An Ultimate Frustration in Classical Lattice-Gas Models

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A classical lattice-gas model is called frustrated if not all of its interactions can attain their minima simultaneously. The antiferromagnetic Ising model on the triangular lattice is a standard example.[1, 29] However, in all such models known so far, one could always find nonfrustrated interactions having the same ground-state configurations. Here we constructed a family of classical lattice-gas models with finite-range, translation-invariant, frustrated interactions and with unique ground-state measures which are not unique ground-state measures of any finite-range, translation-invariant, nonfrustrated interactions.

Our ground-state configurations are two-dimensional analogs of one-dimensional, "most homogeneous,"[13] nonperiodic ground-state configurations of infinite-range, convex, repulsive interactions in models with devil's staircases.

Our models are microscopic (toy) models of quasicrystals which cannot be stabilized by matching rules alone; competing interactions are necessary.

KEY WORDS: Frustration; nonperiodic tilings; dynamical systems of finite type; classical lattice-gas models; ground states; quasicrystals; devil's staircase.

1. INTRODUCTION

We will discuss two families of systems of interacting objects located at vertices of the square lattice. Our first family consists of two-dimensional classical lattice-gas models. In such models, sites of the square lattice are occupied by particles interacting through translation-invariant, finite-range potentials. Configurations of particles minimizing the energy density of their interactions are called ground-state configurations. It is an old and still unsolved problem in solid-state physics, the so-called crystal problem,[2-8]

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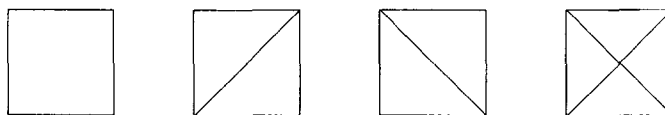
Fig. 1.   Tiles without horizontal and vertical markings.

to understand why ground-state configurations should have a perfect periodic order of crystals or at least nonperiodic order of recently discovered quasicrystals.[9, 10]

A tiling system consists of a finite set of prototiles, the so-called Wang tiles. Wang tiles are squares with markings (like notches and dents) on their sides. These markings define matching rules which tell us which tiles can be nearest neighbors. For example, in tiles in Figs. 1–3, markings are represented by vertical, horizontal, and diagonal lines. Then the matching rules say that these lines cannot be broken on common sides of nearest-neighbor tiles and at common corners of next-nearest-neighbor tiles. Using an infinite number of copies of given prototiles, one can tile the plane completely (centers of tiles form the square lattice) and without overlaps (except boundaries of tiles) such that all matching rules are satisfied. Like ground-state configurations, tilings are structures optimizing (maximizing) the sum of local terms—satisfied matching rules. It is an outstanding problem to understand why such structures are always ordered in some sense.[11]

A natural generalization of tiling systems are systems of finite type. Tiling systems are defined by specifying which pairs of tiles cannot be nearest neighbors. In systems of finite type, we specify which finite patterns of a fixed bounded size are not allowed.

For a given tiling system with n prototiles, we can construct the following lattice-gas model with n types of particles corresponding to tiles. Two nearest-neighbor particles which do not match as tiles have a positive interaction energy, say 1; otherwise the energy of interaction is equal to zero. Such interactions are obviously nonfrustrated; there are ground-state configurations minimizing all of them simultaneously. There is a one-to-one correspondence between such ground-state configurations and tilings of the plane. In the same manner, a classical lattice-gas model can be constructed
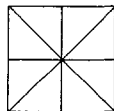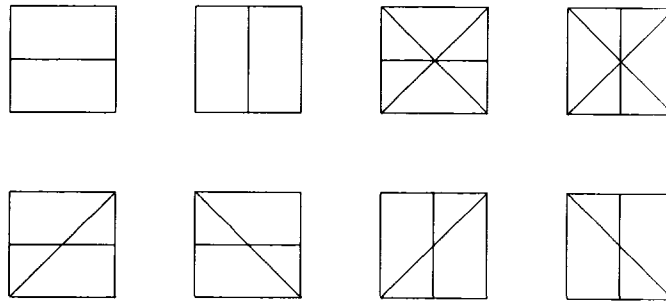
Fig. 2.   A cross.

