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Ground States of Lattice Gases with "Almost" Convex Repulsive Interactions

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To the best of our knowledge there is only one example of a lattice system with long-range two-body interactions whose ground states have been determined exactly: the one-dimensional lattice gas with purely repulsive and strictly convex interactions. Its ground-state particle configurations do not depend on any other details of the interactions and are known as the generalized Wigner lattices or the most homogeneous particle configurations. The question of the stability of this beautiful and universal result against certain perturbations of the repulsive and convex interactions is interesting in itself. Additional motivations for studying such perturbations come from surface physics (adsorption on crystal surfaces) and theories of correlated fermion systems (recent results on ground-state particle configurations of the one-dimensional spinless Falicov–Kimball model). As a first step, we studied a one-dimensional lattice gas whose two-body interactions are 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 showed that such a modification makes the ground-state particle configurations sensitive to the tail of the interactions; if the sum of the strengths of the interactions from the distance 3 on is small with respect to the strength of the interaction at distance 2, then particles form two-particle lattice-connected aggregates that are distributed in the most homogeneous way. Consequently, despite breaking of the convexity property, the ground state exhibits the feature known as the complete devil's staircase.

KEY WORDS: Classical lattice-gas models; ground states; nonconvex interactions; most homogeneous configurations; devil's staircase.

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1. INTRODUCTION

The class of most thoroughly investigated models of present day equilibrium statistical mechanics consists almost exclusively of lattice gases with translation-invariant short-range interactions. On the top of this class there is certainly the lattice gas known as the two-dimensional Ising model. The first step in a study of low-temperature properties of such systems amounts usually to determining their ground states.(1) Provided that the underlying interactions are short-range, numerous methods of searching for ground-state configurations are available. In the case of one-dimensional lattice systems, there is even an algorithmic method.(2, 3) In higher dimensions, let us mention the powerful method of *m*-potential which is successful in many cases of interest.(1)

However, if the translation-invariant interactions are long-range ones, the situation is drastically different. Rigorous results are scarce. To the best of our knowledge there exist only two kinds of interactions for which rigorous results have been obtained: (1) a version of one-dimensional Frenkel–Kontorova model (results of Aubry(4)) and (2) a one-dimensional lattice-gas model with strictly convex repulsive two-body interactions (results of Hubbard(5) and Pokrovsky and Uimin(6)). The continuous systems with more intricate classes of two-body interactions which include the Lennard-Jones type interactions, have been studied first by Ventevogel;(7) an overview of the results by Ventevogel and other authors together with corresponding references can be found in a review paper by Radin.(8)

We would like to point out here that studying these one-dimensional systems involves important scientific issues, well supported by the physics of quasi-one-dimensional materials,(9) highly anisotropic layered systems,(10) and adsorption of molecules on crystal surfaces.(11–14)

The lattice-gas models with purely repulsive and strictly convex two-body interactions emerged from considerations of orderings of electrons in quasi-one-dimensional conductors by Hubbard(5, 9) and orderings of monolayers of atoms adsorbed on solids by Pokrovsky and Uimin.(6) The model still appears to be a cameo in this field. The periodic groundstate particle configurations of this model have been characterized exactly in refs. 5 and 6. Particles are distributed as far as possible from each other, respecting restrictions imposed on their locations by the underlying lattice. These configurations, called by Hubbard the *generalized Wigner lattices*,(5) are independent of any further details of the interaction potential. Moreover, the ground-state exhibits an interesting feature known as the complete devil's staircase.(15, 4)

In view of such an impressing universality of the result obtained independently by Hubbard and by Pokrovsky and Uimin, the question of the stability of this result against some perturbations of the interactions seems natural and interesting from the point of view of statistical mechanics.

Moreover, the interest in this question is supported by other domains of physics. In surface physics a remarkable activity consists in studying, both experimentally and theoretically, orderings of molecules adsorbed on crystal surfaces.(16) The phenomenon can be modelled by means of one-dimensional lattice gases(11–14) with specific two-body interactions, which sometimes constitute certain local perturbations of strictly convex repulsive interactions.(11, 12) One of the often asked questions in this context is whether a non-convex interaction can have a ground-state with the complete devil's staircase property. Let us also mention here some other models, where effects of nonconvexity for the occurrence of modulated order in condensed matter was studied: Frenkel–Kontorova models(17, 18) and one-dimensional Holstein model.(19)

Another motivation for studying effects of modifications of repulsive and strictly convex two-body interactions stems from the recent results concerning ground states of a version of the Falicov–Kimball model(20)—the one-dimensional spinless Falicov–Kimball model. The model can be thought of as a model of quantum itinerant electrons and classical localized particles called f-electrons, nuclei or ions,(21, 22) with only on-site interactions whose strength is the unique parameter of the model—a sort of the Ising model in the field of correlated fermion systems. Such a system can be transformed into a classical lattice-gas model with fairly complicated long-range and many-body interactions.(22) Many years after the discovery of the generalized Wigner lattices, Lemberger(23) found the periodic ground-state configurations of the localized particles in the large-coupling one-dimensional spinless Falicov–Kimball model. He named them the *most homogeneous configurations* because of the special role they play in his ingenious procedure of differentiation and integration of particle configurations. It turns out that the configurations found by Lemberger are just the generalized Wigner lattices. Despite the complicated nature of the effective interaction between electrons and ions, for some details see ref. 24, there is a numerical evidence(25, 26) (based on the approximate method of restricted phase diagrams) that in the strong-coupling regime it can be approximated by a repulsive and strictly convex two-body potential that has the same set of periodic ground-state configurations. Further studies of the ground-state phase diagram of the one-dimensional spinless Falicov–Kimball model, carried out in refs. 25 and 26, revealed for medium and small couplings a number of new families of good candidates for ground-state configurations. Among them are the so-called *n-molecule most homogeneous* configurations, found for the first time and studied it detail in ref. 25. Roughly speaking, they are obtained from the most homogeneous configurations by replacing single particles by lattice-connected aggregates of $n = 2, 3,...$ particles. The arguments in favor of the existence of n-molecule most homogeneous configurations, provided in ref. 25, are based not only on the approximate method of restricted phase diagrams but also on the study of the interaction energy between a few ions only. It has been found that for large values of the unique parameter, for which the most homogeneous configurations are the ground-state configurations, the interaction energy between a few, say two or three, ions is strictly convex. On the other hand, for those values of the unique parameter for which the n-molecule most homogeneous configurations are the ground-state configurations, the interaction energy between two or three ions gets considerably lowered at short distances (which apparently encourages forming n-molecules) and consequently it becomes non-convex at short distances. These results led us naturally to the question whether it is possible to obtain the n-molecule most homogeneous configurations as ground-state configurations of a lattice gas with two-body interactions, by modifying, at short distances only, the two-body interactions whose ground-state configurations are the most homogeneous ones.

What we have said above explains, hopefully, why one-dimensional lattice gases with non-convex two-body interactions are of interest. Let us overview now our results. It seems that for the first time after the papers(5, 6) concerned with ground states of strictly convex two-body interactions on the one-dimensional lattice, we succeeded in describing rigorously the ground state of a non-convex interaction. The convexity property is destroyed up to distance $n = 2$, at distance 1 the value of the considered interactions is set near zero. We prove that if the sum of the strengths of the interactions from distance 3 on is small with respect to the strength of the interaction at distance 2, then its ground-state configurations appear to be close analogs of the most homogeneous configurations, the so called 2-molecule most homogenous configurations (most homogeneous configurations of dimers). As a consequence the ground state has the complete devil's staircase property. Thus, we answer positively the above questions, at least in the case $n = 2$ which we have considered as a first step of our investigations.

Needless to say that we believe the sort of result we obtained to be valid for any n, that is for interactions with values near zero for distances up to $n - 1$ and strictly convex from distance n on. However, a proof along the lines of the case $n = 2$ seems to be technically complicated.

The paper is organized as follows. In Section 2, we introduce the system under consideration and give basic definitions. Then, in Section 3 we formulate our hypothesis. provide examples that reveal problems that have to be solved on the way towards the final result, and sketch our strategy of proving the hypothesis. A relatively simple part of this strategy, Lemma 0, is proved in this section. After that we prove our main theorem, Theorem 1, by means of Lemma 0, 1, and 2. The proofs of Lemma 1 and 2 are given in Section 4 and constitute the major part of the paper. Finally, in Section 5 we provide a discussion of the obtained results, describe limitations and possible extensions. Some technical definitions and statements that are used throughout the text are collected in the Appendix.

2. LATTICE-GAS MODELS AND DEVIL'S STAIRCASES

A classical lattice-gas model, considered here, is a system in which every site of a one-dimensional lattice $\mathbf{Z}$ can be occupied by one particle or be empty. Then, an infinite-lattice configuration is an assignment of particles to lattice sites, i.e., an element of $\Omega = \{1, 0\}^{\mathbf{Z}}$. If $X \in \Omega$ and $\Lambda \subset \mathbf{Z}$, then we denote by X_Λ a restriction of X to Λ. We assume that the particles interact only through two-body forces and to a pair of particles at lattice sites i and j, whose distance is $|i-j|$, we assign the translation-invariant *interaction energy* $V(|i-j|)$. The corresponding two-body *potential* reads: $V(|i-j)|)\, s_i(X)\, s_j(X)$, where $\{s_i(X), i \in \mathbf{Z}\}$ are occupations of sites in a configuration X; $s_i(X)$ assumes value 1 if in the configuration X the site i is occupied by a particle and otherwise value 0. In terms of the above defined potential, the Hamiltonian of our system in a bounded region Λ amounts to the sum of the potential over all pairs of sites having nonempty intersection with Λ:

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

For $Y, X \in \Omega$, we say that Y is a *local excitation* of X, and write $Y \sim X$, if there exists a bounded $\Lambda \subset \mathbf{Z}$ such that $X = Y$ outside Λ.

For $Y \sim X$, the *relative Hamiltonian* is defined by

$$H(Y, X) = \sum_{\{\{i,j\} : \{i,j\} \cap \Lambda \neq \varnothing\}} (V(|i-j|)\, s_i(Y)\, s_j(Y) - V(|i-j|)\, s_i(X)\, s_j(X)) \tag{2}$$

We say that $X \in \Omega$ is a *ground-state configuration* of H if

$$H(Y, X) \geqslant 0 \qquad \text{for any} \quad Y \sim X$$

That is, we cannot lower the energy of a ground-state configuration by changing it locally.

