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Classical Lattice Gas Model with a Unique Nondegenerate but Unstable Periodic Ground State Configuration

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Abstract. We construct a classical lattice gas model with a unique periodic ground state configuration such that the Peierls' condition is not satisfied. The ground state configuration is nondegenerate, which means that for any fixed energy E and any integer n, the diameter of the support of all n-connected local excitations, with energy less than E, is bounded. Nevertheless the configuration is not stable: it does not give rise to a low temperature phase. Any translation invariant Gibbs state of our model corresponds to quasiperiodic ground state configurations. This requires the modification of a recent hypothesis of Dobrushin and Shlosman.

1. Introduction

In their recent paper Dobrushin and Shlosman [1] formulated a hypothesis concerning the stability of ground state configurations of classical lattice systems. They addressed the question: which ground state configurations give rise to the low temperature phases? One of their suggestions was the following. Assume all periodic ground state configurations be related by the symmetry of the Hamiltonian. Then a ground state configuration should be stable if and only if it is nondegenerate, where by nondegeneracy it is meant that for any fixed energy E and any integer n the diameter of the support of all n-connected local excitations with energy less than E is bounded.

Here we provide a counterexample to this assertion. Our model is a two-dimensional lattice gas system with nearest neighbor interaction. The construction is based on Robinson's tiles [2, 3]. There is a family of 56 square-like tiles which tile the plane only in a nonperiodic fashion. This can be translated into a lattice gas model without any periodic ground state configurations in the following way [4, 5, 3]. Every site of the square lattice can be occupied by one of the 56 different particle-tiles. Two nearest neighbor particles which do not "match" contribute positive energy; otherwise the energy is zero. Such model does not have periodic ground state configurations. It does possess, however, "quasiperiodic" ground state configurations. A configuration of particles is quasiperiodic if when a certain fraction of them is ignored the rest of the configuration is periodic; the smaller the fraction, the larger the period. Such quasiperiodic ground state configurations are unstable: arbitrary small changes in chemical potential lead to changes in stoichiometries, in distinction with all previous known models [6]. The low temperature behavior of classical lattice systems with quasiperiodic ground state configurations was studied recently in [3]. It appears that such systems can have many Gibbs states. The existence of quasiperiodic Gibbs state, however, has not been determined. We will demonstrate here that even in the presence of periodic ground state configurations the low temperature behavior may still be of quasicrystalline nature. In order to do that we introduce another particle (which we call square) which does not "match" any square-like particle but "matches" itself. In addition every square-like particle is furnished with one of the two "orientations": $+1$ or -1. The square particle acquires 0 orientation. Two nearest neighbor particles contribute positive energy if their orientations are either not the same or are both -1; otherwise the energy is zero. The interaction of our model is then the sum of the two interactions described above.

It is easy to see that such a lattice gas model has a unique nondegenerate periodic ground state configuration—every lattice site occupied by the square particle. Nevertheless it does not satisfy the Peierls' condition because of the existence of nonperiodic ground state configurations with all bonds "satisfied." (Systems with a finite number of periodic ground state configurations and violating the Peierls' condition were first introduced by Pecherski [7, 8].)

We will prove here that the unique, nondegenerate ground state configuration of our model is not stable: it does not give rise to the low temperature phase. The proof is based on a method developed in [9, 8, 10, 11]. The basic idea is the following. We fix the energy coupling constants in such a way that the lowest excitation energy of the nonperiodic ground state configurations is smaller than the lowest excitation energy of the periodic ground state configuration. Therefore the leading term of the low temperature expansion of the free energy is smaller for the nonperiodic ground state configuration than for the periodic one. The nonperiodic ground state configurations are then dominant [9]. This perturbation argument was made rigorous by Slawny [8] for systems to which Pirogov–Sinai theory applies: finite number of periodic ground state configurations satisfying the Peierls' condition; i.e., not in the present example. One can find a very nice exposition of the proof for the case of the Blume–Capel model in the paper of Bricmont and Slawny [10]. The proof can be applied almost directly in our case. In fact, our model is a variation of the Blume–Capel model incorporating nonperiodic ground state configurations.

