Kepler’s conjecture and phase transitions in the high-density hard-core model on $\mathbb{Z}^3$

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Abstract

We perform a rigorous study of the identical sphere packing problem in $\mathbb{Z}^3$ and of phase transitions in the corresponding hard-core model. The sphere diameter $D > 0$ and the fugacity $u \gg 1$ are the varying parameters of the model. We solve the sphere packing problem for values $D^2 = 2, 3, 5, 8, 9, 10, 12, 2\ell^2$, $\ell \in \mathbb{N}$. For values $D^2 = 2, 3, 5, 8, 9, 10, 12, 2\ell^2$, $\ell \in \mathbb{N}$ and $u > u^0(D)$ we establish the diagram of periodic pure phases, completely or partially. For the case $D^2 = 2\ell^2$, $\ell \in \mathbb{N}$ we use results from Hales’ proof of Kepler’s conjecture.

1 Introduction

In this work we study the hard-core (HC) model of statistical mechanics on the integer lattice $\mathbb{Z}^3$. Lattice hard-core models attracted a considerable interest \cite{baker, bender, brown, bueken, debruijn2, debruijn1, esteban, freyn, freyn2, freyn3, freyn4, freyn5, freyn6, freyn7, freyn8, freyn9, freyn10, freyn11, freyn12, freyn13, freyn14, freyn15, freyn16, freyn17, freyn18, freyn19, freyn20, freyn21, freyn22, freyn23, freyn24, freyn25, freyn26}. The model is characterized by the value of fugacity $u$ and the (Euclidean) hard-core diameter $D$. The latter specifies the space of admissible configurations of the model. A configuration in $\mathbb{Z}^3$ (or simply, a configuration) is a map $\phi : x \in \mathbb{Z}^3 \mapsto \{0, 1\}$ which is identified with the set $\{x \in \mathbb{Z}^3 : \phi(x) = 1\}$. It is convenient to think that a site $x \in \mathbb{Z}^3$ with $\phi(x) = 1$ is occupied by a particle and a site $x \in \mathbb{Z}^3$ with $\phi(x) = 0$ is vacant in configuration $\phi$. Given $D > 0$, a configuration $\phi$ is called $D$-admissible (or admissible, for short) if $\rho(x, x') \geq D$ for any pair of distinct occupied sites $x, x' \in \phi$ where $\rho$ stands for the Euclidean distance. An admissible configuration is referred to as AC or D-AC; it is interpreted as a configuration of non-overlapping open hard balls (HC particles) of diameter $D$. The set of ACs in $\mathbb{Z}^3$ is denoted by $A_D(\mathbb{Z}^3)$.

It suffices to consider attainable $D \geq 1$ for which $D^2$ is integer, with $D^2 = m^2 + n^2 + k^2$ where $m, n, k \in \mathbb{Z}$, as the model with a non-attainable $D$ is equivalent to the one with the nearest larger attainable value. A distance is attainable if it can be realized on $\mathbb{Z}^3$; throughout the paper we assume attainability without stressing it every time again.

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The other parameter characterizing the HC model is the fugacity (or activity) \( u > 0 \). The energy of a finite configuration \( \phi \in \{0, 1\}^{Z^3} \) for fugacity \( u \) is defined as

\[
H(\phi) = \begin{cases} 
( -\ln u ) \cdot \sharp(\phi), & \phi \in A_D(Z^3), \\
+\infty, & \phi \notin A_D(Z^3).
\end{cases}
\]

(1.1)

Here and below, \( \sharp(\phi) \) stands for the number of particles/occupied sites in \( \phi \); a configuration \( \phi \) with \( \sharp(\phi) < \infty \) is referred to as finite.

A standard question in statistical physics is to describe a complete phase diagram (the structure of pure phases) for all \( u \) and \( D \), which seems to be a problem beyond the reach for the existing methods. In this paper we study periodic pure phases and focus on the case \( u \gg 1 \) when the system shows a tendency to have high particle density. This question is intrinsically related to the dense-packing problem of spheres of diameter \( D \) on lattice \( Z^3 \). Note that in the literature exist several terms: dense-packing, optimal dense-packing, close-packing, densest packing. In Section 2 we provide a formal definition of an equivalent notion of a perfect configuration; this term stresses the fact that such an AC has no local defects. For \( u > 1 \), a periodic dense-packing gives a periodic ground state (PGS) of the model (1.1).

The concept of a PGS carries a particular importance from the statistical physics point of view, as it is used in the Pirogov–Sinai theory \[11, 12, 17\] for generating periodic pure phases (i.e., extreme periodic Gibbs measures, EPGMs for short) by means of polymer expansions. The identification of EPGMs is one of the principal goals of this paper. This identification describes the high-density periodic phase diagram of the model. The phenomenon of non-uniqueness of EPGMs corresponds to a phase transition \[18\] which is a central question in the equilibrium statistical mechanics.

Compared to the continuous cases of \( R^2 \) and \( R^3 \), the respective dense-packing problems on lattices \( Z^2 \) and \( Z^3 \) are more complex, as the structure of dense-packings on \( Z^2 \) and \( Z^3 \) depends on arithmetic properties of \( D \), whereas on \( R^2 \) and \( R^3 \) one can simply let \( D = 1 \). The disk-packing problem on \( Z^2 \) and other 2D lattices has been recently solved in \[36, 37, 38\]. The problem in \( Z^3 \) appears to be harder than in \( Z^2 \); it is related to famous Kepler’s conjecture in \( R^3 \) solved in \[21, 22, 35\]. At present, there is no analog of Kepler’s conjecture for \( Z^3 \), and, as the current paper shows, it is a non-trivial task to suggest the structure of dense-packings for an arbitrary value of \( D \). Our work could be considered as an initial step in studying the problem of sphere-packings in \( Z^3 \) and their random perturbations.

We begin with available analogies between the HC model in \( Z^3 \) and those in \( Z^2 \) and \( R^3 \); one such analogy is the appearance of a sub-lattice as a PGS. Up to Euclidean motions, the only dense-packing of identical spheres in \( R^3 \) which is a lattice is the FCC (face-centered cubic) lattice. Accordingly, the FCC lattice gives rise to a continuum family of layered dense-packing configurations in \( R^3 \); see \[21, 22, 35\]. One of these layered dense-packing configurations is known as HCP (hexagonal closed-packing).

A natural question is: for what values of \( D \) there exist \( D \)-FCC sub-lattices in \( Z^3 \), since in this case the entire family of \( Z^3 \)-PGSs is inherited from \( R^3 \). This question can be answered by means of algebraic number theory. In particular, a dense-packing AC in \( Z^3 \) which is a \( D \)-FCC sub-lattice exists iff \( D^2 = 2\ell^2 \) where \( \ell \in N \) \[25, 26, 28\]. Moreover, for \( D^2 = 2\ell^2 \) there are finitely many \( D \)-FCC sub-lattices in \( Z^3 \), typically more than one. In
both $\mathbb{R}^3$ and $\mathbb{Z}^3$ it is natural to partition dense-packing ACs in general and dense-packing sub-lattices in particular into equivalence classes generated by isometries of $\mathbb{R}^3$ and $\mathbb{Z}^3$, respectively. In contrast to FCC in $\mathbb{R}^3$, not every $D$-FCC sub-lattice in $\mathbb{Z}^3$ generates a continuum of layered dense-packing ACs. It occurs iff $D^2 = 2\ell^2$ where $\ell \in \mathbb{N}$ and $\ell = 0 \mod 3$. Furthermore, for a given $\ell$ there may be one or several equivalence classes of $D$-FCC sub-lattices, and their number depends again on arithmetic properties of $\ell$. In the present work these classes and their symmetries have been studied in detail.

A direct analogy with the case of $\mathbb{R}^3$ stops here; the structure of $\mathbb{Z}^3$-PGSs for a general $D^2 \neq 2\ell^2$ remains unclear. Some of our examples show that $\mathbb{Z}^3$-PGSs are not necessarily layered. Nevertheless, one would like to believe that for any attainable $D$ there are PGSs that are sub-lattices in $\mathbb{Z}^3$ (as it is in the case of $\mathbb{Z}^2$ [36]) but this remains an open (and probably, rather difficult) question. In the case of an affirmative answer, the next question would be how to specify the PGS sub-lattices in terms of $D$.

As was mentioned before, in statistical physics the EPGMs are typically generated by some PGSs, but not necessarily by all of them. Due to the symmetries of the HC model, if a PGS generates an EPGM, then each PGS from the same equivalence class also generates an EPGM. Therefore, an important question is: which of those classes generate EPGMs? This question is naturally connected with the theory of dominant PGSs [6, 43, 47]. Our expectation is that in general only one PGS-equivalence class is dominant (i.e., generates EPGMs), but such a conjecture is far from being proven.

A popular tool for identifying EPGMs is the Pirogov-Sinai (PS) theory. If there are only finitely many PGSs – which happens in a number of cases considered in this paper – then it suffices to verify the Peierls bound in a standard form proposed in [41, 42, 47]; see (2.5) below. However, we also discuss more subtle cases where there are countably many PGSs (and a continuum of dense packings in total). Here we use the approach proposed in [6].

The problem of identifying the dense-packing ACs and the resulting high-density phase diagram for the HC model on $\mathbb{Z}^3$ seems to be rather involved. This work makes steps in this direction: for $D^2 = 2, 3, 5, 8, 9, 10, 12$, and for $D^2 = 2^{2n+1}$, $n \in \mathbb{N}$, we establish the complete diagram of periodic pure phases when $u$ is large enough ($u > u^0(D^2)$). The considered cases already demonstrate a richer variety of answers, compared with $\mathbb{Z}^2$ and $\mathbb{R}^3$.

For $D^2 = 3$ and $D^2 = 12$, the PGSs in $\mathbb{Z}^3$ turn out to be $D$-BCC (body-centered cubic) sub-lattices and their $\mathbb{Z}^3$-shifts; such structures are inherited by the EPGMs. However, this pattern seems exceptional, and we think that $D$-BCC sub-lattices do not arise as PGSs for larger values of $D$. For $D^2 = 8, 9, 10$ the PGSs in $\mathbb{Z}^3$ turn out to be deformed $D$-FCC sub-lattices and their $\mathbb{Z}^3$-shifts; again, such structures persist in the corresponding EPGMs. In contrast to $\mathbb{R}^3$, these sub-lattices do not generate additional layered dense-packings.

However, for $D^2 = 5$ the deformed $D$-FCC sub-lattices do generate additional layered dense-packings. Consequently, there is an infinite degeneracy of PGSs. The ordered EPGMs are generated by deformed $D$-HCP configurations which form the only dominant PGS class. Surprisingly, it is deformed $D$-HCPs, rather than deformed $D$-FCCs, that generate EPGMs. This is due to the fact that $D$-HCPs have a larger density of a specific low-energy excitation. Such a phenomenon seems to be of a generic nature and is observed in other cases discussed below.
For $D^2 = 6$ the situation resembles the case of $D^2 = 5$ but is more involved. Similarly to $D^2 = 5$, there is a single class of dense-packing sub-lattices: it consists of deformed $D$-FCC sub-lattices and their $Z^3$-shifts. However, in contrast to $D^2 = 5$, it generates two rather than one continuum families of layered dense-packings.

For $D^2 = 4, 11$ we have a phenomenon of sliding: here there are countably many PGSs that are not separated enough from each other. The sliding phenomenon has been extensively studied for the HC model in 2D ([36, 37, 34, 20]); in particular, it was established that on $Z^2$ there are only 39 values of $D$ with sliding. A relatively short analytic argument proves sliding for the case $D^2 = 4$. The case of $D^2 = 11$ is considerably more complicated. It requires a chain of analytical constructions which reduce the problem to a non-trivial computer enumeration. A complete list of sliding values of $D$ on $Z^3$ remains open.

For $D^2 = 2\ell^2, \ell \in \mathbb{N}$, the structure of PGSs is inherited from $\mathbb{R}^3$. It is the proof of Kepler’s conjecture by Hales [21, 22, 35] which allows us to obtain the results listed below. In particular, for $D^2 = 2^{2n+1}, n \in \mathbb{N} \cup \{0\}$, there is a single PGS class: it consists solely of $D$-FCC sub-lattices and their $Z^3$-shifts, and there are no other dense-packings. Consequently, for $D^2 = 2^{2n+1}$ each PGS generates an EPGM. For all remaining values of $D^2 = 2\ell^2$ there exist at least two but finitely many PGSs classes, each consisting of $D$-FCC sub-lattices and their $Z^3$-shifts.

If $\ell \neq 0 \mod 3$ then at least one of these classes generates EPGMs. We conjecture that there is always a unique dominant class, but we do not have a generic argument covering all possible values of $\ell$.

If $\ell = 0 \mod 3$ then each class of $D$-FCC sub-lattices gives rise to a continuum family of layered dense-packings. For each class of $D$-FCC sub-lattices the corresponding family contains a class of $D$-HCP configurations. The type of excitations removing infinite degeneracy (similar to the one for $D^2 = 5$) does exist in each of these layered families, and therefore we expect that the corresponding $D$-HCP configurations are the only PGSs that can generate EPGMs when $u$ is large enough. We conjecture that among them only one class of $D$-HCP configurations is dominant.

All in all, we observe two types of infinite degeneracy of PGSs in $Z^3$. In the first case, all dense-packings are split into one or more layered continuum families. In this case we expect the system to be ordered and have a non-unique EPGM for $u$ large enough. In the current paper this fact is proved for $D^2 = 5$, but we believe that our proof reveals the core of the phenomenon and in principle can be extended to all values of $D$ with this type of PGS degeneracy. In the second case, the set of dense-packings is considerably wider and contains both layered and non-layered configurations. For example, such a situation occurs for the value $D^2 = 4, 11$ with sliding. Note that on $Z^2$ the purely layered infinite degeneracy already constitutes sliding.

A summary of our results/conjectures on PGSs and EPGMs is presented in Table 1.

In our opinion, a further progress in the understanding the HC model in $Z^3$ may include answering the following open questions.

1) Is it true that for every attainable $D$ there exists at least one dense-packing AC in $Z^3$ which is periodic?
2) Is it true that for every attainable $D$ there exists at least one dense-packing AC which is a sub-lattice of $\mathbb{Z}^3$?

3) In the case of an affirmative answer to the previous question, is it possible to develop a number-theoretical description of those sub-lattices, similarly to the two-dimensional case?

4) What are the exact values of $D$ with sliding on $\mathbb{Z}^3$? Are there finitely many of them?

5) Does there exist an m-potential representation of the energy in $\mathbf{11}$ for all attainable values of $D$?

6) Does some sort of a Peierls bound hold true for all values of $D$?

7) Is it true that the dominant class of ground states is always unique?

| $D^2$ | ♯ of PGS classes | total ♯ of PGSs | PGS type | density | total ♯ of EPGMs | EPGM type |
|-------|------------------|----------------|----------|---------|----------------|-----------|
| 1     | 1                | 1              | $\mathbb{Z}^3$ | 1       | 1              | $\mathbb{Z}^3$ |
| 2     | 1                | 2              | FCC      | 1/2     | 2              | FCC       |
| 3     | 1                | 4              | BCC      | 1/4     | 4              | BCC       |
| 4     | $\mathbb{N}_0$  | $\mathbb{N}_0$ | sliding  | 1/8     |                |            |
| 5     | $\mathbb{N}_0$  | $\mathbb{N}_0$ | layered  | 1/9     | 72             | dHCP      |
| 6     | $\mathbb{N}_0$  | $\mathbb{N}_0$ | layered  | 1/12    |                |            |
| 8     | 1                | 16             | FCC      | 1/16    | 16             | FCC       |
| 9     | 1                | 120            | dFCC     | 1/20    | 120            | dFCC      |
| 10    | 1                | 208            | dFCC     | 1/26    | 208            | dFCC      |
| 11    | $\mathbb{N}_0$  | $\mathbb{N}_0$ | sliding  | 1/32    |                |            |
| 12    | 1                | 32             | BCC      | 1/32    | 32             | BCC       |
| $2^{2n+1}$ | 1                | $2^{3n+1}$    | FCC      | $1/2^{4n+4}$ | $2^{4n+4}$ | FCC       |
| $2l^2$, $3/l$ | finite | finite | FCC | $1/(2l^4)$ | finite | FCC       |
| $2l^2$, $3/l$ | $\mathbb{N}_0$ | $\mathbb{N}_0$ | layered | $1/(2l^3)$ | finite * | HCP * |

Table 1: A summary of results and conjectures on $\mathbb{Z}^3$
Here ♯ stands for cardinality, * marks a conjectured prediction, prefix d means deformed and an empty cell means that the question is open. The table shows the number of PGS equivalence classes, followed by the total number of PGSs and their type, together with the density of occupied sites in PGSs (the maximal packing density). Next, it indicates the total number of periodic pure phases/EPGMs and their types.

This paper includes 11 sections. In Section 2 we introduce necessary technical concepts. In Sections 3 - 8 we consider the cases of values of $D^2 \leq 12$. Section 9 contains the analysis for $D^2 = 2l^2$, $l \in \mathbb{N}$. Section 10 is an appendix containing the description of cubic and FCC $\ell$-sub-lattices in $\mathbb{Z}^3$, depending on arithmetic properties of $\ell$. Section 11 is an appendix containing a note on the PS theory for an infinite/hard-core potential.
2 The HC model: m-potentials, local repelling forces, perfect configurations, sub-lattices and meshes

We start with the definition of the HC model of statistical mechanics. The model is defined on the unit cubic lattice \( \mathbb{Z}^3 \). The configuration space is

\[
A_D(\mathbb{Z}^3) := \{ \phi \in \{0, 1\}^{\mathbb{Z}^3} : \rho(x', x'') \geq D, \text{ whenever } \phi(x')\phi(x'') = 1, \ x', x'' \in \mathbb{Z}^3 \}. \tag{2.1}
\]

The energy \( H(\phi) \) of a finite configuration \( \phi \in A_D(\mathbb{Z}^3) \) is given by (1.1), and the model is characterized by two varying parameters, \( u \) and \( D \). If \( \phi \in A_D(\mathbb{Z}^3) \) is not finite then (1.1) should be understood as a formal sum.

We analyze the phase diagram of the model focusing on periodic pure phases in a large fugacity regime. The goal is to identify the set \( \mathcal{E}(D, u) \) of EPGMs \[18\] for given values of \( u \) and \( D \). The main assumption throughout the paper is that the value \( u \) is large: \( u \geq u^0 \) where \( u^0 = u^0(D^2) \in (1, \infty) \). Our approach follows the PS theory \[41, 42\] and its developments \[6, 24, 47\]. The PS theory is based on the concept of a ground state (GS). For the model (1.1), a GS is an AC \( \varphi \in A_D(\mathbb{Z}^3) \) such that the energy \( H(\varphi) \) cannot be diminished by admissible perturbations localized in some lattice ball \( B_s(x) = \{ y \in \mathbb{Z}^3 : \rho(x, y) < s \} \). Observe, that for \( u > 1 \), a GS \( \varphi \) is an AC in which one cannot increase the number of particles in any ball \( B_s(x) \).

Typically, the PS theory works with PGSs and aims at constructing EPGMs with the help of absolute convergent polymer expansions around a PGS \[47\]. In this case we say that a PGS generates an EPGM and an EPGM is generated by a PGS. We want to stress that the EPGMs generated by different PGSs are mutually singular \[18\].

A convenient way to identify GSs is to represent the energy in terms of a suitable \( m \)-potential \[24\]: for any finite \( \phi \in \{0, 1\}^{\mathbb{Z}^3} \)

\[
H(\phi) = \sum_{x \in \mathbb{Z}^3} U(\phi |_{B_s(x)}) \tag{2.2}
\]

Here and below \( | \) stands for restriction. The constant \( s \geq D \) is independent of \( \phi \) and \( x \) but may vary with \( D \). By definition, in the HC model \( U(\phi |_{B_s(x)}) = +\infty \) if \( \phi |_{B_s(x)} \) is not admissible. It takes finite values if \( \phi \in A_D(\mathbb{Z}^3) \). We would like to stress that the summation in (2.2) is over all \( x \in \mathbb{Z}^3 \), including the vacant sites in AC \( \phi \). Following \[24\], we say that \( U(\cdot) \) is an \( m \)-potential (for the HC model with given \( u, D \)) if there exists a configuration \( \varphi \in \{0, 1\}^{\mathbb{Z}^3} \), such that

\[
U(\varphi |_{B_s(x)}) = U^0 \ \forall \ x \in \mathbb{Z}^3, \text{ where } U^0 := \min_{x \in \mathbb{Z}^3, \phi \in \{0, 1\}^{\mathbb{Z}^3}} U(\phi |_{B_s(x)}) < +\infty. \tag{2.3}
\]

In particular, \( \varphi \in A_D(\mathbb{Z}^3) \). In what follows we always choose \( U(\cdot) \) to be translation invariant. Hence, \( U^0 = \min\left[ U(\psi) : \psi \in A_D(B_s(o)) \right] \), where \( o \) denotes the origin, and

\[
A_D(B_s(x)) := \{ \phi \in \{0, 1\}^{B_s(x)} : \rho(x', x'') \geq D, \text{ whenever } \phi(x')\phi(x'') = 1, \ x', x'' \in \mathbb{Z}^3 \}. \tag{2.4}
\]

Equivalently, \( \psi \in A_D(B_s(x)) \) is expressed as \( \psi \subseteq B_s(x) \) as an AC is identified with the corresponding set of occupied sites.
We call an AC $\varphi$ satisfying (2.3) a perfect configuration (PC). It is clear that if $\varphi$ is a PC then all its $\mathbb{Z}^2$-shifts $\varphi + x$, $x \in \mathbb{Z}^3$, are PCs. Next, if $\varphi$ is a periodic PC then the collection of its shifts is finite and consists of $v(\mathcal{P}(\varphi))$ distinct PCs, where $\mathcal{P}(\varphi)$ denotes a (lattice) fundamental parallelepiped for $\varphi$ and $v(\mathcal{P}(\varphi))$ stands for the Euclidean volume of $\mathcal{P}(\varphi)$. Observe, that for the HC model, the notion of a PC coincides with the notion of a dense-packing. Consequently, the notion of a periodic PC coincides with the notion of a PGS.

The representation (2.2) of $H$ in terms of an m-potential $U(\cdot)$ (if it exists) is non-unique, but the set of PCs does not depend on the specific choice of the m-potential. Furthermore, if an m-potential exists then a PC is always a GS. Conversely, if an m-potential exists then a PGS is always a PC. Owing to this fact, we will freely pass from periodic PCs to PGSs and back. However, we note that a non-periodic GS is not necessarily a PC.

An advantage of representing $H$ in terms of an m-potential $U(\cdot)$ is that it leads to a convenient description of possible perturbations of a given PC $\varphi$. Suppose an AC $\phi$ differs from $\varphi$ on a finite set in $\mathbb{Z}^3$ and consider the union $V$ of balls $B_s(x)$ such that $U(\phi|_{B_s(x)}) > U^0$. Then, according to [6], the restriction $X := \phi|_V$ is called an elementary excitation, when $V$ has a single connected component. In this case, the set $V$ is called the support of $X$ and is denoted by $\text{Supp}(X)$; its cardinality is denoted by $v(\text{Supp}(X))$. (See definitions on pp. 104-105 and comment 5 on p. 118 in [6].) This matches the definition of a contour in [11, 12, 17]. Owing to a discrete character of our HC model, the quantity

$$U^1 := \min \left[U(\psi) : \psi \in \mathcal{A}_D(B_s(o)), U(\psi) > U^0\right]$$

yields $U^1 > U^0$.

For an elementary excitation $X$, we denote by $v(X)$ the cardinality of the set of $x \in \text{Supp}(X)$ such that $U(\phi|_{B_s(x)}) > U^0$; see p. 106 in [6]. Also, denote by $v(B_s(o))$ the cardinality of the lattice ball $B_s(o)$. Consider a PGS $\varphi$ and an AC $\phi$ which differs from $\varphi$ in a single elementary excitation $X$. Then (cf. the last equation on p. 106 in [6]):

$$H(X) := H(\phi) - H(\varphi) = \sum_{\mathbb{Z}^3 \subseteq X} \left(U(\phi|_{B_s(x)}) - U(\varphi|_{B_s(x)})\right) \geq \frac{(U^1 - U^0)v(X)}{v(B_s(o))} \geq \frac{(U^1 - U^0)v(\text{Supp}(X))}{(v(B_s(o)))^2}.$$  \hspace{1cm}(2.5)

The bound (2.5) is known as the Peierls bound and the value $\frac{U^1 - U^0}{(v(B_s(o)))^2} > 0$ as the Peierls constant (in our case it is proportional to $\ln u$). The Peierls bound is a key ingredient in the PS theory [11, 12, 17]. In this paper, the form of Peierls bound (2.5) suffices for all considered cases, except for $D^2 = 5$. For $D^2 = 5$, the PGS family is countably infinite which requires a more involved version of the Peierls bound; cf. (2.9) in [6].

Let $\varphi'$ and $\varphi''$ be different PCs. Take a parallelepiped $\mathcal{P}$ and consider $\varphi'|_{\mathbb{Z}^3 \setminus \mathcal{P}} \cup \varphi''|_{\mathcal{P}}$. The resulting configuration is not necessarily admissible and some uniquely defined set of particles $\alpha = \alpha(\varphi', \varphi'') \in \varphi'|_{\mathbb{Z}^3 \setminus \mathcal{P}}$ needs to be removed from this configuration to restore the admissibility. Suppose there exist PCs $\varphi'$ and $\varphi''$ such that one can construct a monotonically increasing sequence of parallelepipeds $\mathcal{P}_n$, with $\mathcal{P}(\alpha_n) < C$, where $\alpha_n$ is the
corresponding set of removed particles, $\sharp(\alpha_n)$ is its cardinality and $C$ does not depend on $n$. Then we say that the phenomenon of sliding is exhibited for the corresponding value $D$. A typical scenario of sliding is when some straight line of occupied sites in a PC can be shifted (along itself) without breaking the admissibility of the configuration (and consequently resulting in another PC).

With m-potential at hand without lost of generality one can restrict all considerations to admissible configurations only. Having this in mind throughout this paper we use the following formalism to construct m-potentials $U(\cdot)$. Given an attainable value $D^2$, a local repelling force family (LRFF) is defined as a real function $(x, y) \in \mathbb{Z}^3 \times \mathbb{Z}^3 \mapsto f(x, y) \geq 0$ such that $\forall x, y \in \mathbb{Z}^3$: (i) $f(x, y) \neq 0$, (ii) $f(x, y) = f(y, x)$, (iii) $f(x, y) = 0$ if $\rho(x, y) \geq D$. In all cases under consideration in this paper, $\hat{f}(x, y) = f(\rho(x, y)^2)$, i.e., the local force depends only on the Euclidean distance between $\mathbb{Z}^3$-sites. Consequently, an LRFF is identified with the collection of real values $f(D^2) = \{f(\rho(x, y)^2) : 0 \leq \rho(x, y) < D\}$.

