Three-dimensional lattice ground states for Riesz and Lennard-Jones–type energies

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Abstract
The Riesz potential \( f_s(r) = r^{-s} \) is known to be an important building block of many interactions, including Lennard-Jones–type potentials \( f_{n,m}^{\text{LJ}}(r) := ar^{-n} - br^{-m} \), \( n > m \) that are widely used in molecular simulations. In this paper, we investigate analytically and numerically the minimizers among three-dimensional lattices of Riesz and Lennard-Jones energies. We discuss the minimality of the body-centered-cubic (BCC) lattice, face-centered-cubic (FCC) lattice, simple hexagonal (SH) lattices, and hexagonal close-packing (HCP) structure, globally and at fixed density. In the Riesz case, new evidence of the global minimality at fixed density of the BCC lattice is shown for \( s < 0 \) and the HCP lattice is computed to have higher energy than the FCC (for \( s > 3/2 \)) and BCC (for \( s < 3/2 \)) lattices. In the Lennard-Jones case with exponents \( 3 < m < n \), the ground state among lattices is confirmed to be an FCC lattice whereas an HCP phase occurs once added to the investigated structures. Furthermore, phase transitions of type “FCC-SH” and “FCC-HCP-SH” (when the HCP lattice is added) as the inverse density \( V \) increases are observed for a large spectrum of exponents \((n,m)\). In the SH phase, the variation of the ratio \( \Delta \) between the...
interlayer distance $d$ and the lattice parameter $a$ is studied as $V$ increases. In the critical region of exponents $0 < m < n < 3$, the SH phase with an extreme value of the anisotropy parameter $\Delta$ dominates. If one limits oneself to rigid lattices, the BCC-FCC-HCP phase diagram is found. For $-2 < m < n < 0$, the BCC lattice is the only energy minimizer. Choosing $-4 < m < n < -2$, the FCC and SH lattices become minimizers.

KEYWORDS
Epstein zeta function, ground states, Lennard-Jones potential, lattices, Riesz potential

1 INTRODUCTION, SETTING AND MAIN RESULTS

1.1 Motivation

From the first attempt by Huygens\(^1\) to describe solids as periodic assemblies of objects to the formalization of the crystallization conjecture by Blanc and Lewin,\(^2\) the mathematical journey to rigorously justify the emergence of periodic structures in crystal solids never stopped to attract new travelers. Nevertheless, only few rigorous results showing the global minimality, that is, among all possible configurations, of lattice structures for interaction energies are available. Besides the one-dimensional case\(^3–7\) where the optimality of the equidistant configuration $\mathbb{Z}$ is easily derivable, the only known results in dimension $d = 2$\(^8–15\) and $d = 3$\(^10,16\) rely on perturbations of hard-sphere potentials and specific angular dependence.

In dimension $d \in \{8, 24\}$, the linear programming method initiated by Cohn and Elkies\(^17\) has lead to recent important results for packings\(^18,19\) and crystallization at fixed density.\(^20–22\) In particular they showed the universal optimality, at any fixed density and for pairwise energies with interaction potentials $f(r) = F(r^2)$ where $F$ is a completely monotone function, of the densest packings in these dimensions—namely, the Gosset lattice $\mathbb{E}_8$ and the Leech lattice $\Lambda_{24}$. These are the only crystallization results that apply at any fixed density to Riesz energies, where the interaction potential is

$$f_\psi(r) = \frac{1}{r^\psi},$$

and at sufficiently high fixed density for Lennard-Jones–type energies (see Ref. \(^22\), Theorem 2.17) for which the interaction potential is defined by