2. The Model

Each site of the square lattice is occupied by one of the 113 particles. 112 of them are Robinson's square-like particles (the complete description of them can be found in [2, 3]) furnished with one of the two orientations: $+1$ or -1, and one is the square particle with 0 orientation. If $X(a)$ is a particle at site a, then we denote by $X^{or}(a)$ and $X^{t}(a)$ its orientation and its tile component respectively. If the tile components of two adjacent particles do not match the energy is E_t. If the orientations of two neighboring particles are $+1$ and -1 respectively they contribute the energy E_{+-}; if the orientations are 0 and -1 or $+1$ or if both orientations are -1 the energy is E_0. In all remaining cases the energy is zero. We set $0 < 12E_t < E_{+-} < (4/5)E_0$. Observe that the interaction between particles decouples into the sum of the interaction H^{or} between their orientations and H^t between their tile components.

The model just described has a unique periodic ground state configuration Q—all lattice sites occupied by the square particle, and many nonperiodic ones (corresponding to all nonperiodic tilings of the plane) with all bonds "satisfied." The Peierls' condition is not satisfied. To see that let us insert an island of a nonperiodic ground state configuration into the periodic one. The energy of this excitation is proportional to the length of the boundary of the island. On the other hand following Pirogov–Sinai definition one has to include the nonperiodic ground state configuration in the contours. This makes the area of the contour in our example equal to the area of the island.

Q is nondegenerate in the sense of Dobrushin and Shlosman [1], where nondegeneracy means the following. Let G be a ground state configuration and X equal to G except at the finite number of lattice sites denoted by $\operatorname{supp}(X\,|\,G)$. Then X is a "local excitation" of G. The excitation X is said to be n-connected if $\operatorname{supp}(X\,|\,G)$ is n-connected, where two lattice sites are n-connected if their distance is less than n. Let us denote the set of all local n-connected excitations of G by $\Sigma_n(G)$. If

$$H_\Lambda = \sum_{A \subset \Lambda} U_A \tag{2.1}$$

is the finite volume Λ Hamiltonian then

$$E(X\,|\,G) = \sum_{A \subset \mathbb{Z}^2} (U_A(X) - U_A(G)) \tag{2.2}$$

is the excitation energy.

The ground state configuration G is nondegenerate if for any $n > 0$, $E > 0$

$$\max_{\substack{X \in \Sigma_n(G) \\ E(X|G) < E}} (\text{diam. supp}(X\,|\,G)) < \infty. \tag{2.3}$$

It is easy to see that Q is nondegenerate.

3. The Instability of the Periodic Ground State Configuration Q

Using the contour method developed by Bricmont and Slawny [10, 11] we will prove the following theorem.

Theorem. *In any translation invariant Gibbs state of our model the probability of having the square particle at any fixed lattice site goes to zero as $\beta \to \infty$.*

This means that the unique nondegenerate periodic ground state configuration of our model is not stable. It does not give rise to a low temperature phase. The hypothesis of Dobrushin and Shlosman should therefore be modified.

First we define the restricted ensemble corresponding to the nonperiodic ground state configurations. We follow [10] closely.

Let $\mathscr{X} = \mathscr{S}^{\mathbb{Z}^2}$ be the configuration space of the model; $|\mathscr{S}| = 113$. Q is the unique periodic ground state configuration: $Q(a) = q$ (the square particle) for all $a \in \mathbb{Z}^2$. Let

$$\mathscr{X}_R^+ = \{X \in \mathscr{X} : X^{or}(a) = \pm 1, \text{ and if } X^{or}(a) = -1, \\ \text{then } X^{or}(b) = +1 \text{ for every adjacent } b\}.$$

$\mathscr{X}_{R,\Lambda}^+$ are the sets of restrictions to $\Lambda \subset \mathbb{Z}^2$ of the configurations of $\mathscr{X}_R^+$.

