The hard-core model on planar lattices: the disk-packing problem and high-density Gibbs distributions

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Abstract

We study dense packings of disks and related phase transitions in the hard-core model of statistical mechanics on unit triangular, honeycomb and square lattices. The model is characterized by a Euclidean exclusion distance \( D > 0 \) and a value of fugacity \( u > 0 \). We use the Pirogov-Sinai theory to study the Gibbs distributions for a general \( D \) in a high-density regime \( u > u_*(D) \). For infinite sequences of values \( D \) we describe a complete phase diagram: it exhibits a first-order phase transition where the number \( E(D) \) of coexisting pure phases grows as \( O(D^2) \). For the remaining values of \( D \), except for those with sliding, there is still a first-order phase transition, and \( E(D) \geq O(D^2) \). However, the exact identification of the pure phases requires an additional analysis. Such an analysis is performed for a number of typical examples, which involves computer-assisted proofs.

The crucial steps in the study are (i) the identification of periodic ground states and (ii) the verification of the Peierls bound. This is done by using connections with algebraic number theory. In particular, a complete list of sliding values of \( D \) has been specified. As a by-product, we solve the disk-packing problem on the lattices under consideration. The number and structure of maximally-dense packings depend on the disk-diameter \( D \), unlike the case of \( \mathbb{R}^2 \).

All assertions have been proved rigorously, some of the proofs are computer-assisted.

1 Introduction

1.1. The hard-core model emerged in XIX Century in an attempt to describe a system of particles viewed as non-overlapping spheres of a non-negligible diameter (Boltzmann, 1872). The model became popular in various areas of theoretical and applied science. In this work, we focus on aspects of the model which are within the remit of the theory of phase transitions.

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We analyze the hard-core (H-C) model on a planar lattice and study configurations, or packings, of hard-disks of diameter $D$ representing particles with the Euclidean exclusion distance $D$ and centers at lattice sites. When the particle density is low, the particle system is in a gaseous phase which is highly disordered, corresponds to low values of fugacity/activity $u$ and is mathematically described in terms of a unique Gibbs distribution (GD).

An important question is how the system evolves when the density/fugacity increases, e.g., whether it undergoes phase transitions. In a high-density regime (where $u$ is large) the H-C model is intrinsically related to the optimal (i.e., maximally-dense) disk-packing problem. On a lattice, a high-density H-C particle system is expected to become ordered, i.e., to be in a crystalline/solid phase (one or several). This is the principal question addressed in the current paper.

Mathematically, the above question is about the structure of high-density GDs for the H-C model on a lattice in a large-fugacity regime. We focus on unit triangular, honeycomb and square lattices, $A_2$, $H_2$ and $Z^2$. It turns out that only attainable values of $D$ are of interest, i.e., those that can be realized on the corresponding lattice. On $A_2$ and $H_2$ the values $D^2$ are of the form $D^2 = a^2 + b^2 + ab$, while on $Z^2$ they obey $D^2 = a^2 + b^2$, where $a, b$ are non-negative integers. (For a non-attainable disk diameter $D'$ one has to apply our results for the smallest attainable $D$ such that $D > D'$.)

A complete description of the high-density phase diagram requires the determination of all pure phases; mathematically it means an identification of extreme Gibbs distributions (EGDs). A popular tool here is the Pirogov-Sinai (PS) theory based on (i) a specification of periodic ground states (PGSs) and (ii) verification of the Peierls bound for the statistical weight of a deviation of an admissible particle configuration from a PGS.

Lattice H-C models attracted a considerable interest and have a history in statistical mechanics. The existence of multiple EGDs in a high-density regime has been established (i) in $[2]$ on $Z^d$ ($d > 1$) for $D = \sqrt{2}$, (ii) in $[6]$ on $A_2$ for a family of values $D$ and (iii) for a class of non-sliding H-C lattice particle systems in $[7]$. In relation to the H-C model on $A_2$, $H_2$ and $Z^2$, our work includes these results as partial cases of a general theory covering all attainable values of $D$.

The set of attainable values of $D$ is partitioned into groups characterized by different structures of EGDs. For some explicitly determined infinite sequences of numbers $D$ we provide a complete picture of the set of the EGDs. It yields a first-order phase transition where every PGS generates an EGD, and the number $E(D)$ of the EGDs grows as $O(D^2)$. For the remaining infinite sets of values $D$, except for 39 particular numbers on $Z^2$ and 4 on $H_2$, there is still a first-order phase transition, and $E(D) \geq O(D^2)$, but not all PGSs generate EGDs. Here the problem is reduced to an identification of dominant PGSs, which is done for a selection of typical examples. The 43 values of $D$ excluded from our considerations exhibit a phenomenon of sliding, and for them the PS theory is not applicable.

1.2. In the course of identifying ground states we solve the disk-packing problem on the lattices under consideration. For any attainable $D$ we establish the supremum of the disk-packing density among all packings (both periodic and non-periodic) and show that it is achievable.

