known to have phase transitions, the equilibrium state at high activity is not unique. For an open lattice in two or more dimensions there are at least two equilibrium states at high density, corresponding to different sublattice occupation. But for $M \geqslant 3$ the number of geometric arrangements of the filled lattice is infinite (for an open lattice), as shown, for example, by the residual entropy of square ice.

This *may* be an important factor bearing on the question of the existence or absence of a phase transition of the system, and on the uniqueness of the equilibrium state. It is certainly true that those lattice systems for which phase transitions have been proved directly by the Peierls argument can be characterized by the statement that the high-activity phase has finite degeneracy. Other systems with infinite geometrical degeneracy in the high-activity phase have been shown (by other techniques) to be devoid of phase transitions[8–10]—leading to the obvious conjecture. There are, however, counterexamples[11,12] that show the conjecture to be false as a general

principle; it is possible for a system to have a unique equilibrium state on both sides of a phase transition and to be disordered on both sides. Each of these counterexamples, however, is a dual of a more conventional system with finite degeneracies.

The complete solution of the AWR model for arbitrary M might shed light on these questions. For the present, however, the only conclusion we will establish is the absence of a phase transition for sufficiently large (but finite) M; whether or not the same conclusion applies to any M greater than two is at present unknown.

2. DEFINITIONS AND NOTATION

We begin with a finite collection Λ of "sites," which for the present will be quite general. At a later point we will specialize to the case of a regular "lattice" of sites. We shall use lower case letters near the end of the alphabet to denote the individual sites, such as $x \in \Lambda$, and similar capital letters $Y \subset \Lambda$ for subsets of Λ. For the collection of "bonds" we shall use $\mathscr{B}$—this is a subset of $\Lambda \times \Lambda$—with typical element $B \in \mathscr{B}$, more explicitly written as $B = (x, y)$, where x and y are the "end points" of the bond. We shall use a Greek letter early in the alphabet for a subset of $\mathscr{B}$, such as $\beta \subset \mathscr{B}$. If $Y \subset \Lambda$, we shall denote by $\mathscr{B}_Y = \mathscr{B} \cap (Y \times Y)$ the bonds with end points restricted to Y.

It is sometimes convenient to have an explicit notation for the end points of a bond $B = (x, y)$, that is, the vertices upon which B is incident. We write for this $v(B) = \{x\} \cup \{y\}$, and for $\beta \subset \mathscr{B}$ we have $v(\beta) = \bigcup_{B \in \beta} v(B)$.

Any collection β of bonds has a unique decomposition into *connected components* β_j, given formally by

$$\beta = \bigcup \beta_j, \qquad \beta_j \subset \mathscr{B}, \qquad v(\beta_i) \cap v(\beta_j) = \varnothing \quad \text{if} \quad i \neq j$$

and the requirement that each subcollection β_i have no such (nontrivial) decomposition. For one of these connected components β_j, we define its *closure* $\bar{\beta}_j$ by

$$\bar{\beta}_j = \bigcup_{x, y \in v(\beta_j)} [(x, y) \cap \mathscr{B}]$$

and for any $\beta \subset \mathscr{B}$ we define the closure by $\bar{\beta} = \bigcup \bar{\beta}_j$. A central role is played by those subsets of $\mathscr{B}$ that are identical to their closures; we denote by $\mathscr{P}_f^+(\mathscr{B})$ this collection: $\beta \in \mathscr{P}_f^+(\mathscr{B})$ if and only if $\beta = \bar{\beta}$. In this and the preceding paragraph $\mathscr{B}$ may be replaced by $\mathscr{B}_Y$ for definitions restricted to bonds incident upon a subset $Y \subset \Lambda$.

Keeping some such subset Y fixed, we now discuss a configuration on Y, by which we mean a mapping $f: Y \to I_m$, where $I_m = \{1, 2,..., M\}$, such

that $f(x)$ denotes the type of particle at site x. It should be noticed that no site of Y is empty; summation over all sets Y of occupied sites comes later. It should also be noted that f may or may not be a configuration allowed by the AWR rules.