For $Y \in \mathscr{X}_{R,\Lambda^c}^+$ and a fixed arrangement Z of the tile components of the particles in Λ

$$Z_R^+(\Lambda \mid Y, Z) = \sum e^{-\beta H^{or}_{\Lambda \cup \partial \Lambda}(X)}, \tag{3.1}$$

where the sum is over all $X \in \mathscr{X}_R^+$ such that $X(a) = Y(a)$ for all $a \in \Lambda^c \equiv \mathbb{Z}^2 \backslash \Lambda$ and $X^t(a) = Z(a)$ for all $a \in \Lambda$; $\partial \Lambda$ is the set of the sites in the complement of Λ which have nearest neighbors in Λ. $Z_R^+(\Lambda \mid Y, Z)$ is a partition function of a hard-square lattice gas (at each lattice site we can have a particle with -1 orientation and no two particles can be adjacent) with the activity of the particle equal to $e^{-4E_{+-}\beta}$. Let

$$\beta P_R^+(\beta) = -\lim_{\Lambda \to \mathbb{Z}^2} \frac{1}{|\Lambda|} \log Z_R^+(\Lambda \mid Y, Z). \tag{3.2}$$

We have a convergent low-temperature expansion:

$$\beta P_R^+(\beta) = e^{-4E_{+-}\beta} + O(e^{-8E_{+-}\beta}). \tag{3.3}$$

Observe that there are no local excitations of the ground state configuration Q with energy less or equal to E_{+-}.

Let X be a local excitation of any configuration with the orientations of all particles equal to $+1$. We define its retouch by changing the orientation of a particle at a to $+1$ if $X^{or}(a) = -1$ and $X^{or}(b) = +1$ for every adjacent b. Now following an idea of Bricmont and Slawny [10] we introduce two kinds of contours: small-scale contours and large (temperature-dependent) scale contours. A small-scale contour γ of a configuration X is a pair $\gamma = ([\gamma], X_{[\gamma]})$, where $[\gamma]$ is a maximal connected subset of the set of nearest neighbors (a, b) such that

$$(\operatorname{ret} X(a))^{or} \neq (\operatorname{ret} X(b))^{or} \quad \text{or} \quad (\operatorname{ret} X(a))^{or} = (\operatorname{ret} X(b))^{or} = -1.$$

Now let

$$L(\beta) = e^{5E_{+-}\beta/2}.$$

$B(0)$ is a square of side $L(\beta)$ centered at the origin; $B(a) = B(0) + (1/2)L(\beta)a$, $a \in \mathbb{Z}^2$. $B(a)$ is a "regular box" of a configuration X if $X|_{B(a)} \in \mathscr{X}_{R,B(a)}^+$ and it is irregular otherwise. We have two types of irregular boxes $B(a)$ of a configuration X:

type 1 if $X|_{B(a)} = Q|_{B(a)}$,

type 2 if the support of a small-scale contour of X intersects $B(a)$.

A large-scale contour Γ is a connected family of irregular boxes. $\|\Gamma\|$ is the number of boxes in Γ. Given the above definition of contours and having the convergent low temperature expansion (3.3) one can repeat the proof of Bricmont and Slawny [10] and have the following lemma.

Lemma [10]. *If β is large enough there exists a constant c such that for all finite $\Lambda \subset \mathbb{Z}^2$, all boundary condition $S \in \mathscr{X}^+_{R,\Lambda^c}$ and all contours $\Gamma \subset \Lambda$,*

$$P_\Lambda(\Gamma|S) \leqq e^{-c\beta\|\Gamma\|},$$

where $P_\Lambda(\cdot|S)$ is the finite volume Λ Gibbs state with the boundary conditions S.

Sketch of the proof. The proof is based on the fact that the interaction between two particles decouples into the sum of the interaction between the tile components of the particles and the orientations of the particles. We will use the conditional probabilities with respect to all arrangements of the tile components of the particles and reduce everything to the system with the ground state configuration Q and another dominant periodic ground state configuration corresponding to $+1$ orientation of the particles. That system can be handled by the method of Bricmont and Slawny [10].

