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Devil's staircase for nonconvex interactions

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Abstract. – We study rigorously ground-state orderings of particles in one-dimensional classical lattice gases with nonconvex interactions. Such systems serve as models of adsorption on crystal surfaces. In the considered models, the energy of adsorbed particles is a sum of two components, each one representing the energy of a one-dimensional lattice gas with two-body interactions in one of the two orthogonal lattice directions. This feature reduces two-dimensional problems to one-dimensional ones. The interaction energy in each direction is assumed here to be repulsive and strictly convex only from distance 2 on, while its value at distance 1 can be positive or negative, but close to zero. We show that if the decay rate of the interactions is fast enough, then particles form 2-particle lattice-connected aggregates (dimers) which are distributed in the same most homogeneous way as particles whose interaction is strictly convex everywhere. Moreover, despite the lack of convexity, the density of particles *vs.* the chemical potential appears to be a fractal curve known as the complete devil's staircase.

Lattice systems (or lattice gases), where the space available to particles is discretized and only configurational potential energy is taken into account, are typically used as a testing ground for many ideas developed in statistical mechanics. But they are also capable of describing real physical systems encountered in experiments. On the one hand, they serve with success as models of some generic properties of the three basic states of matter: gaseous, liquid and solid. On the other hand, they can be used for describing some specific properties of magnets, alloys etc.

However, it seems that nowadays the domain of physics, where the lattice gases are most vigorously studied, is surface science and in particular the physics of adsorbed layers [1]. One of the important problems of the physics of adsorbed layers is to study orderings of atoms (adatoms) adsorbed on crystal surfaces. This phenomenon can be modelled by certain classical lattice gases [1–5]. Adatoms are assumed to sit on top of substrate atoms of the square lattice [2,3]. Substrate deformation causes effective, long-range interactions between adatoms. In many cases of interest, the Hamiltonian of such system can be decomposed into two parts, one involving two-body interactions between particles located along the *x*-direction and the other one along the perpendicular *y*-direction of the square lattice. Such one-dimensional

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interactions constitute sometimes certain local perturbations of repulsive and strictly convex interactions. Knowing one-dimensional ground-state configurations, we can easily construct two-dimensional ground-state configurations of the original model, as observed in [2] and discussed in the end of our paper. Therefore, in what follows we deal exclusively with one-dimensional systems.

The first step towards understanding the effects of interactions between particles of considered systems amounts to determining their ground-state configurations. Provided the underlying interactions are short-range, numerous methods of searching for ground-state configurations are available [6, 7]. However, if the interactions are long-range ones, the situation is drastically different. Rigorous results are, to the best of our knowledge, limited to a one-dimensional lattice-gas model with strictly convex repulsive two-body interactions (results of Hubbard [8] and Pokrovsky and Uimin [9]).

In classical lattice-gas models, considered in the sequel, every site of a one-dimensional lattice \mathbf{Z} can be occupied by one particle or be empty. Then, a (infinite-lattice) configuration is an assignment of particles to lattice sites. We assume that particles interact only through two-body forces and to a pair of particles at lattice sites i and j , whose distance is $r = |i - j|$, we assign the translation-invariant *interaction energy* $V(r)$. The Hamiltonian of our system in a bounded region Λ can then be written in the following form:

$$H_{\Lambda}(X) = \sum_{\{\{i,j\}:\{i,j\} \cap \Lambda \neq \emptyset\}} V(|i - j|) s_i(X) s_j(X), \quad (1)$$

where $s_i(X)$ assumes value 1 if in the configuration X the site i is occupied by a particle and otherwise value 0.

By *ground-state configurations* we mean infinite-lattice configurations such that no local change of the assignment of particles to lattice sites can decrease the energy. It follows that they have the minimum energy density. In the following we will consider only ground-state configurations with uniformly defined densities of all local particle configurations. Moreover, if a local particle configuration occurs, then it occurs with a positive density. That is to say, we do not consider ground-state configurations with interfaces (like kink ground-state configurations in the Ising model).

If we assume that $V(r)$ is positive for every $r \geq 1$ and strictly convex, that is $V(r) + V(r + 2) > 2V(r + 1)$, then we obtain a model used by Hubbard to study orderings of electrons in quasi-one-dimensional conductors [8, 10] and by Pokrovsky and Uimin to study orderings of monolayers of atoms adsorbed on crystal surfaces [9]. For any given particle density ρ , Hubbard found the energy density $e(\rho)$ of ground-state configurations. He also showed that any ground-state configuration has the following remarkable property. Let $x_i \in \mathbf{Z}$ be a coordinate of the i -th 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 $j \in \mathbf{N}$, *i.e.*, the distances between the first (second, etc.) nearest neighbors can differ by at most one lattice constant. Configurations with such property are known as the *generalized Wigner lattices* [8] or the *most homogeneous configurations* [11].