We denote by $\mathscr{X}_Y$ the space of such configurations, which space clearly has cardinality $M^{|Y|}$, where $|Y|$ is the number of sites in Y. There is a natural mapping (which we call χ) from $\mathscr{X}_Y$ onto $\mathscr{P}_f^\dagger(\mathscr{B}_Y)$, given by

$$B = (x, y) \subset \chi(f) \qquad \text{if and only if} \quad f(x) = f(y) \quad \text{and} \quad (x, y) \in \mathscr{B}_Y$$

That is, $\chi(f)$ is the collection of bonds joining sites with identical types of particles. The function χ is many-to-one; in fact, the multiplicity of the inverse function is of sufficient importance to warrant a definition:

$$G_Y(\beta) = \sum_{f : \chi(f) = \beta} 1, \qquad (\beta \in \mathscr{P}_f^\dagger(\mathscr{B}_Y)) \qquad (1)$$

In particular, $G_Y(\varnothing)$ is the number of *allowed* configurations of Λ for which Y is the set of occupied sites.

The partition function now may be written as

$$\overline{M}(\Lambda, M, z) = \sum_{Y \subset \Lambda} z^{|Y|} [M^{-|Y|} G_Y(\varnothing)] \equiv \sum_{Y \subset \Lambda} z^{|Y|} \Omega(Y)$$

if each type of particle has the same activity $\zeta = z/M$. It is clear that $\Omega(Y)$ is no greater than one and plays the role of the negative exponential of an effective potential function.

3. URSELL FUNCTIONS OF THE POTENTIAL

The Ursell functions ψ of the (effective) potential are defined recursively by

$$\Omega(Y) = 1 + \sum_{\substack{\beta \in \mathscr{P}^\dagger_f(\mathscr{B}_Y) \\ \beta \neq \varnothing}} \prod_j \psi(\beta_j) \qquad (2)$$

where the β_j are the connected components of β. The ψ functions are defined only on the nonvoid connected components. For example, if $Y = \{x, y\}$ and $(x, y) \in \mathscr{B}_Y$, we find $G_Y(\varnothing) = M(M - 1)$ and $\psi(Y) = -M^{-1}$. The Ursell functions ψ provide a criterion for the existence and analyticity of the correlation functions in the thermodynamic limit $\Lambda \to \infty$ (in the sense of van Hove); it is in fact that[8]

$$|1 + z^{-1}| > \min_{\xi > 0} \xi^{-1} R(\xi) \qquad (3)$$

where $R(\xi)$ is an upper bound on the sum

$$R_1(\xi) = \max_{x_0}\left[1 + \sum_{\beta\in\mathscr{P}^\dagger_f(\mathscr{B}):v(\beta)\,\ni\,x_0}|\psi(\beta)|\,\xi^{|v(\beta)|}\right] \tag{4}$$

The summation is restricted to connected sets β equal to their closures. This criterion then establishes analyticity for sufficiently small activity, in the general case. If, however, the Ursell functions decay sufficiently rapidly with increasing $|v(\beta)|$, the region of analyticity can contain the entire positive activity axis.

To study the behavior of the ψ functions we introduce an integrated version of Eq. (1),

$$H_Y(\beta) = \sum_{f:x(f)\,\supset\,\beta} 1, \qquad \beta \in \mathscr{P}_f^\dagger(\mathscr{B}_Y) \tag{5}$$

so that

$$H_Y(\beta) = \sum_{\gamma\,\supset\,\beta} G_Y(\gamma) \tag{6}$$

We can write an explicit formula for $H_Y(\beta)$. Each function f contributing to $H_Y(\beta)$ in Eq. (5) must be constant on each connected component of β, so that

$$H_Y(\beta) = M^{|Y| - v(\beta)| + v(\beta)} \tag{7}$$

where $v(\beta)$ is the number of connected components of β.

It is shown in the appendix, based on the theory of Möbius functions on partially ordered sets,[13] that Eq. (6) may be inverted to give

$$G_Y(\varnothing) = \sum_\beta a_\beta H_Y(\beta) \tag{8}$$

where for $\beta \in \mathscr{P}_f^\dagger(\mathscr{B}_Y)$

$$a_\beta = \sum_{\gamma\subset\mathscr{B}_Y:\,\bar\gamma\,=\,\beta}(-1)^{|\gamma|}, \qquad a_\phi = 1 \tag{9}$$

where $|\gamma|$ is the number of bonds in γ. In other words, if β is regarded as a graph with vertices $v(\beta)$ and connected components β_j, the summation in Eq. (9) is over subgraphs that within each β_j are also connected and incident at each vertex of $v(\beta_j)$. It follows easily from Eq. (9) that the coefficients a_β can be factored according to the $v(\beta)$ connected components β_j of β as

$$a_\beta = \prod_j a_{\beta_j} \tag{10}$$

It also follows that

$$|a_{\beta_j}| \leqslant 2^{|\beta_j|} \tag{11}$$

since the sum is over connected subgraphs and there are a total of $2^{|\beta_j|}$ subgraphs, connected or not.