Fig. 3. Arms.

for any system of finite type. Details of this construction are given in Section 2.

Here we restrict ourselves to models in which there may be many tilings or ground-state configurations but there is only one translation-invariant probability measure supported by them. Such systems are called uniquely ergodic (one may prove that their unique measures are necessarily ergodic with respect to space translations). In case of tilings, we say that they form a single isomorphism class. In lattice-gas models, these unique measures are called ground states. They are zero-temperature limits of translation-invariant Gibbs states describing an equilibrium behavior of systems of many interacting particles.[12]

It follows from the above construction that the family of uniquely ergodic systems of finite type is contained in the family of uniquely ergodic classical lattice-gas models with translation-invariant, finite-range interactions. There are countably many different bounded patterns of tiles or particles on the lattice and therefore countably many different finite-type conditions and hence countably many uniquely ergodic systems of finite type. The main result of this paper is a construction of an uncountable family of lattice-gas models with finite-range interactions and with unique ground states which are not unique ground states of any nonfrustrated, translation-invariant, finite-range interactions and consequently not uniquely ergodic measures of any system of finite type. These are measures with an irrational density of different types of particles and are supported by nonperiodic ground-state configurations. On the other hand, measures supported by a periodic configuration and its translates are necessarily of finite type.

Ground-state configurations of our models are two-dimensional analogs of one-dimensional, "most homogeneous," nonperiodic configurations present in models with infinite-range, convex, repulsive interactions.[13] Such models exhibit a devil's staircase structure of ground states.[14–16] In

ground-state configurations of our models, particles of certain types occupy lattice sites along vertical and horizontal lines. Distances between these lines follow the rule of the most homogeneous configurations.

In Section 2, we describe systems of finite type and general classical lattice-gas models with unique ground states. In Section 3, we discuss a one-dimensional model with a devil's staircase. Section 4 contains our construction of a classical lattice-gas model with an ultimate frustration. A short discussion follows in Section 5.

2. TILINGS, SYSTEMS OF FINITE TYPE, AND LATTICE-GAS MODELS

We begin by discussing *tilings* with square-like tiles. Our tiles are squares with markings on their sides. These markings define matching rules which tell us which tiles can be nearest neighbors. In every tiling, centers of squares form the square lattice Z^2. Tilings can be therefore represented by assignments of tiles to the sites of Z^2, i.e., by elements of $\Omega = \{1,...,n\}^{Z^2}$, where n is the number of different types of tiles, the so-called prototiles. We are interested in uniquely ergodic tiling systems. In such systems, although there are possibly many tilings, using the same family of prototiles, there are unique translation-invariant probability measures on Ω which are supported by them. If matching rules allow only translates of one periodic tiling, then the unique tiling measure assigns an equal probability to all of these translates. Generally, a unique tiling measure, μ, gives equal weights to all tilings and can be obtained as the limit of averaging over a given tiling X and its translates $\tau_a X$ by lattice vectors $a \in Z^d$: $\mu = \lim_{A \to Z^d}(1/|A|)\sum_{a \in A}\delta(\tau_a X)$, where $\delta(\tau_a X)$ is the probability measure assigning probability 1 to $\tau_a X$. There are examples of tiling systems with unique measures supported by nonperiodic tilings.[17-20]

A natural generalization of tiling systems are systems of finite type. Let G be a translation-invariant, closed subset of Ω and μ a uniquely ergodic, translation-invariant measure supported by G.

(Ω, G, μ) is a *dynamical system of finite type*, if there exist $C_i \in \{1,...,n\}^{A_i}$ for some finite $A_i \subset Z^d$ and $i = 1,...,m$ such that

$$G = \{X: X(\tau_a A_i) \neq C_i \text{ for all } a \in Z^d \text{ and any } i = 1,...,m\}$$

In other words, G is defined by the absence of a finite number of certain local configurations.

In *classical lattice-gas models*, every site of the Z^d lattice, $d \geq 1$, can be occupied by one of n different particles. Configurations of lattice models are assignments of particles to the lattice sites, i.e., elements of $\Omega = \{1,...,n\}^{Z^d}$.