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

$$e(X) = \liminf_{\Lambda \to \mathbf{Z}} \frac{H_\Lambda(X)}{|\Lambda|} \tag{3}$$

where $|\Lambda|$ is the number of lattice sites in Λ. In a similar way we define the *particle density* in a configuration X, denoted by $\rho(X)$—the Hamiltonian in (3) has to be replaced by the number of particles in the region Λ.

It can be shown that any ground-state configuration has the minimal energy density which means that local conditions present in the definition of a ground-state configuration enforce global minimum of the energy density.$^{(27)}$

For certain values of external parameters, like the chemical potential or the particle density (depending on the used Gibbs ensemble), our models do not have periodic ground-state configurations. However, for any fixed value of such an external parameter, all ground-state configurations belong to one *local isomorphism class*. It means that they cannot be locally distinguished one from another. Every local pattern of particles present in one ground-state configuration appears in any other within a bounded distance. More formally, there exists a unique *translation-invariant probability measure* supported by ground-state configurations. It is then necessarily the zero-temperature limit of *equilibrium states* (i.e., translation-invariant Gibbs states).$^{(28)}$

In this paper, by the *ground state* of a model we mean precisely the above defined probability measure.

If a system has a unique periodic ground-state configuration and its translations (this happens in our models for those values of the chemical potential that fix a rational particle density), then a unique ground-state measure assigns an equal probability to all these translations. For example, the Ising antiferromagnet has two alternating ground-state configurations but only one ground-state measure which assigns probability 1/2 to both of them.

In the non-periodic case, a probability ground-state measure P gives equal weights to all ground-state configurations and can be obtained as a limit of averaging over a given ground-state configuration X and its translations $\tau_{\mathbf{a}} X$ by lattice vectors $\mathbf{a} \in \mathbf{Z}$: $P = \lim_{\Lambda \to \mathbf{Z}} (1/|\Lambda|) \sum_{\mathbf{a} \in \Lambda} \delta(\tau_{\mathbf{a}} X)$, where $\delta(\tau_{\mathbf{a}} X)$ is a probability measure assigning probability 1 to $\tau_{\mathbf{a}} X$.

One more remark concerning ground states discussed here is in order. We consider exclusively the ground-state measures that are *strictly ergodic*.$^{(29, 30)}$ In particular, every ground-state configuration in their support has 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).

We say that a set $\Lambda \subset \mathbf{Z}$ is *lattice-connected* if for every pair of lattice sites $i, j \in \Lambda$ there is a sequence $i_1,..., i_n$ such that $i_1 = i$, $i_n = j$ and i_k, i_{k+1}, $k = 1,..., n-1$ are the nearest-neighbor sites.

In the sequel, in order to describe some local configurations X_Λ, Y_Λ, for a lattice-connected Λ, we find it convenient to introduce on $\mathbf{Z}$ a *coordinate-axis* with lattice sites located at integer points and to call the positive direction the right one while the opposite direction—the left one. The *environment of* Λ, $\mathbf{Z} - \Lambda$, splits naturally into the *left environment*, consisting of the sites preceding Λ, and the *right environment*, consisting of the sites following Λ. It will also be convenient to set the zero of the axis at the last occupied site of the left environment so that the position of a particle in Λ is positive and coincides with its distance to the left environment. The coordinate-axis introduced will be briefly called *x-axis*.

We assume that the *interaction energy* of two particles separated by distance r, $V(r)$, is summable and for $r \geqslant r_0$ it is positive and strictly convex (see the Appendix), hence decreasing. Such an interaction energy is denoted by $V_{r_0}(r)$. It is convenient to normalize $V_{r_0}(r)$ in such a way that $\lim_{r \to \infty} V_{r_0}(r) = 0$.

Then, we define the interaction energy of a particle at a site r in Λ with the left environment of Λ, $V^L_{r_0}(r)$, as the sum of interaction energies $V_{r_0}(r - j)$ over all occupied sites j in the left environment. The properties of the interaction energy V_{r_0} imply that, for $r \geqslant r_0$, the function $V^L_{r_0}(r)$ is positive, strictly convex, and decreasing.

In what follows some particle configurations play a distinguished part. Among local configurations that appear frequently in our considerations are *atoms*, i.e., occupied sites whose nearest-neighbor sites are empty. The *location of an atom* is identified with the location of the occupied site. Another local configuration is a lattice-connected set of n, $n \geqslant 2$, occupied sites whose left and right nearest-neighbor sites are empty. It is called the *n-molecule*. The *location of a n-molecule* is identified with the location of the first particle of the molecule, i.e., the one with the smallest x-coordinate. Consequently, the *distance between two n-molecules* is identified with the distance between the first particle of one n-molecule and the first particle of the other n-molecule.

However, our attention is focused on global participle configurations which can be characterized as follows. For every particle density ρ, there is a unique sequence of natural numbers d_n, such that the separations between any pair of n-th nearest-neighbor particles are d_n or $d_n + 1$. Such configurations have been called the *generalized Wigner lattices*$^{(5)}$ or the *most homogeneous configurations*.(23) If the particle density is rational, then the corresponding most homogeneous configurations are periodic (the particle locations can be given by means of a construction given for instance in ref. 5) while for irrational densities they are non-periodic.

At least in this paper, the main reason of interest in the most homogeneous configurations stems from the following theorem:

Theorem 0 (Most homogeneous ground-state configurations). In the canonical ensemble, i.e., for a given particle density ρ, the ground-state configurations of a lattice gas (1) with an interaction energy V_1 are the most homogeneous configurations.

This statement has been proven (or at least a proof has been outlined) by Hubbard(5) and Pokrovsky and Uimin.(6) The ground-state phase diagram in the grand-canonical ensemble has been calculated heuristically by Bak and Bruinsma(15) while a proof for the related Frenkel–Kontorova model has been provided by Aubry(4) and adapted to the lattice-gas model case by Mięķisz and Radin;(31) it is outlined below.

In the grand-canonical ensemble, to find the energy density of a ground state we have to minimize

$$f(\rho) = e(\rho) - \mu\rho \tag{4}$$

Now, $e(\rho)$, i.e., the ground-state energy density for the particle density ρ, is differentiable at every irrational ρ and is nondifferentiable at any rational ρ.(4, 31) 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.

As we have already mentioned, for any rational ρ, 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 ρ, there are uncountably many ground-state configurations which are the most homogeneous configurations. It has been shown in ref. 32 that there is still the unique ground-state measure supported by them.

The particle density versus the chemical potential of particles, $\rho(\mu)$, is constant in each set of this partition. Moreover, it is a continuous function on the real line and is inversion symmetric with respect to the point $(\mu_0, \rho(\mu_0))$, where μ_0 is the chemical potential for which the free energy density is hole-particle symmetric ($\rho(\mu_0) = 1/2$). The curve $\rho(\mu)$ is classified as a fractal one and named the *complete devil's staircase.*(4)

The last remark is that without any loss of generality we can restrict our considerations to systems whose particle density ρ does not exceed 1/2. Then the most homogeneous configurations consist exclusively of atoms.

3. BASIC IDEAS AND THE MAIN RESULT

Whether we follow the argument of Hubbard(5) (based on a version of our Lemma A1) or the argument of Pokrovsky and Uimin(6) that proves Theorem 0, we find that such a proof consists essentially of two stages. In the first stage we "chop" configurations that contain n-molecules with some $n = 2, 3,\dots$ off the set of all configurations with particle density ρ, so we are left only with configurations that are composed of atoms whose density is ρ. The second stage is like a "fine tuning" that amounts to precise adjusting the positions of atoms in order to minimize the energy density.

Is the strategy outlined above useful if the two-body strictly convex for $r \geqslant 1$ interaction energy V_1, that appears in Theorem 0, is replaced by an interaction energy V_{r_0} which is strictly convex only for $r \geqslant r_0$, $r_0 = 2, 3,\dots$?

Consider first the second stage. Suppose that the set of configurations composed of atoms only is replaced by the set of configurations that consist exclusively of n-molecules with fixed n, separated by at least distance $r_0 + n - 1$. Let the particle density of these n-molecule configurations be ρ. This class of configurations we denote by $C^n_{r_0, \rho}$. Clearly, the problem of determining the ground-state configurations in $C^n_{r_0, \rho}$ can be reduced to the analogous problem but in the class $C^1_{r_0, \rho/n}$ and with V_{r_0} replaced by the *effective two-body interaction between n-molecules*, $V^{(2)}_{r_0}$. This effective interaction can be naturally defined as the sum of interactions V_{r_0} between ordered pairs of particles such that the first member of a pair belongs to one n-molecule while the second member—to the other n-molecule:

$$\begin{aligned} V^{(2)}_{r_0}(r) = {} & n V_{r_0}(r) + (n-1)(V_{r_0}(r+1) + V_{r_0}(r-1)) \\ & + (n-2)(V_{r_0}(r+2) + V_{r_0}(r-2)) + \cdots + (V_{r_0}(r-n+1) \\ & + V_{r_0}(r+n-1)) \end{aligned} \tag{5}$$

where r stands for the distance between the two considered n-molecules. Since the function $V^{(2)}_{r_0}(r)$ is a sum of functions that are strictly convex for $r \geqslant r_0$, it is also strictly convex for $r \geqslant r_0$. This implies that in the ground-state configurations, the first particles of n-molecules form the most homogeneous configurations with particle density ρ/n, and the same holds true for the second particles of n-molecules, etc. Thus, it is natural to call the obtained ground-state configurations the *n-molecule most homogeneous configurations* of particle density ρ. We summarize the above considerations in the following lemma:

Lemma 0 (Ground-state configurations restricted to $C^n_{r_0,\rho}$). In a lattice gas (1) with an interaction energy V_{r_0}, the ground-state configurations restricted to $C^n_{r_0,\rho}$ are the n-molecule most homogeneous configurations.

Having generalized successfully the stage two, it is tempting to turn to the stage one. Can we modify V_1 in such a way that the ground-state configurations are in $C^n_{r_0,\rho}$? The general suggestion that comes from studies of the Falicov–Kimball model(25) is to set the values of the two-body interaction energy at short distances close to zero. One might expect that setting $V_1(1)=0$ will force the system to form 2-molecules exclusively in the ground-state configurations. However, in order to arrive at such a result, one has to deal with other features of the interaction energy. At this point it is instructive to turn to examples.