Let $W = A_2, H_2, Z^2$ and $\Lambda_l$ be a square of side-length $l$ on $\mathbb{R}^2$. We define the maximal
disk-packing density by

\[ \delta(D, \mathbb{W}) := \sup_\Phi \left\{ \limsup_{l \to \infty} \frac{\text{Area}(\Phi \cap \Lambda_l)}{\text{Area}(\Lambda_l)} \right\}, \]

where \( \Phi \) is a packing of disks of diameter \( D \) with centers at sites of \( \mathbb{W} \).

For any attainable \( D \) on \( \mathbb{A}_2 \) and for any attainable \( D \) such that \( D^2 \) is divisible by 3 on \( \mathbb{H}_2 \)

\[ \delta(D, \mathbb{A}_2) = \delta(D, \mathbb{H}_2) = \frac{\pi}{2\sqrt{3}}, \]

(which is the maximal disk-packing density on \( \mathbb{R}^2 \)).

For all attainable \( D \) with \( D^2 \notin \mathcal{N} := \{1, 4, 7, 13, 16, 28, 31, 49, 64, 67, 97, 133, 157, 256\} \) and \( D^2 \) is non-divisible by 3 on \( \mathbb{H}_2 \)

\[ \delta(D, \mathbb{H}_2) = \frac{\pi D^2}{2\sqrt{3}(D^*)^2}, \]

where \( D^* > D \) is the closest attainable number with \((D^*)^2\) divisible by 3. For the case \( D^2 \in \mathcal{N} \) on \( \mathbb{H}_2 \), we refer the reader to [8].

For all attainable \( D \) on \( \mathbb{Z}^2 \)

\[ \delta(D, \mathbb{Z}_2) = \frac{\pi D^2}{4S(D)} , \]

where \( S(D)/2 \) is the solution to optimization problem (5); see below.

Furthermore, for any attainable non-sliding \( D \) we describe all periodic optimizers, i.e., periodic packings achieving the maximal density. On \( \mathbb{A}_2 \) these are \( D \)-sub-lattices and their shifts (see sub-section 3.2), while on \( \mathbb{Z}_2 \) they are the so-called MDA-sub-lattices and their shifts (see sub-section 3.5). On \( \mathbb{H}_2 \) the optimizers are \( D \)-sub-lattices and their shifts when \( D^2 \) is divisible by 3, and \( D^* \)-sub-lattices and their shifts when \( D^2 \notin \mathcal{N} \) and \( D^2 \) is not divisible by 3 (see sub-section 3.4). For \( D^2 \in \{1, 13, 16, 28, 49, 64, 67, 97, 157, 256\} \) the optimal packings are not necessarily sub-lattices: cf. [8]. For the 43 sliding values \( D \) (on \( \mathbb{Z}_2 \) and \( \mathbb{H}_2 \)), we construct infinitely many maximally-dense periodic packings.

We would like to note that, for each of \( \mathbb{A}_2, \mathbb{Z}_2 \) and \( \mathbb{H}_2 \), there are infinitely many values of \( D \) for which the optimizer is unique up to lattice symmetries, and there are also infinitely many values of \( D \) with multiple, but finitely many, optimizers up to lattice symmetries. Moreover, these alternatives exhausts all attainable non-sliding values of \( D \). The number of optimal packings depends upon \( D \); on \( \mathbb{Z}_2 \) and \( \mathbb{H}_2 \) the disks in these packings do not necessarily touch their ‘neighbors’. Dense-packings on \( \mathbb{A}_2 \) have been also considered in [1].

### 2 Gibbs distributions

#### 2.1 A D-admissible configuration (D-AC) on \( \mathbb{W} \) is a map \( \phi : \mathbb{W} \to \{0, 1\} \) such that dist(\( x, y \)) ≥ \( D \), for all \( x, y \in \mathbb{W} \) with \( \phi(x) = \phi(y) = 1 \). Sites \( x \in \mathbb{W} \) with \( \phi(x) = 1 \) are treated as occupied, those with \( \phi(x) = 0 \) as vacant. The set of D-ACs is denoted by \( \mathcal{A}_D(\mathbb{W}) \). Similar definitions can be introduced for a subset \( \mathbb{V} \subseteq \mathbb{W} \). Cf. Fig. 1.
Given $V \subseteq W$, we say that configuration $\psi \in \mathcal{A}(D, V)$ is compatible with $\phi \in \mathcal{A}$ if the concatenation $\psi \vee (\phi|_{W\setminus V}) \in \mathcal{A}$. Define the probability distribution $\mu_V(\cdot || \phi)$ on $\mathcal{A}(D, V)$:

$$
\mu_V(\psi || \phi) := \begin{cases} 
u^\psi, & \text{if } \psi \text{ is compatible with } \phi, \\ 0, & \text{otherwise}. \end{cases}
$$

(1)

Here $\sharp \psi$ stands for the number of occupied sites in $\psi \in \mathcal{A}(D, V)$ and $Z(V || \phi)$ is the partition function in $V$ with the boundary condition $\phi \in \mathcal{A}$:

$$
Z(V || \phi) := \sum_{\psi \in \mathcal{A}(D, V)} u^{\sharp \psi} 1(\psi \text{ is compatible with } \phi).
$$

(2)

$\mu_V(\cdot || \phi)$ is called an H-C Gibbs distribution in ‘volume’ $V$ with the boundary condition $\phi$ at fugacity $u > 0$.