Working with balls $B_s(x)$ we omit subscript $s$ when its value is irrelevant or clear from the context. Given $x \in \mathbb{Z}^3$ and an AC $\psi \in A_D(B(x))$, define
\[
F(\psi) := \sum_{y \in \psi} f(\rho(x, y)^2) \equiv \sum_{y \in B(x)} \psi(y) f(\rho(x, y)^2),
\]
the total force acting on site $x$ in $\psi$. Next, set
\[
F^*(x) := \max \left[ F(\psi) : \psi \in A_D(B(x)) \right].
\]
If there exists an AC $\varphi \in A_D(\mathbb{Z}^3)$ such that $F(\varphi \mid B(x)) = F^*(x)$ for all $x \in \mathbb{Z}^3$ then $-F(\phi \mid B(x))$ is an m-potential. In this case we say that an LRFF $f(D^2)$ generates an m-potential $F(\phi \mid B(x))$ or, in brief, that $f = f(D^2)$ is an m-LRFF (for a given $D^2$).

Observe that for any finite AC $\phi$
\[
\sum_{x \in \mathbb{Z}^3} F(\phi \mid B(x)) = \sum_{x \in \mathbb{Z}^3} \sum_{y \in \phi} f(\rho(x, y)^2) = \sum_{\psi \in \phi} \sum_{x,y \in \mathbb{Z}^3} f(\rho(x, y)^2) = C\sharp(\phi),
\]
where
\[
C := \sum_{x \in \mathbb{Z}^3} f(\rho(x, y)^2) = \sum_{x \in B(y)} f(\rho(x, y)^2).
\]
Let
\[
U(\phi \mid B(x)) := -\ln(u) \frac{1}{C} F(\phi \mid B(x))
\]
then $U(\phi \mid B(x))$ gives an m-potential for $H(\phi)$ from (1.1).

It is convenient to select $f$ in such a way that $F^* = 1$. The motivation comes from the following way of constructing elementary excitations of a PC. Take a PC $\varphi$, insert particles at a finite collection of sites $\xi = \{x_i\} \in A_D(\mathbb{Z}^3)$, and remove those particles from $\varphi$ that have been repelled. (A repelled particle $y \in \varphi$ is the one at distance $< D$ from an inserted site $x \in \xi$.) Let $\eta$ denote the collection of sites where the repelled particles are located: $\eta = \eta(\varphi, \xi) \subseteq \varphi$. Then the resulting AC is $\phi = (\varphi \setminus \eta) \cup \xi$. 

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Let \( \tilde{z}(\xi) \) and \( \tilde{z}(\eta) \) be the numbers of inserted and repelled particles in a PC \( \varphi \), respectively. The difference \( \tilde{z}(\xi) - \tilde{z}(\eta) \), i.e. the energy of the excitation, is counted as follows. Let \( x \in \xi \) be an inserted site and suppose it repels particles located in \( Y(x) = Y(x, \varphi) \subseteq \varphi \), so that \( \eta = \bigcup Y(x) \). Take an LRFF \( f = \{f(\rho(x,y)^2)\} \), then

\[
\sum_{y \in \eta} \left( 1 - \sum_{x \in \xi} f(\rho(x,y)^2) \right) = \tilde{z}(\eta) - \tilde{z}(\xi)
\]

because for a PC \( \varphi \) one has \( \sum_{y \in \eta} f(\rho(x,y)^2) = F^* = 1 \). The quantity

\[
E(y) := 1 - \sum_{x \in \xi} f(\rho(x,y)^2) \geq 0
\]

is called an excess for the repelled particle \( y \in \varphi \) (under insertion \( \xi \)). In the bound \((2.11)\) we use the symmetry of function \( \hat{f} \) and, consequently, of \( f \). Correspondingly,

\[
\tilde{z}(\eta) - \tilde{z}(\xi) = \sum_{y \in \eta} E(y).
\]

The above argument provides a motivation for calling the quantity \( f(\rho(x,y)^2) \) a local repelling force.

The majority of PCs considered below have specific layered structures. One of them is the densest FCC sub-lattice of \( \mathbb{Z}^3 \): which we refer to as \( A_3 \) (with a slight mishandle of notation):

\[
A_3 := \{ \{m(1,1,0) + n(1,0,1) + k(0,1,1) : m, n, k \in \mathbb{Z} \} \}.
\]

Here and below we write a point \( x \in \mathbb{R}^3 \) as a vector with a triple of Cartesian coordinates \((x_1, x_2, x_3)\) where \( x_i \in \mathbb{R} \). The addition of vectors and multiplication by scalars are done in the usual manner, and the shift of a set \( \chi \subset \mathbb{R}^3 \) by a vector \( x \in \mathbb{R}^3 \) is represented as \( \chi + x \). We use the term a mesh for a subset of \( \mathbb{R}^3 \), congruent to a two- or three-dimensional lattice but not necessarily containing the origin. A mesh congruent to a two-dimensional lattice where generating vectors form an equilateral triangle is referred to as triangular. If the equilateral triangle has side-length \( b \), we call it a triangular \( b \)-mesh or – if it is a lattice – a triangular \( b \)-lattice. More generally, a mesh congruent to a lattice with two generating vectors of equal length is called rhombic. A mesh with orthogonal generating vectors is referred to as rectangular; if in addition the generating vectors are of equal length, we say it is a square mesh. The term a square \( b \)-mesh is used when generating vectors have length \( b \).

Layered PCs considered in this paper are unions of equidistant parallel two-dimensional meshes. The first kind of such PCs uses planes orthogonal to a main diagonal in \( \mathbb{R}^3 \). We use index \( i = 0, 1, 2, 3 \) to enumerate the 4 main diagonals \((1, s_2(i), s_3(i))\):

\[
(1, s_2(0), s_3(0)) = (1, 1, 1), \quad (1, s_2(1), s_3(1)) = (1, -1, 1),
(1, s_2(2), s_3(2)) = (1, -1, -1), \quad (1, s_2(3), s_3(3)) = (1, 1, -1).
\]

Given \( k \in \mathbb{Z} \), denote by \( T_{i,k} \) the projection of \( \mathbb{Z}^3 \) into the affine plane

\[
x_1 + s_2(i)x_2 + s_3(i)x_3 = k, \quad k \in \mathbb{Z},
\]
allowing us to obtain a PC for a given $q$ with a finite family of triangular
orthogonal to $(1, s_2(i), s_3(i))$. Then

$$T_{i,k} = \left\{ m \left( \frac{1}{3}, \frac{2s_2}{3}, \frac{s_3}{3} \right) + n \left( -\frac{1}{3}, -\frac{s_2}{3}, \frac{2s_3}{3} \right), \ m, n \in \mathbb{Z} \right\} + \frac{k}{3}(1, s_2, s_3), \quad (2.15)$$

is a triangular $\sqrt[3]{2/3}$-mesh; we refer to it as basic. Given $q \in \mathbb{N}$ and $i, k$ as above, we work with a finite family of triangular $\sqrt[q]{q}$-sub-meshes $\tau^{(q)}_{i,k,j} \subset T_{i,k}$, labelled by $j = 0, 1, \ldots, r$.

Sub-meshes $\tau^{(q)}_{i,k,j}$ forming this collection are obtained as some $\mathbb{Z}^3$-shifts of each other. In addition, we fix an $h = h(q) \in \mathbb{N}$, and, given a double-infinite sequence $\{j_k, k \in \mathbb{Z}\}$ with digits $j_k = 0, 1, \ldots, r$, consider the layered AC

$$\bigcup_{k \in \mathbb{Z}} \tau^{(q)}_{i,hk,j_k} \quad (2.16)$$

and its $\mathbb{Z}^3$-shifts. In case when we use the above construction we specify the corresponding values $q$, $h(q)$, the family of meshes $\tau^{(q)}_{i,hk,j}$, $0 \leq j \leq r$, and the type of sequence $\{j_k\}$ allowing us to obtain a PC for a given $D^2$ via $(2.16)$. An important class is formed by periodic layered PCs where the corresponding sequence $\{j_k\} = j_0 \ldots j_p$ is obtained by repeating a finite string $j_0 \ldots j_p$.

The second kind of layered PCs uses planes orthogonal to non-main diagonals. As above, we use index $i = 0, \ldots, 5$ to enumerate the 6 non-main diagonals $(s_1(i), s_2(i), s_3(i))$:

$$
\begin{align*}
(s_1(0), s_2(0), s_3(0)) &= (1, 1, 0), \quad (s_1(1), s_2(1), s_3(1)) = (-1, 1, 0); \\
(s_1(2), s_2(2), s_3(2)) &= (1, 0, 1), \quad (s_1(3), s_2(3), s_3(3)) = (-1, 0, 1), \\
(s_1(4), s_2(4), s_3(4)) &= (0, 1, 1), \quad (s_1(5), s_2(5), s_3(5)) = (0, -1, 1). \\
\end{align*} \quad (2.17)
$$

Similarly to the previous construction, given $k \in \mathbb{Z}$, we denote by $Q_{i,k}$ the projection of $\mathbb{Z}^3$ to the affine plane

$$s_1(i)x_1 + s_2(i)x_2 + s_3(i)x_3 = k, \quad k \in \mathbb{Z},$$

orthogonal to non-main diagonal $(s_1(i), s_2(i), s_3(i))$. Then

$$Q_{i,k} = \{ m \cdot a + n \cdot b, \ m, n \in \mathbb{Z} \} + \frac{k}{2}(s_1(i), s_2(i), s_3(i)) \quad (2.18)$$

where

$$a := (1 - |s_1(i)|, 1 - |s_2(i)|, 1 - |s_3(i)|) \quad (2.19)$$

and

$$b := \frac{1}{2} \left( s_2(i) - s_2(i)|s_3(i)| - s_3(i) + s_3(i)|s_2(i)|, \\
s_3(i) - s_3(i)|s_1(i)| - s_1(i) + s_1(i)|s_3(i)|, \\
s_1(i) - s_1(i)|s_2(i)| - s_2(i) + s_2(i)|s_1(i)| \right). \quad (2.20)$$

It is not hard to see that $Q_{i,k}$ is a rectangular $(1 \times \sqrt{2}/2)$-mesh which we again call basic. Given $q_1, q_2 \in \mathbb{N}$ and $i, k$ as above, we work with a finite family of rhombic $\sqrt[q_1]{q_1}, \sqrt[q_2]{q_2}$-sub-meshes $\tau^{(q_1,q_2)}_{i,k,j} \subset Q_{i,k}$, $j = 0, 1, \ldots, t$. Here $\sqrt[q_1]{q_1}, \sqrt[q_2]{q_2}$ are the lengths of the diagonals
in a rhombus with side-length $\sqrt{q_1 + q_2}/2$ emerging in the analysis. As above, sub-meshes $\alpha_{i,hk,j}^{(q_1,q_2)}$ are obtained as some $\mathbb{Z}^3$-shifts of each other. Next, we fix an $h = h(q_1, q_2) \in \mathbb{N}$ and, given a double-infinite sequence $\{j_k, k \in \mathbb{Z}\}$ with digits $j = 0, 1, \ldots, t$, consider the layered AC

$$\bigcup_{k \in \mathbb{Z}} \alpha_{i,hk,j_k}^{(q_1,q_2)}$$

and its $\mathbb{Z}^3$-shifts. The value $h$ and the precise form of meshes $\alpha_{i,hk,j}^{(q_1,q_2)}$ are chosen so that the ensuing layered configuration (2.21) gives a PC. In case when we use the above construction we specify the corresponding values $q_1, q_2, h(q_1, q_2)$, the family of meshes $\alpha_{i,hk,j}^{(q_1,q_2)}$, $0 \leq j \leq t$, and the type of sequence $\{j_k\}$ allowing us to obtain a PC for a given $D^2$ via (2.21).

Finally, an analogous construction can be performed when we choose planes $x_i = 0$, $i = 1, 2, 3$, orthogonal to the coordinate axes. The projection $Z_{i,k}$ of $\mathbb{Z}^3$ to the affine plane $x_i = k$ is congruent to the two-dimensional square lattice $\mathbb{Z}^2$, and, given $q \in \mathbb{N}$, we work with a finite family of square $\sqrt{q}$-sub-meshes $\theta_{i,k}^{(q)} \subset Z_{i,k}$, $j = 0, 1, \ldots, u$. As before, sub-meshes $\theta_{i,k}^{(q)}$ are obtained as some $\mathbb{Z}^3$-shifts of each other. Again, we fix an $h = h(q) \in \mathbb{N}$ and, given a double-infinite sequence $\{j_k, k \in \mathbb{Z}\}$ with digits $j_k = 0, 1, \ldots, u$, consider the layered AC

$$\bigcup_{k \in \mathbb{Z}} \theta_{i,hk,j_k}^{(q)}$$

and its $\mathbb{Z}^3$-shifts. The value $h$ and the precise form of meshes $\theta_{i,hk,j_k}^{(q)}$ are chosen so that the ensuing layered configuration (2.22) gives a PC. In case when we use the above construction we specify the corresponding values $q$, $h(q)$, the family of meshes $\theta_{i,hk,j_k}^{(q)}$, $0 \leq j \leq u$, and the type of sequence $\{j_k\}$ allowing us to obtain a PC for a given $D^2$ via (2.22).

In the forthcoming sections we establish a number of theorems and put forward some conjectures on PCs and EPGMs by following a standardized scheme. The main step in the analysis of PCs is the identification of an LRFF $f(D^2)$ generating an m-potential $U(\cdot)$ for a given $D^2$. First, we select the values $f(\rho(x,y)^2)$. Next, we verify that $F^* = 1$; it includes – for $D^2 = 5, 6, 8, 9, 10, 12$ – the use of a computer routine VerifyForces.java. Then we present a single PC which justifies the m-potential property of the proposed family $f(D^2)$. Finally, we use results of VerifyForces.java combined with appropriate analytic arguments to enlist all PCs for $f(D^2)$ and, consequently, for the value $D^2$. This solves the sphere-packing problem on $\mathbb{Z}^3$ for the values of $D^2 = 2, 3, 4, 5, 6, 8, 9, 10, 12$. The case of $D^2 = 11$ uses an alternative computer-assisted approach. A different scheme is used for the values $D^2 = 2\ell^2$, $\ell \in \mathbb{N}$, where the m-potential emerges from results of [21, 22, 35]. In both cases the ensuing analysis of the EPGMs is based on the PS theory and its extensions.

Finally, we would like to note a difference between HC models on $\mathbb{Z}^2$ and $\mathbb{Z}^3$ which is that on $\mathbb{Z}^3$ – in contrast to $\mathbb{Z}^2$ – there are non-periodic extreme Gibbs measures. The analysis of such Gibbs measures can be carried similarly to [13], but this is outside of the scope of this paper.
3 Cases $D^2 = 2, 3, 4$

3.1 $D^2 = 2$.

This is historically the first case, considered in [12]. For $D^2 = 2$, an LRFF family $f = f^{(2)}$ has

$$f(0) = 1, f(1) = \frac{1}{6}. \quad (3.1)$$

Here the balls $B(x) = B_{\sqrt{2}}(x)$ contain 7 sites. Each $\psi \in A_{\sqrt{2}}(B(x))$ contains at most 6 particles. Consider the potential function $U(\psi) = U^{(2)}(\psi)$:

$$U(\psi) = \frac{1}{2} \sum_{y \in B(x)} \psi(y) f(\rho(x, y)^2). \quad (3.2)$$

The normalizing constant $C$ from (2.9) equals 2. For any finite $\phi \in A_{\sqrt{2}}(\mathbb{Z}^3)$, we have $\sharp(\phi) = \sum_{x \in \mathbb{Z}^3} U(\phi_{|B(x)})$, in agreement with (2.8).

A direct calculation shows that the lattice

$$\varphi^{(2)} := \{ m(1, 1, 0) + n(1, 0, 1) + k(0, 1, 1) : m, n, k \in \mathbb{Z} \} = A_3 \quad (3.3)$$

is a PC. The fundamental parallelepiped for $\varphi^{(2)}$ has volume 2. Consider the collection $S^{(2)}$ of $\mathbb{Z}^3$-shifts of $\varphi^{(2)}$.

**Theorem 3.1A.** Set $S^{(2)}$ exhausts all PC$s for $D^2 = 2$. The cardinality of $S^{(2)}$ is 2. Every PC is periodic. The PCs are $\mathbb{Z}^3$-symmetric to each other. The particle density of any PC equals 1/2.

**Proof.** The assertion follows directly from (3.1) and (3.3). ■

**Theorem 3.1B.** [12] Let $u$ be large enough: $u \geq u^0(2)$. Then there are 2 EPGMs, i.e., $\sharp(\mathcal{E}(\sqrt{2}, u)) = 2$, and each EPGM is generated by a PGS from $S^{(2)}$.

**Proof.** Follows from Theorem 3.1A, the Peierls bound (2.5) and the PS theory. ■

The original proof of Theorem 3.1B was given in [12] before the notion of an m-potential and the PS theory had been invented.

3.2 $D^2 = 3$.

For $D^2 = 3$, an LRFF family $f = f^{(3)}$ has

$$f(0) = 1, f(1) = f(2) = \frac{1}{6}. \quad (3.4)$$

Here the balls $B(x) = B_{\sqrt{3}}(x)$ contain 19 sites. Each $\psi \in A_{\sqrt{3}}(B(x))$ contains at most 6 particles. Consider the potential function $U(\psi) = U^{(3)}(\psi)$:

$$U(\psi) = \frac{1}{4} \sum_{y \in B(x)} \psi(y) f(\rho(x, y)^2). \quad (3.5)$$
It is not hard to see that \( \phi \) possibility of constructing a continuum of PCs. For example, take PC a finite subset in \( \mathbb{Z}^3 \).

A direct calculation shows that the lattice

\[
\varphi^{(3)} := \{ m(2,0,0) + n(0,2,0) + k(1,1,1) : m,n,k \in \mathbb{Z} \} \quad (3.6)
\]
is a PC: it is a \( \sqrt{3} \)-BCC sub-lattice in \( \mathbb{Z}^3 \). The fundamental parallelepiped for \( \varphi^{(3)} \) has volume 4. Consider the collection \( S^{(3)} \) of \( \mathbb{Z}^3 \)-shifts of \( \varphi^{(3)} \).

**Theorem 3.2A.** Set \( S^{(3)} \) exhausts all PCs for \( D^2 = 3 \). The cardinality of \( S^{(3)} \) is 4. Every PC is periodic. The PCs are \( \mathbb{Z}^3 \)-symmetric to each other. The particle density of any PC equals \( 1/4 \).

**Proof.** The assertion follows directly from (3.4) and (3.6).

**Theorem 3.2B.** Let \( u \) be large enough: \( u \geq u^0(3) \). Then there are 4 EPGMs, i.e., \( \sharp(\mathcal{E}(\sqrt{3}, u)) = 4 \), and each EPGM is generated by a PGS from \( S^{(3)} \).

**Proof.** Follows from Theorem 3.2A, the Peierls bound (2.5) and the PS theory.

### 3.3 \( D^2 = 4 \).

For \( D^2 = 4 \), an LRFF family \( f = f^{(4)} \) has

\[
f(0) = 1, f(1) = \frac{1}{2}, f(2) = \frac{1}{4}, f(3) = \frac{1}{8}. \quad (3.7)
\]

Here the balls \( B(x) = B_2(x) \) contain 27 sites. Each \( \psi \in \mathcal{A}_2 \) contains at most 8 particles. Consider the potential function \( U(\psi) = U^{(4)}(\psi) \):

\[
U(\psi) = \frac{1}{8} \sum_{y \in B(x)} \psi(y) f(\rho(x,y)^2). \quad (3.8)
\]

The normalizing constant \( C \) from (2.9) equals 8. For any finite \( \phi \in \mathcal{A}_2(\mathbb{Z}^3) \), we have \( \sharp(\phi) = \sum_{x \in \mathbb{Z}^3} U(\phi|_{B(x)}) \), in agreement with (2.8).

Straightforward examples of PCs are a cubic sub-lattice \( \varphi^{(4)}_\varnothing = 2\mathbb{Z}^3 \) and its shifts \( \varphi^{(4)}_\varnothing + x, x \in \mathbb{Z}^3 \), giving 8 PCs in total, of particle density 1/8. However, there is a possibility of constructing a continuum of PCs. For example, take PC \( \varphi^{(4)}_\varnothing \) and let \( S \) be a finite subset in \( \{ x = (x_1, x_2, x_3) \in \varphi^{(4)}_\varnothing : x_3 = 0 \} \). Denote by \( \varphi^{(4)}_S \) an AC obtained from \( \varphi^{(4)}_\varnothing \) by shifting all occupied sites \( y = (y_1,y_2,y_3) \) with \( (y_1,y_2,0) \in S \) to \( y = (y_1,y_2,y_3+1) \). It is not hard to see that \( \varphi^{(4)}_S \) is also a PC.

**Theorem 3.3.** The HC model for \( D^2 = 4 \) exhibits sliding.

**Proof.** Let \( \varphi' = \varphi^{(4)}_\varnothing \), take a square \( S \) of fixed side-length \( l \), and let \( \varphi'' = \varphi^{(4)}_S \). Denote by \( \mathcal{P}_n \) the parallelepiped with the base \( S \) and the height \( n \in \mathbb{N} \). Then the sequence \( \mathcal{P}_n \) is monotonically increasing, while \( \sharp(\alpha_n) \leq 2l^2 \).
Let us now describe the set of all PCs for $D^2 = 4$. Fix one of the coordinate directions, say along the $x_3$-axis. The construction uses two-dimensional PCs $\varphi_k$ in the horizontal affine planes $x_3 = k$; let us first recall that such PCs are described in the following way, in general, not uniquely. See [36]. We take a square 2-mesh in $\mathbb{Z}_3 := \mathbb{Z}^2 + (0,0,k)$ and put the particles in every site of the mesh. Next, choose a direction, $x_1$ or $x_2$. Then select a collection of one-dimensional 2-meshes parallel to the chosen direction, with particles on them, and shift them in this direction by a unit length. In total, there is a continuum of two-dimensional PCs $\varphi_k$.

Let us now describe the set of all PCs for $D^2 = 4$. Fix one of the coordinate directions, say along the $x_3$-axis. The construction uses two-dimensional PCs $\varphi_k$ in the horizontal affine planes $x_3 = k$. Such PCs are described in the following way, in general, not uniquely (cf. [36]). We take a square 2-mesh in $\mathbb{Z}_3 := \mathbb{Z}^2 + (0,0,k)$ and put the particles in every site of the mesh. Next, choose a direction, $x_1$ or $x_2$. Then select a collection of one-dimensional 2-meshes parallel to the chosen direction, with particles on them, and shift the selected 2-meshes in this direction by a unit length. This gives a continuum of two-dimensional PCs $\varphi_k$.

The obtained PCs on $\mathbb{Z}^3$ form two disjoint categories: $x_3$-even-complete and $x_3$-odd-complete (e-complete and o-complete for short). An e-complete PC has, at each level $x_3 = 2k$, $k \in \mathbb{Z}$, a two-dimensional PC $\varphi_k$ of the above form. The resulting PC on $\mathbb{Z}^3$ is denoted by $\varphi := \bigcup_{k \in \mathbb{Z}} \varphi_k$. An o-complete PC is constructed in a similar manner, with odd layers $x_3 = 2k + 1$ in place of even ones. In addition, every e-complete or o-complete PC $\varphi$ can generate a family of descending PCs obtained by shifting $x_3$-directed copies of $\mathbb{Z}$, with particles at sites of $\varphi$ on it, by a unit length. The same construction can be done for other co-ordinate directions.

In short, we (i) fix one of the co-ordinate directions; (ii) select an e-complete or o-complete PC corresponding to this co-ordinate axis; (iii) finally, construct a PC descending from the selected e-complete or o-complete one. Let $\mathcal{S}^{(4)}$ denote the set of all PCs obtained by the above construction.

**Theorem 3.4.** Set $\mathcal{S}^{(4)}$ exhausts all PCs for $D^2 = 4$. The cardinality of $\mathcal{S}^{(4)}$ is continuum. There are countably many periodic PCs. The particle density of any PC equals 1/8.

**Proof.** Note that open $2 \times 2 \times 2$-cubes $C(x)$ centered at occupied sites $x \in \varphi \in \mathcal{A}_2(\mathbb{Z}^3)$ are pair-wise disjoint. Correspondingly, a PC emerges iff the union of the closures of these cubes covers the entire $\mathbb{R}^3$.

Take an arbitrary PC $\varphi$ and choose one of the co-ordinate directions, say along the $x_3$-axis. Denote by $\Pi(y)$ the ortho-projection of cube $C(y)$ to the horizontal plane $P_{3,0} : x_3 = 0$ in $\mathbb{R}^3$. Let us partition the occupied sites $y = (y_1, y_2, y_3) \in \varphi$ into even and odd categories: even if $y_3$ is even and odd if $y_3$ is odd. We will refer to them as even and odd particles in $\varphi$ and also call the corresponding cubes even or odd, respectively. We claim that two occupied sites, $y_1, y_2 \in \varphi$ such that one of them is even and the other is odd cannot have the intersection $\Pi(y_1) \cap \Pi(y_2)$ with a positive area. In fact, suppose that $\Pi(y_1) \cap \Pi(y_2)$ covers an open unit square $S$. Then either the (infinite) vertical prism $\mathcal{R}$ projected to $S$ has no intersection with a cube $C(y)$ or their intersection is a vertical parallelepiped of height 2 (a vertical 2-brick, for brevity). Thus, we have to cover the piece of $\mathcal{R}$ between $C(y_1)$ and $C(y_2)$ with vertical 2-bricks while the distance between $y_1$
and $y_2$ is odd. This is impossible without having an empty space which implies that $\varphi$ is not a PC. This justifies the claim.

As a result, we get that even and odd cubes are projected into disjoint open $2 \times 2$-squares in plane $P_{3,0}$. In other words, $P_{3,0}$ is partitioned into a pair of even and odd subsets, $V_E$ and $V_O$, and a collection of continuous broken lines representing the boundary between $V_E$ and $V_O$.

Consider a $\mathbb{Z}^2$-site $y \in P_{3,0}$ and the two lines containing $y$ and parallel to the $x_1$- and $x_2$- coordinate axes. If both these lines intersect the boundary between $V_E$ and $V_O$ then for any two cubes $C(\tilde{y}_1), C(\tilde{y}_2)$ with $\Pi(\tilde{y}_i) \ni y$ one has $\Pi(\tilde{y}_1) = \Pi(\tilde{y}_2)$. This is because the projection $\Pi(\tilde{y}_i)$ is at even distances (along the $x_1$- and $x_2$- coordinate axes) from the boundary.

If site $y \in P_{3,0}$ does not have the above property then we have the following cases. (i) None of the above two lines intersects the boundary. (ii) Only one of these lines intersects the boundary.