The ground-state phase diagram in the grand-canonical ensemble has been calculated heuristically by Bak and Bruinsma [12], while a proof for the related Frenkel-Kontorova model has been provided by Aubry [13] and adapted to the lattice-gas model case by Miękisz and Radin [14]; it is outlined below.

In the grand-canonical ensemble, with the fixed chemical potential μ , to find the energy density of a ground state we have to minimize

$$f(\rho) = e(\rho) - \mu\rho. \quad (2)$$

Now, $e(\rho)$ is differentiable at every irrational ρ and is nondifferentiable at any rational ρ [13, 14]. However, as a convex function, it has a left derivative $d^-e(\rho)/d\rho$ and a right derivative $d^+e(\rho)/d\rho$ at every ρ . It follows that to have a ground state with an irrational density ρ of particles, one has to fix $\mu(\rho) = de(\rho)/d\rho$. For any rational ρ , there is a closed interval of chemical potentials $[d^-e(\rho)/d\rho, d^+e(\rho)/d\rho]$, where the most homogeneous configurations of density ρ are the ground-state configurations. One can show that the sum of lengths of these intervals amounts to the length of the interval beginning at the end of the half-line, where the vacuum is the only ground-state configuration, and ending at the beginning of the half-line, where the completely filled configuration is the only ground-state configuration. The particle density *vs.* the chemical potential of particles, $\rho(\mu)$, is constant on each of the above-described intervals. Moreover, it is a continuous function on the real line. The curve $\rho(\mu)$ is classified as a fractal one and named the *complete devil's staircase*, a term introduced first for incommensurate structures by Aubry [15]; see also [13, 16, 17].

For any rational ρ , there is a unique (up to translations) periodic ground-state configuration with that density of particles. For any irrational ρ , there are uncountably many ground-state configurations which are the most homogeneous configurations. It has been shown in [18] that they all belong to one local isomorphism class. It means that they cannot be locally distinguished from one another. Every local pattern of particles present in one ground-state configuration appears in any other within a bounded distance, in other words (more formally), there exists a unique ground-state measure supported by them.

However, it appears that in the models of adsorption [2, 3], $V(1)$ is very small (positive, negative or zero) as compared with $V(2)$, violating therefore the convexity property of interactions. It may seem that the smallness of $V(1)$ together with the repelling nature of remaining interactions will force particles to form 2-particle lattice-connected aggregates, called 2-molecules, allowing the remaining particles to be farther apart. Then, because the interaction between 2-molecules is strictly convex, we would obtain a molecular devil's staircase. However, as the following example shows, one cannot hope to obtain such a universal result, independent of the details of interactions, as in the case of strictly convex interactions.

Example 1. – Consider the potential $V(r)$ which in some units is given by $V(1) = 0$, $V(2) = 4$, $V(3) = 2$, $V(4) = 1$, and $V(r) = 0$ for $r \geq 5$. Clearly $V(r)$ is convex on the half-line $r \geq 2$. Consider also two periodic configurations (period 17) of particle density $\rho = 8/17$ whose elementary cells are of the form: $[\bullet \circ \circ \circ \circ \bullet \bullet \circ \circ \circ \bullet \bullet \circ \circ \circ]_1$ and $[\bullet \circ \bullet \circ \bullet \circ \circ \bullet \circ \circ \bullet \circ \circ \circ]_2$, where \bullet stands for a particle while \circ for an empty site. The energy per elementary cell in the first case is $2V(2) + 3V(4) = 11$ while in the second case it is $3V(3) + 7V(4) = 13$. Thus the configuration $[\cdot]_2$ that consists exclusively of 2-molecules loses against the configuration $[\cdot]_1$ that consists of 2-molecules and 3-molecules. This remains true if we do not set $V(r) = 0$ for $r \geq 5$, but require that $V(r)$ be positive and strictly convex from $r = 2$ on and sufficiently fast decaying from $r = 5$ on.

Now, in order to get rid of n -molecules, $n \geq 3$, we restrict the family of considered potentials, demanding that $V(2)$ be relatively strong with respect to all other $V(r)$'s. We have arrived at the following result:

There are no n -molecules with $n \geq 3$ in any ground-state configuration in a lattice gas (1) with an interaction energy V such that $V(1) > -2V(2)$ and $V(2) \geq (7W + V(1))/2$, where $W = \sum_{r=3}^{\infty} V(r)$.