$$f^{\text{LJ}}_{n,m}(r) = \frac{a}{r^n} - \frac{b}{r^m},$$

where $(a, b) \in (0, \infty)$ and $n > m > d$. The same minimality property is conjectured by Cohn and Kumar\(^5\) to hold in dimension $d = 2$ for the triangular lattice $\mathbb{A}_2$ whereas it is known that no universal minimizer exists in dimension $d = 3$.\(^23\)
The potentials studied in this paper are of high importance in mathematics and physics, and their lattice ground states are known to be fundamental in many domains. On the one hand, Riesz-type energies arise in mathematical physics and number theory in many ways. For instance, in the Coulomb case \( s = d - 2 \) (or \( f(r) = -\log r \) in dimension \( d = 2 \)), the Wigner Conjecture for Jellium\(^{24}\) states that electrons embedded in an uniform background of positive charges must crystallize on a triangular and a body-centered-cubic (BCC) lattice in dimensions 2 and 3, respectively (see also Refs. 2, 25). This is also called the Abrikosov Conjecture\(^{26}\) or Vortices Conjecture\(^{27}\) in the two-dimensional setting related to the vortices in the Ginzburg-Landau theory of superconductors of type II. An equivalent problem can be stated in higher dimension and for general Riesz interaction.\(^{21,25,28–32}\) The general Riesz energy and its related minimization problem also appear in the theory of random point configurations\(^{33}\) as well as approximation theory\(^{34}\) and number theory.\(^{23,35,36}\) On the other hand, Lennard-Jones potentials have been introduced by Mie\(^{37}\) and popularized by Jones\(^{38}\) in its classical \((n, m) = (12, 6)\) form, that is, when the interaction is of Van der Waals type \( \sim br^{-6} \) for large \( r \), initially for studying gas argon. The repulsion at short distance of type \( \sim ar^{-n} \) is here to mimic Pauli exclusion principle. Because \( f_{n,m}^{\text{LJ}} \) is a bonding potential, that is, it has an equilibrium distance, it has been widely used in molecular simulation (see, e.g., Refs. 39–41). It also appears to be a good model for social aggregation\(^{42}\) and has many other applications, like in robotics.\(^{43}\) In dimension \( d = 2 \), numerical investigations suggest that the ground state of the classical Lennard-Jones energy (i.e., \((n, m) = (12, 6)\)) is a triangular lattice,\(^{44}\) whereas the hexagonal close-packing (HCP) structure is expected to be the one in dimension \( d = 3.\)\(^{45}\) Notice also that the ground states of three-dimensional finite-range Lennard-Jones energy among a finite number of structures has been also studied in Ref. 46 for different truncation, cutoff distances, pressure, and exponents. Notice also that the lattice ground states for Lennard-Jones–type energies have been recently proven to be related to the one of the embedded-atom models with Riesz-type electron density and Riesz or Lennard-Jones nuclei interaction, see Ref. 47.

1.2 Minimization among lattices and setting

The goal of this paper is to investigate the possible lattice ground states for Riesz and Lennard-Jones energies in dimension \( d = 3 \), but in the case where simple periodicity is assumed. Indeed, once restricted to the class of lattices

\[
\mathcal{L}_d := \left\{ L = \bigoplus_{i=1}^d \mathbb{Z}u_i \subset \mathbb{R}^d : \{u_i\} \text{ is a basis of } \mathbb{R}^d \right\},
\]

the above minimization problem becomes simpler and the Riesz and Lennard-Jones–type lattice energies are, respectively, defined by

\[
\zeta_L(s) := \frac{1}{2} \sum' \frac{1}{|p|^s}, \quad \text{and} \quad E_{n,m}[L] := \frac{1}{2} \sum' f_{n,m}^{\text{LJ}}(|p|) = a\zeta_L(n) - b\zeta_L(m),
\]

where \( \zeta_L(s) \) is the Epstein zeta function\(^{48}\) associated to the lattice \( L \) and \( \sum' \) means that we sum on all the points excepted the origin. Notice that a factor \( 1/2 \) has been added to identify the Epstein zeta function with the energy per point of \( L \) with interaction potential \( f_s(r) = r^{-s} \). Recall that
s \mapsto \zeta_L(s) \text{ admits an analytic continuation on } \mathbb{C}\setminus \{d\} \text{ (see also Ref. 49)} \text{ and can therefore be defined for any } s < d. \text{ In particular, the value of } \zeta_L(s) \text{ when } s \in (d - 4, d) \text{ is the Jellium energy of the lattice } L \text{ for general Riesz interaction}^{22}, \text{ Theorem 3.1} \text{ including the Coulomb case } s = d - 2, \text{ originally proved by Cotar and Petrache for } s \in [d - 2, d) \text{ in Ref. 30, Lemma 2.6 (see also Ref. 31)}. \text{ Notice that the equivalence between analytic continuation and renormalized energy (of Jellium type) has been recently investigated in a broader framework by Lewin in its review on Riesz and Coulomb gases see Section IV in Ref. 25.}

Whereas in dimension } d = 2, \text{ the triangular lattice has been shown to be minimal for } L \mapsto \zeta_L(s) \text{ for all } s > 0 \text{ in the set of lattices }