Example 1. Consider the convex two-body interaction energy V that in some units is given by $V(1)=0$, $V(2)=4$, $V(3)=2$, $V(4)=1$, $V(r)=0$, for $r \geqslant 5$, and two periodic configurations (period 17) of particle density $\rho=8/17$ whose elementary cells are of the form: $[\bullet\bullet\circ\circ\circ\bullet\bullet\bullet\circ\circ\circ\bullet\bullet\bullet\circ\circ\circ]_1$ and $[\bullet\bullet\circ\circ\bullet\bullet\circ\circ\bullet\bullet\circ\circ\bullet\bullet\circ\circ\circ]_2$, 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 $[\,.\,]_2$, which consists exclusively of 2-molecules, looses against the configuration $[\,.\,]_1$, which consists of 2-molecules and 3-molecules. While the interaction energy chosen is not strictly convex, it is easy to see that the above result remains true if we do not set $V(r)=0$ for $r \geqslant 5$ but extend $V(r)$ to some V_1, with $V_1(r)$ positive and arbitrarily small from $r=6$ on. We deal with the above problem in Lemma 2 which tells us that to exclude n-molecules with $n \geqslant 3$ from competition one should impose a condition on the relative strength of $V_1(2)$ with respect to $V_1(r)$ with $r \geqslant 3$. Namely, it is sufficient to require that the energy of the "tail" of V_2, defined as $W=\sum_{r=3}^{\infty} V_2(r)$, is weak enough compared to $V_2(2)+V_2(1)/2$, i.e., $V_2(2)+V_2(1)/2 \geqslant 7W/2$.

Example 2. This example shows that configurations containing atoms are unlikely to be the ground-state ones. Let the two periodic configurations of particle density $\rho = 3/11$ be of the form: $[\bullet\bullet(5\circ)\bullet\bullet(5\circ)\bullet\bullet(6\circ)]_3$ (period 22) and $[\bullet\bullet(4\circ)\bullet(4\circ)]_4$ (period 11). The notation "$(5\circ)$" stands for five empty sites in a row, etc. If $V(r) = 0$ for $r > 8$, then the energy per cell of 22 sites amounts to $2V(6) + 5V(7) + 4V(8)$, in the case of $[\,.\,]_3$, and to $4V(5) + 4V(6)$, in the case of $[\,.\,]_4$. Now, let the interaction energy V_2 be chosen to coincide with the finite-range interaction energy defined as follows: $V(1)$ is non-positive, $V(2) = 28$, $V(3) = 21$, $V(4) = 15$, $V(5) = 10$, $V(6) = 6$, $V(7) = 3$, $V(8) = 1$, in some units, while for $r \geqslant 9$, $V_2(r)$ is an arbitrarily small positive extension of this function to a strictly convex function. For such V_2 the configuration $[\,.\,]_3$ wins overwhelmingly.

Summing up, in order to implement the stage two in the case of a non-convex interaction energy V_2, we have to force the system, by modifying its interactions, to make the configurations containing n-molecules with $n \geqslant 3, 4, \ldots$ unfavorable energetically, and to show generally that for such interactions the configurations containing atoms cannot be ground-state ones. The latter problem is dealt with in Lemma 1.

Lemma 1 applied for instance to the configuration $[\,.\,]_4$ tells us that, for any V_2 such that $V_2(1) \leqslant 0$, if we take twice larger elementary cell and rearrange the two atoms and the 2-molecule separating them, so that they form two 2-molecules distributed as follows: $[\bullet\bullet(6\circ)\bullet\bullet(4\circ)\bullet\bullet(6\circ)]_5$, then we lower the energy. By Lemma 0, we can farther lower the energy by adjusting the distances between the 2-molecules so that the resulting configuration is the 2-molecule most homogeneous one: $[\bullet\bullet(5\circ)\bullet\bullet(6\circ)\bullet\bullet(5\circ)]_6$.

What we have said above, summarized in Lemma 0, 1, and 2, shows that the strategy that lead to the proof of Theorem 0, which was concerned with strictly convex interaction energies, can be applied also to some non-convex interaction energies V_2.

Theorem 1 (2-molecule most homogeneous ground-state configurations). Consider a lattice gas (1) with a non-convex interaction energy V_2 and a particle density $\rho \leqslant 1/2$. If $V_2(1) = 0$ and $V_2(2) \geqslant 7W/2$, where $W = \sum_{r=3}^{\infty} V_2(r)$, then the ground-state configurations in the support of the strictly ergodic ground-state measure are the 2-molecule most homogeneous configurations of particle density ρ.

Corollary (Complete devil's staircase). In a lattice gas (1) whose interaction energy V_2 satisfies the conditions given in Theorem 1, the particle density versus the chemical potential of particles, $\rho(\mu)$, exhibits the complete devil's-staircase structure.

4. TWO LEMMAS ON ELIMINATING ATOMS AND n-MOLECULES WITH $n \geqslant 3$

Lemma 1 (Eliminating atoms). Consider a lattice gas (1) with an interaction energy V_2, such that $V_2(1) \leqslant 0$. Let X be a configuration that does not contain n-molecules with $n \geqslant 3$. Suppose that the local configuration X_Λ, where Λ is a bounded lattice-connected subset of Z, contains two atoms separated by $k = 0, 1, 2,...$ molecules. Then, by rearranging the positions of particles in X_Λ, it is possible to construct a configuration Y such that $\rho(Y) = \rho(X)$, $Y_{Z-\Lambda} = X_{Z-\Lambda}$, Y_Λ consists exclusively of $k+1$ 2-molecules and $e(Y) < e(X)$.

Corollary. Among configurations that do not contain n-molecules with $n \geqslant 3$, the lowest energy configurations consist exclusively of 2-molecules.

Proof. We propose a proof by reductio ad absurdum. Let Λ be a bounded lattice-connected subset of $\mathbf{Z}$ and suppose that a local configuration X_Λ contains two atoms separated by $k = 0, 1, 2,...$ 2-molecules while $X_{Z-\Lambda}$ is arbitrary. The idea is to construct another configuration Y, with $Y_{Z-\Lambda} = X_{Z-\Lambda}$ and Y_Λ consisting of $k+1$ 2-molecules exclusively, such that the total energy change, $H(Y, X)$, is negative.

We start with describing X_Λ. Going from left to right, its 1st (or left) atom is separated by a empty sites from the left environment, after the first atom we meet the 1st 2-molecule separated from the 1st atom by n_1 empty sites, later on—the second 2-molecule separated from the 1st one by n_2 empty sites and so on. The $(i-1)$th and the ith 2-molecules are separated by n_i empty sites. Finally the 2nd (or right) atom is separated from the last 2-molecule, i.e., the kth 2-molecule, by n_{k+1} empty sites and by b empty sites from the right environment.

As it has been said above, in the new configuration Y, the configurations of the left and right environments remain unchanged while Y_Λ is obtained as follows. We start with the 1st atom and the left particle of the 1st 2-molecule in X_Λ and put them at the two nearest-neighbor sites located in the center of the gap of n_1 empty sites. Clearly, if n_1 is even, then the position of the new 2-molecule (the 1st 2-molecule in Y_Λ)) is defined uniquely, the center of gravity of the 2-molecule coincides with the geometric center of the gap. On the other hand, if n_1 is odd, then we can speak of the left and right central positions of the 2-molecule. In the first case the center of gravity of the 2-molecule is shifted by half the lattice constant to the left of the geometric center of the gap while in the second case—to the right. In the next step we create the 2nd 2-molecule of Y_Λ by taking the right particle of the 1st 2-molecule and the left particle of the 2nd 2-molecule in X_Λ and putting them in the center of the gap made by n_2 empty sites. The procedure described is continued until $k+1$ 2-molecules in Y_Λ is created. Each time the gap between the 2-molecules in X_Λ is odd we have a choice of two central positions. Therefore we may end up with as much as 2^{k+1} different configurations. In the sequel we shall restrict ourselves to two simple choices, namely either we always choose the left central position and the corresponding Y is labeled Y_L or we always choose the right central position what leads to the configuration Y_R.

Our aim is to estimate the energy changes related to passing from X to Y_L, $H(Y_L, X)$ and from X to Y_R, $H(Y_R, X)$. It is convenient to split the total energy of X_Λ, $E_\Lambda(X)$, into two parts: $E_\Lambda(X) = E_\Lambda^{\text{int}}(X) + E_\Lambda^{\text{ext}}(X)$. Here $E_\Lambda^{\text{int}}(X)$ is the *internal energy*, that is the sum of pair interaction energies $V_{r_0}(r)$ over all pairs of particles in X_Λ. The *external energy* of X_Λ, $E_\Lambda^{\text{ext}}(X)$, can in turn be represented as $E_\Lambda^{\text{ext}}(X) = E_\Lambda^L(X) + E_\Lambda^R(X)$, where $E_\Lambda^L(X)$ is the sum of pair interaction energies over all pairs of particles consisting of one particle in the left environment at configuration $X_{Z-\Lambda}$ and one particle in Λ at configuration X_Λ, and $E_\Lambda^R(X)$ is defined similarly. Therefore

$$\begin{aligned} H(Y, X) &= E_\lambda(Y) - E_\Lambda(X) \\ &= E_\Lambda^L(Y) - E_\Lambda^L(X) + E_\Lambda^R(Y) - E_\Lambda^R(X) + E_\Lambda^{\text{int}}(Y) - E_\Lambda^{\text{int}}(X) \qquad (6) \end{aligned}$$

for some Y.

The remaining part of our proof consists of two stages. In the stage one we study only the external energy differences while in the stage two the internal energy differences.