Let ω be a family of small-scale contours in $[\Gamma] = \bigcup_{B \in \Gamma} B$, $[\omega] = \bigcup_{\gamma \in \omega} [\gamma]$, and $[\Gamma] \backslash [\omega] = \bigcup_i M_i$, be the decomposition into connected components. Let $A = \bigcup M_i$, where the union is over all M_i's on which we can have the restricted ensemble $\mathscr{X}^+_{R,M_i}$. First we condition on the particles in $\partial[\Gamma]$:

$$P_\Lambda(\Gamma|S) = \sum P_\Lambda(\Gamma|S, S')P_\Lambda(\Gamma, S'|S), \tag{3.4}$$

where the sum is over all $S' \in \mathscr{X}^+_{R,\partial[\Gamma]}$, and the ensembles defining the probabilities are indicated after the vertical bar. Now we have

$$P_\Lambda(\Gamma|S, S') = P_{[\Gamma]}(\Gamma|S, S') = \sum_{\Gamma^2, \omega} P_{[\Gamma]}(\Gamma^2, \omega|S, S'), \tag{3.5}$$

where the sum is over all possible families Γ^2 of type 2 boxes of Γ and families ω of small-scale contours in $[\Gamma]$ such that for each box of Γ^2 there is a contour of ω with support intersecting the box. We do not include the type 1 boxes in the sum in (3.5). These boxes are, however, included in the definition of $[\Gamma]$ and they are taken into the account to estimate $P_{[\Gamma]}(\Gamma^2, \omega|S, S', W)$ when using (3.10) [10]. Now we condition on W, the tile components of particles in A,

$$P_{[\Gamma]}(\Gamma^2, \omega|S, S') = \sum_W P_{[\Gamma]}(\Gamma^2, \omega|S, S', W)P_{[\Gamma]}(\Gamma^2, \omega, W|S, S'), \tag{3.6}$$

$$P_{[\Gamma]}(\Gamma^2, \omega|S, S', W) = \frac{Z([\Gamma]|\Gamma^2, \omega, S, S', W)}{Z([\Gamma]|S, S', W)}. \tag{3.7}$$

Now we have the following estimates:

$$Z([\Gamma]|\Gamma^2, \omega, S, S', W) \leqq e^{-\beta E(\omega)} \prod_{M_i \subset A} Z^+_R(M_i|S_i, W)e^{-\beta H^t_{A\cup\partial A}(W|S^t_i)}, \tag{3.8}$$

where S_i is the configuration on ∂M_i determined by S, S' and W and $E(\omega) = \Sigma_{\gamma \in \omega} E(\gamma)$ and energy is calculated with respect to H^{or};

$$\begin{aligned} Z([\Gamma]|S, S', W) &\geqq Z'([\Gamma]|S, S', W) \\ &\geqq Z^+_R([\Gamma]|S, S', W')e^{-\beta H^t_{A\cup\partial A}(W'|S^t_i)}e^{-\beta|\partial[\omega]|E_t}, \end{aligned} \tag{3.9}$$

where in Z' the sum does not include the square particles, and W' is the configuration of the tile components of particles in $[\Gamma]$ constructed in the following way:

$$W'|_A = A|_A,$$
$$W'|_{[\Gamma]\setminus A} \text{ is such that } H^t_{[\Gamma]\setminus A}(W') = 0.$$

This can introduce an energy with respect to H^t not bigger than $|\partial[\omega]|E_t$. Because $E(\omega) \geqq E_{+-}|\omega|$, where $|\omega|$ is the number of bonds in ω, and $|\omega| \geqq (1/6)|\partial[\omega]|$, then if $E_t \leqq (1/12)E_{+-}$ then $|\partial[\omega]| \cdot E_t \leqq (1/2)E(\omega)$. Finally

$$P_{[\Gamma]}(\Gamma^2, \omega | S, S', W) \leqq \frac{e^{-\beta E(\omega)/2} \prod_{M_i \in A} Z_R^+(M_i | S_i, W')}{Z_R^+([\Gamma] | S, S', W')}. \tag{3.10}$$

Now to prove the lemma we proceed exactly as in [10]. ■

Following the technique in [10, 12] we may then prove the theorem.

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