In case (i), for any site $z \in P_{3,0}$ of the opposite parity to $y$, both corresponding lines intersect the boundary. Consequently, for any such $z$ the projection $\Pi(\tilde{z})$ containing site $z$ is uniquely determined.

In case (ii), assume for definiteness that the line through $y$ which does not intersect the boundary is parallel to the $x_2$-axis. Then for any $z \in P_{3,0}$ of the opposite parity, the line through $z$ parallel to the $x_1$-axis does intersect the boundary. If for any site $z \in P_{3,0}$ of the opposite parity the line through $z$ parallel to the $x_2$-axis also intersects the boundary then the projection $\Pi(\tilde{z})$ containing site $z$ is uniquely determined for such $z$.

In the opposite case we have at least one $z' = (z'_1, z'_2, 0) \in P_{3,0}$ of the opposite parity to $y$ such that the line through $z'$ and parallel to the $x_2$-axis does not intersect the boundary. Moreover, there exists an entire strip of non-uniqueness sites

$$\{z'' = (z''_1, z''_2, 0) \in P_{3,0}, \ z''_2 \in \mathbb{Z}\}. \quad (3.9)$$

Then take all occupied sites $\hat{\varphi} \in \varphi$ such that $\Pi(\hat{\varphi}) \ni z$ where $z \in P_{3,0}$ has the projection-uniqueness property, shift $\hat{\varphi} \mapsto \hat{\varphi} + (0, 0, 1)$, and recalculate the boundary (as such sites $z$ will change their parity). Observe that after this operation the non-uniqueness strip (3.9) remains intact. Among all such strips consider the one which is closest to $y$. Then the vertical line separating this strip from the half of $P_{3,0}$ containing $y$ is necessarily a part of the new boundary. Consequently, the PC $\varphi$ consists of layers orthogonal to the $x_1$-axis.

### 4 Case $D^2 = 5$

For $D^2 = 5$, an LRFF $f = f^{(5)}$ has

$$f(0) = 1, \ f(1) = \frac{2}{3}, \ f(2) = \frac{3}{4}, \ f(3) = f(4) = 0. \quad (4.1)$$

Here the balls $B(x) = B_{\sqrt{3}}(x)$ contain 19 sites. Each $\psi \in \mathcal{A}_{\sqrt{5}}(B(x))$ contains at most 3 particles. Consider the potential function $U(\psi) = U^{(5)}(\psi)$:

$$U(\psi) = \frac{1}{9} \sum_{y \in B(x)} \psi(y)f(\rho(x, y)^2). \quad (4.2)$$
The normalizing constant $C$ from (2.9) equals 9. For any finite $\phi \in A_\sqrt{3}(\mathbb{Z}^3)$, we have

$$f(\phi) = \sum_{x \in \mathbb{Z}^3} U(\phi | B(x)) ,$$

in agreement with (2.8).

The PCs for $D^2 = 5$ are layered ACs emerging from the first construction proposed in Section 2, cf. (2.16). Here $q = 6$, $h = 3$ and $r = 2$, and every $\tau_{i,k,j}^{(6)}$ is a triangular $\sqrt{6}$-sub-mesh in $\mathbb{Z}^3 \cap T_{i,3k}$ where $T_{i,3k}$ is the basic $\sqrt{2}/3$-mesh defined in (2.15). Further, for $i = 0, 1, 2, 3$ and $s_1 = s_1(i), s_2 = s_2(i)$ given by (2.14) we define

$$
\begin{align*}
\tau_{i,3k,0}^{(6)} &:= \{ m(1, -2s_2, s_3) + n(-1, -s_2, 2s_3), m, n \in \mathbb{Z} \} + k(1, s_2, s_3) \\
\tau_{i,3k,1}^{(6)} &:= \tau_{i,3k,0}^{(6)} + (0, s_2, -s_3), \\
\tau_{i,3k,2}^{(6)} &:= \tau_{i,3k,0}^{(6)} + (0, -s_2, s_3).
\end{align*}
$$

(4.3)

It is instructive to note that the occupied sites in meshes $\tau_{i,3k,1}^{(6)}$ and $\tau_{i,3k,2}^{(6)}$ cover the centers of triangles in mesh $\tau_{i,3k,0}^{(6)}$ in an alternating manner: the centers of two neighboring triangles in $\tau_{i,3k,0}^{(6)}$ (sharing a common side) are occupied by particles from two different meshes. In fact, the same is true for any two meshes: their occupied sites cover the centers of triangles in the third mesh, alternately. The allowed sequences $\{ j_k, k \in \mathbb{Z} \}$ have digits $j_k = 0, 1, 2$ with $j_0 = 0$ and $j_k \neq j_{k+1}$. The set $S^{(5)}$ consists of all layered PCs $\bigcup_{k \in \mathbb{Z}} \tau_{i,3k,j_k}^{(6)}$ (see (2.16)) with the allowed sequences $\{ j_k \}$ and $\mathbb{Z}^3$-shifts of these configurations. We also introduce the subset $S^{(5)}_{\text{per}}$ consisting of PCs $\varphi^{(5)}_{i,j_k}$ with periodic allowed sequences $\{ j_k \}$ and the $\mathbb{Z}^3$-shifts of these PCs. (To prevent a confusion, let us emphasize that the superscript (5) for $\varphi$ refers to $D^2$ while the superscript (6) for $\tau$ refers to the mesh size.)

**Theorem 4.1A.** Set $S^{(5)}_{\text{per}}$ exhausts all PCs for $D^2 = 5$. The cardinality of $S^{(5)}$ is continuum. Set $S^{(5)}_{\text{per}}$ is countable and exhausts all periodic PCs for $D^2 = 5$. The particle density of any PC equals $1/9$.

**Proof.** The set of ACs $\psi$ on $B(x)$ which give $U(\psi) = 1/9$ is partitioned into 3 subsets where each subset is characterized by a fixed collection of values $f(\cdot)$ participating in the sum $U(\psi)$

$$
\{ f(0) \}, \{ f(1), f(2) \}, \{ f(2), f(2), f(2) \}.
$$

(4.4)

Assume that a PC $\varphi$ does not contain a pair of particles at distance $\sqrt{6}$. According to (1.4), the only possibility is $\{ f(1), f(2) \}$ and therefore there are two particles at distance $\sqrt{3}$ from each other. For definiteness, take particles at sites $x_1 = (0, 0, 0)$ and $x_2 = (1, 2, 0)$. Consider the vacant site $x_3 = (1, 1, 1)$. The only way to implement the set $\{ f(1), f(2) \}$ is to place a particle at site $(1, 1, 2)$ which is at distance $\sqrt{6}$ from $x_1$ and hence contradicts the assumption. The possible ways to implement the subset $\{ f(2), f(2), f(2) \}$ are to place a particle either at the site $(2, 0, 1)$ or at the site $(2, 1, 2)$. However, both $(2, 0, 1)$ and $(2, 1, 2)$ are at distance $\sqrt{6}$ from $x_2$, which again contradicts the assumption.

Now, take a PC $\varphi$ and a pair of particles at distance $\sqrt{6}$, for definiteness, say $x_1 = (0, 0, 0)$ and $x_2 = (2, 1, 1)$. Consider the vacant site $x_3 = (1, 0, 1)$ which implies $\{ f(2), f(2), f(2) \}$. The only possibility to implement this subset is to place a particle at site $(1,-1,2)$ that forms an equilateral triangle with $x_1$ and $x_2$. Repeating this argument we obtain a triangular mesh. The densest combination of such triangular meshes leads to our family $S^{(5)}$. 

\[\square\]
To state our results on EPGMs for $D^2 = 5$, we introduce a subset $\mathcal{H}(5) \subset \mathcal{S}(5)$ formed by the deformed HCP configurations. These are periodic PCs $\varphi^{(5)}_{1,01}$, $\varphi^{(5)}_{1,02}$ and their $\mathbb{Z}^3$-shifts.

**Theorem 4.1B.** Let $u$ be large enough: $u \geq u^0(5)$. Then there are 72 EPGMs, i.e., $\sharp(E(\sqrt{5}, u)) = 72$, and each EPGM is generated by a PGS from $\mathcal{H}(5)$.

**Proof.** The proof is an application of results of [6]. Applicability of these results needs verification of several conditions, including the bound (2.9) from [6].

We begin this verification starting with Sect 2.1 of [6]. In the definition of the $l$-boundary we use $l = \sqrt{2}$ in contrast to $l = 2$ as chosen in [6], because [6] uses the max-distance metric. Next, in the terminology of Sect 2.2 in [6], a local GS in a domain $\Lambda$ is a configuration $\varphi \in \mathcal{A}(\Lambda)$ such that $U(\varphi|_{B(x)}) = \frac{1}{9}$ for every $x$ with $B(x) \subset \Lambda$.

Next, we need to check the property that two local ground states coinciding on the $l$-boundary coincide on the whole of $\Lambda$. This follows from the argument in the proof of Theorem 4.1A.

For the HC model the statistical weight of any local excitation is of the form $u^{-n}$ where $n$ is a positive integer. Furthermore, the inverse temperature $\beta = \ln u$, and possible values of the excitation energy are positive integers. We choose $E_D = 2$, where $E_D$ is a notation taken from [6]; the subscript $D$ is unrelated to our admissibility distance $D$.

Now, we need to verify the retouch property from [6]. To this end, we have to list all elementary excitations of energy $\leq E_D$, i.e., of energy 1 and 2. Removing a single particle yields an elementary excitation $\gamma_1$ of energy 1. Removing two particles close enough from each other (see the definition of $\text{Supp}(X)$ in Section 2) gives an elementary excitation $\gamma_2$ of energy 2.

**Lemma 4.1.** Elementary excitations $\gamma_1$ have the same density in all PCs. Elementary excitations $\gamma_2$ also have the same density in all PCs.

**Proof.** A direct calculation shows that the density of $\gamma_1$ is $1/9$. The density of $\gamma_2$ is the same for all PCs $\varphi^{(5)}_{i, (j_k)}$ by construction. Namely, if two removed particles are located in the same mesh $\tau^{(6)}_{i, 3k, j_k}$, then the density is the same for all meshes and therefore for all PCs. Similarly, if the removed particles belong to two different meshes at a fixed distance from each other then the density does not depend on the choice of the pair of meshes.

The next excitation of energy 2, $\gamma_2^*$, is constructed as follows. Consider three subsequent meshes $\tau' := \tau^{(6)}_{i, 3(k-1), j_{k-1}}$, $\tau := \tau^{(6)}_{i, 3k, j_k}$, $\tau'' := \tau^{(6)}_{i, 3(k+1), j_{k+1}}$ and assume that in the middle mesh $\tau$ there is a triangle $\Delta_0$ and in meshes $\tau'$, $\tau''$ there are triangles $\Delta_{\pm 1}$, and the centers of $\Delta_{\pm 1}$ are projected to the center of $\Delta_0$. Then, if we place a particle at the center of $\Delta_0$ and remove the particles from the vertices of $\Delta_0$, we obtain excitation $\gamma_2^*$. See Figure 4.1.
Figure 4.1. A dominating excitation for $D^2 = 5$.

The figure shows the projection to plane $x_1 + x_2 + x_3 = 0$ of a PC $\varphi \in \mathcal{H}^{(5)}$. The thin lines in the background form the triangular $\sqrt{2/3}$-lattice $T_{0,0}$. The green lines and circles indicate the triangular $\sqrt{6}$-mesh $\tau_{0,0,0}^{(6)} \subset T_{0,0}$ and the positions of particles in $\tau_{0,0,0}^{(6)}$. The red lines and circles indicate the projections of the triangular $\sqrt{6}$-meshes $\tau_{0,\pm 3,1}^{(6)} \subset T_{0,\pm 3}$ and the positions of particles in $\tau_{0,\pm 3,1}^{(6)}$. The brown lines of length $\sqrt{5}$ join sites from neighboring meshes $\tau_{0,0,0}^{(6)}$ and $\tau_{0,\pm 3,1}^{(6)}$. A hexagon with brown sides encircles the projection of an octahedron, and triples of brown segments indicate the projections of sides of tetrahedrons. None of the octahedrons or tetrahedrons are equilateral: they are all oblate in the direction orthogonal to the plane. The pink circle at the center of the green triangle indicates the position of a local $u^{-2}$-excitation of type (IIa) which removes three particles at the vertices of the corresponding green triangle. Such an excitation has the highest frequency of occurrence in PC $\varphi \in \mathcal{H}^{(5)}$ among all periodic PCs.

The most elaborate part of our argument is

**Lemma 4.2.** The excitations of types $\gamma_1, \gamma_2$ and $\gamma_2^*$ exhausts all elementary excitations of energies 1 and 2.
There is a site $y$ contains 24 inserted particles and leads to 36 repelled particles. See Figure 4.2.

by subsequently throwing away sites $x$ irreducible collection $\xi$ or to a reducible collection $\eta$ is non-feasible, as one cannot add a new insertion site to $\tau$; these two edges have length $\sqrt{6}$ each and the angle between them equals $\pi/3$. Furthermore, the length of the segment that is orthogonal to each of them equals $\sqrt{3}$ and the end-points of this segment divide the edges at the ratio $2 : 1$. Among the remaining four edges of $\mathcal{T}$ (which join $\tau$ and $\tau'$), three have length $\sqrt{5}$ and one has length $\sqrt{11}$. See a tetrahedron with 4 blue edges on Figure 4.2.

(II) Another situation emerges when the site of insertion belongs to the plane containing $\tau$; it happens iff this site is a center of a triangle in $\tau$. Then consider three subsequent meshes $\tau', \tau, \tau''$ as above. Correspondingly, three situations can occur, depending upon the mutual position of $\tau', \tau$ and $\tau''$. (IIa) The inserted particle repels only three particles at the vertices of the triangle in $\tau$. See the pink circle on Figure 4.1. (IIb) The inserted particle repels four particles at the vertices of a tetrahedron whose base is a triangle from $\tau$ and the fourth vertex belongs to $\tau'$ or $\tau''$; three base edges of the tetrahedron have length $\sqrt{6}$ and three other length $\sqrt{5}$. (IIc) The inserted particle repels five particles at the vertices of a triangular bi-pyramid with one vertex in $\tau'$, one in $\tau''$ and three at the vertices of a triangle in $\tau$.

The inserted collection $\xi$ is called reducible if in the corresponding repelled collection $\eta$ there is a site $y$ repelled by a single site $x \in \xi$. For the reduced collection $\xi' = \xi \setminus \{x\}$, the corresponding set $\eta' = (\eta \setminus \{y\})$, and hence $E(\xi') = z(\eta') - z(\xi) - z(\eta) = E(\xi)$.

The next observation is that any reducible collection $\xi$ of energy 2 can be reduced, by subsequently throwing away sites $x_m, \ldots, x_1$ from $\xi$, either to an irreducible inserted collection $\xi_0$ or to a reducible collection $\xi_1$ of type (IIa), both of energy 2. The second option is non-feasible, as one cannot add a new insertion site to $\xi_1$ without increasing the energy. We now show that the first option is also non-feasible, by verifying that any irreducible $\xi$ has energy at least 8. The inserted collection $\xi_0$ with the minimal energy contains 24 inserted particles and leads to 36 repelled particles. See Figure 4.2.

Furthermore, $\xi_0$ is located in 4 consecutive basic $\sqrt{3}/2$-meshes $T_{i,k}, T_{i,k+1}, T_{i,k+2}, T_{i,k+3}$ (more precisely, in the intersections $T_{i,k} \cap \mathbb{Z}^3, T_{i,k+1} \cap \mathbb{Z}^3, T_{i,k+2} \cap \mathbb{Z}^3$ and $T_{i,k+3} \cap \mathbb{Z}^3$), with the distance $1/\sqrt{3}$ between any two neighboring planes containing these meshes. The repelled collection $\eta_0$ is located in triangular meshes $\tau_L \subset T_{i,k}$, and $\tau_U \subset T_{i,k+3}$, (with distance $\sqrt{3}$ between the planes containing $T_{i,k}$ and $T_{i,k+3}$). Figure 4.2 shows the ortho-projection of $\xi_0$ to the plane containing the lower mesh $T_{i,k}$ endowed with this basic triangular mesh of size $\sqrt{2}/3$; the edges of the basic mesh are drawn in thin lines. The green and red circles mark insertions of type (IIa) in $T_{i,k} \cap \mathbb{Z}^3$ and $T_{i,k+3} \cap \mathbb{Z}^3$, respectively. Each such circle is located at the center of a triangle of the same color with the side-length $\sqrt{6}$ and repels the 3 vertices of this triangle. In the figure there are 7 green and 7 red such triangles.
Figure 4.2. The smallest non-removable local excitation for $D^2 = 5$.

The irreducible insertion collection $\xi_0$ is located in 4 consecutive meshes $T_{i,k}, T_{i,k+1}, T_{i,k+2}, T_{i,k+3}$ (more precisely, in the intersections $T_{i,k} \cap \mathbb{Z}^3, T_{i,k+1} \cap \mathbb{Z}^3, T_{i,k+2} \cap \mathbb{Z}^3$, and $T_{i,k+3} \cap \mathbb{Z}^3$), with the distance between neighboring planes $1/\sqrt{3}$. The repelled configuration $\eta_0$ is located in triangular $\sqrt{6}$-meshes $\tau_L \subset T_{i,k}$, and $\tau_U \subset T_{i,k+3}$, (with distance $\sqrt{3}$ between the planes containing $T_{i,k}$ and $T_{i,k+3}$). The figure shows the ortho-projection of $\xi_0$ to the lower mesh $T_{i,k}$ endowed with this basic triangular mesh of size $\sqrt{2}/3$; the edges/links of the basic mesh are drawn in thin lines. The green and red circles mark insertions of type (IIa) in $T_{i,k} \cap \mathbb{Z}^3$ and $T_{i,k+3} \cap \mathbb{Z}^3$, respectively. Each green or red circle removes the 3 vertices of the corresponding green or red triangle of side-length $\sqrt{6}$; the figure contains 7 green and 7 red such triangles.

The blue edges join a repelled site from mesh $\tau_L$ and a repelled site from mesh $\tau_U$, the shorter between these edges have length $\sqrt{5}$ and the longer $\sqrt{11}$. The blue trapezes indicate the ortho-projections of tetrahedrons; each tetrahedron, in addition to 4 blue edges, includes two non-adjacent/skewed edges, one green and one red. The faint green/pink circles indicate insertions that repel the vertices of the tetrahedrons; the faint green circles mark the insertion sites located in $T_{i,k+1} \cap \mathbb{Z}^3$ (there are 3 of them), while the pink circles (another 3) mark the insertion sites located in $T_{i,k+2} \cap \mathbb{Z}^3$. 
The blue edges join a repelled site from mesh $\tau_L$ and a repelled site from mesh $\tau_U$, the shorter between these edges have length $\sqrt{5}$ and the longer $\sqrt{11}$. The blue trapezes indicate the ortho-projections of tetrahedrons; each tetrahedron, in addition to 4 blue edges, includes two non-adjacent/skewed edges, one green and one red. The faint green/pink circles indicate insertions that repel the vertices of the tetrahedrons; the faint green circles mark the insertion sites located in $T_{i,k+1} \cap \mathbb{Z}^3$ (there are 3 of them), while the faint pink circles (another 3) mark the insertion sites located in $T_{i,k+2} \cap \mathbb{Z}^3$. Both the faint green and faint pink insertions are of type (I).

The above collection $\xi_0$ is minimal irreducible due to the following argument. The ortho-projection of any irreducible collection $\xi$ to $T_{i,k}$ has the boundary that is a continuous broken line, possibly with self-intersections. In a standard way we can define the orientation of this line. It is not hard to check that the only way to make a turn along this line is by angle $\pi/6$, from a long blue segment to a green or red one, or vice versa, from a green or red segment to a long blue one. In other words, to make a turn, one needs to combine a triangle and a tetrahedron. The common site $y$ of the pair (triangle, tetrahedron) has $E(y) = 2/3$. The minimal amount of tetrahedrons needed for a full turn is 6, which yields 12 sites $y$ with $E(y) = 2/3$, i.e., the energy of $\xi$ is at least 8.

**Lemma 4.3.** Among all PCs, $\varphi_{i_1,j_k} \in S_{\text{per}}^{(5)}$ the maximal density $1/9$ of excitations $\gamma_2^*$ of type (IIa) is achieved on $\varphi_{i_1,j_k} \in \mathcal{H}^{(5)}$.

**Proof.** By construction, an excitation of type (IIa) is present in a layer $\tau$ iff its neighboring layers $\tau'$ and $\tau''$ are the same, i.e., are labeled by the same digit from $\{0, 1, 2\}$, which implies the assertion of the lemma. A direct calculation verifies that the density of excitations of type (IIa) in $\varphi_{i_1,j_k} \in \mathcal{H}^{(5)}$ equals $1/9$.

To complete the proof of Theorem 4.1B, observe that Lemma 4.3 implies that the PCs (equivalently PGSs) from $\mathcal{H}^{(5)}$ are dominant in the sense of [6], pp. 111–112 (which includes the Peierls bound (2.9) from [6]). Also, for $u$ large enough, (2.10b) from [6] holds true with $c = u^{-2}/18$. This completes the verification of conditions required in [6].

A direct calculation shows that $\sharp(\mathcal{H}^{(5)}) = 4 \cdot 3 \cdot 3 \cdot 2 = 72$.

**5 Case $D^2 = 6$**

For $D^2 = 6$, an LRFF $f = f^{(6)}$ has

$$f(0) = 1, \quad f(1) = \frac{2}{3}, \quad f(2) = \frac{1}{3}, \quad f(3) = \frac{1}{8}, \quad f(4) = \frac{1}{6}, \quad f(5) = \frac{1}{24}. \quad (5.1)$$

Here the balls $B(x) = B_{\sqrt{6}}(x)$ contain 57 sites. Each $\psi \in \mathcal{A}_{\sqrt{6}}(B(x))$ contains at most 7 particles. Consider the potential function $U(\psi) = U^{(6)}(\psi)$:

$$U(\psi) = \frac{1}{12} \sum_{y \in B(x)} \psi(y)f(\rho(x,y)^2). \quad (5.2)$$
The normalizing constant $C$ from (2.9) equals 12. For any finite $\phi \in A_{\sqrt{\pi}}(\mathbb{Z}^3)$, we have $\hat{z}(\phi) = \sum_{x \in \mathbb{Z}^3} U(\phi|_{B(x)})$, in agreement with (2.8).

The set $S^{(6)}$ comprises two families of layered PCs emerging from the constructions proposed in Section 2 cf. (2.16), (2.21). One family consists of layered PCs as in (2.16), with $q = 6$, $h = 4$ and $r = 6$; here every $\tau_{i,4k,j_k}$ is a triangular $\sqrt{6}$-sub-mesh in $\mathbb{Z}^3 \cap T_{i,4k}$ where $T_{i,4k}$ is a basic $\sqrt{2}/3$-mesh defined as in (2.15). For $i = 0, 1, 2, 3$ and $s_2 = s_2(i), s_3 = s_3(i)$ given by (2.14) we set

$$\gamma_{i,0,0} := \{m(1, -2s_2, s_3) + n(-1, -s_2, 2s_3), m, n \in \mathbb{Z}\}.$$ (5.3)

Consider the following 6 sites at distance $\sqrt{6}$ from the origin:

$$w_{i,1} = (1, -2s_2, s_3), \; w_{i,2} = (-1, -s_2, 2s_3), \; w_{i,3} = (-2, s_2, s_3),$$
$$w_{i,4} = -w_{i,1}, \; w_{i,5} = -w_{i,2}, \; w_{i,6} = -w_{i,3}.$$

Additionally, set $w_{i,0} := (0, 0, 0)$. Define 7 meshes $\gamma_{i,j} \subset T_{i,0}$:

$$\gamma_{i,j} := \gamma_{i,0,0} + \frac{1}{3}w_{i,j}, \; j = 0, \ldots, 6.$$ 

Next, for $k \in \mathbb{Z}$, we say that $j_k = j$ if

$$\tau_{i,4k,j_k} := \frac{4k}{3}(1, s_2, s_3) + \gamma_{i,j}.$$ (5.4)

The sequence $\{j_k\}$ satisfies the following conditions. First, $j_0 = 0$ and $j_k \neq j_{k+1}$. Further,

$$\tau_{i,4k,j_k+1} - \tau_{i,4k,j_k} = \frac{1}{3}w_{i,j'}, \; j' \in \{2, 4, 6\}.$$

The second family consists of layered PCs as in (2.21), with $q_1 = 8$, $q_2 = 16$, $h = 3$ and $t = 2$, where every $\alpha_{i,3k,j_h}$ is a rhombic $(\sqrt{8}, \sqrt{16})$-sub-mesh in $\mathbb{Z}^3 \cap Q_{i,3k}$ with $Q_{i,3k}$ being a basic rectangular $1 \times \sqrt{2}/2$ mesh defined as in (2.18).

Namely, for $i = 0, 1, 2, 3, 4, 5$ labeling the non-main diagonals and $s_1 = s_1(i), s_2 = s_2(i), s_3 = s_3(i)$ given by (2.17) we set

$$\alpha_{i,0,0} := \{m(2a + 2b) + n(2a - 2b) : m, n \in \mathbb{Z}\}.$$ (5.5)

where vectors $a$ and $b$ are defined in terms of $s_1, s_2, s_3$ in (2.19), (2.20). The rhombic lattice $\alpha_{i,0,0}$ lies in $Q_{i,0}$.

Further, consider the following 2 sites at distance $\sqrt{3}/2$ from the origin:

$$v_{i,1} = a + b, \; v_{i,2} = a - b,$$

Additionally, set $v_{i,0} := (0, 0, 0)$. Define 3 meshes $\beta_{i,j} \subset Q_{i,0}$:

$$\beta_{i,j} = \alpha_{i,0,0} + v_{i,j}, \; j = 0, 1, 2.$$
Next, given $k \in \mathbb{Z}$, we say that $j_k = j$ if
\[
\alpha_{i,3k,j_k}^{(8,16)} = \frac{3k}{2}(s_1, s_2, s_3) + \beta_{i,j}. \tag{5.6}
\]

The sequence $\{j_k\}$ satisfies the following conditions. First, $j_0 = 0$ and $j_k \neq j_{k+1}$. Further,
\[
\alpha_{i,3(k+1),j_{k+1}}^{(8,16)} - \alpha_{i,3k,j_k}^{(8,16)} = v_{i,j'}, \quad j' \in \{1, 2\}.
\]

Figure 5.1. Neighboring triangular meshes for $D^2 = 6$.