\mathcal{L}_d(V) := \{L \in \mathcal{L}_d : |\det(u_1, \ldots, u_d)| = V \subset \mathcal{L}_d, \text{ for any fixed covolume } V > 0 \text{ (also called “inverse density”), see Refs. 50–54}, \text{ no such optimality result is shown in dimension } d = 3. \text{ Only conjectures}^{23} \text{ and local minimality results}^{55–58} \text{ are available (see Section 2 for more details).}

The same holds for the Lennard-Jones–type energy } E_L^{n,m}. \text{ Indeed, the two-dimensional ground state of } E_L^{n,m} \text{ in } \mathcal{L}_2 \text{ has been proven to be a triangular lattice for many exponents } (n, m) \text{ by the first author.}^{59,60} \text{ Furthermore, we have observed and partially proved a phase transition of type “triangular-rhombic-square-rectangular” for the minimizer of } E_L^{n,m} \text{ in } \mathcal{L}_2(V) \text{ as } V \text{ increases, see Refs. 61, 62. Only asymptotic and local minimality results have been shown in dimension } d = 3 \text{ in Refs. 58, 63, 64 (see Section 3 for more details). Notice that similar problems have been investigated by the first author in Refs. 65–67 concerning charged systems and related lattice optimality for frame bounds in time-frequency analysis.}

We aim to present a complete picture of the lattice ground states of } L \mapsto \zeta_L(s) \text{ and } E_L^{n,m} \text{ in } \mathcal{L}_3 \text{ and } \mathcal{L}_3(V). \text{ In particular, we want to show minimality properties of the following important three-dimensional lattices (given here with unit density):}

\text{The SC lattice } \mathbb{Z}^3 := \mathbb{Z}(1, 0, 0) \oplus \mathbb{Z}(0, 1, 0) \oplus \mathbb{Z}(0, 0, 1) \quad (1)

\text{The FCC lattice } \mathbb{D}_3 := 2^{-\frac{1}{3}} [\mathbb{Z}(1, 0, 1) \oplus \mathbb{Z}(0, 1, 1) \oplus \mathbb{Z}(1, 1, 0)] \quad (2)

\text{The BCC lattice } \mathbb{D}_3^* := 2^{\frac{1}{3}} \left[\mathbb{Z}(1, 0, 0) \oplus \mathbb{Z}(0, 1, 0) \oplus \mathbb{Z} \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)\right] \quad (3)

\text{The SH lattice } \mathbb{A}_t(\Delta) := \left(\frac{2}{\sqrt{3}\Delta}\right)^{\frac{1}{3}} \left[\mathbb{Z}(1, 0, 0) \oplus \mathbb{Z} \left(\frac{1}{2}, \frac{\sqrt{3}}{2}, 0\right) \oplus \mathbb{Z}(0, 0, \Delta)\right]. \quad (4)

Notice that the SH lattices are nonshifted stacking of triangular lattices with lattice constant } a > 0 \text{ and interlayer distance } d > 0 \text{ and we set } \Delta = d/a. \text{ Furthermore, we also want to investigate the particular role of the unit density hexagonal close-packed structure, which is not a lattice as
Main configurations of $\mathcal{E}_3$: the SC lattice $\mathbb{Z}^3$ (up left), the FCC lattice $D_3$ (up middle), the BCC lattice $D_3^*$ (up right), the SH lattice $A_3(\Delta)$ (down left), the anisotropy parameter $\Delta = d/a$, and the HCP lattice $A_3$ (down right)

defined above, defined by

The HCP structure $A_3 := \Lambda \cup \left( \Lambda + \left( \frac{1}{2}, \frac{1}{\sqrt{12}}, \sqrt{\frac{2}{3}} \right) \right)$

$\Lambda := \mathbb{Z}(1,0,0) \oplus \mathbb{Z} \left( \frac{1}{2}, \frac{\sqrt{3}}{2}, 0 \right) \oplus \mathbb{Z} \left( 0,0, \sqrt{\frac{8}{3}} \right)$.

All the abovementioned periodic structures are depicted in Figure 1. Notice that the names chosen for the SH and HCP structures are the one given by the Strukturbericht designation. Furthermore, we define for convenience the new sets, that is the sets of lattices with added HCP structure,

$\widetilde{\mathcal{E}}_3(V) := \mathcal{E}_3(V) \cup V^{\frac{1}{3}} A_3$, and $\widetilde{\mathcal{E}}_3 := \bigcup_{V > 0} \widetilde{\mathcal{E}}_3(V)$.