![Figure 1: An admissible configuration](image)

2.2. A Gibbs distribution $\mu$ on $W$ is defined as a (weak) limiting point of $\mu_{V_n}(\cdot || \phi)$ as $V_n \nearrow W$ in the Van Hove sense (the boundary condition $\phi$ may vary with $V$). It is a (Borel) probability measure on $\mathcal{A}$. The Gibbs distribution

$$
\lim_{V_n \nearrow W} \mu_{V_n}(\cdot || \phi),
$$

(3)

if it exists, is denoted by $\mu_\phi$; we say that $\mu_\phi$ is generated by $\phi \in \mathcal{A}$.

The set of Gibbs distributions $\mathcal{G}(D) = \mathcal{G}(D, u, W)$ is a Choquet simplex, so $\mathcal{G}(D)$ is defined by the set $\mathcal{E}(D) = \mathcal{E}(D, u, W)$ of its extreme elements. An extreme Gibbs distribution $\mu \in \mathcal{E}$ has the property that $\mu$ cannot be written as a non-trivial mixture over $\mathcal{G}(D)$.

2.3. This work studies the H-C EGDs for values $u$ large enough; such an assumption is in force throughout the paper and not stressed every time again. The structure of set $\mathcal{E}(D)$ depends both on the choice of lattice $W$ and arithmetic properties of $D$ and is studied by using the PS theory based on the notion of a PGS.

A ground state is defined as a $D$-$\text{AC}$ $\varphi \in \mathcal{A}$ with the property that one cannot remove finitely many particles from $\varphi$ and replace them by a larger number of particles without breaking admissibility. A PGS is a ground state invariant under two non-collinear lattice shifts, hence under their convolutions. A parallelogram spanned by the corresponding vectors is called a period of a PGS. We let $\mathcal{P}(D) = \mathcal{P}(D, W)$ denote the set of PGSs for given $D$ and $W$. 

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The PS theory \cite{10}, \cite{11}, states that, under certain assumptions, (a) every periodic EGD $\mu$ is generated by a PGS $\varphi$ in the sense of Eqn (3): $\mu = \mu_\varphi$, and (b) every periodic EGD $\mu$ has a list of properties stressing its pure-phase character. See items (P1) – (P5) below. According to general results from \cite{3}, in dimension two non-periodic ground states do not generate EGDs. So, identifying the PGSs allows us to describe all EGDs. The assumptions that we need to verify are that (I) there are finitely many PGSs, and (II) a deviation from a PGS is controlled by a suitable Peierls bound based on a suitable notion of a contour. Verifying these assumptions is the central part of this work.

3 Periodic ground states

3.1. Let us consider assumption (I). It turns out that, apart from a few exceptional values of $D$ on $\mathbb{H}_2$ and $\mathbb{Z}^2$ which have to be analyzed separately, the PGSs on $\mathbb{W} = \mathbb{A}_2, \mathbb{H}_2, \mathbb{Z}^2$ are constructed from maximally-dense admissible (MDA) sub-lattices $\mathbb{E} \subset \mathbb{W}$ by means of $\mathbb{W}$-shifts. Non-periodic ground states are commented on in sub-section 3.6.

The $\mathbb{W}$-symmetries ($\mathbb{W}$-shifts and $\mathbb{W}$-reflections/rotations) define a partition of set $\mathcal{P}(D, \mathbb{W})$ into PGS-equivalence classes. Let $K = K(D, \mathbb{W})$ denote the number of PGS-equivalence classes, then $K < \infty$ since each class is represented by MDA-sub-lattice(s). Next, let $\sigma$ stand for the discrete area of the fundamental parallelogram of an MDA-sub-lattice and $m_k$ denotes the number of distinct MDA-sub-lattices within a given PGS-equivalence class, $k = 1, \ldots, K$. Thus, for the cardinality $\sharp \mathcal{P}(D, \mathbb{W})$ of the set of PGSs $\mathcal{P}(D, \mathbb{W})$ we have

$$\sharp \mathcal{P}(D, \mathbb{W}) = \sigma \sum_{k=1}^{K} m_k. \quad (4)$$

Further specifications for $K$, $\sigma$ and $m_k$ depend on the choice of $\mathbb{W}$ and $D$ and are provided below. In particular, dependence upon $D$ is non-monotonic and exhibits connections with algebraic number theory.

3.2. On $\mathbb{A}_2$, for any $D$, every MDA sub-lattice is a $D$-sub-lattice, for which a fundamental parallelogram is formed by two equilateral triangles with side-length $D$ ($D$-triangles). This is due to the fact that a triangular arrangement solves the dense-packing problem in $\mathbb{R}^2$. Consequently, on $\mathbb{A}_2$ the value $\sigma = D^2$.

The number $K$ of PGS-classes is related to the number of solutions $a, b \in \mathbb{Z}, 0 \leq a \leq b$, to the Diophantine equation $D^2 = a^2 + b^2 + ab$, for a given value $D$. A helpful fact is that a solution exists (i.e., $D^2$ is a Löshian number) iff the prime decomposition of $D^2$ has primes of the form $3v + 2$ in even powers.