The figure shows two neighboring meshes in a PC $\bigcup_{k \in \mathbb{Z}} \tau_{i,4k,j_k}^{(6)}$ for $D^2 = 6$. The thin lines in the background form the triangular $\sqrt{2/3}$-lattice $T_{i,0}$ in the plane $x_1 + s_2(i)x_2 + s_3(i)x_3 = 0$. The green lines and circles indicate the triangular $\sqrt{6}$-mesh $\tau_{i,0,0}^{(6)} \subset T_{i,0}$ and the positions of occupied sites in this mesh. The red lines and circles indicate the projections of the triangular $\sqrt{6}$-mesh $\tau_{i,4,1}^{(6)} \subset T_{i,4}$ lying in the parallel plane $x_1 + s_2(i)x_2 + s_3(i)x_3 = 4$ and of the positions of occupied sites in this mesh.
Figure 5.2. Neighboring rhombic meshes for $D^2 = 6$.

The figure shows two neighboring rhombic meshes in a PC $\bigcup_{k \in \mathbb{Z}} \alpha_{i,3k,jk}^{(6,16)}$ for $D^2 = 6$. The thin lines in the background form the rectangular $(1 \times \sqrt{2}/2)$-lattice $Q_{i,0}$ in the plane $s_1(i)x_1 + s_2(i)x_2 + s_3(i)x_3 = 0$ orthogonal to the non-main diagonal $(s_1(i), s_2(i), s_3(i))$. The green lines and circles indicate the positions of particles in the rhombic $(\sqrt{8}, \sqrt{16})$-mesh $\alpha_{i,0,0}^{(8,16)} \subset Q_{i,0}$ in this plane, with rhombus diagonals of lengths $\sqrt{8}$ and $\sqrt{16}$. The red lines and circles indicate the projections of the rhombic $(\sqrt{8}, \sqrt{16})$-mesh $\alpha_{i,3,1}^{(8,16)} \subset Q_{i,3}$ lying in the parallel plane $s_1(i)x_1 + s_2(i)x_2 + s_3(i)x_3 = 3$ and of the positions of occupied sites in this mesh.

The set $S^{(6)}$ consists of all layered configurations $\bigcup_{k \in \mathbb{Z}} \tau_{i,4k,jk}^{(6)}$ and $\bigcup_{k \in \mathbb{Z}} \alpha_{i,3k,jk}^{(8,16)}$, with the allowed sequences $\{j_k\}$ and $\mathbb{Z}^3$-shifts of these configurations. We also introduce the subset $S_{\text{per}}^{(6)}$ consisting of PCs with periodic allowed sequences $\{j_k\}$, and $\mathbb{Z}^3$-shifts of these configurations.

**Theorem 5.1.** Set $S^{(6)}$ exhausts all PCs for $D^2 = 6$. The cardinality of $S^{(6)}$ is continuum. Set $S_{\text{per}}^{(6)}$ is countable and exhausts all periodic PCs for $D^2 = 6$. The particle density of any PC from $S^{(6)}$ equals 1/12.

**Proof.** The set of ACs $\psi$ on $B(x)$ which give $U(\psi) = 1/12$ is partitioned into 8 subsets; each subset is characterized by a fixed collection of values $f(\cdot)$ participating in the sum $U(\psi)$

$$
\{f(0)\}, \{f(1), f(3), f(3), f(5), f(5)\}, \{f(1), f(3), f(5), f(5), f(5), f(5)\}, \{f(1), f(4), f(5), f(5), f(5), f(5)\}, \{f(2), f(2), f(2), f(2)\}, \{f(2), f(2), f(4), f(4)\}, \{f(2), f(4), f(4), f(4)\}, \{f(4), f(4), f(4), f(4), f(4)\}.
$$

Suppose that a PC $\varphi$ contains two particles at distance $\sqrt{5}$ from each other. The only corresponding subset is characterized by the collection $\{f(1), f(4), f(5), f(5), f(5), f(5)\}$. Any $\psi$ from this subset is congruent to the AC with occupied sites at

$$(0, 0, -1), (0, 0, 2), (2, 1, 0), (1, -2, 0), (-2, -1, 0), (-1, 2, 0).$$

24
Then the vacant site $(0, 1, 0)$ is at distances $\sqrt{2}$, $\sqrt{2}$, $\sqrt{4}$ and $\sqrt{5}$ from some of the particles above but there is no subset in $(5,7)$ which contains $\{f(2), f(2), f(4), f(5)\}$. Therefore, a PC $\varphi$ does not contain two particles at distance $\sqrt{9}$ from each other.

Among the remaining ACs $\psi$ with $U(\psi) = 1/12$, only the subset $\{f(2), f(2), f(2)\}$ does not contain a pair of particles at distance $\sqrt{8}$ from each other, but one cannot construct the entire PC solely with subset $\{f(2), f(2), f(2)\}$, as the regular $\sqrt{6}$-tetrahedron does not belong to $\mathbb{Z}^3$. Thus, some other subset from $(5,7)$ must be utilized. Consequently, a PC $\varphi$ contains a pair of particles, say $(2, 1, 1)$ and $(2, -1, -1)$, at distance $\sqrt{8}$ from each other. Then the vacant site $(2, 0, 0)$ is at distance $\sqrt{2}$ from both of them (it is located in the middle of the joining segment) and the only containing subset from $(5,7)$ is $\{f(2), f(2), f(4), f(4)\}$ with the only implementation containing the particles at $(0, 0, 0)$ and $(4, 0, 0)$. Next, the vacant site $(1, 0, 1)$ is at distance $\sqrt{2}$ from both $(0, 0, 0)$ and $(2, 1, 1)$. The corresponding subsets from $(5,7)$ are $\{f(2), f(2), f(2)\}$ and $\{f(2), f(2), f(4), f(4)\}$.

First, consider the case $\{f(2), f(2), f(4), f(4)\}$. The only possible implementation contains particles at $(1, 0, 3)$ and $(1, -2, 1)$, both at distance $\sqrt{4}$ from $(1, 0, 1)$. These two particles are at distance $\sqrt{8}$ from each other which implies the particles at $(-1, -1, 2)$ and $(3, -1, 2)$ by the earlier argument. The result is the parallelepiped with vertices

$$(0, 0, 0), (2, 1, 1), (4, 0, 0), (2, -1, -1), (-1, -1, 2), (1, 0, 3), (3, -1, 2), (1, -2, 1),$$

where two faces are rhombuses with diagonals $\sqrt{8}$, $\sqrt{16}$, two faces are rhombuses with diagonals $\sqrt{6}$, $\sqrt{18}$, and two faces are rhombuses with diagonals $\sqrt{10}$, $\sqrt{14}$.

Second, consider the case $\{f(2), f(2), f(2)\}$. The only possible implementation contains a particle at $(1, -1, 2)$. Then consider a vacant site $(2, 0, 1)$ which is at distances $\sqrt{1}$, $\sqrt{3}$, $\sqrt{5}$, $\sqrt{5}$, $\sqrt{5}$ from other particles. The only corresponding subset from $(5,7)$ is $\{f(1), f(3), f(5), f(5), f(5), f(5)\}$, and its only implementation contains particles at $(3, 0, 3)$ and $(3, -2, 1)$. Now, the vacant site $(3, -1, 1)$ is at distances $\sqrt{1}$, $\sqrt{3}$, $\sqrt{5}$, $\sqrt{5}$, $\sqrt{5}$, $\sqrt{5}$ from other particles. This leads to the subset $\{f(1), f(3), f(5), f(5), f(5), f(5)\}$, and its only implementation contains a particle at $(5, -1, 2)$. The result is the parallelepiped with vertices

$$(0, 0, 0), (2, 1, 1), (4, 0, 0), (2, -1, -1), (1, -1, 2), (3, 0, 3), (5, -1, 2), (3, -2, 1),$$

where, as in the previous case, two faces are rhombuses with diagonals $\sqrt{8}$, $\sqrt{16}$, two faces are rhombuses with diagonals $\sqrt{6}$, $\sqrt{18}$, and two faces are rhombuses with diagonals $\sqrt{10}$, $\sqrt{14}$.

Thus, a PC $\varphi$ is a concatenation of parallelepipeds congruent to the above one. Consider all pairs of parallelepipeds in $\varphi$ having a common $\sqrt{8}$, $\sqrt{16}$-rhombic face. They necessarily form disjoint double-infinite sequences which we call beams. If all parallelepipeds in a beam are not the shifts of each other (i.e. some pairs of them are symmetric reflections of each other) then each parallelepiped adjacent to the beam can be glued to the beam in a unique way (via the common face), which keeps all $\sqrt{8}$, $\sqrt{16}$-rhombuses parallel to each other. Continuing this process, we reconstruct the entire PC $\varphi$ which is a stack of parallel $\sqrt{8}$, $\sqrt{16}$-rhombic meshes by construction.

If every next parallelepiped in a beam is a shift of the previous one then the beam contains two flat faces constructed solely from $\sqrt{6}$-equilateral triangles. A parallelepiped
glued to such face does not necessarily have a common face with a parallelepiped from the beam. It may have one common triangle with two consecutive parallelepipeds from the beam. Nevertheless, the $\sqrt{10}$, $\sqrt{14}$-rhombic faces can be glued in a unique way, which extends a single beam into a pair of parallel $\sqrt{6}$-triangular meshes. Finally, such pairs of meshes can be combined into the entire PC $\varphi$ which is a stack of parallel $\sqrt{6}$-triangular meshes by construction.

The rigorous analysis of EPGMs for $D^2 = 6$ large $u$ remains an open problem.

6 Cases $D^2 = 8, 9, 12$

6.1 $D^2 = 8$.

For $D^2 = 8$, an LRFF family $f^{(8)}$ has

$$f(0) = 1, \quad f(1) = \frac{1}{2}, \quad f(2) = f(3) = \frac{1}{4}, \quad f(4) = \frac{1}{6}, \quad f(5) = f(6) = \frac{1}{8}. \quad (6.1)$$

Here the balls $B(x) = B(\sqrt{7}(x))$ contain 81 sites. Each $\psi \in \mathcal{A}_{\sqrt{7}}(B(x))$ contains at most 6 particles. Consider the potential function $U(\psi) = U^{(8)}(\psi)$:

$$U(\psi) = \frac{1}{16} \sum_{y \in B(x)} \psi(y) f(\rho(x, y)^2). \quad (6.2)$$

The normalizing constant $C$ from (2.9) equals 16. For any finite $\phi \in \mathcal{A}_{\sqrt{7}}(\mathbb{Z}^3)$, we have $z(\phi) = \sum_{x \in \mathbb{Z}^3} U(\phi|_{B(x)})$, in agreement with (2.8).

A direct calculation shows that the lattice

$$\varphi^{(8)} := \{ m(2, 2, 0) + n(2, 0, 2) + k(0, 2, 2) : m, n, k \in \mathbb{Z} \} = 2A_3 \quad (6.3)$$

is a PC. The fundamental parallelepiped for $\varphi^{(8)}$ has volume 16. Consider the collection $S^{(8)}$ of $\mathbb{Z}^3$-shifts of $\varphi^{(8)}$.

**Theorem 6.1A.** Set $S^{(8)}$ exhausts all PCs for $D^2 = 8$. The cardinality of $S^{(8)}$ is 16. Every PC is periodic. The PCs are $\mathbb{Z}^3$-symmetric to each other. The particle density of any PC equals 1/16.

**Proof.** The set of ACs $\psi$ on $B(x)$ which give $U(\psi) = 1/16$ is partitioned into 6 subsets; each subset is characterized by a fixed collection of values $f(\cdot)$ participating in the sum $U(\psi)$

$$\{ f(0) \}, \{ f(1), f(5), f(5), f(5), f(5) \}, \{ f(1), f(5), f(6), f(6), f(6) \},$$

$$\{ f(2), f(2), f(6), f(6), f(6) \}, \{ f(3), f(3), f(3), f(3) \},$$

$$\{ f(4), f(4), f(4), f(4), f(4) \}. \quad (6.4)$$

Assume that a PC $\varphi$ contains two particles at distance $\sqrt{10}$. For definiteness, consider sites $(0, 0, 0)$ and $(3, 1, 0)$. Then the vacant site $(1, 1, 0)$ is at distance $\sqrt{2}$ and $\sqrt{4}$,
respectively, from our chosen sites. The above list of subsets does not contain a subset which includes both \( f(2) \) and \( f(4) \). This contradicts the fact that \( \varphi \) is a PC. Therefore, there is no PC containing a pair of sites at distance \( \sqrt{10} \). A direct enumeration shows that each of the ACs \( \psi \) with \( U(\psi) = 1/16 \) which does not have a pair of sites at distance \( \sqrt{10} \) contains a pair of sites at distance \( \sqrt{8} \).

Assume that a PC \( \varphi \) contains two sites at distance \( \sqrt{8} \). For definiteness, consider sites \((0, 0, 0)\) and \((2, 2, 0)\). Then the vacant site \((1, 1, 0)\) is at distance \( \sqrt{2} \) from both chosen sites. There is only one subset in the list \((6.4)\) containing \( f(2) \) twice. Consequently, the only possibility to implement this subset is to place particles at sites \((2, 0, \pm 2), (0, 2, \pm 2)\).

The above argument can be repeated for sites \((1, 0, \pm 1), (0, 1, \pm 1)\), etc., and consequently \( \varphi \) is uniquely recovered.

**Theorem 6.1B.** Let \( u \) be large enough: \( u \geq u^0(8) \). Then there are 16 EPGMs, i.e., \( \sharp(\mathcal{E}(\sqrt{8}, u)) = 16 \), and each EPGM is generated by a PGS from \( G^8 \).

**Proof.** Follows from Theorem 6.1A, the Peierls bound \((2.5)\) and the PS theory.

The PC \( \varphi^8 \) is another example of a \( D\)-FCC sub-lattice in \( \mathbb{Z}^3 \). The cases \( D^2 = 2, 8 \) are also covered by general Theorems 8.1A and 8.1B. The LRFF based proofs presented above are more elementary.

### 6.2 \( D^2 = 9 \).

For \( D^2 = 9 \), an LRFF family \( f^{(9)} \) has

\[
\begin{align*}
    f(0) &= 1, \quad f(1) = \frac{2}{3}, \quad f(2) = \frac{1}{2}, \quad f(3) = \frac{1}{4}, \quad f(4) = f(5) = \frac{1}{6}, \quad f(6) = \frac{1}{12}, \quad f(8) = 0. \quad (6.5)
\end{align*}
\]

Here the balls \( B(x) = B_{\sqrt{r}}(x) \) contain 81 sites. Each \( \psi \in \mathcal{A}_3(B(x)) \) contains at most 6 particles. Consider the potential function \( U(\psi) = U^{(9)}(\psi) \):

\[
U(\psi) = \frac{1}{20} \sum_{y \in B(x)} \psi(y) f(\rho(x, y)^2). \quad (6.6)
\]

The normalizing constant \( C \) from \((2.9)\) equals 20. For any finite \( \phi \in \mathcal{A}_3(\mathbb{Z}^3) \), we have \( \sharp(\phi) = \sum_{x \in \mathbb{Z}^3} U(\phi|_{B(x)}) \), in agreement with \((2.8)\).

Consider the set \( S^{(9)} \) formed by 6 congruent lattices \( \varphi^{(9)}_{i,l} \), \( i = 1, 2, 3 \), \( l = 0, 1 \), defined below, and their \( \mathbb{Z}^3 \)-shifts. Set

\[
\begin{align*}
    \varphi^{(9)}_{1,0} &:= \left\{ m(0, 3, 1) + n(0, -1, 3) + k(2, 1, 2) : m, n, k \in \mathbb{Z} \right\}, \\
    \varphi^{(9)}_{1,1} &:= \left\{ m(0, 3, -1) + n(0, -1, -3) + k(2, 1, -2) : m, n, k \in \mathbb{Z} \right\}, \quad (6.7)
\end{align*}
\]

with \( \varphi^{(9)}_{1,1} \) obtained from \( \varphi^{(9)}_{1,0} \) via the reflection about the plane \( x_3 = 0 \). Lattices \( \varphi^{(9)}_{2,l} \) and \( \varphi^{(9)}_{3,l} \) are obtained from \( \varphi^{(9)}_{1,l} \) via the rotation in \( \mathbb{R}^3 \) by \( \pi/2 \) about the \( x_3 \)- and \( x_2 \)-axis, respectively. The fundamental parallelepiped for each lattice has volume 20.
Observe that \( \varphi^{(9)}_{1,0} = \bigcup_{k \in \mathbb{Z}} \theta^{(10)}_{1,2k,j_k} \) where
\[
\theta^{(10)}_{1,0,0} = \left\{ m(0, 3, 1) + n(0, -1, 3) : m, n \in \mathbb{Z} \right\}
\]
is a square \( \sqrt{10} \)-lattice in the plane \( x_1 = 0 \) and \( \theta^{(10)}_{1,2k,0} := \theta^{(10)}_{1,0,0} + k(2, 0, 0) \) is the square \( \sqrt{10} \)-mesh in the affine plane \( x_1 = 2k, k \in \mathbb{Z} \). Correspondingly, \( \theta^{(10)}_{1,2k,1} := \theta^{(10)}_{1,0,0} + k(0, 1, 2) \), that is, the sites of \( \theta^{(10)}_{1,2k,1} \) are located at the centers of the \( (\sqrt{10} \times \sqrt{10}) \)-squares of \( \theta^{(10)}_{1,2k,0} \) and vice versa. Then \( \varphi^{(9)}_{1,0} = \bigcup_{k \in \mathbb{Z}} \theta^{(10)}_{1,2k,j_k} \), where \( j_k = 01 \). Cf. (2.22), with \( q = 10 \), \( h = 2 \) and \( u = 1 \).

A representation of PC \( \varphi^{(9)}_{1,1} \) as a union of square \( (\sqrt{10} \times \sqrt{10}) \)-meshes can be constructed in a similar way.

**Theorem 6.2A.** Set \( S^{(9)} \) exhausts all PCs for \( D^2 = 9 \). The cardinality of \( S^{(9)} \) is 120. Every PC is periodic. The PCs are \( \mathbb{Z}^3 \)-symmetric to each other. The particle density of any PC equals 1/20.

**Proof.** The set of \( \psi \) on \( B(x) \) which give \( U(\psi) = 1/20 \) is partitioned into 8 subsets; each subset is characterized by a fixed collection of values \( f(\cdot) \) participating in the sum \( U(\psi) \)
\[
\{ f(0), \{ f(1), f(5), f(6), f(6), f(6), f(6), f(6), f(6) \}, f(1), f(6), f(6), f(6), f(6), f(6), f(6), f(6) \},
\{ f(2), f(3), f(5), f(6), f(6), f(2), f(4), f(5), f(5) \},
\{ f(2), f(5), f(5), f(5), f(2), f(5), f(5), f(6), f(6) \},
\{ f(4), f(4), f(5), f(5), f(5), f(5), f(5), f(5) \}. \tag{6.8}
\]

Assume that a PC \( \varphi \) contains two particles at distance \( \sqrt{12} \). For definiteness, consider sites \( x_1 = (0, 0, 0) \) and \( x_2 = (2, 2, 2) \). Then the vacant site \( (1, 1, 1) \) is at distance \( \sqrt{3} \) from both \( x_1 \) and \( x_2 \). However, the above list (6.8) does not contain collections with at least 2 distances between occupied sites equal to \( f(3) \). This contradicts the fact that \( \varphi \) is a PC. Therefore, there is no PC containing a pair of sites at distance \( \sqrt{12} \). A direct enumeration shows that each of the ACs \( \psi \) with \( U(\psi) = 1/20 \) which does not have a pair of sites at distance \( \sqrt{12} \) contains a pair of sites at distance \( \sqrt{10} \).

Assume that a PC \( \varphi \) contains two particles at distance \( \sqrt{10} \). For definiteness, consider sites \( x_1 = (0, 0, 0) \) and \( x_2 = (1, 3, 0) \). Then the vacant site \( (0, 1, 0) \) is at distance 1 from \( x_1 \) and at distance \( \sqrt{5} \) from \( x_2 \). The only corresponding subset in (6.8) is \( \{ f(1), f(5), f(6), f(6) \} \); therefore two sites \( (-1, 2, \pm 2) \) are occupied in \( \varphi \). Now consider a vacant site \( (0, 3, 0) \) which is at distance 1 from \( (1, 3, 0) \) and at distance \( \sqrt{6} \) from sites \( (-1, 2, \pm 2) \). The only possibility for site \( (0, 3, 0) \) to implement one of the subsets from (6.8) is when there is an occupied site \( (-2, 4, 0) \).

Repeating this argument for the vacant site \( (-2, 3, 0) \) leads to the occupied site \( (-3, 1, 0) \). Thus, we obtain a square by-pyramid whose 4 base side-lengths are \( \sqrt{10} \), and the remaining 8 side-lengths are \( \sqrt{5} \). Iterating this construction yields three square \( \sqrt{10} \)-meshes in horizontal planes where \( x_3 = -2, 0, 2 \). Iterating the construction, we get similar structures at levels \(-4 \) and \( 4 \). And so on: as a result, PC \( \varphi \) is identified as a member of collection \( S^{(9)} \).
\textbf{Theorem 6.2B.} Let \( u \) be large enough: \( u \geq u^0(9) \). Then there are 120 EPGMs, i.e., \( \sharp(\mathcal{E}(\sqrt{9}, u)) = 120 \), and each EPGM is generated by a PGS from \( S^{(9)} \).

**Proof.** Follows from Theorem 6.2A, the Peierls bound (2.5) and the PS theory. \( \blacksquare \)

\subsection{6.3 \( D^2 = 12 \)}

For \( D^2 = 12 \), an LRFF family \( f^{(12)} \) has

\[
\begin{align*}
    f(0) &= 1, \\
    f(1) &= 1, \\
    f(2) &= 3, \\
    f(3) &= f(4) = \frac{1}{2}, \\
    f(5) &= \frac{1}{4}, \\
    f(6) &= \frac{1}{8}, \\
    f(8) &= f(9) = f(10) = f(11) = 0. \\
\end{align*}
\]

(6.9)

Here the balls \( B(x) = B_{\sqrt{7}}(x) \) contain 81 sites. Each \( \psi \in \mathcal{A}_{\sqrt{7}}(B(x)) \) contains at most 4 particles. Consider the potential function \( U(\psi) = U^{(12)}(\psi) \):

\[
U(\psi) = \frac{1}{32} \sum_{y \in B(x)} \psi(y) f(\rho(x, y)^2). 
\]

(6.10)

The normalizing constant \( C \) from (2.9) equals 32. For any finite \( \phi \in \mathcal{A}_{\sqrt{7}}(\mathbb{Z}^3) \), we have \( \sharp(\phi) = \sum_{x \in \mathbb{Z}^3} U(\phi|_{B(x)}) \), in agreement with (2.5).

A direct calculation shows that the lattice

\[
\varphi^{(12)} := \{ m (4, 0, 0) + n (0, 4, 0) + k (2, 2, 2) : m, n, k \in \mathbb{Z} \}
\]

(6.11)

is a PC: it is a \( \sqrt{12} \)-BCC sub-lattice in \( \mathbb{Z}^3 \). The fundamental parallelepiped for \( \varphi^{(12)} \) has volume 32. The set \( S^{(12)} \) is formed by the \( \mathbb{Z}^3 \)-shifts of \( \varphi^{(12)} \).

\textbf{Theorem 6.3A.} Set \( S^{(12)} \) exhausts all PC\s for \( D^2 = 12 \). The cardinality of \( S^{(12)} \) is 32. Every PC is periodic. The PCs are \( \mathbb{Z}^3 \)-symmetric to each other. The particle density of any PC equals 1/32.

**Proof.** The set of ACs \( \psi \) on \( B(x) \) which give \( U(\psi) = \frac{1}{32} \) is partitioned into 9 subsets; each subset is characterized by a fixed collection of values \( f(\cdot) \) participating in the sum \( U(\psi) \)

\[
\{ f(0) \}, \{ f(1) \}, \{ f(2), f(5) \}, \{ f(2), f(6), f(6) \}, \{ f(3), f(3) \}, \{ f(4), f(4) \}, \\
\{ f(4), f(5), f(5) \}, \{ f(4), f(5), f(6), f(6) \}, \{ f(5), f(5), f(5), f(5) \}. 
\]

(6.12)

Consider an occupied site in a PC and, for definiteness, assume that it is \( (0, 0, 0) \). Take the vacant site \( (1, 1, 1) \). The list (6.12) contains a single subset containing \( f(3) \); therefore the site \( (2, 2, 2) \) is also occupied.

A similar argument asserts that we must put a particle in all 8 sites \( (\pm 2, \pm 2, \pm 2) \). We can repeat this step for every of these 8 sites, then for their \( \sqrt{12} \)-neighbors and so on. \( \blacksquare \)

\textbf{Theorem 6.3B.} Let \( u \) be large enough: \( u \geq u^0(12) \). Then there are 32 EPGMs, i.e., \( \sharp(\mathcal{E}(\sqrt{12}, u)) = 32 \), and each EPGM is generated by a PGS from \( S^{(12)} \).

**Proof.** Follows from Theorem 6.3A, the Peierls bound (2.5) and the PS theory. \( \blacksquare \)

The PCs \( \varphi^{(3)} \) and \( \varphi^{(12)} \) are examples of \( D \)-BCC sub-lattices in \( \mathbb{Z}^3 \). We think that \( D^2 = 3, 12 \) are the only cases where a \( D \)-BCC sub-lattice is a PC in \( \mathbb{Z}^3 \).
7 Case $D^2 = 10$

For $D^2 = 10$, an LRFF $f^{(10)}$ has

$$f(0) = 1, f(1) = \frac{5}{6}, f(2) = f(3) = \frac{1}{2}, f(4) = \frac{1}{3}, f(5) = f(6) = \frac{1}{6}, f(8) = f(9) = 0. \quad (7.1)$$

Here the balls $B(x) = B(\sqrt{D} x)$ contain 81 sites. Each $\psi \in A_{\sqrt{10}}(B(x))$ contains at most 6 particles. Consider the potential function $U(\psi) = U^{(10)}(\psi)$:

$$U(\psi) = \frac{1}{26} \sum_{y \in B(x)} \psi(y) f(\rho(x,y)^2). \quad (7.2)$$

The normalizing constant $C$ from (2.13) equals 26. For any finite $\phi \in A_{\sqrt{10}}(\mathbb{Z}^3)$, we have $\sharp(\phi) = \sum_{x \in \mathbb{Z}^3} U(\phi|_{B(x)})$, in agreement with (2.8).

To identify the PCs, consider the following 8 congruent lattices $\varphi^{(10)}_{i,l}$, $i = 0, 1, 2, 3$, $l = 0, 1$

$$\varphi^{(10)}_{i,0} := \left\{ m(-1, -3s_2(i), 4s_3(i)) + n(3, -4s_2(i), s_3(i)) + k(0, 3s_2(i), -s_3(i)) : m, n, k \in \mathbb{Z} \right\},$$

$$\varphi^{(10)}_{i,1} := \left\{ m(-1, 4s_2(i), -3s_3(i)) + n(3, s_2(i), -4s_3(i)) + k(0, -s_2(i), 3s_3(i)) : m, n, k \in \mathbb{Z} \right\}, \quad (7.3)$$

where $s_2(i), s_3(i)$ are given by (2.11), and $\varphi^{(10)}_{i,1}$ is obtained from $\varphi^{(10)}_{i,0}$ via the reflection about the plane $x_2 = (-1)^i x_3$. The fundamental parallelepiped of each sub-lattice $\varphi^{(10)}_{i,l}$ has volume 26. As in previous cases, we denote by $S^{(10)}$ the set formed by the $\mathbb{Z}^3$-shifts of $\varphi^{(10)}_{i,l}$.