If $X \in \Omega$ and $A \subset \mathbf{Z}^d$, then $X(A) \in \Omega_A = \{1,...,n\}^A$ is a projection of X on A. Particles interact through generally many-body potentials. A *potential* Φ is a family of real-valued functions, Φ_A on Ω_A, for all finite $A \subset \mathbf{Z}^d$. If $\Phi_A = 0$ when $\mathrm{diam}(A) > r$ for a certain $r > 0$, then we say that Φ has a finite range r. We assume that Φ is translation invariant, i.e., $\Phi_{A+a}(\tau_a X) = \Phi_A(X)$, where τ_a is the translation by the lattice vector $a \in \mathbf{Z}^d$ and $\Phi_A(X) \equiv \Phi_A(X(A))$.

For a finite $A \subset \mathbf{Z}^d$, a *Hamiltonian* of particles in A can be written as

$$H_A^\Phi = \sum_{V \subset A} \Phi_V$$

Y is a *local excitation* of X, $Y \sim X$, Y, $X \in \Omega$, if there exists a finite $A \subset \mathbf{Z}^d$, such that $Y = X$ outside A.

The *relative Hamiltonian* is defined as

$$H^\Phi(Y, X) = \sum_{A \subset \mathbf{Z}^d} (\Phi_A(Y) - \Phi_A(X)) \qquad \text{for} \quad Y \sim X$$

Observe, that for finite-range potentials, there are only a finite number of nonzero terms in the above sum.

$X \in \Omega$ is a *ground-state configuration* of a potential Φ if

$$H^\Phi(Y, X) \geqslant 0$$

for every $Y \sim X$, i.e., one cannot lower the energy of a ground-state configuration by its local change (on a finite subset of lattice sites).

The *energy density* $e(X)$ of a configuration X is defined as

$$e(X) = \liminf_{A \to \mathbf{Z}^d} \frac{H_A^\Phi(X)}{|A|}$$

where $A \to \mathbf{Z}^d$ in some certain sense.

One can prove that if X is a ground-state configuration, then X has the minimal energy density, i.e., $e(X) \leqslant e(Y)$ for every $Y \in \Omega$. It means that local conditions contained in the definition of a ground-state configuration force the global minimization of the energy density.

Although, for any given Hamiltonian, the set of ground-state configurations is nonempty, it may not contain any periodic configuration.[21-24]

In our models, there is a unique translation-invariant probability measure on Ω, supported by ground-state configurations. It is then necessarily the zero-temperature limit of equilibrium states (translation-invariant Gibbs states).[12] We call it the *ground state* of a given model.

A potential Φ, for which there exists a configuration minimizing simultaneously all interactions Φ_A, is called nonfrustrated. Such a configuration is of course a ground-state configuration.

Formally, a potential Φ is nonfrustrated or is called an m-potential,[25, 26] if there exists a configuration $X \in \Omega$ such that

$$\Phi_A(X) = \min_Y \Phi_A(Y)$$

for every finite $A \subset \mathbf{Z}^d$.

Theorem 1. There is one-to-one correspondence between dynamical systems of finite type and uniquely ergodic ground states of classical lattice-gas models with nonfrustrated, translation-invariant, finite-range potentials.

Proof. Let (Ω, G, μ) be a dynamical system of finite type defined by the absence of C_i, $i = 1,..., m$. We define a translation-invariant potential Φ such that $\Phi_A(X(A)) = 1$, if A is a translate of A_i for some i and $X(A) = C_i$, and zero otherwise. Φ is obviously nonfrustrated and μ is the unique ground state of Φ.

Conversely, let Φ be a nonfrustrated, translation-invariant, finite-range potential with a unique ground state μ supported by a set G of ground-state configurations. Let $X \in \Omega$ be such that

$$\Phi_A(X) = \min_Y \Phi_A(Y) \qquad \text{for any finite } A$$

G is then defined by the absence of local configurations $X(A)$ such that $\Phi_A(X(A)) \neq \min_Y \Phi_A(Y)$. Hence (Ω, G, μ) is a dynamical system of finite type. $\blacksquare$

The goal of this paper is to construct a classical lattice-gas model with a frustrated, translation-invariant, finite-range potential and with a uniquely ergodic ground state μ which is not a uniquely ergodic measure of any dynamical system of finite type or equivalently not a ground state of any nonfrustrated, translation-invariant, finite-range potential.