Stage One: Estimating External Energy Variation. Consider the pair of particles that constitute the ith 2-molecule in Y_L. Let $E_i^L(Y_L)$ and $E_i^L(X)$ stand for the external interaction energy of that pair of particles with the left environment at configurations Y_L and X, respectively. Then

$$E_\Lambda^L(Y_L) - E_\Lambda^L(X) = \sum_{i=1}^{k+1} (E_i^L(Y_L) - E_i^L(X)) \qquad (7)$$

and similarly

$$E_\Lambda^R(Y_L) - E_\Lambda^R(X) = \sum_{i=1}^{k+1} (E_i^R(Y_L) - E_i^R(X)) \qquad (8)$$

Therefore we are left with estimating the energy differences $E_i^L(Y_L) - E_i^L(X)$ and $E_i^R(Y_L) - E_i^R(X)$ what requires a detailed description of positions, in configurations X and Y_L, of the two particles that constitute the

ith 2-molecule in Y_L. In X, the particles mentioned are the right particle of the $(i-1)$th 2-molecule whose position according to the x-axis is denoted by x_i and the left particle of the ith 2-molecule whose position is then x_i+n_i+1. Let us recall that the positions mentioned coincide with the distances between the particles considered and the left environment. In Y_L the corresponding positions are $x_i+[n_i/2]$ and $x_i+[n_i/2]+1$. Now we are ready to express the energies $E_i^L(Y_L)$ and $E_i^L(X)$ in terms of the interaction energy, $V_{r_0}^L(r)$, of a particle at $r\in\Lambda$ with the left environment (see Section 2 for the definition and properties). Then

$$E_i^L(X)=V^L(x_i)+V^L(x_i+n_i+1) \tag{9}$$

and

$$E_i^L(Y_L)=V^L(x_i+[n_i/2])+V^L(x_i+[n_i/2]+1) \tag{10}$$

Therefore

$$\begin{aligned}E_i^L(Y_L)-E_i^L(X)&=(V^L(x_i+[n_i/2])-V^L(x_i))\\&\quad+(V^L(x_i+[n_i/2]+1)-V^L(x_i+n_i+1))\end{aligned} \tag{11}$$

Since $V^L(r)$ is a decreasing function of distance r, the inspection of the distances that appear in Eq. (11) shows that the first energy difference is negative while the second one is positive. Hence the net outcome can only be established by calling additional properties of $V^L(r)$. We use the convexity property of $V^L(r)$ (for $r\geqslant 2$). Estimating $E_i^L(Y_L)-E_i^L(X)$ amounts to estimating the variations of $V^L(r)$ at the intervals $[x_i, x_i+[n_i/2]]$ and $[x_i+[n_i/2]+1, x_i+n_i+1]$ (see Sect. 2). First suppose that n_i is even. Then both intervals are of the same length, $n_i/2$, but the second one is shifted to the right with respect to the first one. Therefore by convexity

$$V^L(x_i+n_i/2+1)-V^L(x_i+n_i+1)\leqslant V^L(x_i)-V^L(x_i+n_i/2) \tag{12}$$

and consequently

$$E_i^L(Y_L)-E_i^L(X)\leqslant 0 \tag{13}$$

which is the desired result. However if n_i is odd, one of the intervals, the one located more to the right, is longer by 1 and an analogous reasoning does not reproduce inequality (13). Translating the longer interval to the left, so that its left end coincides with the left end of the shorter one, we obtain by convexity

$$E_i^L(Y_L) - E_i^L(X) \leqslant V^L(x_i + [n_i/2]) - V^L(x_i + \{n_i/2\}) \tag{14}$$

Remark. In a similar way one can derive a stronger inequality, namely the r.h.s. of (14) can be replaced by $V(x_i + n_i) - V(x_i + n_i + 1)$.

To get an estimate of the external energy $E_\Lambda^{\text{ext}}(Y_L) - E_\Lambda^{\text{ext}}(X)$ it remains to find the counterparts of inequalities (13) and (14) in the case of the right environment. For this purpose it is convenient to introduce a second coordinate-axis, the y-axis, similar to the x-axis but pointing in the opposite direction. We keep using the notions of left and right according to the x-axis. The zero of the y-axis is set at the 1st (i.e., most to the left) particle of the right environment, so that again the y-position of a particle in Λ coincides with the distance between that particle and the right environment. Now a while of reflection enables us to realize that the interaction energies with the right environment can be obtained from the interaction energies with the left environment by replacing x_i by y_i and interchanging the square and curly brackets. Thus the counterparts of (9) and (10) read

$$E_i^R(X) = V^R(y_i) + V^R(y_i + n_i + 1) \tag{15}$$

and

$$E_i^R(Y_L) = V^R(y_i + \{n_i/2\}) + V^R(y_i + \{n_i/2\} + 1) \tag{16}$$

respectively, and the counterpart of (11) is

$$\begin{aligned} E_i^R(Y_L) - E_i^R(X) = (&V^R(y_i + \{n_i/2\}) - V^R(y_i)) \\ &+ (V^R(y_i + \{n_i/2\} + 1) - V^R(y_i + n_i + 1)) \end{aligned} \tag{17}$$

Again, if n_i is even we find

$$E_i^R(Y_L) - E_i^R(X) \leqslant 0 \tag{18}$$

and if n_i is odd:

$$E_i^R(Y_L) - E_i^R(X) \leqslant V^R(y_i + \{n_i/2\}) - V^R(y_i + [n_i/2]) \tag{19}$$

Summing up, the external energy variation on passing from X to Y_L has an upper bound of the form

$$\begin{aligned}E^{\mathrm{ext}}_{\Lambda}(Y_L)-E^{\mathrm{ext}}_{\Lambda}(X) &= E^{L}_{\Lambda}(Y_L)-E^{L}_{\Lambda}(X)+E^{R}_{\Lambda}(Y_L)-E^{R}_{\Lambda}(X)\\ &= \sum_{i=1}^{k+1}\left(E^{L}_{i}(Y_L)-E^{L}_{i}(X)\right)+\sum_{i=1}^{k+1}\left(E^{R}_{i}(Y_L)-E^{R}_{i}(X)\right)\\ &\leqslant \sum_{i=1}^{k+1}\left(V^{L}(x_i+[n_i/2])-V^{L}(x_i+\{n_i/2\})\right)\\ &\quad +\left(V^{R}(y_i+\{n_i/2\})-V^{R}(y_i+[n_i/2])\right)\end{aligned} \tag{20}$$

Again a while of reflection enables us to write down the upper bound for the change in the total external energy on passing from X to Y_R, that represents a counterpart of (20). It is enough to interchange in (20) x_i with y_i and R with L:

$$\begin{aligned}E^{\mathrm{ext}}_{\Lambda}(Y_R)-E^{\mathrm{ext}}_{\Lambda}(X) &= E^{L}_{\Lambda}(Y_R)-E^{L}_{\Lambda}(X)+E^{R}_{\Lambda}(Y_R)-E^{R}_{\Lambda}(X)\\ &= \sum_{i=1}^{k+1}\left(E^{L}_{i}(Y_R)-E^{L}_{i}(X)\right)+\sum_{i=1}^{k+1}\left(E^{R}_{i}(Y_R)-E^{R}_{i}(X)\right)\\ &\leqslant \sum_{i=1}^{k+1}\left(V^{R}(y_i+[n_i/2])-V^{R}(y_i+\{n_i/2\})\right)\\ &\quad +\left(V^{L}(x_i+\{n_i/2\})-V^{L}(x_i+[n_i/2])\right)\end{aligned} \tag{21}$$

By inspection of (20) and (21) one finds that the upper bound given in (20) is just the opposite of the upper bound given in (21). Thus, if $E^{\mathrm{ext}}_{\Lambda}(Y_L)-E^{\mathrm{ext}}_{\Lambda}(X)>0$, then its upper bound (20) is strictly greater than zero, consequently the upper bound (21) is strictly less than zero what implies that $E^{\mathrm{ext}}_{\Lambda}(Y_R)-E^{\mathrm{ext}}_{\Lambda}(X)<0$ and vice versa. Therefore we proved that either $E^{\mathrm{ext}}_{\Lambda}(Y_L)-E^{\mathrm{ext}}_{\Lambda}(X)$ or $E^{\mathrm{ext}}_{\Lambda}(Y_R)-E^{\mathrm{ext}}_{\Lambda}(X)$ is non-positive.

Remark. Let us note here that the lemma is valid also if $k=0$.

Stage Two: Estimating Internal Energy Variation. Now we are going to estimate the internal energy difference $E^{\mathrm{int}}_{\Lambda}(Y_L)-E^{\mathrm{int}}_{\Lambda}(X)$, which appears to be a considerably more laborious task than it was the case for the external energy difference. To arrive at a satisfactory upper bound of $E^{\mathrm{ext}}_{\Lambda}(Y_L)-E^{\mathrm{ext}}_{\Lambda}(X)$ we represented the external energy $E^{\mathrm{ext}}_{\Lambda}(Y_L)$ and $E^{\mathrm{ext}}_{\Lambda}(X)$ by a sum of external energies of pairs of particles in Λ that constitute 2-molecules in the configuration $Y_L(Y_R)$. Such a partition of the external energy led to energy differences that could be estimated by means of the convexity property of the interaction involved. We shall need a counterpart of this partition for $E_\Lambda^{\text{int}}(Y_L)$ and $E_\Lambda^{\text{int}}(X)$. This time a natural object is not a pair of particles but two pairs of particles that constitute two 1st nearest-neighbor 2-molecules in $Y_L(Y_R)$, two 2nd nearest-neighbor 2-molecules, and so on, until a pair of $(k+1)$th nearest-neighbor 2-molecules. We can define in a natural way the internal interaction energy of those objects, in terms of $V(r)$. First consider a pair of 1st nearest neighbor 2-molecules in Y_L, say the ith and $(i+1)$th one, $i=2,..., k-1$ (so that the boundary molecules, the 1st and the $(k+1)$th one, are excluded from our consideration for a moment). To build up the ith 2-molecule in Y_L, we pick up the right particle of the $(i-1)$th molecule in X and move it to the right by distance $[n_i/2]$, then the left particle of the ith molecule in X and move it by distance $\{n_i/2\}$ to the left. Thus the ith and $(i+1)$th molecules in Y_L are separated by the distance $x_i^{(1)}+1$, where

$$x_i^{(1)} := g(n_i, n_{i+1}) = \{n_i/2\} + [n_{i+1}/2] \tag{22}$$

and we used the function $g(s, t)$ defined in the Appendix. The internal interaction energy of the pair of molecules considered is defined as the sum of all the four interaction energies $V(r)$ between the particles separated only by the gap $x_i^{(1)}$:

$$\begin{aligned} E_i^{(1)}(Y_L) = E_{Y_L}(n_i, n_{i+1}) &:= (V(x_i^{(1)}+1) + V(x_i^{(1)}+2)) \\ &\quad + (V(x_i^{(1)}+2) + V(x_i^{(1)}+3)) \end{aligned} \tag{23}$$

While according to our description above the definitions (22) and (23) do not apply to these cases $i=1$ and $i=k$, a direct inspection shows that

$$x_1^{(1)} = g(n_1, n_2), \qquad x_k^{(1)} = g(n_k, n_{k+1}) \tag{24}$$

and

$$\begin{aligned} E_1^{(1)}(Y_L) &= E_{Y_L}(n_1, n_2) \\ &:= (V(x_1^{(1)}+1) + V(x_1^{(1)}+2)) + (V(x_1^{(1)}+2) + V(x_1^{(1)}+3)) \\ E_k^{(1)}(Y_L) &= = E_{Y_L}(n_k, n_{k+1}) \\ &:= (V(x_k^{(1)}+1) + V(x_k^{(1)}+2)) + (V(x_1^{(k)}+2) + V(x_k^{(1)}+3)) \end{aligned} \tag{25}$$

i.e., these definitions apply to all $i=1,..., k$. The quantities $x_i^{(1)}$ and $E_i^{(1)}(Y_L)$ can be thought of as the values of the functions g and E_{Y_L} evaluated at the pairs (n_i, n_{i+1}), $i=1,..., k$, of two consecutive gaps in X_Λ, respectively.