Observe that $\varphi^{(10)}_{i,0} = \bigcup_{k \in \mathbb{Z}} \tau^{(26)}_{i,2k,jk}$, where

$$\tau^{(26)}_{i,0,0} = \left\{ m(-1, -3s_2(i), 4s_3(i)) + n(3, -4s_2(i), s_3(i)) : m, n \in \mathbb{Z} \right\}$$

is a triangular $\sqrt{26}$-lattice in the plane $x_1 + x_2 s_2 + x_3 s_3 = 0$, and

$$\tau^{(26)}_{i,2k,0} := \tau^{(26)}_{i,0,0} + \frac{2k}{3}(1, s_2, s_3)$$

is the triangular $\sqrt{26}$-mesh in the plane $x_1 + x_2 s_2 + x_3 s_3 = 2k$, $k \in \mathbb{Z}$. Correspondingly,

$$\tau^{(26)}_{i,2k,1} := \tau^{(26)}_{i,2k,0} + \frac{1}{3}(-2, 7s_2, -5s_3),$$

that is, the sites of $\tau^{(26)}_{i,2k,1}$ are located at the centers of the $\sqrt{26}$-triangles of $\tau^{(26)}_{i,2k,0}$ and vice versa. Similarly, the sites of

$$\tau^{(26)}_{i,2k,2} := \tau^{(26)}_{i,2k,0} + \frac{1}{3}(-5, -2s_2, 7s_3)$$
are located at the centers of the \( \sqrt{26} \)-triangles of \( \tau_{i,2k,1}^{(26)} \) and vice versa. Then \( \varphi_{i,0}^{(10)} = \bigcup_{k \in \mathbb{Z}} \tau_{i,2k,jk}^{(26)} \) where \( \{jk\} = \overline{012} \). Cf. (2.10), with \( q = 26 \), \( h = 2 \) and \( r = 2 \).

A representation of \( PC \varphi_{i,1}^{(10)} \) as a union of \( \sqrt{26} \)-triangular meshes can be constructed in a similar way.

**Theorem 7A.** Set \( S^{(10)} \) exhausts all PCs for \( D^2 = 10 \). The cardinality of \( S^{(10)} \) is 208. Every PC is periodic. The PCs are \( \mathbb{Z}^3 \)-symmetric to each other. The particle density of any PC equals 1/26.

**Proof.** It is convenient to take \( \varphi_{0,0}^{(10)} \) as a representative for \( S^{(10)} \). The distance between the planes containing meshes \( T_{0,2k} \) and \( T_{0,2(k+1)} \) is equal to \( \sqrt{4/3} \). The occupied sites from meshes \( \tau_{k-1} := \tau_{0,2k-2,jk-1}^{(26)} \) and \( \tau_{k+1} := \tau_{0,2k+2,jk+1}^{(26)} \) are projected into centers of equilateral triangles from the mesh \( \tau_k := \tau_{0,2k,jk}^{(26)} \). Moreover, for each occupied site from \( \tau_k \) there are:

(i) 3 occupied sites at distance \( \sqrt{10} \) from mesh \( \tau_{k-1} \),
(ii) 3 occupied sites at distance \( \sqrt{14} \) from mesh \( \tau_{k+1} \),
(iii) 3 occupied sites at distance \( \sqrt{14} \) from mesh \( \tau_{k-2} \),
(iv) 3 occupied sites at distance \( \sqrt{14} \) from mesh \( \tau_{k+2} \),
(v) 1 occupied site at distance \( \sqrt{12} \) from mesh \( \tau_{k-3} \),
(vi) 1 occupied site at distance \( \sqrt{12} \) from mesh \( \tau_{k+3} \).

Here \( \tau_{k \pm n} \) are defined similarly to \( \tau_{k \pm 1} \).

E.g., for the occupied site \((0,0,0) \in \tau_0 \), the above collection (i) is \( I_{(i)} = \{(1,0,-3), (0,-3,1), (-3,1,0)\} \), collection (ii) is \( I_{(ii)} = \{(-1,0,3), (0,3,-1), (3,-1,0)\} \), collection (iii) is \( I_{(iii)} = \{(1,-3,-2), (-3,-2,1), (-2,1,-3)\} \) collection (iv) is \( I_{(iv)} = \{(-1,3,2), (3,2,1), (2,-1,3)\} \), the single-site collections described in (v) and (vi) are \( I_{(v)} = \{(-2,-2,-2)\} \) and \( I_{(vi)} = \{(2,2,2)\} \), respectively.

The vertices listed in \( I_{(i)} \), \( I_{(iii)} \) and \( I_{(v)} \), together with \((0,0,0)\), span a parallelepiped \( P_- \) where all edges have length \( \sqrt{10} \), all faces are rhombuses with diagonals of length \( \sqrt{14} \) and \( \sqrt{26} \), and the shortest diagonal of \( P_- \) has length \( \sqrt{12} \). A congruent parallelepiped, \( P_+ \), is spanned by \((0,0,0)\) and the vertices listed in \( I_{(ii)} \), \( I_{(iv)} \) and \( I_{(vi)} \). Both \( P_\pm \) are fundamental parallelepipeds for \( \varphi_{0,0}^{(10)} \). Each of \( P_\pm \) can be uniquely partitioned into 6 congruent tetrahedrons. For each of the tetrahedrons the corresponding 3 pairs of opposite sides have the following lengths: \( \sqrt{10} \) and \( \sqrt{12} \), \( \sqrt{10} \) and \( \sqrt{14} \), \( \sqrt{10} \) and \( \sqrt{14} \). Thus, the entire sub-lattice \( \varphi_{0,0}^{(10)} \) is the union of congruent tetrahedrons. (Such a tetrahedron has the following dihedral angles: \( \frac{\pi}{2}, \frac{\pi}{2}, \pi - 2 \cdot \arccos \left( \frac{\sqrt{2}}{\sqrt{7}} \right), \frac{\pi}{3}, \arccos \left( \frac{\sqrt{2}}{\sqrt{7}} \right), \arccos \left( \frac{\sqrt{2}}{\sqrt{7}} \right) \); it is a member of the first infinite family of rational tetrahedrons from Theorem 1.8 in [33].)

The set of ACs \( \psi \) on \( B(x) \) which give \( U(\psi) = \frac{1}{26} \) is partitioned into 15 subsets; each subset is characterized by a fixed collection of values \( f(\cdot) \) participating in the sum \( U(\psi) \).
\{f(0), \{f(1), f(5)\}, \{f(1), f(6)\}, \{f(2), f(4), f(6)\}, \\
\{f(2), f(5), f(6), f(6)\}, \{f(2), f(6), f(6), f(6)\}, \\
\{f(3), f(3)\}, \{f(3), f(4), f(5)\}, \{f(3), f(4), f(6)\}, \\
\{f(3), f(5), f(5), f(5)\}, \{f(3), f(5), f(5), f(6)\}, \\
\{f(3), f(5), f(6), f(6)\}, \{f(3), f(6), f(6), f(6)\}, \\
\{f(4), f(6), f(6), f(6), f(6)\}, \{f(6), f(6), f(6), f(6), f(6)\}, f(6), f(6), f(6)\}.  \quad (7.4)

Assume that a PC \( \varphi \) contains two particles at distance \( \sqrt{11} \). For definiteness consider sites \( x_1 = (0, 0, 0) \) and \( x_2 = (1, 1, 3) \). Then the vacant site \( x_3 = (1, 0, 1) \) is at distance \( \sqrt{2} \) from \( x_1 \) and \( \sqrt{5} \) from \( x_2 \). Similarly, the vacant site \( x_4 = (1, 0, 2) \) is at distance \( \sqrt{5} \) from \( x_1 \) and at distance \( \sqrt{2} \) from \( x_2 \). According to the list (7.4), the only possible subset containing those distances is \( \{f(2), f(5), f(6), f(6)\} \). It is not hard to see that it is impossible to add two more sites at distance \( \sqrt{6} \) from \( x_3 \) without breaking admissibility and the same is true for \( x_4 \). This contradicts the fact that \( \varphi \) is a PC. Therefore, there is no PC containing a pair of sites at distance \( \sqrt{11} \).

A similar argument establishes that a PC \( \varphi \) cannot contain occupied sites at distance \( \sqrt{13} \) from each other. For this case \( x_1 = (0, 0, 0), x_2 = (2, 3, 0) \) and \( x_3 = (1, 1, 0), x_4 = (1, 2, 0) \).

Next, we verify that a PC \( \varphi \) must contain a pair of occupied sites at distance \( \sqrt{12} \). Suppose that in \( \varphi \) there is no pair of particles at distance \( \sqrt{12} \) from each other. Then, a direct enumeration shows that, taking into account lattice symmetries, there are only 5 distinct ACs \( \psi \in A_{\sqrt{10}}(B(x)) \) which do not contain a pair of particles at distances \( \sqrt{11}, \sqrt{12} \) or \( \sqrt{13} \):

\[
\psi_1 = \{(-2, -1, 0), (1, 0, 0)\}, \psi_2 = \{(-2, -1, -1), (0, 0, 2), (1, 0, -1)\},
\psi_3 = \{(-2, -1, 0), (0, 2, -1), (1, -1, -1), (1, 0, 2)\},
\psi_4 = \{(-2, -1, -1), (-1, -1, 2), (0, 2, 0), (1, -1, -2), (2, -1, 1)\},
\psi_5 = \{(-2, -1, 1), (-1, -1, 2), (-1, 2, 1), (1, -2, -1), (1, 1, -2), (2, 1, 1)\}.
\]

The corresponding collections of values \( f(\cdot) \) are, respectively:

\[
\{f(1), f(5)\}, \{f(2), f(4), f(6)\}, \{f(3), f(5), f(5), f(5)\},
\{f(4), f(6), f(6), f(6), f(6)\}, \{f(6), f(6), f(6), f(6), f(6)\}.
\]

It turns out that for each of the last 4 ACs \( \psi_i, i = 2, 3, 4, 5 \), in (7.5) there is a vacant site \( x_i \) such that it is impossible to have \( \phi \supset \psi_i \) such that \( U(\phi |_{B(x_i)}) = 1/26 \). Namely, \( x_5 = (0, -1, 0), x_4 = (0, -1, 0), x_3 = (0, 0, 1), x_2 = (-1, 0, 0) \). Note that there is a possibility for \( U(\phi |_{B(x_2)}) = \frac{1}{26} \) if the site \( \bar{x} = (-2, 2, 0) \in \phi \). However, in this case the distance between occupied sites \( (-2, 2, 0) \) and \( (0, 0, 2) \) is \( \sqrt{12} \) which contradicts the assumption. The last possibility is an AC \( \phi \) which contains \( \psi_1 \) and does not contain any of \( \psi_i, i = 2, 3, 4, 5 \). Such a configuration must contain 8 occupied sites forming a parallelepiped congruent to \( \mathcal{P}_\pm \). But \( \mathcal{P}_\pm \) contains a pair of particles at distance \( \sqrt{12} \) which again contradicts the assumption.

Finally, consider two occupied sites \( x_1 \) and \( x_2 \) in a PC \( \varphi \) at distance \( \sqrt{12} \). For definiteness consider sites \( x_1 = (0, 0, 0) \) and \( x_2 = (-2, 2, 2) \). Take the vacant site \( x_3 =
(0, 2, 1). For \( \varphi \ni x_1, x_2 \), the only possibilities to have \( U(\varphi|_{B(x_3)}) = \frac{1}{26} \) are when either the site \((1, 3, 0)\) or \((1, 3, 2)\) is occupied since the subset \(\{f(5), f(5)\}\) implies either the subset \(\{f(3), f(5), f(5)\}\) or the subset \(\{f(3), f(5), f(5), f(6)\}\), both of which contain \(f(3)\). Due to symmetry, it suffices to consider the site \((1, 3, 0)\) only. The unique way to obtain the subset \(\{f(3), f(5), f(5), f(6)\}\) is to place a particle at site \((1, 1, 3)\). However, a particle at \((1, 1, 3)\) is at distance \(\sqrt{11}\) from \(x_1\) which is impossible in a PC. The unique way to obtain the subset \(\{f(3), f(5), f(5), f(5)\}\) is to place a particle at site \((1, 2, 3)\).

Repeating the argument with \(x_3 = (0, 1, 2)\) in place of \((0, 2, 1)\), we obtain another occupied site \((0, -1, 3)\). Continuing this process with \(x_3 = (-1, 0, 2), (-2, 0, 1), (-2, 1, 0)\) and \((-1, 2, 0)\), we add other four occupied sites \((-3, -1, 2), (-3, 0, -1), (-2, 3, -1)\) and \((1, 3, 0)\). These 8 occupied sites form the vertices of a parallelepiped congruent to \(\mathcal{P}_\pm\), where all sides have length \(\sqrt{10}\).

Now take the vacant site \(\overline{x} = (1, 1, 1)\). The only possibility to have \(U(\varphi|_{B(\overline{x})}) = 1/26\) is when the site \((3, 0, 1)\) is occupied, as the set \(\{f(3), f(5), f(5)\}\) implies either the set \(\{f(3), f(5), f(5)\}\) or the set \(\{f(3), f(5), f(5), f(6)\}\); the latter combination is again impossible without breaking admissibility. This produces another pair of occupied sites \((1, 2, 3)\) and \((3, 0, 1)\) at distance \(\sqrt{12}\) from each other. Therefore, the previous construction can be repeated, to recover another parallelepiped congruent to \(\mathcal{P}_\pm\), adjacent to the first one. This process can be iterated further, until all of \(\varphi\) is recovered. That is, we obtain that any PC \(\varphi\) is a member of \(S^{(10)}\).

**Theorem 7B.** Let \(u\) be large enough: \(u \geq u^0(10)\). Then there are 208 EPGMs, i.e., \(\sharp(\mathcal{E}(\sqrt{10}, u)) = 208\), and each EPGM is generated by a PGS from \(S^{(10)}\).

**Proof.** Follows from Theorem 7A, the Peierls bound [25] and the PS theory.

## 8 Case \(D^2 = 11\)

The case \(D^2 = 11\) is interesting because it is the first case where the Voronoi cell of the minimal volume does not tessellate the space (it is true for \(D\) large enough). To identify the PCs for \(D = \sqrt{11}\) we develop a new technique that was not used in previous sections. It is an analytic argument combined with a computer enumeration. A part of the difficulty was to make such enumeration efficient enough to be completed in a reasonable time.

A part of the technique is the concept of a discrete Voronoi cell (DVC); it is meaningful for any exclusion distance \(D\). Given \(y \in \mathbb{Z}^3\) and an AC \(\phi \in \mathcal{A}_D(\mathbb{Z}^3), \phi \neq \emptyset\), we calculate

\[
m(y) = m(y, \phi) := \min \{\rho(x', y), x' \in \phi\}.
\]

Define the DVC of site \(x \in \phi\) as the set

\[
\mathcal{C}(x) = \mathcal{C}(x, \phi) := \{y \in \mathbb{Z}^3 : \rho(y, x) = m(y)\}.
\]

Further, let \(\sharp(y)\) denote the cardinality of the set \(\{x' \in \phi : \rho(x', y) = m(y)\}\). The volume of DVC \(\mathcal{C}(x)\) is defined as

\[
v(\mathcal{C}(x)) := \sum_{y \in \mathcal{C}(x)} \frac{1}{\sharp(y)}.
\]
Observe that the intersection \( C(x') \cap C(x'') \) can be non-empty for some \( x' \neq x'' \) but for \( \phi \in A_D(\mathbb{Z}^3) \) we have a formal equality

\[
\sum_{x \in \phi} v(C(x)) \equiv \sharp(\mathbb{Z}^3),
\]

where \( \sharp(\mathbb{Z}^3) \) stands for the number of lattice sites in \( \mathbb{Z}^3 \).

Due to the discreteness, the minimal DVC volume

\[
v_o := \min \left[ v(C(x, \phi)) : x \in \phi, \phi \in A_D(\mathbb{Z}^3) \right]
\]

is well-defined. If there exists a configuration \( \varphi \in A_D(\mathbb{Z}^3) \) such that for all \( x \in \varphi \)

\[
v(C(x)) = v_o
\]

then \( \varphi \) is a PC.

Indeed, for any saturated \( \phi \in A_D(\mathbb{Z}^3) \) define the potential

\[
U(\phi|_{B_{4D}(y)}) := -\frac{1}{\sharp(y)} \sum_{x \in \phi : C(x) \ni y} \frac{1}{v(C(x))}.
\]

Then for any \( \phi \in A_D(\mathbb{Z}^3) \) we have a formal equality

\[
-\sum_{y \in \mathbb{Z}^3} U(\phi|_{B_{4D}(y)}) = \sum_{y \in \mathbb{Z}^3} \frac{1}{\sharp(y)} \sum_{x \in \phi : C(x) \ni y} \frac{1}{v(C(x))} = \sum_{x \in \phi} \frac{1}{v(C(x))} \sum_{y \in C(x)} \frac{1}{\sharp(y)} = \sharp(\phi),
\]

i.e., \( U \) is a potential counting the number of particles in \( \phi \). Clearly,

\[
U(\phi|_{B_{4D}(y)}) \geq -\frac{1}{v_o},
\]

and therefore the particle density in \( \phi \in A_D(\mathbb{Z}^3) \) does not exceed \( \frac{1}{v_o} \).

For \( D = \sqrt{12} \) the minimal DVC volume is equal to 32, and there exists a unique PC \( 4\mathbb{Z}^3 \cup (2, 2, 2) + 4\mathbb{Z}^3 \), up to \( \mathbb{Z}^3 \)-shifts and \( \mathbb{Z}^3 \)-symmetries. Correspondingly, the maximal particle density is \( \frac{1}{32} \). Our aim is to show that for \( D = \sqrt{11} \) the maximal particle density is also \( \frac{1}{32} \). Unfortunately, for \( D = \sqrt{11} \) there exist DVCs \( C(x) \) having \( v(C(x)) < 32 \), which prevents a direct application of the above argument based on minimal DVCs. However, we will show that a neighborhood of an exceptionally small DVC \( C(x) \) always contains one or more DVCs \( C(x') \) with \( v(C(x')) \) large enough to compensate for the volume deficiency \( 32 - v(C(x)) \).

To establish these facts we need an appropriate lower bound for the DVC volume. More specifically, it is enough to consider 57 sites \( y \in B_{\sqrt{5}}(x) \), where \( B_{\sqrt{5}}(x) \) is the closed lattice ball of radius \( \sqrt{5} \) centered at site \( x \in \mathbb{Z}^3 \). The intersection

\[
c(x)(= c(x, \phi)) := C(x) \cap B_{\sqrt{5}}(x)
\]

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is called a bounded DVC (BDVC). The maximal possible BDVC volume is equal to 1 + 6 + 12 + 8 + 6 + 24 = 57, where we counted the number of sites \(y\) with \(\rho(x,y)^2 = 0, 1, 2, 3, 4, 5,\) respectively. Note that

\[
v(c(x)) \leq v(C(x)).
\]

Therefore, the bound

\[
v(c(x)) \geq 32, \quad x \in \phi,
\]

implies that for \(D = \sqrt{\Pi}\) the particle density in \(\phi \in A_{\sqrt{\Pi}}(\mathbb{Z}^3)\) is \(\leq \frac{1}{32}\).

In the arising context, two particles \(x', x'' \in \phi\) are called neighbors if \(c(x') \cap c(x'') \neq \emptyset\). Later on, we use a more restrictive notion of a ‘true neighbor’.

**Lemma 8.1.** For \(D = \sqrt{\Pi}\) there exist, up to \(\mathbb{Z}^3\)-symmetries and \(\mathbb{Z}^3\)-shifts, 38 BDVCs of volume \(\frac{380}{12}\), 106 BDVCs of volume \(\frac{382}{12}\), and 14 BDVCs of volume \(\frac{383}{12}\). All these BDVCs are listed in the output of program BDVC.java.

**Proof.** Without loss of generality we investigate only BDVCs centered at the origin \(o = (0, 0, 0)\). It is not hard to see that all 24 \(\mathbb{Z}^3\)-symmetric images of \(x = (2, 2, 3)\) do not affect \(v(c(o))\) as for any contributing \(y\) the distance \(\rho(o,y) < \rho(x,y)\). The same is true for all 24 \(\mathbb{Z}^3\)-symmetric images of \(x = (1, 3, 3)\), as well as of any \(x\) with \(\rho(o,x)^2 > 20\). Thus, we only need to consider \(x\) which are \(\mathbb{Z}^3\)-symmetric images of

\[(1,1,3), (2,2,2), (0,2,3), (1,2,3), (0,3,3), (0,0,4), (0,1,4), (1,1,4), (0,2,4).
\]

The rest of the proof uses an exhaustive computer enumeration taking into account the above remarks.

Together with the origin \(o\), an admissible configuration of \(n - 1\) neighbors forms an \(n\)-site tuple (a term used in programs BDVC.java and BDVCNeighbors.java; see below). A part of the proof is that we enumerate such tuples recursively, exhaustively and without repetitions. Any tuple with the DVC volume < 32 must have at least one particle at distance \(\sqrt{\Pi}\) from the origin. Without loss of generality we assume that this is a particle at \((-3, -1, -1)\). Accordingly, we initialize the BDVC enumeration by fixing the 2-tuple

\[(0,0,0), (-3, -1, -1).
\]

A search for an admissible tuple of a larger size is confined to sites inside the lattice ball \(\overline{B}_{\sqrt{\Pi}}(o)\). To streamline the search, we index all sites in \(\overline{B}_{\sqrt{\Pi}}(o)\) so that the two above sites, \((0,0,0)\) and \((-3, -1, -1)\), have indices 0 and 1, respectively. To eliminate repetitions (encountering a tuple more than once), we list the elements of a tuple (particles) in an increasing order of site indices.

We begin enumerating the admissible tuples with adding a third particle to the initial 2-tuple. The search for such a particle is done by sequential trying all sites in \(\overline{B}_{\sqrt{\Pi}}(o)\), beginning with the site with index 3. Afterwards, we add a fourth particle in a similar manner and so on, until it becomes impossible to add one more particle without breaking admissibility.

In the latter situation we remove the last 2 particles from the obtained tuple and attempt to add an additional particle whose site index is larger than the site index of
the second to the last between the removed particles. To be more specific, if the indices of the removed particles are \( i'' \) and \( i' > i'' \) then we start our search from the site with index \( i'' + 1 \). If this search is unsuccessful, we remove another (the third from the last) particle having site index \( i''' < i'' \) and again attempt a forward search starting with site index \( i'' + 1 \). If the consecutive searches fail and we end up removing all particles except for the initial two then all possible admissible tuples are enumerated.

An opposite situation is when, after removing several particles from the tuple, we are able to add a new particle to it. Subsequently, we proceed as in the beginning by adding more and more particles until the particle addition process gets stuck. At that moment we again perform the removal of particles from the tuple and so forth.

The total amount of different tuples encountered during the exhaustive enumeration equals 7758631864. Each tuple with the corresponding BDVC volume \( < 32 \) is printed out as soon as it is discovered. The corresponding counts match those listed in the lemma.

In the corollary below we extend the assertion of Lemma 8.1 to DVCs.

**Corollary 8.2.** For \( D = \sqrt{11} \), up to \( \mathbb{Z}^3 \)-symmetries and \( \mathbb{Z}^3 \)-shifts, there exist 38 DVCs of volume \( \frac{380}{12} \), 106 DVCs of volume \( \frac{382}{12} \) and 14 DVCs of volume \( \frac{383}{12} \). All these DVCs are listed in the output of BDVC.java.

**Proof.** It is a direct calculation to verify that each BDVC from Lemma 8.1 is actually a DVC.

Next, we establish that, among neighbors of a particle \( x \in \phi \) with \( v(c(x)) < 32 \), there always exist one or several particles such that the total volume of their BDVCs is large enough to compensate for the volume deficiency \( 32 - v(c(x)) \). To this end, consider the following definition. Given a configuration \( \phi \in \mathcal{A}_{\sqrt{11}}(\mathbb{Z}^3) \) and a particle \( x' \in \phi \), we say that \( x' \) is a **true neighbor** of particle \( x \in \phi \setminus \{x'\} \) if either \( c(x', \phi) \) contains a site \( y \in \mathbb{Z}^3 \) with \( \rho(y, x') = \rho(y, x) \), or ball \( \overline{B}_{\sqrt{11}}(x) \) contains a site \( y \in \mathbb{Z}^3 \) with \( \rho(y, x') < \rho(y, x) \) and \( \rho(y, x) < \rho(y, x'') \) for all \( x'' \in \phi \setminus \{x, x'\} \). The property of being a true neighbor means that removing \( x' \) from \( \phi \) changes BDVC \( c(x) \). As was mentioned at the beginning of the proof of Lemma 8.1 each true neighbor \( x' \) of \( x \) belongs to \( \overline{B}_{\sqrt{11}}(x) \). Consequently, the true neighbor property is determined by the restriction \( \phi |_{\overline{B}_{\sqrt{11}}(x)} \).

A particle \( x \in \phi \) with \( v(c(x)) > 32 \) is called a **donor**. A particle \( x \in \phi \) with \( v(c(x)) < 32 \) is called an **acceptor**. For a particle \( x \in \phi \) denote by \( n(x) \) the number of true acceptor neighbors of \( x \). Given a donor \( x \), we wish to distribute the excess volume \( v(c(x)) - 32 \) evenly among its true acceptor neighbors. To distribute evenly means that a true acceptor neighbor \( x' \) receives an increment in the volume \( v(c(x')) = \frac{v(c(x)) - 32}{n(x)} \) and referred to as an excess donation (from \( x \) to \( x' \)). After a donation procedure is performed for every donor, we obtain a re-distributed BDVC volume \( \hat{v}(c(x)) \) for every particle \( x \in \phi \); if \( x \) is an acceptor (from one or more donors) then \( \hat{v}(c(x)) \) will be \( > v(c(x)) \). By construction, \( \hat{v}(c(x)) = 32 \) for each non-acceptor \( x \in \phi \).

**Lemma 8.3.** Let \( \phi \in \mathcal{A}_{\sqrt{11}}(\mathbb{Z}^3) \) and \( x \in \phi \) be an acceptor particle. Then

\[
\hat{v}(c(x)) \geq 32.
\]
The presented proof is computer assisted. Its analytical argument yields an algorithm implemented in program \textsf{BDVCNeighbors.java}. Observe that all possible acceptor BDVCs are listed in Lemma 8.1. We analyze tuples for med by acceptor particles an algorithm implemented in program \textsf{BDVCNeighbors.java}.