3. ONE-DIMENSIONAL DEVIL'S STAIRCASES AND THE MOST HOMOGENEOUS CONFIGURATIONS

One of the examples of a frustrated potential is provided by the following lattice-gas model with infinite-range interactions.[13] Every site of the one-dimensional lattice $\mathbf{Z}$ can be occuppied by one particle or be empty. Particles at a distance n interact through a convex, repulsive potential V_n: $V_n > 0$, $V_{n+1} + V_{n-1} \geqslant 2V_n$ for $n > 1$, and $V_n \to 0$ as $n \to \infty$. For any given density p of particles, one can find the energy density $e(p)$ of ground-state configurations.[13] For any rational p, there is a unique (up

to translations) periodic ground-state configuration with that density of particles. It has the following property. Let $x_i \in \mathbf{Z}$ be a coordinate of the ith particle. Then there exists a sequence of natural numbers d_j such that $x_{i+j} - x_i \in \{d_j, d_j + 1\}$ for every $i \in \mathbf{Z}$ and $j \in \mathbf{N}$. Configurations with such property are called the *most homogeneous configurations*.

Of course, if we do not fix the density, particles want to be as far one from another as possible, so the vacuum is the only ground state. Now we introduce a chemical potential $h > 0$ and pass to the grand-canonical ensemble. Particles are now frustrated—they do not want to be on the lattice because of the interactions between them and at the same time they want to be on the lattice because of the chemical potential. To find the energy density of a ground state we have to minimize

$$f(p) = e(p) - hp \tag{1}$$

Now, $e(p)$ is differentiable at every irrational p and is nondifferentiable at any rational p.[15] However, as a convex function, it has a left derivative $d^- e(p)/dp$ and a right derivative $d^+ e(p)/dp$ at every p. It follows that to have a ground state with an irrational density, p, of particles, one has to fix $h(p) = de(p)/dp$. For any rational p, one has the interval of chemical potentials $h \in [d^- e(p)/dp, d^+ e(p)/dp]$. One can show that the sum of lengths of these intervals has the length of the interval of all considered values of chemical potentials. We have obtained a *complete devil's staircase*.[14, 15]

As we have already mentioned, for any rational p, there is a unique (up to translations) periodic ground-state configuration with that density of particles—there is a unique ground-state measure. For any irrational p, there are uncountably many ground-state configurations which are the most homogeneous configurations. Now we will show that there is still the unique ground-state measure supported by them.

Proposition 1. For any $0 \leqslant p \leqslant 1$, there exists a unique sequence d_n such that the corresponding most homogeneous configurations have p as their density of particles.

Proof. Let $p^n(d_n)$ be the density of pairs of particles which are the nth neighbors at a distance d_n in the most homogeneous configurations. The following system of equations have unique solutions for d_n and $0 \leqslant p^n(d_n)$, $p^n(d_n + 1) \leqslant 1$, for any $n \geqslant 1$:

$$p^n(d_n) + p^n(d_n + 1) = p \tag{2}$$

$$d_n p^n(d_n) + (d_n + 1) p^n(d_n + 1) = n \tag{3}$$

Theorem 2. For any $0 \leqslant \rho \leqslant 1$, there is a unique translation-invariant probability measure (the ground state of the corresponding Hamiltonian) supported by the most homogeneous configurations such that ρ is their density of particles.

Proof by the Induction. Assume that there two such measures, μ_1 and μ_2. Denote by $\mu_1(d_1)$ the density, in μ_1, of pairs of two successive particles at a distance d_1, by $\mu_1(d_1, d_1 + 1)$ the density of triples of three successive particles with successive distances d_1 and $d_1 + 1$, and generally, by $\mu_1(P_n)$ with $P_n = (p_1,..., p_n)$, $p_i \in \{d_1, d_1 + 1\}$, $i = 1,..., n$, the density of $(n + 1)$th tuples of $n + 1$ successive particles with p_i as successive distances between them. Analogously, we introduce densities for μ_2. We will show that $\mu_1(P_n) = \mu_2(P_n)$ for every P_n and every $n \geqslant 1$. We will use the induction on n.

The above equality for $n = 1$ follows from the fact that both μ_1 and μ_2 have the same density of particles.