1.3 Method

Whereas different rigorous techniques exist for studying lattice energies in dimension $d = 2$ (see, e.g., Refs. 22, 54, 59, 66, 67), where $\dim \mathcal{L}_2 = 3$ and $\dim \mathcal{L}_2(V) = 2$ for all $V > 0$, the situation in dimension $d = 3$ is much more complicated. Indeed the so-called fundamental domain containing only one copy of each lattice (up to dilation, isometry, and symmetry) is five-dimensional for $\mathcal{L}_3(1)$ and has a complicated shape (see, e.g., Terras). Very few rigorous results have been proven in dimension 3. Let us recall as an example the computer-assisted proof of Sarnak and
Strömbergsson where the FCC lattice is shown to be minimal for the height of the flat torus (i.e., the derivative of \( s \mapsto \zeta_L(s) \) at \( s = 0 \)).

In our work, we parameterize any lattice \( L \in \mathcal{L}_3 \) by six real numbers \((u, v, x, y, z, V)\) where \( V \) is the covolume of \( L \) and, following, \[ L = V^\frac{1}{3} [\mathbb{Z}u_1 \oplus \mathbb{Z}u_2 \oplus \mathbb{Z}u_3], \]

\[ u_1 = 2^\frac{1}{6} \left( \frac{1}{\sqrt{u}}, 0, 0 \right), \quad u_2 = 2^\frac{1}{6} \left( \frac{x}{\sqrt{u}}, \frac{v}{\sqrt{u}}, 0 \right), \quad u_3 = 2^\frac{1}{6} \left( \frac{y}{\sqrt{u}}, \frac{vz}{\sqrt{u}}, \frac{u}{v\sqrt{2}} \right). \]

This parameterization appears to be the same as in Ref. 23, Eq. (27), where \((t_{12}, t_{13}, t_{23}) = (x, y, z)\), \(y_1 = v^{-2}\), and \(y_2 = 2u^{-3}v^4\). We therefore use the corresponding three-dimensional Grenier’s fundamental domain shifted by one half to have only one copy of the unit density FCC point in it, that is, \((u, v, x, y, z) \in \mathcal{G}_3\) defined by the following nine inequalities:

\[ \begin{align*}
   & (i) \quad 1 \leq (1 + x - y)^2 + v^2 \left( (1 - z)^2 + \frac{u^3}{2v^4} \right), \\
   & (ii) \quad 1 \leq (x - y)^2 + v^2 \left( (1 - z)^2 + \frac{u^3}{2v^4} \right), \\
   & (iii) \quad 1 \leq x^2 + v^2, \\
   & (iv) \quad 1 \leq y^2 + v^2 \left( z^2 + \frac{u^3}{2v^4} \right), \\
   & (iv') \quad 1 \leq (y - 1)^2 + v^2 \left( z^2 + \frac{u^3}{2v^4} \right), \\
   & (v) \quad 1 \leq z^2 + \frac{u^3}{2v^4}, \\
   & (vi) - (viii) \quad 0 \leq x \leq \frac{1}{2}, 0 \leq y \leq 1, 0 \leq z \leq \frac{1}{2}.
\end{align*} \]

Our goal is then to investigate the minimizers of the following type of energy per point:

\[ E_f[L] := \frac{1}{2} \sum_{p \in L} f(|p|^2) = \frac{1}{2} \sum_{j,k,l} f \left( \frac{1}{2} V^\frac{2}{3} \left[ (j + xk + yl)^2 + v^2(k + zl)^2 + \frac{u^3}{2v^2} l^2 \right] \right), \]

when \((u, v, x, y, z) \in \mathcal{G}_3, V > 0\) and \(f(r) \in \{ r^{-\frac{s}{2}}, ar^{-\frac{n}{2}} - br^{-\frac{m}{2}} \}\). Notice that when our potential \(f\) is not summable (i.e., when \(m, n, s \leq 3\)), we have used the analytic continuation of the Epstein zeta function (see, e.g., Ref. 49), but the corresponding expression can always be written in terms of energies of type \(E_f\).

To compute numerically the minimizers, we have used the optimization tool FindMinimum in Mathematica, which includes ConjugateGradient, PrincipalAxis, LevenbergMarquardt, Newton, QuasiNewton, InteriorPoint, and LinearProgramming methods. It has to be noticed that, as in Ref. 23, we can systematically restrict our study to a compact domain of \(\mathcal{G}_3\) because our energy diverges or goes to zero as the parameters \((u, v)\) go to infinity (see also Ref. 60 for such an example in two dimensions).