We will consider three disjoint groups of values of $D$ (or $D^2$) deemed TA1, TA2 and TB, and based on further conditions upon prime factors of $D^2$. The first character in the labels TA1, TA2 and TB reflects the choice of a lattice ($T$ stands for triangular).

First, take the case TA1: here $D^2$ is of the form $D^2 = a^2$ or $D^2 = 3a^2$ where $a \in \mathbb{N}$ has only prime factors 3 or prime factors of the form $3v + 2$, i.e., the prime decomposition of $D^2$ has no primes of form $3v + 1$. Then the above Diophantine equation has a unique solution, and the $D$-sub-lattice is $\mathbb{A}_2$-reflection invariant; consequently, $K = 1$, $m_1 = 1$ and the number of PGSs is $D^2$. 

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Case TA2 emerges when the equation has a unique solution such that \( a < b \), with \( a, b \in \mathbb{N} \). A value \( D^2 \) belongs to this group iff its prime decomposition has a single prime of form \( 3v + 1 \). In this case \( K = 1 \), the \( D \)-sub-lattice is not \( A_2 \)-reflection invariant, \( m_1 = 2 \), and the number of PGSs is \( 2D^2 \). Cf. Fig. 2.

![Figure 2](image)

Figure 2: PGSs on \( A_2 \), for \( D^2 = 9 \) (Case TA1) (a), and \( D^2 = 13 \) (Case TA2) (b). The number of PGSs is 9 and 26, respectively.

The 3rd case, TB, covers all remaining values of \( D \); in this case the equation has multiple solutions. Each solution \( a, b, 0 \leq a \leq b \), generates a PGS-equivalence class, and its cardinality is \( D^2 \) or \( 2D^2 \), similarly to the above cases TA1 and TA2. Cf. Fig. 3.

![Figure 3](image)

Figure 3: PGSs on \( A_2 \) for \( D^2 = 49 \) (Case TB). There are 49 horizontal PGSs (a) and 98 inclined (b). The horizontal PGSs are the only dominant.

3.3. Now consider \( W = \mathbb{H}_2, \mathbb{Z}^2 \). As was said, for some values \( D^2 \) on \( \mathbb{H}_2 \) and \( \mathbb{Z}^2 \) we encounter a phenomenon of sliding. It occurs when one can pass from one PGS to another without any local loss in 'energy' i.e., without decreasing the local particle numbers. As a result, the Peierls bound does not hold, and the PS theory does not apply.

On \( \mathbb{H}_2 \) there are just 4 sliding values: \( D^2 = 4, 7, 31, 133 \); the proof of this fact is computer-assisted. Cf. Fig. 4 (a).

On \( \mathbb{Z}^2 \) there exist 39 sliding values: \( D^2 = 4, 8, 9, 18, 20, 29, 45, 72, 80, 90, 106, 121, 157, 160, 218, 281, 392, 521, 698, 821, 1042, 1325, 1348, 1517, 1565, 2005, 2792, 3034, 3709, 4453, 4756, 6865, 11449, 12740, 13225, 15488, 22784, 29890, 37970 \). Cf. Fig. 4 (b). This was first conjectured by the authors [8], then in [4] it was proved that the sliding list is finite, then finally the completeness of the above list was independently established in [9], [5].
We conjecture that for the sliding values of $D$ on $\mathbb{H}_2$ and $\mathbb{Z}^2$, the EGD is unique for all values of fugacity $u$.

In what follows we consider the non-sliding values of $D$ only.

3.4. Additionally, on $\mathbb{H}_2$ there are exceptional values $D^2 = 1, 13, 16, 28, 49, 64, 97, 157, 256$ where the PGS-class is unique but is non-lattice. Cf. Fig. 5. Furthermore, for $D^2 = 67$ there are two classes one of which is non-lattice. These values are analyzed via a special approach and not discussed in this article.

Thus, in what follows, on $\mathbb{H}_2$ we refer to non-exceptional values of $D$: here every PGS is an MDA-sub-lattice. More precisely, if $3|D^2$ then every PGS is a $D$-sub-lattice since
a $D$-triangle can be inscribed in $\mathbb{H}_2$. Accordingly, we define groups of values $D^2$ deemed HA1, HA2 and HB and formed by the values from cases TA1, TA2 and TB divisible by 3. When $D^2$ belongs to one of these H-cases, the theory goes in parallel to the respective T-case. In particular, this yields the same values $K$, $m_k$ while $\sigma = 2/3D^2$. Cf. Fig. 6.

When $D^2$ is not divisible by 3, we pick the nearest Löschian number $(D^∗)^2 > D^2$ divisible by 3: the fact is that every MDA-sub-lattice is a $D^∗$-sub-lattice in $\mathbb{H}_2$, as triangles with area less than that of the $D^∗$-triangle do not generate $D$-admissible PGSs. This defines a group of values $D^2$ called case HC, for which the above theory is repeated with $D$ replaced by $D^∗$. Cf. Fig. 7.