A pair of 2nd nearest-neighbor molecules in Y_L, say the ith and $(i+2)$th one, is separated by two consecutive gaps between 1st nearest-neighbor molecules, $x_i^{(1)}$ and $x_{i+1}^{(1)}$. From the point of view of the interaction energies between the particles constituting these molecules, they are separated by one gap of $x_i^{(2)}$ empty sites, where

$$x_i^{(2)} := x_i^{(1)} + x_{i+1}^{(1)} + 2 = \{n_{i/2}\} + [n_{i+2}/2] + (n_{i+1} + 2) \tag{26}$$

Consequently we can define the internal interaction energy of the pair considered of 2nd nearest-neighbor molecules in Y_L, $E_i^{(2)}(Y_L)$, as the corresponding energy between 1st nearest neighbors, i.e., by replacing simply $x_i^{(1)}$ in Eq. (23) by $x_i^{(2)}$.

While in terms of 1st nearest-neighbor gaps, n_i, the pair of 1st nearest-neighbor molecules, the ith and $(i+1)$th one, was associated with the pair (n_i, n_{i+1}), the pair of 2nd nearest neighbor molecules, ith and $(i+2)$th, is associated with two consecutive pairs of such pairs $((n_i, n_{i+1}), (n_{i+1}, n_{i+2}))$. But from the point of view of the interaction energies between the particles constituting the ith and $(i+2)$th molecules, the transition from 1st nearest-neighbor molecules to 2nd nearest neighbor molecules can be described as a "renormalization process" that maps two consecutive pairs of consecutive 1st nearest-neighbor gaps into a pair of consecutive 2nd nearest-neighbor gaps:

$$((n_i, n_{i+1}), (n_{i+1}, n_{i+2})) \to (n_i + (n_{i+1} + 2), n_{i+2} + (n_{i+1} + 2)) \tag{27}$$

Thus the pair of 2nd nearest-neighbor molecules, the ith and $(i+2)$th one, can also be associated with one pair of gaps—the pair of consecutive 2nd nearest-neighbor gaps $(n_i + (n_{i+1} + 2), n_{i+2} + (n_{i+1} + 2))$. Then in terms of the consecutive 2nd nearest-neighbor gaps

$$x_i^{(2)} = x(n_i + (n_{i+1} + 2), n_{i+2} + (n_{i+1} + 2)) \tag{28}$$

and

$$E_i^{(2)}(Y_L) = E_{Y_L}(n_i + (n_{i+1} + 2), n_{i+2} + (n_{i+1} + 2)) \tag{29}$$

This construction can be naturally continued: the pair of 3rd nearest-neighbor molecules, the ith and $(i+3)$th one, is associated with the pair of consecutive triples of consecutive 1st nearest-neighbor gaps

$$((n_i, n_{i+1}, n_{i+2}), (n_{i+1}, n_{i+2}, n_{i+3})) \tag{30}$$

or, after renormalizing, with the pair of 3rd nearest-neighbor gaps

$$(n_i+(n_{i+1}+2)+(n_{i+2}+2),\ n_{i+3}+(n_{i+1}+2)+(n_{i+2}+2)) \tag{31}$$

Consequently

$$x_i^{(3)}=x(n_i+(n_{i+1}+2)+(n_{i+2}+2),\ n_{i+2}+(n_{i+1}+2)+(n_{i+2}+2)) \tag{32}$$

and

$$E_i^{(3)}(Y_L)=E_{Y_L}(n_i+(n_{i+1}+2)+(n_{i+2}+2),\ n_{i+3}+(n_{i+1}+2)+(n_{i+2}+2)) \tag{33}$$

What we have said above enables us to represent $E_\Lambda^{\mathrm{int}}(Y_L)$ as follows:

$$E_\Lambda^{\mathrm{int}}(Y_L)=\sum_{i=1}^{i=k} E_i^{(1)}(Y_L)+\sum_{i=1}^{i=k-1} E_i^{(2)}(Y_L)+\cdots+E_1^{(k)}(Y_L) \tag{34}$$

where the last component in the above equation stands for the internal interaction energy of the 1st and the last, i.e., $(k+1)$th molecule in Y_L.

Having defined a partition of $E_\Lambda^{\mathrm{int}}(Y_L)$ we have to construct a suitable partition of $E_\Lambda^{\mathrm{int}}(X)$, so that.the energy differences that will appear eventually in $E_\Lambda^{\mathrm{int}}(Y_L)-E_\Lambda^{\mathrm{int}}(X)$ can be shown to be negative, by means of convexity properties. We have in mind Lemma A1 of the Appendix.

We start with the level of 1st nearest neighbors. Since in $E_i^{(1)}(Y_L)$, given by Eq. (23), the energies $V(r)$ group naturally into two pairs, so that each distance involved in one pair has a counterpart differing by 1 in the second pair, it would certainly be convenient to preserve this property in a partition of $E_\Lambda^{\mathrm{int}}(X)$ we are searching for. Then instead of comparing some four energies in $E_\Lambda^{\mathrm{int}}(X)$ with the four energies in $E_i^{(1)}(Y_L)$ we would have to compare only one group of two energies in $E_i^{(1)}(Y_L)$ with a pair of energies in $E_\Lambda^{\mathrm{int}}(X)$.

Let us start with the pair $V(x_i^{(1)}+1)$, $V(x_i^{(1)}+2)$ of $E_i^{(1)}(Y_L)$. In order to be able to apply Lemma A1, the corresponding energies in $E_\Lambda^{\mathrm{int}}(X)$ should be associated with some distances, say $r_1<r_2$, such that $r_1+r_2\leqslant(x_i^{(1)}+1)+(x_i^{(1)}+2)$ and $r_1\leqslant x_i^{(1)}+1<x_i^{(1)}+2\leqslant r_2$. Searching for such distances is facilitated considerably by Lemma A2, which gives lower and upper bounds for a quantity like $x_i^{(1)}$. We note that the bounds are the best ones, since they can be attained. The particles that constitute the ith and $(i+1)$th 2-molecules in Y_L, whose internal energy is $E_i^{(1)}(Y_L)$, come from the ith, $(i+1)$th and $(i+2)$th 2-molecules in X_Λ, separated by the gaps of n_i and n_{i+1} empty sites, or distances n_i+1 and $n_{i+1}+1$, respectively.

In order not to consider from the very beginning the specific behavior of energies at the borders of X_A we limit the index i to the interval $2 \leqslant i \leqslant k-1$. It will be convenient in the sequel to label the particles that constitute the ith, $(i+1)$th and $(i+2)$th 2-molecules in X_A by a, b, c, d, e, f, in the order from the left to the right. Thus $r_{a,b} = r_{c,d} = r_{e,f} = 1$, where $r_{a,b}$ stands for the distance between the particles labelled a, b, etc.

In what follows we shall label even (odd) integers by the subscript "*even*" ("*odd*"). First suppose that $n_i = n_{even}$ and $n_{i+1} = n_{odd}$. Then by Lemma A4, for $n_{even} < n_{odd}$

$$n_{even} + 1 \leqslant x_i^{(1)} + 1 < x_i^{(1)} + 2 \leqslant n_{odd} + 1 \tag{35}$$

and

$$(n_{even} + 1) + (n_{odd} + 1) = (x_i^{(1)} + 1) + (x_i^{(1)} + 2) \tag{36}$$

For $n_{even} > n_{odd}$, n_{even} has to be interchanged with n_{odd} in Ineq. (35). Therefore, according to Lemma A4 there is no other choice than $r_1 = \min\{n_{even} + 1, n_{odd} + 1\}$ and $r_2 = \max\{n_{even} + 1, n_{odd} + 1\}$. Fortunately, there are particles separated by these distances, we can set either $r_1 = r_{b,c}$ and $r_2 = r_{d,e}$ or vice versa. The second group of longer by 1 distances can be realized as either $r_1 + 1 = r_{b,d}$ (or $r_{a,c}$) and $r_2 + 1 = r_{c,e}$ (or $r_{d,f}$) or vice versa. Now, by Lemma A1

$$V(r_{bc}) + V(r_{d,e}) = V(n_{even} + 1) + V(n_{odd} + 1) \geqslant V(x_i^{(1)} + 1) + V(x_i^{(1)} + 2) \tag{37}$$

and a similar inequality is satisfied if $r_{b,c}$, $r_{d,e}$ are replaced by $r_{b,d}$, $r_{c,e}$ (longer by 1) and all other distances in Ineq. (37) are expanded by 1. Summing up, in the case $n_i = n_{even}$ and $n_{i+1} = n_{odd}$ a good candidate for the counterpart of $E_i^{(1)}(Y_L)$ in X_A is

$$\begin{aligned} E_{i,(e,o)}^{(1)} &= (V(r_{b,c}) + V(r_{d,e})) + (V(r_{b,d}) + V(r_{c,e})) \\ &= (V(n_{even} + 1) + V(n_{odd} + 1)) + (V(n_{even} + 2) + V(n_{odd} + 2)) \end{aligned} \tag{38}$$

Note that only interactions between 1st nearest-neighbor 2-molecules enter into $E_{i,(e,o)}^{(1)}$, and two one, out of four possible for each pair of 2-molecules, have been picked up.