The idea of the proof is to start with an arbitrary configuration containing n -molecules, removing $n - 2$ particles from every n -molecule, rearranging the resulting configuration and then putting back the removed particles in the form of 2-molecules. One can show that if the above conditions are satisfied, then the gain in energy caused by removing particles is strictly

larger than its loss associated with inserting back the particles.

The following example shows that configurations containing isolated particles, called atoms, are unlikely to be the ground-state ones.

Example 2. – Consider the following periodic (period 13) configuration: $[\bullet \circ \circ \bullet \bullet \circ \circ \bullet \circ \circ \bullet \circ \circ]_3$. The elementary cell $[\cdot]_3$ contains a local configuration of two atoms separated by a 2-molecule. Let us transform this local configuration into another one, consisting of two 2-molecules only, by moving to each other the left atom and the right particle of the 2-molecule and the right atom and the right particle of the 2-molecule. The resulting elementary cell reads: $[\circ \bullet \bullet \circ \circ \bullet \bullet \circ \circ \circ \bullet \bullet \circ]_4$. One can easily calculate the relative energy change of the local configurations considered above; for a potential described in Example 1 it is negative, showing that the original periodic configuration is not a ground-state one.

We have generalized the above procedure to any local configuration containing two atoms separated by $k = 0, 1, \dots, 2$ -molecules. Particles from neighboring pairs are moved to each other and $k + 1$ 2-molecules are created. Then, it appears that the internal energy of all considered particles strictly decreases and the change is bounded from above by the interaction energy between two atoms taken with the minus sign, while the interaction energy of considered particles with all the rest does not increase. In this way we proved the following statement:

Consider a lattice gas (1) with an interaction energy V such that $V(1) \leq 0$. Among configurations that do not contain n -molecules with $n \geq 3$, the lowest-energy configurations consist exclusively of 2-molecules.

The actual proofs of the two results, discussed above, are fairly technical and for this reason they are included in a separate paper [19].

Combining the above two results we obtain that the ground-state configurations of our model contain only 2-molecules. It is easy to see that the effective interaction between these molecules is strictly convex —it is a sum of strictly convex interactions between particles of the molecules. The latter observation enables us to formulate a theorem that constitutes our main result.

Theorem (2-molecule most homogeneous ground-state configurations). – Consider a lattice gas (1) with a nonconvex interaction energy V and a particle density $\rho \leq 1/2$. If $V(r)$ is strictly convex and positive for $r \geq 2$, $-V(2) < V(1) \leq 0$ and $V(2) \geq (7W + V(1))/2$, then the ground-state configurations (without interfaces) are the 2-molecule most homogeneous configurations of particle density ρ .

Corollary (Molecular devil's staircase). – In a lattice gas (1) whose interaction energy V satisfies the conditions given in the theorem, the particle density *vs.* the chemical potential of particles, $\rho(\mu)$, exhibits the complete devil's-staircase structure.

To summarize, we have proven rigorously the existence of the molecular complete devil's staircase in one-dimensional lattice-gas models with certain nonconvex long-range interactions.

As explained at the very beginning, our main result, concerned with one-dimensional lattice gases, applies directly to a class of two-dimensional lattice gases modelling the adsorption of adatoms on crystal surfaces. Such models have been investigated numerically by Ishimura and Yamamoto [2]. In particular, they posed the question about the possibility of the presence of a devil's staircase in such models. Due to the symmetry of the considered Hamiltonians (1), with respect to space rotations by $\pi/2$, the two-dimensional ground-state adatom configurations are given by the oblique arrangements of one-dimensional ground-state configurations determined above. Namely, the adatom configurations at lattice lines in the x -direction can be chosen as the one-dimensional ground-state configurations, with the condition that, going in the positive

y -direction, the configuration of the next lattice line is shifted by one lattice constant in the positive x -direction. Now, knowing the solution of the ground-state problem, it would be very interesting to investigate the low-temperature stability of such structures.

There is also a numerical evidence [20, 21] that certain nonconvex interactions appear, as effective two-body interactions, in the one-dimensional spinless Falicov-Kimball model [22, 23]; it is known that this quantum model can be transformed into a classical lattice-gas model with fairly complicated long-range and many-body interactions [24, 25].

Another class of systems, where our ground-state results are immediately applicable, consists of three-dimensional layered systems, like those studied by Fisher and collaborators [26]. As in the two-dimensional case, it is highly desirable to study the stability of ground-state orderings against thermal fluctuations.

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