![Figure 7](image)

**Figure 7**: (a) PGSs on $\mathbb{H}_2$ for $D^2 = 147$ (Case HB). The ‘vertical’ PGSs (black) are dominant. (b) PGSs on $\mathbb{H}_2$ for values $D^2$ from Class HC, with $D^∗^2 = D^2 + 2$, and their associated $D^∗$-triangles (black). (i) For $D^2 = 19$, $D^∗^2 = 21$. (ii) For $D^2 = 61$, $D^∗^2 = 63$. (iii) For $D^2 = 217$, $D^∗^2 = 219$. The gray $\mathbb{H}_2$-triangles give the minimal area when the side-lengths are $\geq D$ and the angles $\leq \pi/2$. However, they do not generate PGSs. The PGSs are MDA-lattices constructed from the black $D^∗$-triangles.

3.5. A different situation emerges on $\mathbb{Z}^2$, where a $D$-triangle can never be inscribed. Nevertheless, every PGS-equivalence class is constructed from an MDA-sub-lattice. The MDA-sub-lattices in $\mathbb{Z}^2$ are defined implicitly, via solutions of a discrete optimization problem

$$\text{minimize the area of a } \mathbb{Z}^2\text{-triangle } \triangle \text{ with side-lengths } \ell_i \geq D \text{ and angles } \alpha_i \leq \pi/2.$$ \hspace{1cm} (5)

The term $\mathbb{Z}^2$-triangle means a triangle with vertices in $\mathbb{Z}^2$. Accordingly, $\sigma = S$ where $S/2$ is the minimum achieved in (5). A minimizing triangle in (5) is referred to as an M-triangle. Adjacent pairs of M-triangles form fundamental parallelograms of MDA-sub-lattices generating the PGSs. Cf. Fig. 8.

Problem (5) always has a solution but the M-triangle $\triangle$ may be non-unique. A delicate point is that there are different types of non-uniqueness of an M-triangle $\triangle$: (i) there are $N_0 > 1$ M-triangles, and they are $\mathbb{R}^2$- but not $\mathbb{Z}^2$-congruent; (ii) there are $N_1 > 1$ M-triangles, and they are not $\mathbb{R}^2$-congruent; (iii) a mixture of (i) and (ii). Cf. Fig. 9. The value $K$ is the number of non-$\mathbb{Z}^2$-congruent M-triangles. Next: (a) $m_k = 1$ if $D^2 = 2$, and (b) $m_k = 2$ or 4 when $D^2 > 2$ and the M-triangle $\triangle$ defining the PGS-equivalence class is isosceles or not, respectively.

Similarly to $\mathbb{A}_2$ and $\mathbb{H}_2$, the identification of PGSs on $\mathbb{Z}^2$ is intrinsically connected with algebraic number theory. It turns out that, for a given $D$, one can characterize
the corresponding M-triangles via solutions to norm equations in ring $\mathbb{Z}[\sqrt{-1}]$. Such a connection helps to prove that uniqueness of an M-triangle and each of non-uniqueness types (i)–(iii) occur for infinitely many values $D$, and the degrees of degeneracy $N_0, N_1$ can be arbitrarily large as $D \to \infty$.

![Figure 8](image)

Figure 8: PGSs on $\mathbb{Z}^2$ for (a) $D^2 = 16, S = 15$ and (b) $D^2 = 25, S = 23$. In both cases, the M-triangles are $\mathbb{Z}^2$-congruent, and there is a single PGS-equivalence class. Consequently, $K = 1$. For $D^2 = 16$ the M-triangles are isosceles, and there are 2 MDA-sub-lattices. For $D^2 = 25$ the M-triangles are non-isosceles, and there are 4 MDA-sub-lattices. Accordingly, $\sigma = 15, m = 2$ for $D^2 = 16$ and $\sigma = 23, m = 4$ for $D^2 = 25$. The number of PGSs is 30 and 92, respectively.

![Figure 9](image)

Figure 9: Non-uniqueness of M-triangles on $\mathbb{Z}^2$: (a) for $D^2 = 425, S = 375$ ($\mathbb{R}^2$-but not $\mathbb{Z}^2$-congruent, $N_0 = 2$) and (b) for $D^2 = 65, S = 60$ ($\mathbb{R}^2$-non-congruent, $N_1 = 2$). Which PGS-class generates EGDs is determined by dominance.

3.6. It is possible to check that any non-periodic ground state on $\mathbb{Z}^2$ contains at least one infinite connected component of non-M-triangles and no finite ones. Moreover, the number of non-M-triangles in a $\mathbb{Z}^2$-square $V(L)$ of side-length $L$ can only grow at most linearly with $L$; this means that in a non-periodic ground state, non-M-triangles form, effectively, a one-dimensional array.

A similar pattern for non-periodic ground states emerges on $A_2$ and $\mathbb{H}_2$. Let us repeat once more that non-periodic ground states do not generate EGDs in dimension two \[3\].
4 The Peierls bound

4.1. Contours. Physically speaking, contours describe local perturbations of PGSs. They emerge when we (i) remove some particles from a PGS $\phi$ and (ii) add some new particles at ‘inserted’ sites, maintaining $D$-admissibility.

A formal definition is as follows. First, we define a template as a common period of all MDA-sub-lattices and its shifts by the multiples of the spanning vectors. Cf. Fig. 10.