It now follows that

$$\Omega(Y) = M^{-|Y|}G_Y(\varnothing) = 1 + \sum_{\substack{\beta \in \mathscr{P}_f{}^{\dagger}(\mathscr{B}_Y) \\ \beta \neq \phi}} a_\beta M^{-\delta(\beta)}$$

$$= 1 + \sum_{\substack{\beta \in \mathscr{P}_f{}^{\dagger}(\mathscr{B}_Y) \\ \beta \neq \phi}} \prod_j [M^{-\delta(\beta_j)}a_{\beta_j}] \qquad (12)$$

where we have introduced $\delta(\beta) = |v(\beta)| - \nu(\beta)$. It follows then that for the connected components the Ursell functions are given by

$$\psi(\beta_j) = M^{-(|v(\beta_j)|-1)}a_{\beta_j} \qquad (13)$$

4. ABSENCE OF PHASE TRANSITION

In this section we assume the following properties of Λ and $\mathscr{B}$ as $\Lambda \to \infty$; No site of Λ is an end point of more than c bonds in $\mathscr{B}$, for some fixed $c > 0$, and there is defined some complete ordering of the sites. A "lattice" of sites is a special case.

Proposition 1. The Ursell functions $\psi(\beta_j)$ satisfy the bound

$$|\psi(\beta_j)| \leqslant \gamma^{|v(\beta_j)|} \qquad (14)$$

where $\gamma = \gamma(M)$ decreases to zero as $M \to \infty$.

Proof. By Eqs. (11) and (13),

$$|\psi(\beta_j)| \leqslant M^{-|v(\beta_j)|+1} \cdot 2^{c|v(\beta_j)|/2} = M(2^{c/2}/M)^{|v(\beta_j)|}$$
$$\leqslant [(2^c/M)^{1/2}]^{|v(\beta_j)|}$$

since $|v(\beta_j)| \geqslant 2$. Hence γ may be taken as $(2^c/M)^{1/2}$.

Proposition 2. The number of connected sets β_j such that $x_0 \in v(\beta_j)$ and $|v(\beta_j)| = v$ is no greater than α^v for some positive α.

Proof. Regarding $(\Lambda, \mathscr{B})$ as a graph, we define for any β_j a unique progression of bonds (i.e., a "lattice walk"), beginning at x_0, that contains a bond incident at each vertex of β_j. This walk will turn out to require no more than $2v$ steps. Since there are no more than $c^{(2v)}$ lattice walks of $2v$ steps beginning at a specified site, there are no more than c^{2v} connected sets β_j such that $x_0 \in v(\beta_j)$ and $|v(\beta_j)| = v$.

It is well known that any connected graph contains at least one spanning tree graph—a partial graph that contains no cycles and has an edge incident at each vertex. The ordering of the sites (vertices) induces a natural ordering of the spanning tree graphs, and we select the lowest one in that induced ordering. A unique lattice walk is defined on this lowest spanning tree graph,

beginning at x_0, by the following three rules (where "outward" means away from x_0 and "inward" means toward x_0):

1. A previously visited vertex is never revisited in an outward step.

2. An outward step takes precedence over an inward step; i.e., an inward step is taken only from a vertex of degree one or from a vertex all of whose adjacent vertices have already been visited.

3. A step is always taken in the direction of the accessible vertex lowest in the ordering.

It is clear that the above rules define a unique lattice walk of exactly $2(v - 1) < 2v$ steps, starting and ending at x_0, for each connected set of v bonds containing x_0. The proof is thus complete, with $\alpha = c^2$. We can now state our main result.

Theorem. There is an $M_0 > 0$ such that for $M > M_0$ the AWR model has no phase transition for any positive real activity.

Proof. The sum R_1 in Eq. (4) is dominated by

$$R(\xi) = 1 + \sum_{v > 0} (\gamma \alpha \xi)^v = (1 - \gamma \alpha \xi)^{-1} \tag{15}$$

for $\xi < (\gamma \alpha)^{-1}$, where $\gamma = \gamma(M)$ and α are given in Propositions 1 and 2, respectively. It is trivial to show that

$$\min_{\xi} \xi^{-1} R(\xi) = 4\alpha\gamma \tag{16}$$

and this minimum can be made arbitrarily small by choosing M large enough. According to Eq. (3), analyticity is guaranteed for z in the region $|1 + z^{-1}| > 4\alpha\gamma$. Hence, for $4\alpha\gamma < 1$, the entire positive real axis is included. With the above choices for α and γ, this leads to the condition

$$4(2^c/M_0)^{1/2}c^2 < 1 \tag{17}$$

For the square lattice with $c = 4$, Eq. (17) gives $M_0 > 2^{16}$, a value which is certainly far larger than necessary. It would be most interesting to know if $M_0 = 3$ is large enough.