Let $n = 2$. If $P_2 = (d_1, d_1)$, then let $P'_2 = (d_1, d_1 + 1)$. Then

$$\mu_i(P'_2) = \mu_i(d_1 + 1), \qquad i = 1, 2 \tag{4}$$

and therefore

$$\mu_1(P'_2) = \mu_2(P'_2) \tag{5}$$

We have

$$\mu_1(P_2) + \mu_1(P'_2) = \mu_2(P_2) + \mu_2(P'_2) \tag{6}$$

and therefore

$$\mu_1(P_2) = \mu_2(P_2) \tag{7}$$

All three remaining types of P_2 can be treated in an analogous way.

Now assume the equality for any P_k with fixed $k \geqslant 2$. If P_{k+1} is of the form (d_1, P_{k-1}, d_1) for some P_{k-1} and $P'_{k+1} = (d_1 + 1, P_{k-1}, d_1)$, then

$$\mu_1(P'_{k+1}) = \mu_1(d_1 + 1, P_{k-1}) \tag{8}$$

$$\mu_2(P'_{k+1}) = \mu_2(d_1 + 1, P_{k-1}) \tag{9}$$

By the induction assumption the right-hand sides of (8) and (9) are equal and hence the left-hand sides of (8) and (9) are equal. Now again by the induction assumption we have

$$\mu_1(P_{k-1}, d_1) = \mu_2(P_{k-1}, d_1) \tag{10}$$

and hence

$$\mu_1(P_{k+1}) + \mu_1(P'_{k+1}) = \mu_2(P_{k+1}) + \mu_2(P'_{k+1}) \tag{11}$$

It follows that

$$\mu_1(P_{k+1}) = \mu_2(P_{k+1}) \tag{12}$$

All three remaining types of P_{k+1} can be treated in an analogous way. ∎

To summarize, for every chemical potential, there is a unique ground state of the corresponding Hamiltonian. Therefore, there are uncountably many Hamiltonians with uniquely ergodic ground states.

One of the goals of this paper is to investigate if one can obtain similar results in two-dimensional models with strictly finite-range interactions. Let us mention at this point, that for any finite-range interaction in one dimension, there exists at least one periodic ground-state configuration.[27, 28] Hence a devil's staircase cannot appear in one-dimensional classical lattice gas models with finite-range, translation-invariant interactions.

4. A MODEL WITH AN ULTIMATE FRUSTRATION

Let us first describe particles of our model. They correspond to square tiles with diagonal, horizontal, and vertical markings. There is a tile without any markings and there are tiles with one or two diagonal markings as shown in Fig. 1. A tile with the horizontal, vertical, and two diagonal markings is called a cross and is shown in Fig. 2. All other tiles are called arms and are shown in Fig. 3.

Our first finite-type condition is a nearest-neighbor or a next-nearest-neighbor matching rule which says that a line of markings cannot end. This is translated into a nearest-neighbor or a next-nearest-neighbor interaction between two particles in the standard way. Two nearest-neighbor or next-nearest-neighbor particles which do not match as tiles have a positive interaction energy, $J_2 > 0$; otherwise the energy is equal to zero.

Our second finite-type condition allows only certain patterns of five vertically or horizontally successive tiles. Namely, among five vertically successive tiles there must be at least one arm with the horizontal marking or a cross and there cannot be two such tiles at a distance smaller than four. Analogously, among five horizontally successive tiles there must be at least one arm with the vertical marking or a cross and there cannot be two such tiles at a distance smaller than four. Again, this is translated into a five-body interaction by simply assigning a positive energy, $J_5 > 0$, to all forbidden patterns; allowed five-particle patterns have zero energy.

Finally, we have a three-site condition which forces every arm with diagonal markings to have a cross as one of its nearest neighbors. A respective coupling constant is denoted by $J_3 > 0$.

A *broken bond* is a local configuration of particles which does not satisfy a finite-site condition.