![Figure 10: Templates (gray) and fundamental parallelograms on $A_2$ for $D^2 = 7$ (a) and on $Z^2$ for $D^2 = 25$ (b).](image)

We say that a template $F$ is $\phi$-regular in $\phi$ if, $\forall x \in F$, we have $\phi(x) = \varphi(x)$. A template $F$ is called $\varphi$-correct if $F$ and all 8 of its adjacent templates are $\varphi$-regular. The frustrated set is formed by the union of templates that are not $\varphi$-correct $\forall \varphi \in P(D)$.

A contour $\Gamma$ in a $D$-AC $\phi \in A(D)$ is defined as a pair $(S, \phi|_S)$ where $S = \text{Supp}(\Gamma) \subset W$ is a connected component of the frustrated set. We say $\Gamma$ is finite if the set $\text{Supp}(\Gamma)$ is finite.

Let $\Gamma$ be a finite contour in a $D$-AC $\phi \in A(D)$. The complement $W \setminus \text{Supp}(\Gamma)$ has one infinite connected component which we call the exterior of $\Gamma$ and denote by Ext$(\Gamma)$. In addition, set $W \setminus \text{Supp}(\Gamma)$ may have finitely many interior connected components; they are denoted by Int$_j(\Gamma)$, $j = 1, \ldots, J$, and we set Int$(\Gamma) = \bigcup_{j=1}^J \text{Int}_j(\Gamma)$. Cf. Fig. 11. We say that $\Gamma$ is a $\varphi$-contour in $\phi$ if every template $F \subset \text{Ext}(\Gamma)$ adjacent to $\text{Supp}(\Gamma)$ is $\varphi$-correct in $\phi$. We say that $\Gamma$ is an external contour in $\phi$ if $\text{Supp}(\Gamma)$ does not lie in Int$(\Gamma')$ for any other contour $\Gamma'$.

An important point is that a contour can be considered without a reference to the AC $\phi$: it is enough that we indicate (i) a $D$-AC $\psi_T$ over set $\text{Supp}(\Gamma)$, (ii) an external phase $\varphi$ and the internal phases $\varphi_j$, such that every template $F \subset \text{Ext}(\Gamma)$ adjacent to $\text{Supp}(\Gamma)$ is $\varphi$-correct and every template $F \subset \text{Int}_j(\Gamma)$ adjacent to $\text{Supp}(\Gamma)$ is $\varphi_j$-correct, $j = 1, \ldots, J$.

With the above definitions at hand, we write down the contour representation for the partition function:

$$Z(V_n||\varphi) = u^{\sharp(\varphi|_{V_n})} \sum_{\{\Gamma_i\} \subset V_n} \prod_{i} w(\Gamma_i). \quad (6)$$

Here the summation goes over compatible contour collections $\{\Gamma_i\}$ with pair-wise disjoint $\text{Supp}(\Gamma_i) \subset V_n$, while $w(\Gamma)$ stands for the statistical weight of contour $\Gamma$:

$$w(\Gamma) = u^{\sharp(\psi_T) - \sharp(\varphi|_\Gamma)}. \quad (7)$$
Figure 11: Contour supports on $\mathbb{A}_2/\mathbb{H}_2$ (a) and $\mathbb{Z}^2$ (b). Dark-gray color marks non-correct templates, light-gray templates are their neighbors.

Pictorially, compatibility means that if two of contours, $\Gamma$ and $\Gamma'$, from the collection are not separated by a third contour $\Gamma$ then their external and/or internal phases are coordinated. Formally, it requires two properties. (a) If (i) $\text{Supp}(\Gamma') \subset \text{Int}_j(\Gamma)$ and (ii) there is no contour $\Gamma$ in $\{\Gamma_i\}$ with $\text{Supp}(\Gamma) \subset \text{Int}_j(\Gamma)$ and $\text{Supp}(\Gamma) \subset \text{Int}_j(\Gamma)$ then the internal phase $\varphi_j$ of $\Gamma$ serves as the external phase for $\Gamma'$. (b) If (i) $\text{Supp}(\Gamma') \subset \text{Ext}(\Gamma)$ and (ii) there is no contour $\Gamma$ in $\{\Gamma_i\}$ with $\text{Supp}(\Gamma) \subset \text{Ext}(\Gamma)$ and $\text{Supp}(\Gamma') \subset \text{Int}(\Gamma)$ then $\Gamma$ and $\Gamma'$ have the same external phase. Note that all external contours in a compatible collection $\{\Gamma_i\}$ are $\varphi$-contours for the same $\varphi$.

The condition upon $V_n$ in (6) is that $V_n$ is a finite union of templates.

We then can think of a Gibbs distribution $\mu_{V_n}(\cdot \parallel \varphi)$ as a probability measure on compatible contour collections $\{\Gamma_i\}$ in $V_n$.

### 4.2. The Peierls constant

The next step is to establish a bound

$$\sharp(\psi_{\Gamma}) - \sharp(\varphi |_\Gamma) \leq -p \|\text{Supp}(\Gamma)\|.$$  (8)

Here $\|\text{Supp}(\Gamma)\|$ stands for the number of templates in $\text{Supp}(\Gamma)$ and $p = p(D, \mathbb{W}) > 0$ is a Peierls constant per a template. Then the statistical weight $w(\Gamma)$ will obey $w(\Gamma) \leq u^{-p \|\text{Supp}(\Gamma)\|}$, and a standard Peierls argument will lead to properties (P1-5) below.