In the second step we suppose that both n_i and n_{i+1} are odd, say $n_i = n_{odd}$ and $n_{i+1} = m_{odd}$. Then by Lemma A4, for $n_{odd} < m_{odd}$

$$n_{odd} + 2 \leqslant x_i^{(1)} + 1 < x_i^{(1)} + 2 \leqslant m_{odd} + 1 \tag{39}$$

while for $n_{odd} < m_{odd}$, n_{odd} and m_{odd} have to be interchanged in Ineq. (39) If $n_{odd} = m_{odd}$, then

$$n_{odd} + 1 = x_i^{(1)} + 1 < x_i^{(1)} + 2 = n_{odd} + 2 \tag{40}$$

Whatever the relation between n_{odd} find m_{odd},

$$n_{odd} + m_{odd} + 3 = (x_i^{(1)} + 1) + (x_i^{(1)} + 2) \tag{41}$$

Therefore, the distances r_1 and r_2 are determined uniquely, like in the first step. Trying to realize r_1 and r_2 as interparticle distances we have to be careful not to run into conflict with the choice made previously. The two consecutive gaps of n_{odd} and m_{odd} empty sites can be preceded by an even gap, so two interactions between particles belonging to the pair of 1st nearest-neighbor 2-molecules that are separated by the gap of n_{odd} empty sites might have already been used. Therefore, in the case $n_i = n_{odd}$ and $n_{i+1} = m_{odd}$ we choose for the counterpart of $E_i^{(1)}(Y_L)$ in X_Λ the energy

$$\begin{aligned} E_{i,(o,o)}^{(1)} &= (V(r_{b,d}) + V(r_{d,e})) + (V(r_{a,d}) + V(r_{c,e})) \\ &= (V(n_{odd} + 2) + V(m_{odd} + 1)) + (V(n_{odd} + 3) + V(m_{odd} + 2)) \end{aligned} \tag{42}$$

In the third step we suppose that $n_i = n_{odd}$ and $n_{i+1} = n_{even}$. Then by Lemma A4, for $n_{odd} < n_{even}$

$$n_{odd} + 2 \leqslant x_i^{(1)} + 1 < x_i^{(1)} + 2 \leqslant n_{even} + 2 \tag{43}$$

and

$$(n_{odd} + 2) + (n_{even} + 2) = (x_i^{(1)} + 1) + (x_i^{(1)} + 2) \tag{44}$$

For $n_{odd} > n_{even}$, n_{even} has to be interchanged with n_{odd} in Ineq. (43). Therefore according to Lemma A1 there is no other choice than $r_1 = \min\{n_{even} + 2, n_{odd} + 2\}$ and $r_2 = \max\{n_{even} + 2, n_{odd} + 2\}$. Therefore in the case $n_i = n_{odd}$ and $n_{i+1} = n_{even}$ we choose for the counterpart of $E_i^{(1)}(Y_L)$ in X_Λ the energy

$$\begin{aligned} E_{i,(o,e)}^{(1)} &= (V(r_{b,d}) + V(r_{c,e})) + (V(r_{a,d}) + V(r_{c,f})) \\ &= (V(n_{odd} + 2) + V(n_{even} + 2)) + (V(n_{odd} + 3) + V(n_{even} + 3)) \end{aligned} \tag{45}$$

Our definition of $E_{i,(o,e)}^{(1)}$ is not in conflict with those in the previous two situations.

In the last step we suppose that both n_i and n_{i+1} are even, say $n_i = n_{even}$ and $n_{i+1} = m_{even}$. Then by Lemma A4, for $n_{even} < m_{even}$

$$n_{even} + 2 \leqslant x_i^{(1)} + 1 < x_i^{(1)} + 2 \leqslant m_{even} + 1 \tag{46}$$

while for $n_{even} > m_{even}$, n_{even} and m_{even} have to be interchanged in Ineq. (46). If $n_{even} = m_{even}$, then

$$n_{even} + 1 = x_i^{(1)} + 1 < x_i^{(1)} + 2 = n_{even} + 2 \tag{47}$$

Whatever the relation between n_{even} and m_{even},

$$n_{even} + m_{even} + 3 = (x_i^{(1)} + 1) + (x_i^{(1)} + 2) \tag{48}$$

Therefore, again the distances r_1 and r_2 are determined uniquely. As a counterpart of $E_i^{(1)}(Y_L)$ in X_Λ in the case $n_i = n_{even}$ and $n_{i+1} = m_{even}$ we choose the energy

$$\begin{aligned} E_{i,(e,e)}^{(1)} &= (V(r_{b,c}) + V(r_{c,e})) + (V(r_{b,d}) + V(r_{d,f})) \\ &= (V(n_{even} + 1) + V(m_{even} + 2)) + (V(n_{even} + 2) + V(m_{even} + 3)) \end{aligned} \tag{49}$$

This choice is compatible with the fact that the gap preceding n_{even} and the one following m_{even} can be odd.

So far we have succeeded in selecting a component of $E_\Lambda^{\text{int}}(X)$ that is not less than $\sum_{i=2}^{i=k-1} E_i^{(1)}(Y_L)$. For any sequence of gaps, $n_2, n_3, \ldots, n_k$ we have assigned, by means of definitions (38), (42), (45) and (49), a sum of pair interactions in such a way that all the four pair interactions between the particles constituting 1st nearest-neighbor 2-molecules separated by n_i, $i = 2, 3, \ldots, k$, empty sites enter the sum. So the sum considered can be viewed as the sum over groups of four two-body interactions between particles of 1st nearest neighbor 2-molecules in X.

It remains to take care of boundary terms. Staying at the level of 1st nearest neighbors, in Y_L they consist of eight pair interactions: the four ones being the components of $E_1^{(1)}(Y_L)$ and another four—the components of $E_k^{(1)}(Y_L)$. The interactions named can be compared with the following eight components of $E_\Lambda^{\text{int}}(X)$: two interactions between the left atom and the first 2-molecule, two interactions between the 1st and the 2nd 2-molecules, two interactions between the kth and $(k+1)$th 2-molecules and two interactions between the kth 2-molecule and the right atom. It is sufficient to consider in detail the left end of Λ. The interaction of the left atom separated by n_1 empty sites from the 1st molecule amounts obviously to

$$V(n_1+1)+V(n_1+2) \tag{50}$$

The two still "free" interactions between the 1st and the 2nd molecules are:

$$\begin{aligned} V(r_{b,c})+V(r_{a,c}) &= V(n_2+1)+V(n_2+2), &&\text{if } n_2 \text{ is odd}\\ V(r_{a,c})+V(r_{a,d}) &= V(n_2+2)+V(n_2+3), &&\text{if } n_2 \text{ is even}\end{aligned} \tag{51}$$

Therefore we define the left boundary internal energy as:

$$\begin{aligned} E^{(1)}_{1,o} &= (V(n_1+1)+V(n_2+1))+(V(n_1+2)+V(n_2+2)), &&\text{if } n_2 \text{ is odd}\\ E^{(1)}_{1,e} &= (V(n_1+1)+V(n_2+2))+(V(n_1+2)+V(n_2+3)), &&\text{if } n_2 \text{ is even}\end{aligned} \tag{52}$$

Comparing $E^{(1)}_{1,o}$ and $E^{(1)}_{1,e}$ with the energies $E^{(1)}_{i,(e,o)}$, $E^{(1)}_{i,(o,o)}$, $E^{(1)}_{i,(o,e)}$, and $E^{(1)}_{i,(e,e)}$, defined by Eqs. (38), (42), (45), (49) we find that

$$E^{(1)}_{1,o} \begin{cases} = E^{(1)}_{1,(e,o)}, & \text{if } n_1 \text{ is even}\\ \geqslant E^{(1)}_{1,(o,o)}, & \text{if } n_1 \text{ is odd}\end{cases} \tag{53}$$

and

$$E^{(1)}_{1,e} \begin{cases} = E^{(1)}_{1,(e,e)}, & \text{if } n_1 \text{ is even}\\ \geqslant E^{(1)}_{1,(o,e)}, & \text{if } n_1 \text{ is odd}\end{cases} \tag{54}$$

Thus

$$E^{(1)}_{1,e} - E^{(1)}_{1}(Y_L) \geqslant 0 \tag{55}$$

and

$$E^{(1)}_{1,o} - E^{(1)}_{1}(Y_L) \geqslant 0 \tag{56}$$

At the right end the situation is completely analogous. It is enough to replace n_1 by n_k, n_2 by n_{k+1} and interchange the indices e and o in the formulae (52), (53, (54) to arrive at the right boundary internal energies $E^{(1)}_{k,o}$ and $E^{(1)}_{k,e}$ that are not less than $E^{(1)}_{k}(Y_L)$.

This lengthy sequence of definitions, given above, amounts to the following: by means of definitions (38), (42), (45), (49), (53), (54) and the remark after inequality (56), we defined the function E_X on pairs of consecutive gaps, such that its values on pairs of 1st nearest-neighbor gaps, $E_i^{(1)}(X) := E_X(n_i, n_{i+1})$, $i = 1,..., k$, satisfy the inequalities

$$E_i^{(1)}(X) - E_i^{(1)}(Y_L) \geqslant 0 \tag{57}$$

The $\sum_{i=1}^{k} E_i^{(1)}(X)$ can be taken as the required counterpart of $\sum_{i=1}^{k} E_i^{(1)}(Y_L)$. Now following the inductive procedure developed to define the partition (34) of $E_\Lambda^{\text{int}}(Y_L)$, we apply E_X to pairs of consecutive 2nd nearest-neighbor gaps and define

$$E_i^{(2)}(X) = E_X(n_i + (n_{i+1} + 2), n_{i+2} + (n_{i+1} + 2)) \tag{58}$$

By Lemma A1 the inequality (57) implies that

$$E_i^{(2)}(X) - E_i^{(2)}(Y_L) \geqslant 0 \tag{59}$$

so $\sum_{i=1}^{k-1} E_i^{(2)}(X)$ can stand for the required counterpart of $\sum_{i=1}^{k-1} E_i^{(2)}(Y_L)$. Continuing this process we arrive at the following partition of $E_\Lambda^{\text{int}}(X)$:

$$\begin{aligned} E_\Lambda^{\text{int}}(X) = \sum_{i=1}^{k} E_i^{(1)}(X) + \sum_{i=1}^{k-1} E_i^{(2)}(X) + \cdots + E_1^{(k)}(X) \\ + V\left(n_1 + \sum_{i=2}^{k+1} (n_i + 2) + 1\right) \end{aligned} \tag{60}$$

and moreover we obtain that

$$E_\Lambda^{\text{int}}(X) - E_\Lambda^{\text{int}}(Y_L) \geqslant V\left(n_1 + \sum_{i=2}^{k+1} (n_i + 2) + 1\right) > 0 \tag{61}$$

where $V(n_1 + \sum_{i=2}^{k+1} (n_i + 2) + 1)$ stands for the interaction of the left atom with the right one. Clearly, if we substitute Y_R for Y_L we arrive at the same conclusion as (61).

Remark. The inequality (61) holds true if there are no molecules between two atoms.