Now we will construct ground-state configurations of a lattice-gas model with the above finite-range, translation-invariant interactions. Looking just at horizontal and vertical markings we see an infinite grid of infinite horizontal and vertical lines such that nearest-neighbor parallel lines are at a distance four or five. These are the only configurations of particles corresponding to tilings which satisfy the two-site and five-site conditions described above. Now we will show that the three-site condition forces distances between lines to follow the rule (discussed in Ch. 3) of the most homogeneous configurations of particles on the one-dimensional lattice **Z**.[13]

Proposition 2.   Let X be a configuration which satisfies the two-site and five-site conditions. Let x_i be a double-sided sequence of x coordinates of vertical lines and y_j be a double-sided sequence of y coordinates of horizontal lines in X. Then X satisfies the three-site condition (and therefore it is a ground-state configuration) if and only if there is a sequence of natural numbers d_n such that for every $n \geqslant 1$ either

$$x_{i+n} - x_i, \ y_{j+n} - y_j \in \{d_n, d_n + 1\} \tag{13}$$

or

$$x_{i+n} - x_i = d_n, \ y_{j+n} - y_j \in \{d_n - 1, d_n, d_n + 1\} \tag{14}$$

or

$$x_{i+n} - x_i \in \{d_n - 1, d_n, d_n + 1\}, \ y_{j+n} - y_j = d_n \tag{15}$$

for every i and j.

Proof by the Induction.   The five-site condition forces (13) to be satisfied with $d_1 = 4$. Now let us consider lines which are next-nearest neighbors. Let us assume, without loss of generality, that $x_{i+2} - x_i = 10$ and $y_{j+2} - y_j = 8$. A diagonal line passing through a lattice site (x_i, y_j) intersects a horizontal line at a lattice site (x_{i+8}, y_{j+8}) which violates the three-site condition. Conversely, if condition (13) is satisfied with $d_2 = 8$ or $d_2 = 9$, or (14) or (15) with $d = 9$, then any diagonal line passing through a lattice site (x_i, y_j) intersects nearest and next-nearest horizontal and vertical lines at a distance at most one from a cross.

We will proceed now with the second step of the induction. The following statement is assumed to be true: a diagonal line passing through a lattice site (x_i, y_j) intersects k nearest horizontal and vertical lines at a distance at most one from a cross, if and only if, for every $n = 1, ..., k$, (13) or (14) or (15) is satisfied for every i and j. Now we have to show that this statement is true for $k + 1$. Let us assume, without loss of generality, that $x_{i+k} - x_i = d_k + 1$ and $y_{j+k} - y_j = d_k$. If $x_{i+k+1} - x_{i+k} = 5$ and $y_{j+k+1} - y_{j+k} = 4$, so none of the above conditions are satisfied, then the diagonal line intersects a vertical line at a lattice site $(x_{i+k+1}, y_{j+k+1} + 2)$ and a horizontal line at a lattice site $(x_{i+k+1} - 2, y_{j+k+1})$, so the three-site condition is violated. In all three remaining cases, (13) or (14) or (15) is satisfied and intersections are at a distance at most one from a cross. ∎

Observe, that if at least for one n, (14) or (15) is satisfied for every i and j, then X is periodic, with a period d_n in x or y direction respectively. The density of arms is therefore rational; in fact it is equal to $2n/d_n$. Let us note that our model has ground-state configurations with all possible densities of horizontal and vertical markings (counted together) satisfying following inequalities: $2/5 \leqslant \rho_m \leqslant 1/2$. Therefore, it has uncountably many different ground-state measures. On the other hand, if one fixes the irrational density of horizontal and vertical markings, then our model has a unique ground-state measure which we denote by μ_{ρ_m}. For any rational ρ_m, we have many ground-state measures. In both cases we have that the density of crosses, $\rho_{cr} = (\rho_m/2)^2$. Now we introduce chemical potentials, $h_{cr} < 0$ for crosses and $h_a > 0$ for arms. For fixed ρ_m, the energy density of any configuration satisfying all finite-site conditions is given by a convex function

$$f(\rho_m) = -(h_{cr} - 2h_a)(\rho_m/2)^2 - h_a \rho_m \tag{16}$$

Minimization of f with respect to ρ_m gives us

$$\rho_m = \frac{2h_a}{2h_a - h_{cr}} \tag{17}$$

Now we will show that when the density of horizontal and vertical markings, ρ_m, is fixed, then μ_{ρ_m} is the only ground state of the Hamiltonian including all finite-site conditions and chemical potentials, and its energy density is given by (16) and (17).