By the definition of a contour, every template $F \subset \text{Supp}(\Gamma)$ contains some sort of a defect. A trivial defect is when at least one particle can be added to configuration $\psi_{\Gamma} |_F$; in this case we get at least a factor 1 in place of $p$ in inequality (8).

For a saturated defective template $F \subset \text{Supp}(\Gamma)$, the situation is more complex. Here we use the Delaunay triangulation for $\psi_{\Gamma} |_F$; the fact is that for each of the triangles the area is $\geq \sigma/2$, and for at least one triangle the area is $\geq (1 + \sigma)/2$. (Note that the lattice triangle has a half-integer area.) The number of such triangles is $O(\|\text{Supp}(\Gamma)\|)$. On the other hand, the number of particles inside $\text{Supp}(\Gamma)$ equals the doubled number of triangles. This ultimately leads to (8).

The constant $p(D)$ can actually be lower-bounded by $c/D^2$.

### 5 Dominance, extreme Gibbs distributions

#### 5.1. If for a given $D$, the number $K$ of PGS-equivalence classes equals 1, the number
of EGDs \( \sharp \mathcal{E}(D, W) \) equals the number of PGSs \( \sharp \mathcal{P}(D, W) \). When \( K > 1 \), i.e., there are multiple PGS-equivalence classes, not all PGS-classes generate EGDs, only the dominant ones. The dominant classes are those which maximize a ‘truncated free energy’ for the ensemble of small contours; cf. [11].

Thus, for a given non-sliding \( D \),

\[
\sharp \mathcal{E}(D, W) = \sigma \sum_{k=1}^{L} m_k,
\]

where \( L \leq K \) is the number of dominant PGS-equivalence classes. We conjecture that for the H-C model the value \( L = 1 \), that is, there exist a unique dominant PGS-class.

5.2. As an outcome of the PS theory for the H-C model we have the following properties.

(P1) Each EGD \( \mu \in \mathcal{E}(D, W) \) is generated by a PGS. That is, each EGD is of the form \( \mu_\varphi \) for some \( \varphi \in \mathcal{P}(D, W) \). If PGSs \( \varphi_i \) generate EGDs \( \mu_{\varphi_i} \), \( i = 1, 2 \), and \( \varphi_1 \neq \varphi_2 \) then \( \mu_{\varphi_1} \perp \mu_{\varphi_2} \). The EGDs inherit symmetries between the PGSs.

(P2) Consequently, EGD-generation is a class property: if a PGS \( \varphi \in \mathcal{P}(D, W) \) generates an EGD \( \mu_\varphi \) then every PGS \( \varphi' \) from the same equivalence class generates an EGD \( \mu_{\varphi'} \). Such a class is referred to as dominant. If a PGS-equivalence class is unique, it is dominant.

(P3) Each EGD \( \mu_\varphi \) exhibits the following properties. For \( \mu_\varphi \)-almost all \( \phi \in \mathcal{A} \): (i) all contours \( \Gamma \) in \( \phi \) are finite, (ii) for any site \( x \in W \) there exist only finitely many contours \( \Gamma \) (possibly none) such that \( x \) lies in the interior of \( \Gamma \), (iii) there are countably many disjoint \( D \)-connected sets of \( \varphi \)-correct templates one of which is infinite while all remaining \( D \)-connected sets are finite, (iv) for every \( \varphi' \in \mathcal{P}(D, W) \setminus \{ \varphi \} \), there are countably many \( D \)-connected sets of \( \varphi' \)-correct templates all of which are finite.

(P4) EGD \( \mu_\varphi \) admits a polymer expansion and has an exponential decay of correlations.

(P5) As \( u \to \infty \), \( \mu_\varphi \) converges weakly to a measure sitting on a single \( D \)-AC \( \varphi \).

Property (P3) establishes a percolation picture for EGD \( \mu_\varphi \): there is a ‘sea’ of \( \varphi \)-correct templates with ‘islands’ of non-\( \varphi \)-correct sites inside which there may be ‘lakes’ of templates of different correctness, etc. In such a picture, contours mark ‘coastal/shallow-water strips’.

5.3. Specification of dominant PGS-classes for a general value \( D \) remains an open question; we present a complete answer for values \( D^2 = 49, 147, 169 \) on \( \mathbb{A}_2 \) or \( \mathbb{H}_2 \) by classifying the small contours. In doing so we develop an approach which could be used for other examples.

The simplest small contour occurs when we merely remove a particle from a PGS \( \varphi \). Clearly, all PGSs are ‘equal in rights’ relative to this perturbation type, as they are maximally-dense. The same is true about removing pairs of particles, etc. Then there is a possibility of inserting one and removing three particles, at the vertices of the Delaunay triangle of \( \varphi \); these are single insertions. Continuing, we can think of double insertions where pairs of inserted particles remove four particles at the vertices of covering parallelogram in \( \varphi \), and so on, maintaining the difference 2 between the number
of removed and inserted particles (and, of course, \( D \)-admissibility). This yields a finite collection of admissible \( u^{-2} \)-insertions where we add \( n \) and remove \( n + 2 \) particles.