For each true neighbor \( x'_j \) we calculate the conditionally minimal BDVC volume and conditionally minimal BDVC excess volume this true neighbor is capable to donate to \( x \).

The minimization is done under the condition that the following particles are present in the tuple: \( x, x'_j \) and all other true neighbors \( x'_j \neq x'_j \). In particular, this allows us to identify the true neighbors \( x'_j \) for which the conditionally minimal BDVC volume exceeds 32. Such a neighbor will never be an acceptor. A remaining true neighbor \( x'_j \) has a possibility to become an acceptor at least in some tuples. We treat such \( x'_j \) as acceptors in our lower estimates below.

The sum over \( j \) of all obtained conditionally minimal BDVC excess volume donations gives a lower bound for the total excess volume donated to the acceptor’s BDVC \( c(x) \). Computationally, the above individual minimization (for each \( x'_j \) separately) is considerably less massive than a simultaneous minimization (for all \( x'_j \) collectively).

For each identified donor’s conditional BDVC \( c(x'_j) \) the exact number \( n(x'_j) \) of its neighbor’s BDVCs \( c(x''_{k(j)}) \) with \( v(c(x''_{k(j)})) < 32 \) cannot be known without another massive enumeration. Instead, we estimate \( n(x'_j) \) from above. Given a true neighbor \( x''_{k(j)} \) of particle \( x \), we enumerate tuples consisting of \( x, x'_j \), all other true neighbors \( x'_j \neq x'_j \) of \( x \), and the neighbors \( x''_{k(j)} \) of \( x_j \). Among the \( x''_{k(j)} \) we identify the true neighbors of \( x_j \), and they all are counted as acceptors (which gives an upper estimate for the number of acceptor true neighbors of \( x'_j \)). Among all other true neighbors \( x'_j \neq x'_j \) we count as acceptors only those particles which have been classified earlier as possible acceptors (see above). The particle \( x \) is always counted as an acceptor true neighbor of \( x'_j \). The total estimated number of acceptors is denoted by \( N(x'_j) \). Clearly, \( N(x'_j) \geq n(x'_j) \), and instead of the actual excess donation \( \frac{v(c(x'_j)) - 32}{n(x'_j)} \) we use its lower bound \( \frac{v(c(x'_j)) - 32}{N(x'_j)} \).

The implemented algorithm (see program \textsf{BDVCNeighbors.java}) relies on a classification of \( v(c(x'_j)) \) (as potential acceptors or non-acceptors) which has been performed in advance. However, for the validity of the argument the algorithm double-checks that this classification is correct.

In the resulting output of \textsf{BDVCNeighbors.java} one can see that for every considered tuple the accumulated lower-bounded excess volume is larger than the deficiency of \( v(c(x)) \). Thus, unlike the DVC volume \( v(C(x)) \), the re-distributed BDVC volume \( \hat{v}(c(x)) \) is not smaller than 32 for any particle \( x \).

\begin{corollary}
For \( D = \sqrt{11} \) the particle density in any admissible configuration \( \phi \) is not larger than \( \frac{1}{32} \).
\end{corollary}

\textbf{Proof.} The proof is straightforward.
Lemma 8.3 allows us to use the minimal re-distributed BDVC volume (= 32) instead of the minimal BDVC volume (< 32) to recover the existence of a PC, e.g. \( \varphi = 4\mathbb{Z}^3 \cup \{(2,2,2) + 4\mathbb{Z}^3\} \). Contrary to the case of \( D = \sqrt{12} \), for \( D = \sqrt{11} \) there exist other PCs not taken into each other by \( \mathbb{Z}^3 \)-symmetries and \( \mathbb{Z}^3 \)-shifts. In fact, for \( D = \sqrt{11} \) the cardinality of the set of PCs is continuum.

**Theorem 8.5.** For \( D = \sqrt{11} \) the corresponding hard-core model exhibits sliding.

**Proof.** Consider the BCC configuration \( \varphi = 4\mathbb{Z}^3 \cup \{(2,2,2) + 4\mathbb{Z}^3\} \) as the initial periodic PC. In particular, \( \varphi \) contains particles \( x_k = (2k,2k,2k), k \in \mathbb{Z} \) belonging to the lattice main diagonal. If we shift these particles along this main diagonal by the vector \((1,1,1)\) then instead we obtain the particles at sites \((2k+1,2k+1,2k+1), k \in \mathbb{Z}\). It is not hard to see that the resulting configuration is still an admissible one. Indeed, a particle at site \((2k+1,2k+1,2k+1)\) has 6 neighbors

\[
(2k,2k,2k+4), (2k+2,2k-2,2k+2), (2k+4,2k,2k),
(2k+2,2k+2,2k-2), (2k,2k+4,2k), (2k-2,2k+2,2k+2)
\]

at squared distance 11 from it and 2 neighbors

\[
(2k-1,2k-1,2k-1) (2k+3,2k+3,2k+3)
\]

at squared distance 12 from it. All other particles in \( \varphi \) are further away from \((2k+1,2k+1,2k+1)\). Similarly, one can slide in \( \varphi \) any line of particles parallel to any of main diagonals. This constitutes sliding.

\[\square\]

**9 Case \( D^2 = 2\ell^2 \)**

The case \( D^2 = 2\ell^2 \), \( \ell \in \mathbb{N} \) relies on results about dense-packing configurations in \( \mathbb{R}^3 \) established in \cite{21,22,35}. These results allow us to identify the PCs and establish the corresponding Peierls bound. Our argument utilizes the scoring function \( \overline{\varphi}(\overline{\varphi} | \overline{\varxi}x) \), \( x \in \overline{\varphi} \), which has been constructed in \cite{21}, see (1.4) and Definition 5.12. Here and below, \( \overline{\varphi} \) is a 1-AC in \( \mathbb{R}^3 \) and \( \overline{\varxi}x \) is the closed ball in \( \mathbb{R}^3 \) centered at \( x \in \mathbb{R}^3 \):

\[
\overline{\varphi} \subset \mathbb{R}^3, \rho(y,y') \geq 1 \ \forall \ y \in \overline{\varphi} \ \text{and} \ y' \in \overline{\varphi} \ \setminus \ {y},
\overline{\varxi}x = \overline{\varxi}x_{2.51}(x) := \{y \in \mathbb{R}^3 : \rho(x,y) \leq 2.51\}. \quad (9.1)
\]

The over-line symbol in this notation stresses that the objects under consideration are in \( \mathbb{R}^3 \).

We work with a modified scoring function \( \overline{\varphi} = -\overline{\varphi} + \frac{16\pi}{3} \) which has the following properties.

(I) \( \overline{\varphi}(\overline{\varphi} | \overline{\varxi}x) \) is shift-invariant: \( \overline{\varphi}(\overline{\varphi} | \overline{\varxi}x) = \overline{\varphi}(\overline{\varphi} + u | \overline{\varxi}(x+u)) \), \( \forall u \in \mathbb{R}^3 \) and \( x \in \overline{\varphi} \).

(II) For a 1-FCC configuration \( \varphi \) and any \( x \in \varphi \)

\[
\overline{\varphi}(\varphi | \overline{\varxi}x) = \overline{\varphi} \in (0, \infty).
\]
(III) For any 1-AC $\phi$ in $\mathbb{R}^3$ and $x \in \phi$, 
\[ \mathcal{V}(\phi|_{B(x)}) \leq \mathcal{V}^* \]

Cf. Theorems 1.7, 6.1 and Corollary 6.3 in [21].

(IV) Suppose a 1-AC $\phi$ in $\mathbb{R}^3$ coincides with a 1-FCC configuration $\varphi$ outside a closed cube $C_r(o) \subset \mathbb{R}^3$ of side-length $r$ centered at the origin $o$. Assume $r$ is large enough: $r \gg 2.51$. Then
\[ \sum_{x \in \phi \cap C_{2r}(o)} \mathcal{V}(\phi|_{B(x)}) = \sum_{x \in \varphi \cap C_{2r}(o)} \mathcal{V}(\varphi|_{B(x)}). \]

Cf. Lemma 5.10 and Theorem 5.11 in [21].

For a discrete $\phi \in A_D(\mathbb{Z}^3)$, we define
\[ v(\phi|_{B_r(x)}) := \mathcal{V}(\phi|_{B_r(x)}), \quad \mathcal{V} := \frac{1}{D} \phi, \]
where $r = 2.51D$, and $\phi$ and its $\frac{1}{D}$-scaled version $\mathcal{V}$ are understood as sets of points in space. The condition $D^2 = 2(\ell^2$ is necessary and sufficient to guarantee the existence of $D$-FCC sub-lattices in $\mathbb{Z}^3$. Correspondingly, for this case the function $v$ inherits properties (I)-(IV) from $\mathcal{V}$.

It is convenient for us to use the relative form of (1.1)
\[ H(\phi) = \left( -\ln u \right) \cdot (\sharp(\phi) - \sharp(\varphi)), \quad \phi \in A_D(\mathbb{Z}^3), \varphi \text{ is a PGS}, \quad (9.2) \]
which generates the same Gibbs measures on $\mathbb{Z}^3$ as (1.1). Let
\[ \zeta(\phi|_{B_r(x)}) := \frac{v(\phi|_{B_r(x)})}{v^*} - 1. \]

Then for a $\ell$-FCC sub-lattice $\varphi$ and $\phi \in A_D(\mathbb{Z}^3)$ such that $\varphi$ and $\phi$ coincide outside of $B_s(o)$, where $s \gg r = 2.51D$ and $o$ is the origin, we have
\[ \sharp(\varphi) - \sharp(\phi) = \sum_{x \in \phi} \zeta(\phi|_{B_r(x)}), \]
as follows from the properties (II) - (IV) above. Consequently,
\[ H(\phi) = (\ln u) \sum_{x \in \phi} \zeta(\phi|_{B_r(x)}). \quad (9.3) \]
The above representation is similar (but not equivalent) to (2.2). Consequently, in analogy with condition (2.3), a configuration $\varphi \in A_D(\mathbb{Z}^3)$ is called a PC if $\zeta(\varphi|_{B_r(x)}) = 0$ for all $x \in \varphi$.

According to [21, 22, 35], the only dense-packing configurations in $\mathbb{R}^3$ are FCC, HCP and their layered mixtures, up to Euclidean motions.

**Lemma 9.1.** If a $D$-scaled version of a dense-packing configuration in $\mathbb{R}^3$ exists in $\mathbb{Z}^3$ then all such $D$-scaled configurations existing in $\mathbb{Z}^3$ exhaust the set $S(D^3)$ of $D$-PCs in $\mathbb{Z}^3$. 

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Proof. The assertion follows from Claim 1.16 and Theorem 6.1 in [21] or Theorem 8.1, p. 138 in [35].

Clearly, the $D$-scaled versions of these dense-packing configurations are $D$-FCC, $D$-HCP configurations, their layered mixtures $\varphi^{(D^2)}_{i,j}$ and their $\mathbb{Z}^3$-shifts. For the necessary and sufficient conditions for their existence and for the detailed description of their structures see Appendix A.

Now assume that $D^2 = 2\ell^2$ where $\ell \neq 0 \mod 3$. In this case the set $\mathcal{S}^{(D^2)}$ consists of $D$-FCC sub-lattices and their $\mathbb{Z}^3$-shifts. To apply the PS theory, it remains to establish a suitable Peierls bound for contours. The definition of a contour can be given as a direct generalization of that in Sect. 3.1 of [37]. More specifically, a rhombic template $F_{k,j}$ from [37] is replaced by a parallelepiped with congruent rhombic faces, and the number of occupied sites in a $D$-PC $\varphi$ within such a parallelepiped is re-calculated in a straightforward manner. A contour $\Gamma = (\text{Supp} (\Gamma), \varphi \mid_{\text{Supp} (\Gamma)})$ and its support $\text{Supp} (\Gamma)$ are defined as in Sect 3.1 of [37]. The statistical weight $w(\Gamma)$ is defined as

$$w(\Gamma) = u^{|(\varphi \mid_{\text{Supp} (\Gamma)}) - \varphi \mid_{\text{Supp} (\Gamma)}|};$$

(9.4)

cf. (3.9) from [37].

For a saturated AC $\phi$ the Peierls bound for $w(\Gamma)$ is established similarly to Lemma 5.4 from [37]. The analog of this lemma is

Lemma 9.2. (The Peierls bound) There exists a constant $p = p(D) > 0$ such that for any contour $\Gamma = (\text{Supp} (\Gamma), \varphi \mid_{\text{Supp} (\Gamma)})$ we have

$$w(\Gamma) = \prod_{x \in \varphi \mid_{\text{Supp} (\Gamma)}} u^{-\xi(\varphi \mid_{B(x)})} \leq u^{-p(D)\|\text{Supp} (\Gamma)\|}$$

(9.5)

where $\|\text{Supp} (\Gamma)\|$ stands for the number of templates (see [37]) in $\text{Supp} (\Gamma)$.

Proof. The equality in (9.5) is the result of substituting (9.3) in (9.4). Note that the contribution into the product in (9.5) comes only from sites $x$ where $\upsilon(\varphi \mid_{B(x)}) > \upsilon^*$; otherwise (i.e., when $\upsilon = \upsilon^*$) site $x$ does not contribute into (9.3). Observe that

$$\text{if } \upsilon(\varphi \mid_{B(x)}) - \upsilon^* \geq \upsilon^* \text{ then } \upsilon(\varphi \mid_{B(x)}) - \upsilon^* \geq \frac{1}{2} \upsilon(\varphi \mid_{B(x)}).$$

On the other hand, due to discreteness

$$\text{if } \upsilon(\varphi \mid_{B(x)}) - \upsilon^* < \upsilon^* \text{ then } \upsilon(\varphi \mid_{B(x)}) - \upsilon^* \geq \delta(D) \geq \frac{\delta(D)}{2\upsilon^*} \upsilon(\varphi \mid_{B(x)})$$

where $\delta(D) > 0$. According to the definition of a $\varphi$-correct template, for a saturated AC $\phi$ we have an inequality

$$\sum_{x \in \varphi \mid_{\text{Supp} (\Gamma) : \upsilon(\varphi \mid_{B(x)}) > \upsilon^*}} \upsilon(\varphi \mid_{B(x)}) \geq \frac{1}{27D^3|\text{Supp} (\Gamma)|}.$$

Also, $|\text{Supp} (\Gamma)| = \kappa(D)|\text{Supp} (\Gamma)|$ where $\kappa(D) > 0$ and $|\text{Supp} (\Gamma)|$ denotes the number of sites in $\text{Supp} (\Gamma)$. Thus, we can take

$$p(D) = \frac{\kappa(D)}{27D^3} \min \left(\frac{1}{2}, \frac{\delta(D)}{\upsilon^*}\right).$$

(9.6)
An extension of the Peierls bound to non-saturated ACs is straightforward because each template in $\phi|_{\text{Supp } \Gamma}$ where one can add a particle contributes a factor $\leq u^{-1}$ into the statistical weight $w(\Gamma)$.

The results from Appendix A, together with Lemmas 9.1 and Theorem 10.8, lead to the following theorems.

**Theorem 9.1A.** Suppose that $D^2 = 2^{2n+1}$ where $n \in \mathbb{N} \cup \{0\}$. Let $S^{(D^2)}$ be the collection consisting of $D$-FCC sub-lattice $2^n A_3$ and its $\mathbb{Z}^3$-shifts. Set $S^{(D^2)}$ exhausts all PCs. The cardinality of $S^{(D^2)}$ is $2^{3n+1}$. The particle density of any PC equals $1/2^{3n+1}$. All PCs are $D$-FCC sub-lattices, and they form a single equivalence class.

**Proof.** It is well-known that equation (10.6) has only trivial solutions (where two of the numbers $m, n, k$ vanish), iff $\ell = 2^n$. See Theorem 5 p. 79, in [19]. With this at hand, the assertion of the theorem follows from Lemma 9.1 and Theorem 10.8.

**Theorem 9.1B.** Suppose that $D^2 = 2^{2n+1}$ where $n \in \mathbb{N} \cup \{0\}$. Let $u$ be large enough: $u \geq u^0(D^2)$. Then there are $2^{3n+1}$ EPGMs, i.e., $\sharp(\mathcal{E}(D, u)) = 2^{3n+1}$, and each EPGM is generated by a PGS from $S^{(D^2)}$.

**Proof.** The structure of PGSs for values of $D$ under consideration is given in Theorem 9.1A and consists of a single equivalence class. The Peierls bound (9.3) allows us to complete the proof via the PS theory.

**Theorem 9.2A.** Suppose that $D^2 = 2\ell^2$ where $\ell \in \mathbb{N}$, $\ell \neq 2^n$ and $\ell \neq 0 \mod 3$. Let $S^{(D^2)}$ be the collection consisting of all $D$-FCC sub-lattices and their $\mathbb{Z}^3$-shifts. Set $S^{(D^2)}$ exhausts all PCs. In total, there are finitely many PCs. The particle density of any PC equals $1/2\ell^3$. All PCs are $D$-FCC sub-lattices, and form more than one equivalence class.

The number of equivalence classes of $D$-FCC sub-lattices and the $\mathbb{Z}^3$-symmetries for each class (and hence the cardinality of the class) depend on the rational prime decomposition of $\ell$, as detailed in the Appendix A.

**Proof.** The assertion of the theorem follows from Lemma 9.1 and Theorem 10.8.

**Theorem 9.2B.** Suppose that $D^2 = 2\ell^2$ where $\ell \in \mathbb{N}$, $\ell \neq 2^n$ and $\ell \neq 0 \mod 3$. Let $u$ be large enough: $u \geq u^0(D^2)$. Then there exists at least one dominant PGS-equivalence class. Each PGS $\varphi$ from a dominant class generates an EPGM $\mu_\varphi$. Conversely, every EPGM $\mu$ is generated by a PGS from some dominant class.

**Proof.** The structure of PGSs for values of $D$ under consideration is given in Theorem 9.2A and consists of two or more equivalence classes. The Peierls bound (9.3) allows us to complete the proof via the PS theory.

**Theorem 9.3A.** Suppose $D^2 = 2\ell^2$ where $\ell \in \mathbb{N}$ and $\ell = 0 \mod 3$. Let $S^{(D^2)}$ be the set consisting of layered ACs: $\phi^{(D^2)}_{i, \{j_k\}}$ for $i = 0, 1, 2, 3$ and allowed sequences $\{j_k\}$, all rotations of ACs $\phi^{(D^2)}_{i, \{j_k\}}$ inscribed in $\mathbb{Z}^3$, and the $\mathbb{Z}^3$-shifts of such ACs. Set $S^{(D^2)}$ exhausts all
PCs. The cardinality of $S^{(D^2)}$ is continuum. The particle density in a PC equals $1/2\ell^3$. The subset $S^{(D^2)}_{\text{per}}$ consisting of periodic layered ACs from $S^{(D^2)}$ is countable and exhausts all periodic PCs. Depending on the rational prime decomposition of $\ell$, the sub-lattices in $S^{(D^2)}_{\text{per}}$ are partitioned into more than one but finitely many equivalence classes.

**Proof.** The assertion of the theorem follows from Lemma 9.1 and Theorem 10.8. \hfill $\blacksquare$

It is natural to expect that some analog of Theorem 9.2B holds true also for $D^2 = 2\ell^2$ when $\ell = 0 \mod 3$, and it can be proved by using methods from [6]. The first step here is the identification of the PGSs, and it is completed in Theorem 9.3A. The next step is the identification of the lowest order of the perturbation theory in which the infinite degeneracy of PGSs is removed. It turns out that this order equals 2 (equivalently the statistical weight equals $u^{-2}$), and the smallest excitation removing the degeneracy is described in the following way.

Consider three subsequent meshes $\tau := \tau_{i,2(k-1),j_{k-1}}$, $\tau := \tau_{i,2k,j_k}$, $\tau'' := \tau_{i,2(k+1),j_{k+1}}$ and assume that in the middle mesh $\tau$ there is a triangle $\triangle_0$ and in meshes $\tau'$, $\tau''$ there are triangles $\triangle_{\pm 1}$, and the centers of $\triangle_{\pm 1}$ are projected to the center of $\triangle_0$. Then, if we place a particle at the center of $\triangle_0$ and remove the particles from the vertices of $\triangle_0$, we obtain the desired excitation.

The maximal density of the above $u^{-2}$-excitations is achieved at the $D$-HCP configurations $\varphi^{(D^2)}_{i,\tau}, \varphi^{(D^2)}_{i,\tau'}$ with $i = 0, 1, 2, 3$, their rotations and, subsequently, $\mathbb{Z}^3$-shifts. Consequently, only the $D$-HCP configurations are expected to be dominant. The first difficulty in completing the proof of this claim lies in the verification that there is no other non-trivial excitation of order 2. Second, we need to identify, among all classes of $D$-HCP configurations, the dominant one. In Theorem 4.1B we verified it for a similar case where $D = \sqrt{5}$, but the proof of the claim for a general $D^2 = 2\ell^2$ with $\ell = 0 \mod 3$ is not known. Nevertheless, we put forward the following conjecture.

**Conjecture.** Suppose $D^2 = 2\ell^2$ where $\ell \in \mathbb{N}$ and $\ell = 0 \mod 3$. All EPGMs are generated by PCs from a single equivalence class. This class has cardinality $16\ell^3$ and consists of 8 $D$-HCP configurations and their $\mathbb{Z}^3$-shifts. Consequently, $\sharp\mathcal{E}(\sqrt{2}\ell, u) = 16\ell^3$.

## 10 Appendix A: $D$-FCC sub-lattices in $\mathbb{Z}^3$ and corresponding layered structures

It is known that a $D$-FCC sub-lattice in $\mathbb{Z}^3$ exists iff $D^2 = 2\ell^2$ with $\ell \in \mathbb{N}$, see Proposition 12 in [20], and in this section we focus on such values of $D^2$. A canonical example of a $D$-FCC sub-lattice is the scaled lattice $\Lambda_3$:

$$\ell\Lambda_3 := \left\{ m(\ell, \ell, 0) + n(\ell, 0, \ell) + k(0, \ell, \ell) : m,n,k \in \mathbb{Z} \right\}. \quad (10.1)$$

Cf. (2.13). Depending upon the rational prime decomposition of $\ell$, there may exist other $D$-FCC sub-lattices in $\mathbb{Z}^3$; see below. We also verify that the whole collection of layered structures emerging in $\mathbb{R}^3$ exists in $\mathbb{Z}^3$ iff $\ell = 0 \mod 3$, in which case they fit the construction described in Section 2 and give PCs of the form (2.16).
Let \( \tau_{i,2\ell k,j}^{(D^2)} \) be a triangular \( \sqrt{2}\ell \)-mesh as in (2.16), with \( q = 2\ell^2 \) and \( h = 2\ell, r = 2 \). The dependence on \( j = 0, 1, 2 \) is given by:

\[
\tau_{i,2\ell k,0}^{(D^2)} := \{ m\ell(1,-s_2,0) + n\ell(1,0,-s_3) : m, n \in \mathbb{Z} \} + \frac{2\ell k}{3}(1, s_2, s_3) \\
\tau_{i,2\ell k,1}^{(D^2)} := \tau_{i,2\ell k,0}^{(D^2)} + \frac{\ell}{3}(-2, s_2, s_3), \\
\tau_{i,2\ell k,2}^{(D^2)} := \tau_{i,2\ell k,0}^{(D^2)} + \frac{\ell}{3}(2, -s_2, -s_3),
\]

(10.2)

where \( s_2 = s_2(i) \) and \( s_3 = s_3(i) \) are determined in (2.11). Next, set \( \varphi_{i,(j_k)}^{(D^2)} := \bigcup_{k \in \mathbb{Z}} \tau_{i,2\ell k,j_k}^{(D^2)} \), with a double-infinite sequence \( \{ j_k \} \) such that \( j_0 = 0 \) and \( j_k \neq j_{k+1} \).

Observe that for any \( \ell \in \mathbb{N} \), the layered ACs \( \varphi_{i,012}^{(D^2)} \) and \( \varphi_{i,021}^{(D^2)} \) are FCC \( \ell \)-sub-lattices in \( \mathbb{Z}^3 \). Moreover, all remaining layered ACs \( \varphi_{i,(j_k)}^{(D^2)} \) also belong to \( \mathbb{Z}^3 \) if \( \ell \equiv 0 \mod 3 \). This includes HCP \( \ell \)-configurations \( \varphi_{i,012}^{(D^2)} \) and \( \varphi_{i,021}^{(D^2)} \).

A finite number of additional FCC \( \ell \)-sub-lattices \( R\ell A_3 \), obtained from \( \ell A_3 \) by non-trivial rotations \( R \), may exist for a given \( \ell \); this depends on the rational prime decomposition of \( \ell \). If \( \ell \equiv 0 \mod 3 \) then the corresponding layered ACs \( R\varphi_{i,(j_k)}^{(D^2)} \) are also inscribed in \( \mathbb{Z}^3 \).

For a given \( \ell \), the identification of all FCC \( \ell \)-sub-lattices in \( \mathbb{Z}^3 \) is equivalent to the identification of cubic \( \ell \)-sub-lattices as they are in a 1-1 correspondence.

It is straightforward that a cubic sub-lattice in \( \mathbb{Z}^3 \) with basis \( \{ x_1, x_2, x_3 \} \) contains an FCC sub-lattice with the basis

\[
y_1 = x_1 + x_2, \quad y_2 = x_2 + x_3, \quad y_3 = x_1 + x_3.
\]

Furthermore, all FCC \( \ell \)-sub-lattices of \( \mathbb{Z}^3 \) can be obtained in this way. See Corollaries 2.2 and 2.3 in [28].

The latter fact originates from the connections between both types of sub-lattices and the ring of integer quaternions. Every non-zero integer quaternion \( z = a + b \cdot \mathbf{i} + c \cdot \mathbf{j} + d \cdot \mathbf{k} \neq 0 \), with \( a, b, c, d \in \mathbb{Z} \), defines a non-trivial rotation of \( \mathbb{R}^3 \) given by the ortho-normal Euler-Rodrigues matrix:

\[
R(z) = \frac{1}{\ell} \begin{pmatrix}
a^2 + b^2 - c^2 - d^2 & 2bc - 2ad & 2bd + 2ac \\
2bc + 2ad & a^2 - b^2 + c^2 - d^2 & 2cd - 2ab \\
2bd - 2ac & 2cd + 2ab & a^2 - b^2 - c^2 + d^2
\end{pmatrix},
\]

(10.4)

where

\[
\ell = \ell(z) = ||z||^2 = a^2 + b^2 + c^2 + d^2.
\]

(10.5)

The rotation angle \( \alpha \) is given by

\[
\alpha = 2 \arccos \left( \frac{a}{a^2 + b^2 + c^2 + d^2} \right),
\]

and the rotation axis is along the vector \( (b, c, d) \). The rows of the matrix \( \ell R(z) \), \( \ell = ||z||^2 \), form a basis of a cubic \( \ell \)-sub-lattice of \( \mathbb{Z}^3 \), which we denote by \( \mathbb{Z}^3(z) \), and all such sub-lattices can be obtained in this way [8 9 15 14]. Each basis vector \( m, n, k \) of \( \mathbb{Z}^3(z) \)

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represents a Pythagorean quadruple with

\[ m^2 + n^2 + k^2 = \ell^2. \]  

(10.6)

The columns of the matrix \( \ell R(z) \) form a basis of the conjugated sub-lattice \( \mathbb{Z}^3(z) \) corresponding to the conjugated quaternion \( z \), that is, to the rotation along the same axis but in the opposite direction. The lattice \( \mathbb{Z}^3(z) \) coincides with the original lattice \( \mathbb{Z}^3 \) iff \( \|z\| = 1 \).