Lemma 2 (Eliminating n-molecules with $n \geqslant 3$). Consider a lattice gas (1) with an interaction energy V_2, such that $V_2(1) \geqslant 0$. Let X be a configuration containing triples of particles separated by distance one, whose density is nonzero. Then there is a configuration Y, with $\rho(Y) = \rho(X)$, free of such triples. Moreover, if $V_2(2) \geqslant (7W - V_2(1))/2$, then $e(Y) < e(X)$, where $W = \sum_{r=3}^{\infty} V_2(r)$.

Corollary. In a lattice gas of Lemma 2, if $V_2(2) \geqslant (7W - V_2(1))/2$, then the ground-state configurations in the support of the strictly ergodic ground-state measure do not contain triples of particles separated by distance one. In particular, such ground-state configurations do not contain n-molecules with $n \geqslant 3$.

Proof. The idea of our proof is to start with an arbitrary configuration containing forbidden triples of particles, that is triples of particles separated by distance one, and transform it, using Lemma 1 and some rearrangements of particles, whose energy costs are controlled by simple bounds, into another configuration of the same density but free of the forbidden triples of particles. The proof is completed by showing that the overall energy cost of attaining the final configuration is negative, provided that a suitable condition on the interaction energy is imposed.

Let X be an arbitrary configuration with the particle density $\rho(X) \leqslant 1/2$ and whose density of the forbidden triples, $\rho_3(X)$, satisfies the inequality $\rho_3(X) > 0$. Removing one particle from each forbidden triple we lower the energy by at least $V_2(2) + V_2(1)$ and arrive at a configuration $\tilde{X}$ whose particle density satisfies the double inequality

$$1/2 > \rho(\tilde{X}) \geqslant \rho(X) - \rho_3(X) \tag{62}$$

Consider the class of configurations that consist of 2-molecules and atoms (separated by at least two empty sites) exclusively and whose density if $\rho(\tilde{X})$. The configuration $\tilde{X}$ belongs to this class. Let Y be the lowest energy density configuration in this class, thus $e(Y) \leqslant e(\tilde{X})$. By (62), $\rho(X) - \rho(\tilde{X}) \leqslant \rho_3(X)$, therefore the energy density variation $e(X) - e(\tilde{X})$ is bounded from below by $(V_2(2) + V_2(1))(\rho(X) - \rho(\tilde{X}))$. Consequently, we arrive at the following lower bound for $e(X)$:

$$e(X) > (V_2(2) + V_2(1))(\rho(X) - \rho(\tilde{X})) + e(Y) \tag{63}$$

By Lemma 1 the configuration Y does not contain atoms, thus it consists exclusively of 2-molecules. It is clear that there is only one (up to translations) configuration of density 1/2 that consists exclusively of 2-molecules. It is the periodic configuration whose elementary cell has the form [• • ∘ ∘], where the filled circles stand, say, for occupied sites. The 2-molecules are separated by distances 3, i.e., by 2 unoccupied sites. Obviously, a configuration that consists exclusively of 2-molecules and whose particle density is less than 1/2, contains arrangement of 3 unoccupied sites in a row wit a non-vanishing density. Such a configuration can be thought of as a collection of local particle configurations that are separated by at least 3 unoccupied sites in a row. Shifting the local configurations separated by at least 3 unoccupied sites in a row, while respecting the conditions that they cannot be separated by less than 2 unoccupied sites in a row, we can create arrangement of 6 unoccupied sites in a row. Then in the middle of the 6-site gap obtained we insert a 2-molecule. The whole procedure is repeated until the particle density comes back to the value $\rho(X)$. The result is a configuration $\tilde{Y}$. Now we can try to compare the energy densities $e(\tilde{Y})$ and $e(X)$ and see if $e(X)$ can be strictly larger than $e(\tilde{Y})$, what would prove that ground-state configurations do not contain forbidden arrangements of particles. Suppose that we can bound from above by Δ the energy cost of creating a 6-site gap and inserting there a 2-molecule. Then we can compare $e(\tilde{Y})$ and $e(Y)$:

$$e(\tilde{Y}) - e(Y) \leqslant \Delta(\rho(X) - \rho(\tilde{X}))/2 \tag{64}$$

By means of inequalities (62) and (63), we arrive at the following inequality relating $e(X)$ and $e(\tilde{Y})$:

$$e(X) > e(\tilde{Y}) + (V_2(2) + V_2(1) - \Delta/2)(\rho(X) - \rho(\tilde{X})) \tag{65}$$

Therefore, the ground-state configurations do not contain forbidden arrangements of particles if $V_2(2) + V_2(1) \geqslant \Delta/2$.

It remains to derive the upper bound Δ. For that we first estimate the energy cost of translating a single particle by distance 1. Let a chosen particle be separated from its left nearest neighbor by distance r and from its right nearest neighbor by distance r'. The total interaction energy of the particle can be viewed as the sum of the interaction energies $E_L^{(1)}(r)$ and $E_R^{(1)}(r')$ with all the particles to its left and to its right, respectively. Suppose we shift our particle by distance 1 to the left. Then the change in the total energy of the particle is bounded from above by $E_L^{(1)}(r-1) - E_L^{(1)}(r)$, since $E_R^{(1)}(r'+1) - E_R^{(1)}(r') \leqslant 0$. Let x_i, $i = 1, 2,...,$ be the distance between the ith left nearest neighbor and the $(i+1)$th left nearest neighbor. Then

$$\begin{aligned} &E_L^{(1)}(r-1) - E_L^{(1)}(r) \\ &\quad = (V_2(r-1) + V_2(r-1+x_1) + V_2(r-1+x_1+x_2) + \cdots) \\ &\qquad - (V_2(r) + V_2(r+x_1) + V_2(r+x_1+x_2) + \cdots) \\ &\quad = V_2(r-1) + -(V_2(r) - V_2(r-1+x_1)) - (V_2(r+x_1) \\ &\qquad - V_2(r-1+x_1+x_2)) - \cdots \leqslant V_2(r-1) \end{aligned} \tag{66}$$

By means of inequality (66) we are able to give a simple upper bound for the energy cost of translating a local configuration considered above by distance 1 to the left (right). This energy does not exceed the sum of $V_2(r-1)$ over all distances r, $r \geqslant 4$, between the particles of the configuration considered and the left nearest neighbor particle of this configuration:

$$\sum_{r=4}^{\infty} n_r V_2(r-1) \leqslant \sum_{r=4}^{\infty} V_2(r-1) = W \tag{67}$$

where $n_r = 1$ if the local configuration considered contains a particle separated by distance r from the left nearest-neighbor particle of this configuration, and $n_r = 0$ otherwise. Consider again a configuration that is a collection of local configurations separated by at least 3 unoccupied sites. We can create a 6-site gap between two local configurations by shifting a chosen local configuration by distance one to the left, then shifting its right nearest-neighbor local configuration by distance 1 to the right, what creates a 5-site gap between the configuration chosen and its right nearest-neighbor local configuration, and after that shifting simultaneously the right nearest-neighbor and the right next nearest-neighbor local configurations by distance 1 to the right. Each of the three reshuffles of local configurations increases the energy by no more than W. Thus, a 6-site gap can be created at the cost that does not exceed $3W$. Now inserting a 2-molecule in the middle of the 6-site gap created will cost no more than $4W + V_2(1)$. Therefore, we can set $\Delta = 7W + V_2(1)$.

5. SOME EXTENSIONS OF THE MAIN RESULT AND APPLICATIONS

The both lemmas, formulated and proved in the previous section, set conditions on the value of V_2 at distance one, which go in opposite directions. It is for this reason that in Theorem 1 this value is set to zero. However, it is not hard to see that with some effort this conditions can be relaxed.

First, suppose $V_2(1) < 0$. This condition fits the assumptions of Lemma 1 but not those of Lemma 2. In the latter case, the energy gain on breaking forbidden triples of particles is as before $V_2(2) + V_2(1)$ but is diminished now by the second term and may even become negative. On the other hand, the energy increase on inserting a 2-molecule into a six-site gap, $4W + V_2(1)$, is also diminished, again provided the latter expression is positive. Thus, Theorem 1 holds true also for $V_2(1) < 0$, but such that $V_2(2) \geqslant (7W - V_2(1))/2$, which can only take place if $|V_2(1)| < 2V_2(2)$.

Second, suppose $V_2(1) > 0$. Now, in turn, this condition fits the assumptions of Lemma 2 but not those of Lemma 1, which is a more severe problem to overcome than the previous one. The final conclusion of our proof of Lemma 1 is a consequence of the fact that the energy difference of an initial local configuration, consisting of two atoms separated by some k 2-molecules, and the final one, consisting of $k+1$ 2-molecules, is not smaller than $V_2(r_{atom}) - V_2(1)$, where r_{atom} is an arbitrary distance between the two atoms in the initial local configuration. If, as we have supposed originally, $V_2(1) = 0$, then the lower bound obtained implies that the energy difference considered is positive what completes our proof of Lemma 1. If however $V_2(1) > 0$, to arrive at the same conclusion by means of a similar proof we would have to limit from above r_{atom}, which is not possible. Instead, we can turn to a strategy analogous to that used in Lemma 2.

In order to restrict the set of possible ground-state configurations to the set $C^1_{2,\rho}$ we have to get rid of forbidden pairs of particles, i.e., particles separated by distance 1. We fix distance $r \geqslant 4$ and choose a particle density $\rho < 1/r$. Removing one particle from each forbidden pair we lower the energy by $V_1(1)$ and arrive at a configuration of lower density, consisting of atoms exclusively. The ground-state configuration among such configurations is a most homogeneous configuration, in which the smallest distance d between neighboring atoms is greater than r. Then we insert back the removed particles in such a way that the smallest distance between neighboring atoms is greater than $[d/2]+1$. Now, if $V_1(1) > 2\sum_{r \geqslant [d/1]+1} V_1(r)$, then the obtained configuration has a lower energy density. Therefore, under the stated conditions, any ground-state configuration consists only of atoms and consequently is a most homogeneous configuration.

Finally, we would like to point out that our Theorem 1 and its generalizations discussed above can be used to study properties of two- and three-dimensional lattice gases.

Consider first a two-dimensional lattice gas on the square lattice $\mathbf{Z}^2$. Let (x, y) be an orthogonal coordinate system, such that the its axes coincide with lattice directions with unit lattice constants. Suppose that with respect to this coordinate system the Hamiltonian H_Λ decomposes into $H^x_\Lambda + H^y_\Lambda$, where H^x_Λ is a sum of two-body potentials supported by pairs of sites along the x-direction, and H^y_Λ is an analogous sum but in the y-direction. Then, knowing the one-dimensional ground-state configurations of H^x_Λ, we can easily construct two-dimensional ground-state configurations of H_Λ. For instance, the particle configurations of lattice lines in the x-direction can be chosen as the ground-state configurations of H^x_Λ, 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. The Hamiltonians considered above naturally appear in surface physics.(11)

Another situation, where our results are applicable, is the realm of three-dimensional layered systems, like those studied extensively by Fisher and collaborators, see for instance ref. 10.