Proposition 3. If J_5 is sufficiently big, then the density of broken five-site bonds is equal to zero in any ground state.

Proof. If among five vertically (horizontally) successive particles in a configuration X there are not any particles with the horizontal (vertical) marking or there are particles with the horizontal (vertical) marking at a distance smaller than four, then we either put there a particle with the horizontal (vertical) marking or remove a particle with the horizontal (vertical) marking. In may happen that we have to put or remove nearby some particles with the horizontal (vertical) marking, in order not to create other broken five-site bonds. During this process we may create some broken two-site or three-site bonds. However, if J_5 is sufficiently big, the above procedure decreases the energy and therefore the configuration X is not a ground-state configuration. ∎

Now we will show that also the density of broken two-site and three-site bonds is zero in any ground state with a fixed p_m. Let p be a density of broken bonds in a probability measure μ which has zero density of broken five-site bonds. Let $n = 2^m$ be such that $1/n^2 < p$. Let $S = \{ \mathbf{a} \in \mathbf{Z}^2 : 0 \leqslant a_1, a_2 < n \}$. We call $\tau_{\mathbf{b}} S$, $\mathbf{b} \in \mathbf{Z}^2$, an *r-square* of a configuration X in the support of μ, if the number of vertical markings, n_v, and the number of horizontal markings, n_h, satisfy the following inequalities:

$$(r - 1)n < |n_v - n_h| \leqslant rn \tag{18}$$

for a natural number $r > 1$ and

$$0 \leqslant |n_v - n_h| \leqslant n \tag{19}$$

for $r = 1$.

Proposition 4. If S is an *r*-square of X, $r > 1$, then the number of broken bonds, B, in $X(S)$ is bigger than $r^2/9$.

Proof. If $r = 2$, then it follows from Proposition 2 that there is a broken bond in $X(S)$. If $r > 2$, then we divide S into four squares of the size $n/2$. If a smaller square is a 2-square (with $n/2$ in (18)), then there is a broken bond in it. We call such a square a *good* square. If a smaller square is a 1-square (with $n/2$ in (19)), then we call it a *bad* square. Every *r*-square with $r > 2$ we divide again into four squares. We continue this procedure untill all squares are either good or bad squares. Let $D = \sum_i (r_i/2^{k_i})$, where the summation is with respect to all good and bad squares; $r_i = 2$ for every good square, $r_i = 1$ for every bad one and k_i is the number of divisions to get a given square. We have that $D \geqslant r$. Let G be the number of good squares. Proposition 2 tells us that $B \geqslant G$. Now we have to prove that $G > D^2/9$.

The above division procedure can be represented by a hierarchical directed tree with vertices corresponding to squares and edges joining a square with its four subsquares. Good and bad squares are final vertices of such tree. Among four final squares connected to a common square, there must be at least one good square. Let us notice that when we enlarge a tree by connecting a good square to three bad squares and one good square, we increase D and leave G unchanged. Therefore, to prove the above bound, it is sufficient to consider such trees that all good squares are of the same size and no square is connected to more than one good square. Let k be the smallest number such that all squares of size $n/2^k$ which are not final ones, are connected to three bad squares and one good square. We may also assume that there are no bad squares of sizes bigger than $n/2^k$. Otherwise, we could take a part of a tree connected to a square of size $n/2^k$ (changing this square to a bad one) and connect it to a bad square of size $n/2^{k'}$ with $k' < k$, increasing in this way D and not changing G. Let us assume now that there are s bad squares of size $n/2^k$; $0 \leqslant s < 3 \times 4^{k-1}$. For such a tree

$$G = 4^k - s \tag{20}$$

$$D < s/2^k + 3(4^k - s)/2^k \tag{21}$$

It follows from (20) and (21) that

$$G > D^2/9 \tag{22}$$

hence the induction step is finished.

The equality in (22) is attained in the infinite tree with $k = s = 0$. ∎

Theorem 3. For a fixed density of horizontal and vertical markings, ρ_m, for the Hamiltonian specified by chemical potentials h_{cr} and h_a and all finite-type conditions described above, μ_{ρ_m} is the only ground state.