If the row-vectors of \( \ell R(z) \) are \( x_1, x_2, x_3 \) then \( y_1, y_2, y_3 \) defined as in (10.3) form a basis of the corresponding FCC \( \ell \)-sub-lattice of \( \mathbb{Z}^3 \), denoted by \( A_3(z) \). Note that the length of vectors \( y_i \) is \( \sqrt{2\ell} \); together with the origin, vectors \( y_i \) give the vertices of a regular tetrahedron. The lattice \( A_3(z) \) coincides with the original lattice \( A_3 \) iff \( \|z\| = 1 \). More generally, given an integer quaternion \( z \), we can consider layered ACs \( \varphi^{(D2)}_{i,j_k}(z) \), as images of \( \varphi^{(D2)}_{i,j_k} \) under the rotation \( R(z) \) generated by \( z \).

The rest of this section is devoted to the description of all cubic \( \ell \)-sub-lattices of \( \mathbb{Z}^3 \) including their number and symmetries. Cf. [27]. The symmetries of cubic \( \ell \)-sub-lattices and hence FCC \( \ell \)-sub-lattices are important for our considerations because if a sub-lattice generates an EPGM then every \( \mathbb{Z}^3 \)-symmetric image of this sub-lattice also generates an EPGM. An example of a cubic \( \ell \)-sub-lattice is \( \ell \mathbb{Z}^3 \), with the basis

\[
\{ (\ell, 0, 0), (0, \ell, 0), (0, 0, \ell) \},
\]

(10.7)

where \( \ell \in \mathbb{N} \). In general, we say that a sub-lattice is a cubic \( \ell \)-sub-lattice if it has a basis formed by three mutually orthogonal integer vectors of length \( \ell \).

The facts collected in this section are consequences of classical algebraic number theory, but we were not able to find a single source containing them in the desired form. We present these facts as a series of propositions accompanied with proofs when no direct reference is available.

**Proposition 10.1.** A cubic \( \ell \)-sub-lattice of \( \mathbb{Z}^3 \) exists iff \( \ell \) is a positive integer.

**Proof.** If \( \ell \in \mathbb{Z} \) then \( \ell \mathbb{Z}^3 \) is the desired sub-lattice. If \( \ell \notin \mathbb{Z} \) but there exists a cubic \( \ell \)-sub-lattice of \( \mathbb{Z}^3 \) then \( \ell = \sqrt{d} \) where \( d \in \mathbb{N} \) as all basis vectors of the sub-lattice have integer coordinates. Moreover, the vector product of two basis vectors is a vector of length \( \ell^2 \) with integer coordinates which is collinear to the third basis vector, also with integer coordinates. The ratio of lengths of these two collinear vectors is equal to \( \ell^2 / \ell = \ell \), and it should also be equal to the ratio of the corresponding first coordinates. As both coordinates are integers, their ratio is rational and cannot be equal to an irrational \( \sqrt{d} \). 

Since the HC model under consideration is \( \mathbb{Z}^3 \)-symmetric, we are interested only in the equivalence classes of sub-lattices with respect to \( \mathbb{Z}^3 \)-symmetries. We use the standard notation \( O_h \) for the group of \( \mathbb{Z}^3 \)-symmetries which is of order 48. The group \( O_h \) consist
of:

(i) the identity,
(ii) six rotations by $\pm \frac{\pi}{2}$ with respect to one of the coordinate axis,
(iii) three rotations by $\pi$ with respect to one of the coordinate axis,
(iv) six rotations by $\pi$ with respect to one of the coordinate plane diagonals, 
(v) eight rotations by $\pm \frac{2\pi}{3}$ with respect to one of the main diagonals,
(vi) twenty four composition of the inversion (central symmetry) with each of the previous elements.

The 24 symmetries listed in (i-v) form the subgroup $S_4$ of $O_h$. Item (vi) recognizes the fact that $O_h \cong Z_2 \times S_4$ where the group $Z_2$ consists of the identity and the inversion.

Each cubic $\ell$-sub-lattice of $\mathbb{Z}^3$ is invariant under the inversion, hence under the action of $O_h$ every stabilizer of a cubic $\ell$-sub-lattice contains $Z_2$, and every equivalence class (identified with an orbit of this sub-lattice under the action of $O_h$) contains at most 24 sub-lattices. In the generic case, the stabilizer group is exactly $Z_2$, and the sub-lattices in the class are obtained from each other by symmetries listed in (ii-v). Cf. Proposition 10.7 below.

All non-generic cases are where a cubic $\ell$-sub-lattice is invariant under a larger subgroup. It turns out (cf. Propositions 10.2-10.6 below) that the possible stabilizer groups are $Z_2 \times Z_2$, $Z_6$, Dih$_4$, Dih$_6$ and $O_h$, of orders 4, 6, 8, 12 and 48 respectively. As all listed orders are different, the size of the equivalence class is determined by the type of the corresponding stabilizer. Each of the propositions below characterizes the class corresponding to each stabilizer and exhausts the list of all possible stabilizers.

**Proposition 10.2.** A class with a single cubic $\ell$-sub-lattice is formed only by $\ell \mathbb{Z}^3$, with the basis (10.7), where $\ell \in \mathbb{N}$. This sub-lattice is invariant under all symmetries from $O_h$.

**Proof.** Suppose we have a cubic $\ell$-sub-lattice invariant under all elements of $O_h$ and different from $\ell \mathbb{Z}^3$. Assume it has a basis vector $(m, n, k)$ of length $\ell$ with non-zero components $m, n, k$. Take vector $(n, -m, k)$ obtained via the rotation by $\pi/2$ around the vertical axis; it has length $\ell$ and belongs to the sub-lattice. The scalar product of these two vectors equals $mn - mn + k^2 = k^2 > 0$, whereas it should be either 0 or $-\ell^2$. This is a contradiction.

Assume the sub-lattice contains vector $(m, n, 0)$ of length $\ell$ with non-zero $m, n$. Then vector $(0, m, n)$, of length $\ell$, belongs to the sub-lattice as it is obtained via rotation by $2\pi/3$ around the main diagonal collinear with the vector $(1, 1, 1)$ (referred to as the $(1,1,1)$-diagonal). The scalar product of these two vectors equals $mn$, but as before it should be 0 or $-\ell^2$. We again get a contradiction.

The remaining possibility is that all 6 vectors of length $\ell$ in our $\ell$-sub-lattice have two components 0. Then it coincides with $\ell \mathbb{Z}^3$.

**Proposition 10.3.** (i) A class with 4 cubic $\ell$-sub-lattices exists iff $\ell = 3t$, $t \in \mathbb{N}$, and is unique for a given $t$. Such a class is formed by the sub-lattices obtained via the rotation of $\ell \mathbb{Z}^3$ by the angle $\pi$ about each of the 4 main diagonals. These sub-lattices are spanned
by the following 4 bases

\[
\{(-t, 2t, 2t), (2t, -t, 2t), (2t, 2t, -t)\}; \quad \{(t, 2t, 2t), (-2t, -t, 2t), (-2t, 2t, -t)\};
\]
\[
\{(-t, -2t, 2t), (2t, t, 2t), (2t, -2t, -t)\}; \quad \{(-t, 2t, -2t), (2t, -t, -2t), (2t, 2t, t)\}.
\]

(ii) Each cubic \(\ell\)-sub-lattice from the class is invariant under the rotations by \(2\pi/3\) about the corresponding main diagonal, the reflection about any diagonal plane containing this main diagonal and the inversion, which generate the dihedral stabilizer subgroup \(\text{Dih}_3 \times \mathbb{Z}_2 \simeq \text{Dih}_6 \lt O_h\) of order 12.

**Proof.** It is a direct calculation to verify that the class containing 4 cubic \(\ell\)-sub-lattices (10.9) satisfies the properties in (ii), and each sub-lattice from (10.9) does not have additional symmetries. Therefore, it remains to verify the inverse: if a cubic \(\ell\)-sub-lattice is invariant under symmetries listed in statement (ii) then it is one of the sub-lattices (10.9).

Suppose a cubic \(\ell\)-sub-lattice is invariant under the rotation by \(\pm 2\pi/3\) about a main diagonal. For definiteness, choose the \((1, 1, 1)\)-diagonal and consider the rotation angle \(2\pi/3\). Let a vector \((m, n, k) \neq (\ell, \ell, \ell)\) of length \(\sqrt{3}\ell\) be collinear to a main diagonal of our sub-lattice. Then its image after the rotation, \((k, m, n)\), must give another main diagonal of the sub-lattice. Consequently, the cos of the angle between these two diagonals, \((km + mn + nk)/3\ell^2\), must be equal to \(1/3\). This implies that

\[
(m + n + k)^2 = (m^2 + n^2 + k^2) + 2(km + mn + nk) = 3\ell^2 + 2\ell^2 = 5\ell^2,
\]

which is impossible with integer \(m, n, k, \ell\), due to irrationality of \(\sqrt{5}\). Thus, the only remaining possibility is \((m, n, k) = (\ell, \ell, \ell)\), i.e., that the cubic sub-lattice is obtained by a rotation of \(\ell\mathbb{Z}^3\) around the \((1, 1, 1)\)-diagonal. Let the angle of rotation be \(\alpha\).

Suppose that the sub-lattice is also invariant under the reflection about a diagonal plane. Then it is not hard to see that this diagonal plane must contain vector \((1, 1, 1)\), and the angle \(\alpha\) must be \(\pi\). Moreover, the standard orthogonal basis of \(\ell\mathbb{Z}^3\) is mapped, under the rotation by \(\pi\) around the \((1, 1, 1)\)-diagonal, into \(\{(-t, 2t, 2t), (2t, -t, 2t), (2t, 2t, -t)\}\), where \(t = \ell/3\). The corresponding three vectors belong to \(\mathbb{Z}^3\) only if \(\ell = 0 \mod 3\).

The remaining triples in (10.9) correspond to the other three main diagonals. \(\blacksquare\)

**Proposition 10.4.** (i) A class with 6 cubic \(\ell\)-sub-lattices exists iff \(\ell\) has a prime factor \(p = 1 \mod 4\). The sub-lattices forming such a class are obtained by rotating \(\ell\mathbb{Z}^3\) by the angles \(\pm 2\arctan\left(\frac{b}{a}\right)\) around each of the 3 coordinate axes, and they are spanned by the bases

\[
\{(\ell, 0, 0), (0, n, k), (0, -k, n)\}; \quad \{(\ell, 0, 0), (0, k, n), (0, n, -k)\};
\]
\[
\{(0, n, 0), (n, 0, k), (n, -k, 0)\}; \quad \{(0, n, 0), (n, 0, -k), (n, -k, 0)\};
\]
\[
\{(0, 0, n), (n, k, 0), (-k, n, 0)\}; \quad \{(0, 0, n), (k, n, 0), (n, -k, 0)\}.
\]

(10.10)

Here \(a, b, n, k, t \in \mathbb{N}\) are such that

\[
a > b, \gcd(a, b) = 1, \quad \ell = (a^2 + b^2)t, \quad n = (a^2 - b^2)t, \quad k = 2abt, \quad n^2 + k^2 = \ell^2. \quad (10.11)
\]

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The above pair $a, b \in \mathbb{N}$ is identified with the pair of conjugated Gaussian integers $a \pm b \cdot i$ in the ring $\mathbb{Z} \left[ \sqrt{-1} \right]$. Each conjugated pair from $\mathbb{Z} \left[ \sqrt{-1} \right]$ generates 2 sub-lattices in each row of (10.10). Different triples $a, b, t \in \mathbb{N}$ with $a > b$, $\gcd(a, b) = 1$, $t(a^2 + b^2) = \ell$ determine different classes.

(ii) When the rotation axis is fixed, each of the emerging 2 sub-lattices (listed in the respective row in (10.10)) is invariant under the rotation by $\pi/2$ about the chosen coordinate axis and the inversion, generating the dihedral stabilizer subgroup $\text{Dih}_4 < \text{Oh}$ of order 8.

(iii) If $\ell$ contains distinct prime factors $\rho_i = 1 \mod 4$ with multiplicities $\rho_i \geq 0$ then the corresponding number of classes of cardinality 6 equals

$$\frac{1}{2}s_2(\ell) := \frac{1}{2} \left[ \prod_i (2\rho_i + 1) - 1 \right]. \tag{10.12}$$

**Proof.** (i, ii) It is a direct calculation to verify that the class containing 6 sub-lattices (10.10) satisfies properties (ii), and each sub-lattice from (10.10) does not have additional symmetries. The next step is to check the inverse: if a cubic $\ell$-sub-lattice is invariant under symmetries listed in statement (ii) then it is one of sub-lattices (10.10).

Suppose a cubic $\ell$-sub-lattice is invariant under the rotation by $\pm \frac{\pi}{2}$ around a coordinate axis. Then the sub-lattice is also invariant under the rotation by $\pi$ around the same axis. For definiteness, assume that the sub-lattice is invariant under the rotation by $\pi$ around the vector $(1, 0, 0)$.

Take the collection of 6 vectors of length $\ell$: three forming an orthogonal basis of the sub-lattice plus their opposites obtained via the inversion. Let $(m, n, k)$ be a vector from the collection forming the smallest angle $\alpha$ with $(1, 0, 0)$. By construction, the vector $(m, -n, -k)$ obtained via the rotation must also belong to the sub-lattice. This may happen only if $\alpha = 0, \alpha = \frac{\pi}{4} \text{ or } \alpha = \frac{\pi}{2}$, as two vectors of length $\ell$ from the sub-lattice must be either collinear or orthogonal. The case $\alpha = \frac{\pi}{2}$ is impossible as it implies that all 6 vectors belong to the half-space $m \leq 0$. The case $\alpha = \frac{\pi}{4}$ implies that the angle between $(m, n, k)$ and $(m, -n, -k)$ is $\frac{\pi}{2}$ and therefore $m^2 = n^2 + k^2$ and, consequently, $l = \sqrt{2}m$, violating the requirement $l \in \mathbb{N}$. Thus, $\alpha = 0, \text{ i.e. } (\ell, 0, 0)$ is the basis vector of our sub-lattice, which occurs only if the sub-lattice is $\ell\mathbb{Z}^3$ or is obtained by a rotation of $\ell\mathbb{Z}^3$ around $(\ell, 0, 0)$.

This implies that the basis of the sub-lattice is $\{(\ell, 0, 0), (0, n, k), (0, -k, n)\}$ which is listed first in the top line in (10.10). Here $n, k$ are integers such that $n^2 + k^2 = \ell^2$. The second triple in the top line in (10.10) corresponds to the conjugated sub-lattice obtained via the rotation by the same angle in the opposite direction. The remaining triples in (10.10) correspond to the other coordinate axes.

The next step is to verify representation (10.11). The already established condition $n^2 + k^2 = \ell^2$ in (10.11) means that $n, k, \ell$ form a Pythagorean triple. The structure of such triples is associated with the rotation matrices

$$R = \frac{1}{\sqrt{a^2 + b^2}} \begin{pmatrix} a & b \\ -b & a \end{pmatrix}, \quad R^{-1} = \frac{1}{\sqrt{a^2 + b^2}} \begin{pmatrix} a & -b \\ b & a \end{pmatrix}.$$
The rows of the orthogonal matrix

\[ t(a^2 + b^2)R^2 = t \begin{pmatrix} a^2 - b^2 & 2ab \\ -2ab & a^2 - b^2 \end{pmatrix} \]

parametrize Pythagorean triples in (10.11) through orthogonal pairs \((n, k)\) and \((-k, n)\). It is well-known that this parametrization can be derived from the identification of the matrices \(R\) and \(R^{-1}\) with the pair of conjugated Gaussian integers \(a \pm b \cdot i\).

Given \(\ell \in \mathbb{N}\), the non-trivial representation of \(\ell^2\) as the sum of two positive squares, i.e. as the norm of a Gaussian integer, exists iff the rational prime decomposition of \(\ell\) has a factor \(p = 1 \mod 4\). Here non-trivial means different from the representation \(\ell^2 + 0^2 = \ell^2\). A prime \(p = 1 \mod 4\) is the product of two conjugated Gaussian primes \(a \pm b \cdot i\), where \(a > b > 0\) with \(\gcd(a, b) = 1\) are uniquely defined by \(p\). A rational prime \(p = 3 \mod 4\) is always a Gaussian prime (for example see [19 5]). Denote by \(p_i\), \(i = 1, 2, \ldots\) the set of distinct primes of the form \(4s + 1\) entering the rational prime decomposition of \(\ell\) with multiplicities \(p_i \geq 1\). For each \(i\) we have \(p_i = (a_i + b_i \cdot i)(a_i - b_i \cdot i)\), where integers \(a_i > b_i > 0\) are uniquely defined by \(p_i\). Thus, one can form a multitude of products

\[ \prod_{i=1}^\infty (a_i \pm b_i \cdot i)^{\alpha_i}, \quad 0 \leq \alpha_i \leq p_i, \quad \sum \alpha_i \geq 1 \] (10.13)

by varying the selection of \(\alpha_i\) and the sign in front of \(b_i\). Expanding the product in (10.13), we end up with a Gaussian integer \(a + b \cdot i\) satisfying (after a multiplication by a unit in \(\mathbb{Z}[\sqrt{-1}]\))

\[ a, |b| \in \mathbb{N}, \quad a > |b|, \quad \gcd(a, b) = 1, \quad \ell = (a^2 + b^2)t, \quad t \in \mathbb{N}. \] (10.14)

Note that in (10.13), the value \(b\) can be negative, and the triple \(a, b, t\) defines a unique quadratic \(\ell\)-sub-lattice of \(\mathbb{Z}^2\). Changing the sign of \(b\) implies a conjugated sub-lattice (see the second triple in each row of (10.10)). This completes the verification of (10.11) and therefore the proof of assertions (i) and (ii).

(iii) To establish (10.12), observe that there are \(p_i\) possibilities to choose \(\alpha_i > 0\), and for each of them there are 2 possibilities to choose the sign between \(a_i\) and \(b_i\). An additional possibility is \(\alpha_i = 0\) which amounts to \(2p_i + 1\) choices in total. Since the choices for different \(i\) are done independently, the quantity

\[ s_2(\ell) = \prod_i (2p_i + 1) - 1 \] (10.15)

counts the total amount of possibilities, excluding the case where all \(\alpha_i = 0\). This is exactly the number of distinct square \(\ell\)-sub-lattices in \(\mathbb{Z}^2\) different from \(\ell\mathbb{Z}^2\), because a pair of conjugated square \(\ell\)-sub-lattices of \(\mathbb{Z}^2\) generates cubic \(\ell\)-sub-lattices of \(\mathbb{Z}^3\) from the same class. Hence, the number of classes corresponding to \(\ell\) is equal to \(\frac{s_2(\ell)}{2}\), which establishes (iii).

Remark. The possibilities \(a = b\) or \(b = 0\) excluded by (10.11) give a class with a single sub-lattice considered in Proposition 10.2.
Proposition 10.5. (i) A class formed by 8 cubic \( \ell \)-sub-lattices exists iff \( \ell \) has a prime factor \( p = 1 \mod 3 \). The sub-lattices forming such a class are obtained by rotating \( \ell \mathbb{Z}^3 \) by the angles \( \pm 2 \arctan \left( \frac{b \sqrt{3}}{2a - b} \right) \) around each of the 4 main diagonals, and they are spanned by the bases

\[
\begin{align*}
\{(m,n,k), (k,m,n), (n,k,m)\}, & \quad \{(m,k,n), (n,m,k), (k,n,m)\}, \\
\{(m,-m,k), (m,-m,n), (n,-m,k), (n,-m,n)\}, & \quad \{(k,-m,n), (m,-m,k), (n,-m,k), (n,-m,n)\}, \\
\{(-m,m,n), (-k,m,n), (n,-k,m), (n,-k,n)\}, & \quad \{(k,-m,n), (-m,-k,n), (n,-m,k), (n,-m,n)\},
\end{align*}
\]

(10.16)

Here \( a, b, m, k, n, t \in \mathbb{N} \) are such that

\[
\begin{align*}
(10.17)
\end{align*}
\]

The above pair \( a, b \in \mathbb{N} \) is identified with the pair of conjugated Eisenstein integers \( a + b \cdot \omega \) and \( a + b \cdot \bar{\omega} \) in the ring \( \mathbb{Z}[\omega] \), where \( \omega = (-1 + \sqrt{3} \cdot i)/2 \). Each conjugated pair from \( \mathbb{Z}[\omega] \) generates 2 sub-lattices in each row of (10.16). Different triples \( a, b, t \in \mathbb{N} \) with \( a > 2b \), \( \gcd (a, b) = 1 \), \( t(a^2 + b^2 - ab) = \ell \) determine different classes.

(ii) When the rotation axis is fixed, each of the emerging 2 sub-lattices (listed in the respective row in (10.16)) is invariant under the rotation by \( 2\pi/3 \) about the chosen main diagonal and the inversion, generating the stabilizer subgroup \( Z_3 \times Z_2 \simeq Z_6 < O_h \) of order 6.

(iii) If \( \ell \) contains distinct prime factors \( p_i = 1 \mod 3 \) with multiplicities \( \rho_i \geq 0 \) then the corresponding number of classes of cardinality 8 equals

\[
\begin{align*}
\frac{1}{2} \hat{s}_2(\ell) := \frac{1}{2} \left[ \prod_i (2\rho_i + 1) - 1 \right].
\end{align*}
\]

(10.18)

Proof. (i, ii) It is a direct calculation to verify that the class containing 8 sub-lattices (10.16) satisfies properties (ii), and each sub-lattice from (10.16) does not have additional symmetries. The next step is to check the inverse: if a cubic \( \ell \)-sub-lattice is invariant under symmetries listed in statement (iii) then it is one of sub-lattices (10.16).

Suppose a cubic \( \ell \)-sub-lattice is invariant under the rotation by \( \pm \frac{2\pi}{3} \) about a main diagonal. For definiteness, choose the \((1,1,1)\)-diagonal and consider the rotation angle \( \frac{2\pi}{3} \). Let a vector \((m,n,k) \neq (\ell, \ell, \ell)\) of length \( \sqrt{3} \ell \) define a main diagonal of our cubic \( \ell \)-sub-lattice. Then its image after rotation, \((k,m,n)\), must give another main diagonal of the sub-lattice. Consequently, the cos of the angle between these two diagonals, \((km + mn + nk)/3\ell^2\), must be equal to \(1/3\). This implies that

\[
(m + n + k)^2 = (m^2 + n^2 + k^2) + 2(km + mn + nk) = 3\ell^2 + 2\ell^2 = 5\ell^2,
\]

which is impossible with integer \( m, n, k, \ell \) due to irrationality of \( \sqrt{5} \). Thus, the only remaining possibility is \((m,n,k) = (\ell, \ell, \ell)\), i.e., that the cubic \( \ell \)-sub-lattice is obtained by a rotation of \( \ell \mathbb{Z}^3 \) around the \((1,1,1)\)-diagonal.
This implies that the basis of the sub-lattice is \((m, n, k, (k, m, n), (n, k, m))\), which is listed first in the top line in (10.16). Here \(m, n, k\) are integers such that

\[(m - k)^2 + (n - k)^2 - (m - k)(n - k) = \ell^2\]  

(10.19)

which is the last condition in (10.17). To see the necessity of (10.19), denote by \(A_2\) the intersection of \(Z^4\) and the plane \(x_1 + x_2 + x_3 = 0\). Then \(A_2\) is a triangular lattice with distance \(\sqrt{2}\) between nearest sites. For definiteness, select vectors \(e_1 = (1, -1, 0, 0)\) and \(e_2 = (0, 1, -1)\) as a basis in \(A_2\). Obviously, \(lZ^3 \cap A_2 = lA_2\) is a triangular \(l\)-sub-lattice of \(A_2\). The rotation of \(lZ^3\) around the \((1, 1, 1)\)-diagonal corresponds to the rotation of \(lA_2\) by the same angle around the origin. If under this rotation the vector \((0, 0, 0)\) is mapped to the vector \((m, n, k)\) then vectors \((0, \ell, 0)\) and \((0, 0, \ell)\) are mapped into \((k, m, n)\) and \((n, k, m)\), respectively as a cyclic permutation of coordinates corresponds to a rotation by \(2\pi/3\) mapping one basis vector into another. Consequently, the vector \((1, -\ell, 0)\) is mapped into the vector \((m - k, n - m, k - n) = (m - k)e_1 + (n - k)e_2\). Thus, (10.19) defines an Eisenstein triple which is an \(A_2\)-analogue of a Pythagorean triple \(m^2 + n^2 = \ell^2\) in \(Z^3\) considered in (10.11). The second triple in the top line in (10.16) corresponds to the conjugated sub-lattice obtained via the rotation by the same angle in the opposite direction. The remaining triples in (10.16) correspond to the other main-diagonals.

It remains to verify representation (10.17). The problem of identifying triangular \(l\)-sub-lattices of \(A_2\) is similar to that for square \(l\)-sub-lattices of \(Z^2\), which was discussed in the proof of the previous proposition. The only difference is that, instead of Gaussian integers, one needs to work with Eisenstein integers forming the ring \(Z[\omega]\). The structure of Eisenstein triples in \(A_2\) is associated with the rotation matrices

\[R = \frac{1}{\sqrt{a^2 + b^2 - ab}} \begin{pmatrix} a & b \\ -b & a-b \end{pmatrix}, \quad R^{-1} = \frac{1}{\sqrt{a^2 + b^2 - ab}} \begin{pmatrix} a-b & -b \\ b & a \end{pmatrix}\]

given in \(A_2\)-coordinates \(e_1\) and \(e_2\). The rows of the matrix

\[t(a^2 + b^2 - ab)R^2 = t \begin{pmatrix} a^2 - b^2 & 2ab - b^3 \\ b^2 - 2ab & a^2 - 2ab \end{pmatrix}\]

parametrize the solutions \((m - k), (n - k)\) to (10.19). This parametrization can be derived from the identification of the matrices \(R\) and \(R^{-1}\) with the pair of conjugated Eisenstein integers \(a + b \cdot \omega\) and \(a + b \cdot \bar{\omega}\).