APPENDIX. MÖBIUS FUNCTIONS ON PARTIALLY ORDERED SETS

We review briefly the theory of Möbius functions on partially ordered sets[13,14] and apply that theory to the solution of Eqs. (6) and (7).

Let Q be a finite set partially ordered by the relation $\leqslant$. The Möbius function $\mu(x, y)$ for Q is defined inductively by $\mu(x, x) = 1$ for all $x \in Q$ and

$$\mu(x, y) = - \sum_{x \leqslant z < y} \mu(x, z)$$

for $x < y$. Otherwise, $\mu(x, y) = 0$. The Möbius function μ is inverse to the ζ function, defined by

$$\zeta(x, y) = \begin{cases} 1 & x \leqslant y \\ 0 & \text{otherwise} \end{cases}$$

Since μ is inverse to ζ, a relation of the sort

$$H(x) = \sum_{y \leqslant x} G(y) = \sum_{y \in Q} G(y)\zeta(y, x)$$

defined on Q can be solved for G:

$$G(x) = \sum_{y \in Q} H(y)\mu(y, x) \tag{A.1}$$

This is the Möbius inversion formula.

Now the finite set $\mathscr{P}_f^+(\mathscr{B}_\gamma) = Q$ is partially ordered by inclusion: $\gamma \leqslant \beta$ if $\gamma \supset \beta$, including the case $\gamma = \beta$. Equation (8) is the same as Eq. (18) with $a_\beta = \mu(\beta, \varnothing)$, where the void set $\varnothing$ is the unique *maximal* element (called "1") in Q.

The problem now is in evaluating the Möbius function. One case is easy— if $Q' = \mathscr{P}_f(A) = $ set of all subsets of a finite set A, it is readily shown that

$$\mu(x, y) = (-1)^{|x| - |y|} \quad \text{for} \quad x \leqslant y \tag{A.2}$$

where $|x|$ is the number of elements (of A) in subset x.

It is sometimes possible to obtain one Möbius function from another. An important example uses the notion of a Galois connection between two partially ordered sets P and Q. If $\pi: Q \to P$ and $\rho: P \to Q$ are both order-inverting functions satisfying $\pi(\rho(p)) \geqslant p$ and $\rho(\pi(q)) \geqslant q$ for $p \in P$, $q \in Q$, then the pair (π, ρ) is called a Galois connection.

Proposition. Let P and Q be partially ordered finite sets, each having a unique minimal element (0) and Q having a unique maximal element 1. Let $\pi: Q \to P$ and $\rho: P \to Q$ be a Galois connection, and let μ be the Möbius function for Q and μ^* the Möbius function for P. Suppose furthermore that

$$\pi(x) = 0 \quad \text{if and only if} \quad x = 1$$

and

$$\rho(0) = 1$$

Then the Möbius functions are related by

$$\mu(0, 1) = \sum_{a \in P: \, \rho(a) = 0} \mu^*(0, a) \tag{A.3}$$

For the proof see Ref. 13. Our application is for $Q = \mathscr{P}_f^+(\mathscr{B}_\gamma)$ as before, with

$1 = \varnothing$ and $0 = \mathscr{B}_Y$; also we need $P = \mathscr{P}_f(\mathscr{B}_Y)$ ordered by $\alpha \leqslant \gamma$ if $\alpha \subset \gamma$, so that $0 = \varnothing$ in P. [Notice that the inclusion goes the opposite direction from that in Q.] By Eq. (A.2), $\mu^*(\alpha, \gamma) = (-1)^{|\alpha| - |\gamma|}$ for $\alpha \leqslant \gamma$, $|\alpha|$ denoting now the number of bonds in α.

The mappings π and ρ are defined by

$$\pi(\alpha) = \alpha, \qquad \rho(\gamma) = \bar{\gamma}$$

and are readily seen to be a Galois connection. Equation (A.3) now reads

$$\mu(\mathscr{B}_Y, \varnothing) = \sum_{\gamma \in P:\, \gamma = \mathscr{B}_Y} (-1)^{|\gamma|}$$

which is the same as Eq. (9) with $Y = v(\beta)$.

ACKNOWLEDGMENTS

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