Proof. If the density of horizontal markings, ρ_{hm}, is equal to the density of vertical markings, ρ_{vm}, then in the absence of broken horizontal and vertical lines (broken two-site, nearest-neighbor bonds), $\rho_{cr} = (\rho_m/2)^2$. We may decrease the density of crosses but for every removed cross we have to create a broken horizontal or vertical line and this increases the energy if J_2 is sufficiently big. It shows that in the case of $\rho_{hm} = \rho_{vm}$, μ_{ρ_m} is the only ground state. Let us suppose now that $\rho_{hm} \neq \rho_{vm}$, $\rho_{hm} = \rho_m/2 - \alpha$ and $\rho_{vm} = \rho_m/2 + \alpha$, $\alpha > 0$. Again, let us assume first that there are no broken horizontal and vertical lines. Then

$$\rho_{cr} = (\rho_m/2)^2 - \alpha^2 \tag{23}$$

Denote by ρ_r the density of r-squares and by ρ the density of broken bonds in a configuration X. We have

$$\alpha = (\rho_{vm} - \rho_{hm})/2 \leqslant \frac{1}{2n^2} \sum_r \rho_r rn \qquad (24)$$

and by the Jensen's inequality we obtain

$$\alpha^2 \leqslant \sum_r \rho_r \frac{r^2}{4n^2} \qquad (25)$$

Hence, at most we may decrease the density of crosses by the amount on the right-hand side of (25), so if $J_2, J_3 > (10/4) |h_{cr}|$, then $\rho = 0$, if X is a ground-state configuration. We had to put 10 instead of 9 in the bound in order to deal with 1-squares by using $1/n^2 < \rho$. Of course, we may decrease farther the density of crosses, but as before, for every removed cross we have to create a broken line. ∎

To summarize, for a fixed chemical potential h_a, for every irrational density of horizontal and vertical markings, $2/5 \leqslant \rho_m \leqslant 1/2$, it follows from (16) and (17) that there exists a chemical potential h_{cr} given by

$$h_{cr} = 2h_a(1 - 1/\rho_m) \qquad (26)$$

such that the corresponding Hamiltonian has a unique ground state, μ_{ρ_m}, with ρ_m as the density of horizontal and vertical markings. Therefore, there are uncountably many uniquely ergodic ground states on a phase diagram of our model.

5. CONCLUSIONS

Two potentials are called *equivalent* if they have the same relative Hamiltonians and therefore the same ground states and Gibbs states.

In ref. 29, we constructed a model with a frustrated, translation-invariant, nearest-neighbor potential for which there does not exist an equivalent, nonfrustrated, translation-invariant, finite-range potential. An important feature of that model is the absence of periodic ground-state configurations. However, there is a unique translation-invariant probability measure—ground state—supported by nonperiodic ground-state configurations. It was a first deterministic lattice-gas model in which a global minimum of energy is not a sum of local (in space) minima. To be more precise, one cannot minimize the energy of interacting particles by minimizing their energy in a finite volume and all its translates, no matter how big is the

volume. In fact, if you take a finite box of any size and find a configuration of particles in this box which minimizes the energy of their interactions, then such a configuration, called a local ground-state configuration, cannot be a part of an infinite-lattice ground-state configuration (compare also ref. 30).

Here we constructed models with unique nonperiodic ground states which are not unique ground states of any nonfrustrated potential, equivalent or not. This extends substantially the result of ref. 29. The unique ground state of the model discussed in ref. 29 is the unique ground state of some nonfrustrated, translation-invariant, finite-range potential. Here we have shown that the class of structures which are ground states of finite-range potentials is larger that the family of ground states of nonfrustrated, finite-range potentials. It means that our nonperiodic ground-state configurations are represented by tilings without any local matching rules.

Such situation was investigated in microscopic models of quasicrystals. Gähler and Jeong[31] studied octagonal Amman–Beenker tilings which do not allow for perfect matching rules. They assigned negative energies to certain clusters of tiles and provided some numerical evidence that ground-state configurations of such interactions form a single isomorphism class consisted of octagonal Amman–Beenker tilings.

To summarize, we have constructed a family of lattice-gas models with frustrated, translation-invariant, finite-range interactions and with unique ground states which are not unique ground states of any nonfrustrated, translation-invariant, finite-range interaction.

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