Given \(\ell \in \mathbb{N}\), the non-trivial representation of \(\ell^2\) in the form (10.19), i.e. as the norm of an Eisenstein integer, exists iff the rational prime decomposition of \(\ell\) has a factor \(p = 1\) mod 3. Here non-trivial means different from the representations \(\ell^2 = 0^2 - \ell \cdot 0 = \ell^2\) and \(\ell^2 + \ell^2 - \ell \cdot \ell = \ell^2\). A prime \(p = 1\) mod 3 is the product of two conjugated Eisenstein primes \(a + b \cdot \omega\) and \(a + b \cdot \bar{\omega}\), where \(a > |2b| > 0\) with \(\gcd(a, b) = 1\) are uniquely defined by \(p\). (Note, that for \(p = 3\), \(a = 2\) and \(b = 1\).) A rational prime \(p = 2\) mod 3 is always an Eisenstein prime. Denote by \(p_i\), \(i = 1, 2, \ldots\) the set of distinct primes of the form \(3s + 1\) entering the rational prime decomposition of \(\ell\) with multiplicities \(\rho_i \geq 1\). For each \(i\) we have \(p_i = (a_i + b_i \cdot \omega)(a_i + b_i \cdot \bar{\omega})\), where integers \(a_i > |2b_i|\) are uniquely determined by \(p_i\). Thus, one can form a multitude of products

\[\prod_{i=1}^{\infty} (a_i + b_i \cdot \omega)^{\alpha_i}, \quad 0 \leq \alpha_i \leq \rho_i, \quad \sum_{i=1}^{\infty} \alpha_i \geq 1\]

(10.20)
by varying the selection of $\alpha_i$ and the selection of $\omega$ as either $\omega$ or $-\omega$. Expanding the product in (10.20), we end up with an Eisenstein integer $a + b \cdot \omega$ satisfying (after a multiplication by a unit in $\mathbb{Z}[\omega]$)

$$a, |b| \in \mathbb{N}, a > |2b|, \gcd(a, b) = 1, \ell = (a^2 + b^2 - ab)t, \text{ where } t \in \mathbb{N}. \quad (10.21)$$

Note, that in (10.21) the value $b$ can be negative, and the triple $a$, $b$, $t$ defines a unique triangular $\ell$-sub-lattice of $A_2$. Changing the sign of $b$ and replacing $a$ with $a - b$ implies a conjugated sub-lattice (see the second triplet in given row of (10.16)). This completes the verification of (10.17). To finish the proof of assertions (i) and (ii), we only need to observe that the site $a e_1 + b e_2 \in A_2$ can be written as $\sqrt{2} \left( a - \frac{b}{2}, \frac{b\sqrt{3}}{2} \right)$ in Cartesian coordinates $e_1' = \frac{1}{\sqrt{2}} e_1, e_2' = \frac{2}{\sqrt{6}} e_2 - \frac{1}{\sqrt{6}} e_1$ implying the desired value for the tangent of the rotation angle.

(iii) To establish (10.18), observe that there are $\rho_i$ possibilities to choose $\alpha_i > 0$ and for each of them there are 2 possibilities to choose between $\omega$ and $\overline{\omega}$. An additional possibility is $\alpha_i = 0$ which amounts to $2\rho_i + 1$ choices in total. Since the choices for different $i$ are done independently, the quantity

$$\tilde{s}_2(\ell) = \prod_{i=1}^{\rho_i} (2\rho_i + 1) - 1 \quad (10.22)$$

counts the total amount of possibilities, excluding the case where all $\alpha_i = 0$. This is exactly the number of distinct triangular $\ell$-sub-lattices in $A_2$ different from $\ell A_2$ and its rotation by $\frac{\pi}{6}$ (the case of $a = 2b$ treated in the Proposition 10.3). Because a pair of conjugated triangular $\ell$-sub-lattices of $A_2$ generates cubic $\ell$-sub-lattices of $\mathbb{Z}^3$ from the same class, the number of corresponding classes is equal to $\frac{\tilde{s}_2(\ell)}{2}$. This yields (iii). \hfill \blacksquare

**Remark.** The case $a = 2b$ excluded by (10.17) gives rise to a class with 4 sub-lattices considered in Proposition 10.3. The case $b = 0$ gives rise to a class with a single sub-lattice from Proposition 10.2

**Proposition 10.6.** (i) A class formed by 12 cubic $\ell$-sub-lattices exists iff $\ell$ has a prime factor of the form $8s + 1$ or $8s + 3$. The sub-lattices forming such a class are obtained by rotating $\ell \mathbb{Z}^3$ by the angles $\pm 2 \arctan \left( \frac{\sqrt{2}b}{a} \right)$ around each of the 6 non-main diagonals, and they are spanned by bases

$$\{(m, n, k), (n, m, -k), (-k, k, m - n)\}, \{(m, n, -k), (n, m, k), (k, -k, m - n)\},$$
$$\{(n, m, k), (m, n, -k), (k, m, -n)\}, \{(n, m, -k), (m, n, k), (-k, k, -m - n)\},$$
$$\{(k, m, n), (-k, n, m), (m - n, -k)\}, \{(-k, m, n), (k, n, m), (m - n, k, -k)\},$$
$$\{(k, n, -m), (-k, m, n), (m - n, k, -n)\}, \{(-k, n, -m), (k, m, n), (m - n, -k, k)\},$$
$$\{(n, k, m), (m, -k, n), (k, m - n, -k)\}, \{(n, -k, m), (m, k, n), (-k, m - n, k)\},$$
$$\{(-m, k, n), (-n, -k, m), (k, m - n, k)\}, \{(-m, -k, n), (-n, k, m), (-k, m - n, -k)\}. \quad (10.23)$$
Here \( a, b, m, n, k, t \in \mathbb{N} \) are such that
\[
\begin{align*}
  a & \neq b, \quad a \neq 2b, \quad \gcd(a, b) = 1, \quad (a^2 + 2b^2)t = \ell, \quad m = a^2t, \quad n = 2b^2t, \quad k = 2abt, \\
  (m - n)^2 + 2k^2 &= \ell^2.
\end{align*}
\] (10.24)

The above pair \( a, b \in \mathbb{N} \) is identified with the pair of conjugated algebraic integers \( a \pm b \sqrt{2} \) in the ring \( \mathbb{Z}[\sqrt{-2}] \). Each conjugated pair from \( \mathbb{Z}[\sqrt{-2}] \) generates 2 sub-lattices in each row of (10.23). Different triples \( a, b, t \in \mathbb{N} \) with \( \gcd(a, b) = 1 \), \( t(a^2 + 2b^2) = \ell \) determine different classes.

(ii) Each sub-lattice in a class is invariant under the rotation by \( \pi \) about the corresponding non-main diagonal and the inversion, generating the stabilizer subgroup \( \mathbb{Z}_2 \times \mathbb{Z}_2 \simeq V_4 < O_h \) of order 4.

(iii) If \( \ell \) has distinct prime factors \( p_i \) of the form \( 8s + 1 \) or \( 8s + 3 \) with multiplicities \( \rho_i \), then the number of classes of cardinality 12 equals
\[
\frac{1}{2} S_2(\ell) := \frac{1}{2} \left[ \prod_i (2\rho_i + 1) - 1 \right].
\] (10.25)

**Proof.** (i, ii) It is a direct calculation to verify that the class containing 12 sub-lattices (10.23) satisfies properties (ii), and each sub-lattice from (10.23) does not have additional symmetries. The next step is to check the inverse: if a cubic \( \ell \)-sub-lattice is invariant under symmetries listed in statement (ii) then it is one of sub-lattices (10.23).

Suppose a cubic \( \ell \)-sub-lattice is invariant under the rotation by \( \pm \pi \) about a non-main diagonal. For definiteness, choose the \( (1,1,0) \)-diagonal and consider the rotation angle \( \pi \). Take the collection of 6 vectors of length \( \ell \): three forming an orthogonal basis of the sub-lattice plus their opposites obtained via the inversion. Let \( (m, n, k) \) be a vector from the collection, forming the smallest angle with \( (1,1,0) \). By construction, the vector \( (n, m, -k) \) obtained via the rotation of \( (m, n, k) \) must also belong to the sub-lattice. This may happen only if the angle \( \alpha \) between \( (m, n, k) \) and \( (n, m, -k) \) is 0 or \( \frac{\pi}{2} \), as two vectors of length \( \ell \) from the \( \ell \)-sub-lattice must be either collinear or orthogonal. The case \( \alpha = 0 \) is impossible because in that case \( n = m, k = 0 \) implying \( 2m^2 = \ell^2 \), which contradicts irrationality of \( \sqrt{2} \). Thus, \( \alpha = \frac{\pi}{2} \), and \( (\ell, \ell, 0) \) is a diagonal of the considered cubic \( \ell \)-sub-lattice, i.e. the sub-lattice is obtained by a rotation of \( \ell \mathbb{Z}^3 \) around \( (1,1,0) \)-diagonal.

This implies that the basis of the sub-lattice is \( \{(m, n, k), (n, m, -k), (-k, k, m - n)\} \), which is listed first in the top line in (10.23). Indeed, by construction the length of \( (m, n, k) \) and \( (n, m, -k) \) is \( \ell \) and the angle between them is \( \frac{\pi}{2} \), that is, \( m^2 + n^2 + k^2 = \ell^2 \) and \( 2mn - k^2 = 0 \). Hence, the vector \( (-k, k, m - n) \) is orthogonal to both of them and has length \( \ell \).

Thus, \( m, n, k \) are integers such that
\[
(m - n)^2 + 2k^2 = \ell^2, \quad (-2k)^2 + 2(m - n)^2 = 2\ell^2
\] (10.26)
which is the last condition in (10.24). To see the necessity of (10.26), denote by \( L \) the intersection of \( \mathbb{Z}^3 \) and the plane \( x_1 + x_2 = 0 \). Then \( L \) is a rectangular lattice \( \mathbb{Z} \times \sqrt{2}\mathbb{Z} \). For definiteness, select vectors \( e_1 = (0,0,1) \), \( e_2 = (-1,1,0) = (0,1,0) - (1,0,0) \) as a basis in \( L \). Obviously, \( \ell \mathbb{Z}^3 \cap L = \ell L \) is a rectangular sub-lattice of \( L \). The rotation of \( \ell \mathbb{Z}^3 \)
around the $(1, 1, 0)$-diagonal corresponds to the rotation of $\ell L$ by the same angle around the origin. If under this diagonal the vector $(\ell, 0, 0)$ is mapped into the vector $(m, n, k)$ then vector $(0, \ell, 0)$ is mapped into $(n, m, -k)$ obtained from $(m, n, k)$ via rotation by $\pi$ about the $(1, 1, 0)$-diagonal. Consequently, the vector $(0, 0, \ell)$ is mapped into the vector $(-k, k, m - n) = \frac{1}{m + n}((m, n, k) \times (n, m, -k)) = (m - n)e_1 + ke_2$. Accordingly, the vector $(-\ell, \ell, 0)$ is mapped into $(n - m, m - n, -2k) = -2ke_1 + (m - n)e_2$. Thus, \((10.26)\) is an $\mathbb{L}$-analogue of Pythagorean and Eisenstein triples considered in \((10.11)\) and \((10.17)\), respectively. The second triple in the top line in \((10.23)\) corresponds to the conjugated sub-lattices obtained via the rotation by the same angle in the opposite direction. The remaining triples in \((10.23)\) correspond to the other non-main diagonals.

It remains to verify representation \((10.24)\). The problem of identifying rectangular sub-lattices of $\mathbb{L}$ congruent to $\ell L$ is similar to that for square $\ell$-sub-lattices of $\mathbb{Z}^2$, which was discussed in the proof of Proposition \(10.4\). The only difference is that, instead of Gaussian integers, one needs to work with algebraic integers from the ring $\mathbb{Z}[\sqrt{-2}]$, belonging to the norm-Euclidean quadratic field $\mathbb{Q} [\sqrt{-2}]$. The structure of triples \((10.26)\) is associated with the rotation matrices

$$R = \frac{1}{\sqrt{a^2 + 2b^2}} \begin{pmatrix} a & b \\ -2b & a \end{pmatrix}, \quad R^{-1} = \frac{1}{\sqrt{a^2 + 2b^2}} \begin{pmatrix} a & -b \\ 2b & a \end{pmatrix}$$

given in $\mathbb{L}$-coordinates $e_1$ and $e_2$. The rows of the matrix

$$t(a^2 + 2b^2)R^2 = t \begin{pmatrix} a^2 - 2b^2 & 2ab \\ -4ab & a^2 - 2b^2 \end{pmatrix}$$

parametrize solutions $m - n, k$ and $-2k, m - n$ to the pair of equations \((10.26)\). This parametrization can be derived from the identification of the matrices $R$ and $R^{-1}$ with the pair of conjugated algebraic integers $a \pm b \cdot \sqrt{2i} \in \mathbb{Z} [\sqrt{-2}]$.

Given $\ell \in \mathbb{N}$, the non-trivial representation of $\ell^2$ in the form \((10.26)\), i.e. as the norm of an algebraic integer from $\mathbb{Z} [\sqrt{-2}]$, exists iff the rational prime decomposition of $\ell$ has a factor $p = 1 \mod 8$ or $p = 3 \mod 8$. Here non-trivial means different from the representations $\ell^2 + 2 \cdot 0^2 = \ell^2$, $\ell^2 + 2(2t)^2 = (3t)^2$ and $(2t)^2 + 2(4t)^2 = (6t)^2$. A rational prime $p$ is the product of two conjugated primes $a \pm b \cdot \sqrt{2i} \in \mathbb{Z} [\sqrt{-2}]$, where $a, b > 0$ with $\gcd(a, b) = 1$ are uniquely defined by $p$. A rational prime $p = 5 \mod 8$ or $p = 7 \mod 8$ is always an algebraic prime in $\mathbb{Z} [\sqrt{-2}]$. Denote by $p_i$, $i = 1, 2, \ldots$ the set of distinct rational primes of the form $8s + 1$ or $8s + 3$ entering the rational prime decomposition of $\ell$ with multiplicities $\rho_i \geq 1$. For each $i$ we have $p_i = (a_i + b_i \cdot \sqrt{2i})(a_i - b_i \cdot \sqrt{2i})$, where integers $a_i, b_i > 0$ are uniquely defined by $p_i$. Thus, one can form a multitude of products

$$\prod_{i=1}^{\rho_i} (a_i \pm b_i \cdot \sqrt{2i})^{\alpha_i}, \quad 0 \leq \alpha_i \leq \rho_i, \quad \sum_{i=1}^{\rho_i} \alpha_i \geq 1 \quad (10.27)$$

by varying the selection of $\alpha_i$ and the sign in front of $b_i$. Expanding the product in \((10.27)\), we end up with an algebraic integer $a + b \cdot \sqrt{2i}$ satisfying (after a multiplication by a unit in $\mathbb{Z} [\sqrt{-2}]$)

$$a, b \in \mathbb{N}, \quad \gcd(a, b) = 1, \quad \ell = (a^2 + 2b^2)t, \quad t \in \mathbb{N}. \quad (10.28)$$

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Note, that in (10.28) the value $b$ can be negative, and the triple $a, b, t$ defines a unique rectangular sub-lattice of $L$ congruent to $\ell L$. Changing the sign of $b$ implies a conjugated sub-lattice (see the second triple in given row of (10.23)). This completes the verification of (10.24). To finish the proof of assertions (i) and (ii), we only need to observe that the site $ae_1 + be_2 \in L$ can be written as $(a, \sqrt{2}b)$ in Cartesian coordinates $e'_1 = e_1$, $e'_2 = \sqrt{2}e_2$ implying the desired value for the tangent of the rotation angle.

(iii) To establish (10.25), observe that there are $\rho_i$ possibilities to choose $\alpha_i > 0$, and for each of them there are 2 possibilities to choose the sign between $a_i$ and $b_i$. An additional possibility is $\alpha_i = 0$ which amounts to $2\rho_i + 1$ choices in total. Since the choices for different $i$ are done independently, the quantity

$$s_2(\ell) = \prod_{i=1}^n (2\rho_i + 1) - 1$$

(10.29)

counts the total amount of possibilities, excluding the case where all $\alpha_i = 0$. This is exactly the number of distinct rectangular sub-lattices in $L$ congruent to $\ell L$ but different from $\ell L$ and the rotations of $\ell L$ by $2\arctan(\sqrt{2})$ or $2\arctan\left(\sqrt{\frac{1}{2}}\right)$ (the cases of $a = b$ or $a = 2b$ treated in the Proposition 10.3). Because a pair of conjugated rectangular sub-lattices of $L$ generates cubic $\ell$-sub-lattices of $Z^3$ from the same class, the number of corresponding classes is equal to $\frac{s_2(\ell)}{2}$ which establishes (iii). □

Remark. The cases $a = b$ and $a = 2b$ excluded in (10.24) give rise to a class with 4 sub-lattices considered in Proposition 10.3. The case $b = 0$ gives rise to a class with a single sub-lattice from Proposition 10.2.

Propositions 10.1 - 10.6 are dealing with solutions to the Diophantine equation (10.6) which defines Pythagorean quadruples. This equation is a special case of the classical equation

$$m^2 + n^2 + k^2 = t.$$  

(10.30)

The number of solutions $(m, n, k)$ to (10.30) is usually denoted by $r_3(t)$ and depends on the rational prime decomposition of $t$. If an integer $\ell$ has rational prime representation $\ell = 2^{\rho_2} \prod_{p_j \geq 3} p_j^{\rho_j}$ then the number $r_3(\ell^2)$ is given by (see [10], formula (3.1)):

$$r_3(\ell^2) = 6 \prod_{p_j \geq 3} \left[ \frac{p_j^{\rho_j+1} - 1}{p_j - 1} - (-1)^{(p_j-1)/2} \frac{p_j^{\rho_j} - 1}{p_j - 1} \right].$$  

(10.31)

Proposition 10.7. (i) A class formed by 24 cubic $\ell$-sub-lattices exists iff $r(\ell) > 0$, where

$$r(\ell) := r_3(\ell^2) - 30 + 24(\ell^2 \text{ mod } 3) - 12s_2(\ell) - 24\tilde{s}_2(\ell) - 36\tilde{s}_2(\ell);$$  

(10.32)

the number $r(\ell)$ is computed from the prime decomposition of $\ell$ according to (10.12), (10.18), (10.25), (10.31).

(ii) Each sub-lattice in a class is invariant under the inversion, generating the stabilizer subgroup $Z_2 < O_h$. 

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(iii) The quantity $\frac{r(\ell)}{144}$ gives a lower bound for the number of classes with 24 sub-lattices. It is only a lower bound since sub-lattices from two different classes may share a basis vector.

**Proof.** Each of Propositions 10.2 - 10.6 describes a special collection of solutions to (10.6). Each $\ell$-sub-lattice found in these propositions determines 6 solutions to (10.6) which are the basis of the sub-lattice and its inverse. Each of these 6 solutions is obtained by a rotation of one of the basis vectors from $\ell\mathbb{Z}^3$. Each basis vector belongs to a coordinate axis, and rotations of a coordinate axis trace some cones in $\mathbb{R}^3$.

The following cones are traced when we rotate a coordinate axis in accordance with Propositions 10.4 - 10.6.

(i) The coordinate axes (Proposition 10.4).

(ii) The coordinate planes (Proposition 10.4).

(iii) The diagonal planes (Proposition 10.6).

(iv) Four cones having one of the main diagonals as the rotation axis

\[
(\pm x \pm y + z)^2 - (x^2 + y^2 + z^2) = 0 \quad \text{(Proposition 10.5)}.
\]

(v) Six cones having one of the non-main diagonals as the rotation axis

\[
(\pm x + y)^2 - (x^2 + y^2 + z^2) = 0
\]
\[
(\pm x + z)^2 - (x^2 + y^2 + z^2) = 0 \quad \text{(Proposition 10.6)}.
\]
\[
(\pm y + z)^2 - (x^2 + y^2 + z^2) = 0
\]

Possible intersections between cones from Proposition 10.4 and from Propositions 10.5 or 10.6 are only the coordinate axes, which corresponds to the case from Proposition 10.2. Possible intersections between cones from Proposition 10.5 and from Proposition 10.6 are only the lines along the vectors

\[
(-t, 2t, 2t), (2t, -t, 2t), (2t, 2t, -t), (t, 2t, 2t), (-2t, -t, 2t), (-2t, 2t, -t),
\]
\[
(-t, -2t, 2t), (2t, t, 2t), (2t, -2t, -t), (-t, 2t, -2t), (2t, -t, -2t), (2t, 2t, t),
\]

emerging in Proposition 10.3 which is possible only for $\ell$ divisible by 3. This observation allows us to count distinct solutions to (10.6) originating from different propositions.

Proposition 10.2 describes 6 solutions of (10.6). Proposition 10.3 describes 6 solutions for each of the 4 sub-lattices, resulting in 24 solutions in total. Each sub-lattice in Proposition 10.4 contains 2 solutions included in Proposition 10.2 plus 4 new solutions. This amounts to $4 \cdot 6 \cdot \frac{1}{2} \tilde{s}_2(\ell)$ solutions. Each sub-lattice in Proposition 10.5 describes 6 new solutions. This amounts to $6 \cdot 8 \cdot \frac{1}{2} \tilde{s}_2(\ell)$ solutions. Each sub-lattice in Proposition 10.6 describes 6 new solutions. This amounts to $6 \cdot 12 \cdot \frac{1}{2} \tilde{s}_2(\ell)$ solutions. If there exists at least one solution different from the ones listed above then it necessarily belongs to a class with 24 sub-lattices. The RHS of (10.32) evaluates the amount of such solutions.
This completes the proof of assertion (i). The proofs of (ii) and (iii) are straightforward as each class of 24 sub-lattices has $24 \cdot 6 = 144$ solutions to (10.6).

Due to the 1-1 correspondence (10.3) between the cubic $\ell$-sub-lattices and FCC $\ell$-sub-lattices in $\mathbb{Z}^3$ we arrive at the following theorem.

**Theorem 10.8.** The $D$-FCC sub-lattices in $\mathbb{Z}^3$ exist iff $D^2 = 2\ell^2$ where $\ell \in \mathbb{N}$. For $D^2 = 2\ell^2$, these FCC $\ell$-sub-lattices are grouped into a finite number of disjoint classes, where each class contains 1, 4, 6, 8, 12 or 24 sub-lattices. The sub-lattices in a given class are obtained from each other via $\mathbb{Z}^3$-symmetries. The number of classes of a given cardinality and the coordinate representation of the basis of each sub-lattice in the class depend on the rational prime decomposition of $\ell$ as detailed in Propositions 10.1 - 10.7. Each FCC $\ell$-sub-lattice is $A_3(z)$ for an integer quaternion $z$ with $\|z\|^2 = \ell$.

**Proof.** Follows directly from Propositions 10.1 - 10.7.

11 Appendix B: Hard-core potentials in the Pirogov-Sinai theory

The original Pirogov-Sinai theory ([41], [42], [47]) and its various extensions (e.g., [6]) consider lattice models with a finite spin space and a finite potential of a finite range. Nevertheless, it is straightforward to extend this theory to hard-core models of a finite exclusion radius (which are models with an infinite potential).

Standard notions of a ground state and a periodic ground state are applicable to both finite-potential models and hard-core models of the above type. The first fundamental assumption of the PS theory is that the model has a finite number of PGSs, which remains the requirement for the hard-core models under consideration.

Based on the above requirement, one can partition the entire lattice, say $\mathbb{Z}^n$, into cubes of side-length $l$ such that $l$ is larger than the interaction radius, and every PGS can fit into this cube considered as a torus. This construction is applicable to both finite-potential models and hard-core models.

Denote by $S$ the spin space of a model and by $C$ the lattice cube of side-length $l$. A convenient, though not required, step is to replace the spin space $S$ with the space $S^C$, which reduces the model to the one with a nearest-neighbor interaction. Here the nearest neighbors of a given lattice site are the sites at a distance not larger than $\sqrt{n}$ from this site. The constructed nearest-neighbor interaction takes finite values if the initial model has a finite-value potential. The original hard-core requirement translates into forbidding some pairs of spins at nearest-neighbor sites. Nevertheless, by construction, the PGSs (which are constant configurations in the reduced model) remain admissible. Without loss of generality we assume from now on that the spin space is a finite subset of $\mathbb{N}$, and the PGSs are constant configurations with the spin values $1, 2, \ldots, k$ respectively (i.e., there are $k$ of them).

The next step in the PS theory is a definition of a $q$-correct point ([47], p. 561) in a spin configuration $\phi$, with $q \in \{1, \ldots, k\}$. Note that after the change of the spin space the interaction radius equals $\sqrt{n}$. Consequently, the above definition implies that a $q$-correct point $x$ is a lattice site for which not only $\phi(x) = q$, but $\phi(x') = q$ for all nearest neighbors
$x'$ of $x$ as well. This definition remains applicable to hard-core models. The same is true for the definition of a contour in a given configuration $\phi$, which is a connected component (in the sense of nearest neighbors) of non-correct points (cf. [17], p. 561). Note that such a contour is a pair consisting of a connected component of points called a support of a contour and a spin configuration in this support.

Any spin configuration in a finite volume with a PGS boundary condition is in a one-to-one correspondence with a finite collection of finite contours (called a boundary in [17], p. 561). In particular, a configuration mapped into a single $q$-contour has a constant PGS-value $q$ in the exterior of the contour and some (possibly different) constant PGS-values $q_i$ in the $i$-th connected component of the interior of the contour. Here the exterior and the interior are defined as connected components of the complement of the contour support. (See (1.5) in [17].)

Under this construction, a relative energy of a $q$-contour is defined as the difference between the energy of the PGS $q$ in the considered volume and the energy of the above configuration containing a single contour (see (1.6) in [17]). Without loss of generality one can assume that the pair potential is equal to 0 for any pair of neighboring sites having the same PGS-values, and it is positive for any other pair of spins at neighboring sites (the value $+\infty$ is also allowed). Consequently, a relative energy of a contour is simply the sum of pair interactions over the pairs of neighboring sites belonging to the support of the contour. An energy of a contour represents a contour functional (Section 1.6. in [17]) which, in turn, defines a statistical weight of a contour. The rest of the argument in [17] can be applied verbatim.

Essentially, the hard-core potential has an impact only upon the statistical weight of a contour. Namely, some contours have statistical weight 0. Moreover, the arguments in [17] utilize only upper bounds on the absolute values of statistical weights of contours (see (1.9), (1.23), (1.50), (2.2), (2.28) in [17]). Finally, everything is reduced to the analysis of a polymer model (Section 2.1 in [17]) where a polymer is a connected lattice set, and the associated statistical weight is the sum over statistical weights of the contours having this set as their support. In the hard-core case not all configurations in a given support contribute to this sum, which only makes the sum smaller.

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