APPENDIX

Definition 1. We say that a real function f, defined on integers $n \geqslant n_0$, is *convex*, if for every $n \geqslant n_0 + 1$ the following inequality is satisfied:

$$f(n+1) + f(n-1) \geqslant 2f(n) \tag{68}$$

Lemma A1 (Convexity of decreasing f in $\mathbf{Z}$). Let integers x, y, s, t satisfy the inequalities

$$n_0 \leqslant x \leqslant s < t \leqslant y \qquad \text{and} \qquad x + y \leqslant s + t \tag{69}$$

and let f be a convex and decreasing function for integers $n \geqslant n_o$. Then

$$f(x) + f(y) \geqslant f(s) + f(t) \tag{70}$$

Definition 2. For any positive integer n, $[n/2]$ is the greatest integer that does not exceed $n/2$ while $\{n/2\} = n - [n/2]$.

Lemma A2 (Properties of bracket functions $[\,.\,]$ and $\{\,.\,\}$). For positive integers $n \leqslant m$, $[n/2] \leqslant [m/2]$, and $\{n/2\} \leqslant \{m/2\}$.

Moreover,

$$\left[\frac{m+n}{2}\right] = \begin{cases} \left[\dfrac{m}{2}\right] + \left[\dfrac{n}{2}\right] + 1, & \text{if } m \text{ and } n \text{ are odd} \\ \left[\dfrac{m}{2}\right] + \left[\dfrac{n}{2}\right], & \text{otherwise} \end{cases} \tag{71}$$

and

$$\left\{\frac{m+n}{2}\right\} = \begin{cases} \left\{\dfrac{m}{2}\right\} + \left\{\dfrac{n}{2}\right\} - 1, & \text{if } m \text{ and } n \text{ are odd} \\ \left\{\dfrac{m}{2}\right\} + \left\{\dfrac{n}{2}\right\}, & \text{otherwise} \end{cases} \tag{72}$$

Definition 3. For an ordered pair of positive integers (s, t) we define

$$g(s, t) = \{s/2\} + [t/2] \tag{73}$$

Lemma A3 (Properties of function g). For positive integers $s \leqslant t$,

$$s \leqslant g(s, t) \leqslant t \tag{74}$$

More refined bounds are given in Lemma A4. For positive integers p, s, t

$$g(s+p, t+p) = g(s, t) + p \tag{75}$$

Lemma A4 (Best bounds for function g). Let n_{even} and m_{even} be two positive even integers and n_{odd} and m_{odd}—two positive and odd integers and let $g_{e,o}$ be an abbreviation for $g(n_{even}, n_{odd})$, etc. Then

EO: (n_{even}, n_{odd})

$(EO1)$ If $n_{even} < n_{odd}$, then $n_{even} \leqslant g_{e,o} \leqslant n_{odd} - 1$

$(EO2)$ If $n_{even} > n_{odd}$, then $n_{odd} \leqslant g_{e,o} \leqslant n_{even} - 1$

$$2g_{e,o} = n_{even} + n_{odd} - 1 \tag{76}$$

OO: (n_{odd}, m_{odd})

$(OO1)$ If $n_{odd} < m_{odd}$, then $n_{odd} + 1 \leqslant g_{o,o} \leqslant m_{odd} - 1$

$(OO2)$ If $n_{odd} > m_{odd}$, then $m_{odd} + 1 \leqslant g_{o,o} \leqslant n_{odd} - 1$

$(OO3)$ If $n_{odd} = m_{odd}$, then $g_{o,o} = n_{odd} = m_{odd}$

$$2g_{o,o} = m_{odd} + n_{odd} \tag{77}$$

OE: (n_{odd}, n_{even})

$(OE1)$ If $n_{odd} < n_{even}$, then $n_{odd} + 1 \leqslant g_{o,e} \leqslant n_{even}$

$(OE2)$ If $n_{odd} > n_{even}$, then $n_{even} + 1 \leqslant g_{o,e} \leqslant n_{odd}$

$$2g_{o,e} = n_{odd} + n_{even} + 1 \tag{78}$$

EE: (n_{even}, m_{even})

$(EE1)$ If $n_{even} < m_{even}$, then $n_{even} + 1 \leqslant g_{e,e} \leqslant m_{even} - 1$

$(EE2)$ If $n_{even} > m_{even}$, then $m_{even} + 1 \leqslant g_{e,e} \leqslant n_{even} - 1$

$$2g_{e,e} = m_{even} + n_{even} \tag{79}$$

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REFERENCES

1. J. Slawny, Low Temperature Properties of Classical Lattice Systems: Phase Transitions and Phase Diagrams, in *Phase Transitions and Critical Phenomena*, Vol. 11, C. Domb and J. L. Lebowitz, eds. (Academic Press, London 1987).
2. M. Bundaru, N. Angelescu, and G. Nenciu, On the ground state of Ising chains with finite range interactions, *Phys. Lett.* **43A**:5 (1973).
3. J. Miękisz and C. Radin, Third law of thermodynamics, *Mod. Phys. Lett. B* **1**:61 (1987).
4. S. Aubry, Exact models with a complete devil's staircase, *J. Phys. C: Solid State Phys.* **16**:2497 (1983).
5. J. Hubbard, Generalized Wigner lattices in one-dimension and some applications to tetracyanoquinodimethane (TCNQ) salts, *Phys. Rev. B* **7**:494 (1978).
6. V. L. Pokrovsky and G. V. Uimin, On the properties of monolayers of adsorbed atoms, *J. Phys. C: Solid State Phys.* **11**:3535 (1978).
7. W. J. Ventevogel, Why do crystals exist? *Phys. Lett.* **64A**:463 (1978); On the configuration of a one-dimensional system of interacting particles with minimum potential energy per particle, *Physica A* **92**:343 (1978).
8. C. Radin, Low temperature and the origin of crystalline symmetry, *Int. J. Mod. Phys. B* **1**:1157 (1987).
9. J. Hubbard, Generalized Wigner lattices and band motion efects, in *Quasi One-Dimensional Conductors II*, Lecture Notes in Physics 96, S. Barišić, A. Bjeliš, J. R. Cooper, B. Leontiš, eds. (Springer Verlag, Berlin, Heidelberg, New York, 1979).
10. M. E. Fisher and A. Szpilka, Domain-wall interactions. I. General features and phase diagrams for spatially modulated phases, *Phys. Rev. B* **36**:644 (1987).
11. N. Ishimura and T. Yamamoto, Commensurate structures of adatoms on a square lattice, *J. Phys. Soc. Japan* **58**:2439 (1989).
12. K. Sasaki, Lattice gas model for striped structures of adatom rows on surfaces, *Surf. Sci.* **318**:L1230 (1994).
13. F. Bagehorn, J. Lorenc, and Cz. Oleksy, A model of linear chain submonolayer structures: application to $L_i/W(112)$ and Li/Mo(112), *Surf. Sci.* **349**:165 (1996).
14. Cz. Oleksy and J. Lorenc, Ground states of a one-dimensional lattice-gas model with an infinite-range nonconvex interaction. A numerical study, *Phys. Rev. B* **54**:5955 (1996).
15. P. Bak and R. Bruinsma, One-dimensional Ising model and the complete devil's stair-case, *Phys. Rev. Lett.* **49**:249 (1982).
16. B. N. J. Persson, Ordered structures and phase transitions in adsorbed layers, *Surf. Sci. Rep.* **15**:1 (1992).
17. M. Marchand, K. Hood, and A. Caillé, Nonconvex interactions and the occurrence of modulated phases, *Phys. Rev. Lett.* **58**:1660 (1987).
18. K. Sasaki and R. B. Griffiths, Equivalence of certain convex and nonconvex models of spatially modulated structures, *J. Stat. Phys.* **53**:1031 (1988).

19. J. L. Raimbault and S. Aubry, Non-$2k_f$ charge density wave induced by phonon dispersion in one-dimensional Peierls conductors, *J. Phys.: Condens. Matter* **7**:8287 (1995).
20. L. M. Falicov and J. C. Kimball, Simple model for semiconductor-metal transitions: SmB_6, and transition-metal oxides, *Phys. Rev. Lett.* **22**:997 (1969).
21. U. Brandt and R. Schmidt, Exact results for the distribution of the *f*-level ground state occupation in the spinless Falicov–Kimball model, *Z. Phys. B* **67**:43 (1987).
22. T. Kennedy and E. H. Lieb, An itinerant electron model with crystalline or magnetic long range order, *Physica A* **138**:320 (1986).
23. P. Lemberger, Segregation in the Falicov–Kimball model, *J. Phys. A* **25**:15 (1992).
24. Ch. Gruber, J. L. Lebowitz, and N. Macris, Ground-state configurations of the one-dimensional Falicov–Kimball model, *Phys. Rev. B* **48**:4312 (1993).
25. C. Gruber, D. Ueltschi, and J. Jędrzejewski, Molecule formation and the Farey tree in the one-dimensional Falicov–Kimball model, *J. Stat. Phys.* **76**:125 (1994).
26. Z. Gajek, J. Jędrzejewski, and R. Lemański, Canonical phase diagrams of the 1D Falicov–Kimball model at $T=0$, *Physica A* **223**:175 (1996).
27. Ya. G. Sinai, *Theory of Phase Transitions: Rigorous Results* (Pergamon Press, Oxford, 1982).
28. A. C. D. van Enter, R. Fernandez, and A. D. Sokal, Regularity properties and pathologies of position-space renormalization-group transformations: scope and limitations of Gibbsian theory, *J. Stat. Phys.* **72**:879 (1993).
29. S. Kakutani, Ergodic theory of shift transformations, *Proc. Fifth Berkeley Sympos. Math. Statist. Probability* **II**:405 (1967).
30. M. Keane, Generalized Morse sequences, *Zeit. Wahr.* **10**:335 (1968).
31. J. Miękisz and C. Radin, How common are incommensurate solids, University of Texas preprint, unpublished (1987).
32. J. Miękisz, An ultimate frustration in classical lattice-gas models, *J. Stat. Phys.* **90**:285 (1998).