![Figure 12: Dominance on \( A_2 \), for \( D^2 = 147 \). This figure shows admissible \( u^{-2} \)-insertions for \( D^2 = 147 \) on \( A_2 \). Here we have two PGS-equivalence classes, one ‘inclined’ (a, c) and one ‘vertical’ (b, d). Single admissible \( u^{-2} \)-insertions are marked by brown dots (a, b); gray lenses indicate areas from where a single insertion repels four sites in a PGS and hence yields a \( u^{-2} \)-insertion. The number of single \( u^{-2} \)-insertions is 68 per a \( D \)-rhombus for both PGS-classes. Double, triple and quadruple \( u^{-2} \)-insertions are shown on frames (c, d) by red, green and blue colors, respectively. For the inclined class there is no admissible quadruple \( u^{-2} \)-insertion, and for the neither class there is an admissible \( n \)-particle \( u^{-2} \)-insertion with \( n \geq 5 \). The count of all \( u^{-2} \)-insertions shows that the vertical PGS-class is dominant.

In the above-mentioned examples, it is possible to (a) enumerate the \( u^{-2} \)-insertions, and (b) verify that higher-order insertions (beginning with \( u^{-3} \)) can be discarded when fugacity \( u \) is large enough. It allows us to identify the dominant PGS-classes for these values of \( D \). The most involved part of the argument (requiring a computer-assisted proof) is to check that the maximal number of added particles in admissible \( u^{-2} \)-insertions is \( n = 4 \): here we remove 6 occupied sites from the boundary of a \( 2D \)-triangle in a given PGS.
6 Conclusions

In this work we address a construction of the phase diagram for the hard-core model on $A_2, H_2$ and $Z^2$ in a high-density regime. One can say that the H-C model admits a straightforward application of the PS theory, but the challenge here lies in determining PGSs and verifying a suitable Peierls bound. A zest of the work is that the PGSs have been identified by means of algebraic number theory. Since the PGSs coincide with periodic disk-packings of maximal density, we also obtain the description of the latter, which yields a solution to the disk-packing problem on $A_2, H_2$ and $Z^2$.

A number of questions have been answered, covering the phenomenon of sliding and the complete structure of the phase diagram when there is a single PGS-equivalence class. The only remaining question within the remit of the PS theory is how to identify the dominant class(es) among multiple PGS-equivalence classes.

The work also casts light on several important open problems beyond the PS theory. (1) What is the phase diagram as a function of $u > 0$ for non-sliding $D$, including existence of a Kosterlitz–Thouless transition, presence of amorphous/glassy phases, etc. (2) What is the dependence of the critical value(s) of $u$ upon $D$? If point $u^0 = u^0(D)$ separates the uniqueness and non-uniqueness domains, and $u^1(D)$ is the lower threshold for the PS regime, then do we have $u^0(D) = u^1(D)$ for some/all/no $D$? (3) Is there a phase transition in the presence of sliding, and what is the full phase diagram? (4) Could our results provide hints towards understanding the model in $R^2$?

All assertions in this article are mathematically rigorous. The details can be found in [8], [9].

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References

[1] Connelly, R., W. Dickinson. Periodic planar disc packings. Phil. Trans. Roy. Soc., A372, 20120039. http://dx.doi.org/10.1098/rsta.2012.0039

[2] Dobrushin, R. The problem of uniqueness of a Gibbsian random field and the problem of phase transitions. Funct. Anal. Appl., 4:4 (1968), 302–312

[3] Dobrushin, R. and Shlosman, S. The problem of translation invariance of Gibbs states at low temperatures. In: Math. Phys. Reviews, 5, PP 53-195. Harwood Academic Publ., 1985

[4] Krachun, D. Triangles on $Z^2$ and sliding phenomenon. arXiv:1912.07566v1 (2019)

[5] Krachun, D. Extreme Gibbs measures for high-density hard-core model on $Z^2$. arXiv:1912.07566v2 (2020)

[6] Heilmann, O. and Praestgaard, E. Phase transition of hard hexagons on a triangular lattice. J. Stat. Phys., 9 (1973), 1-22
[7] Jauslin, I. and Lebowitz, J. High-fugacity expansion, Lee-Yang zeros and order-disorder transitions in hard-core lattice systems. *Comm. Math. Phys.*, 364 (2018), 655–682

[8] Mazel, A., Stuhl, I. and Suhov, Y. High-density hard-core model on triangular and hexagonal lattices. [arXiv:1803.04041v2] (2020)

[9] Mazel, A., Stuhl, I. and Suhov, Y. High-density hard-core model on $\mathbb{Z}^2$ and norm equations in ring $\mathbb{Z}[\sqrt{-1}]$. [arXiv:1909.11648v2] (2019)

[10] Pirogov, S. and Sinai, Y. Phase diagrams of classical lattice systems. *Teor. Mat. Fiz.* 25, 26 (1975, 1976), 1185-1192, 61-76

[11] Zahradnik, M. An alternate version of Pirogov-Sinai theory. *Comm. Math Phys.*, 93 (1984), 559-581