When \(L \in \{ \mathbb{Z}^3, D_3, D_3^*, A_4(\Delta), A_3 \}\), the exact formulas of \(E_f[L]\) and their analytic continuations can be found in Section 4. Also, because the shape (i.e., its class up to dilation and isometry) of the global minimizer of \(E_{\text{MJ}}^{14}[n,m]\) is independent of \((a, b)\) (see Ref. 64), we have decided to choose \(a = \frac{m}{n-m}\) and \(b = \frac{n}{n-m}\) as it is usually done in the physics literature. Therefore, our Lennard-Jones–type
energy will be, for any lattice $L$,

$$E_{n,m}^{\text{LI}}[L] = \frac{m}{n-m} \zeta_L(n) - \frac{n}{n-m} \zeta_L(m). \quad (8)$$

### 1.4 Plan of the paper

Sections 2 and 3 are, respectively, devoted to investigate the lattice ground states for Riesz and Lennard-Jones–type energies. The exact formulas used to compute our energies are stated in Section 4.

### 2 MINIMIZERS OF THE RIESZ ENERGY

In this part, we investigate the minimizers of the Epstein zeta function $L \mapsto \zeta_L(s)$ in $L_3(1)$ or $\mathcal{L}_3(1)$ and for any $s \in \mathbb{R}$. The formulas we are using are available in Section 4. It is indeed enough to consider the $V=1$ case because the Epstein zeta function is homogeneous, that is,

$$\zeta_{V^{1/3}L}(s) = V^{-\frac{1}{3}} \zeta_L(s), \quad \forall V > 0, \quad \forall s \in \mathbb{R}. \quad (9)$$

It is already known (see Refs. 55, 57) that $D_3$ and $D_3^*$ are both local minimizers of $L \mapsto \zeta_L(s)$ in $L_3(1)$ for all $s > 0$. Except of the minimality result of $D_3$ for the height of the flat torus $L \mapsto \zeta_L'(0)$ in Ref. 23 (and its very recent application 70 to the optimality of $D_3^*$ for diblock copolymer molecular systems) as well as the optimality of $\mathbb{Z}_d$ among $d$-dimensional orthorhombic lattices following from Montgomery’s work, 54 we are not aware of any other global optimality results in dimension $d = 3$ for the Epstein zeta function.

First, we have rechecked the following well-known observations (see Ref. 23):

- for all $0 < s < \frac{3}{2}$, $D_3^*$ is the unique minimizer of $L \mapsto \zeta_L(s)$ in $L_3(1)$;
- for all $s > \frac{3}{2}$, $D_3$ is the unique minimizer of $L \mapsto \zeta_L(s)$ in $L_3(1)$.

Furthermore, it is easy to show (see, e.g., (33) applied to $s = 3/2$) that $\zeta_{D_3}(\frac{3}{2}) = \zeta_{D_3^*}(\frac{3}{2})$.

#### Minimization for $0 < s < 3$

Here we use the analytic continuation with respect to $s$ of the Epstein zeta function. The energies of $D_3$ and $D_3^*$ have close values, hence we plot their difference in Figure 2. It vanishes for $s \to 0^+$ as $\zeta_L(s) \to -1/2$ for any lattice $L$ and it remains finite for $s \to 3^-$ by the general Kronecker’s Limit Formula 71, Theorem 2.2. The latter value was calculated semi-analytically. We can see that $\zeta_{D_3}(s) - \zeta_{D_3^*}(s)$ is positive for $0 < s < 3/2$ and negative otherwise, as expected.
Minimization for \( s > 3 \)

Recall that for large \( s \) the FCC and HCP lattices could compete as they are closed packed lattices so that they should have common asymptotes. The large \( s \) expansions can be deduced from summation formulas of the type (37) by inspection. For the FCC lattice we get

\[
\zeta_{D_3}(s) \approx \frac{1}{2s/6} \left[ 6 + \frac{3}{2^{s/2}} + \frac{12}{3^{s/2}} + \frac{6}{2^s} + \cdots \right]
\]  

(10)

whereas for the HCP one

\[
\zeta_{A_3}(s) \approx \frac{1}{2s/6} \left[ 6 + \frac{3}{2^{s/2}} + \frac{1}{\left(\frac{8}{3}\right)^{s/2}} + \frac{9}{3^{s/2}} + \cdots \right].
\]  

(11)

We can see that both the leading and subleading terms are equal and for large enough \( s \) the third term decides that \( \zeta_{D_3}(s) < \zeta_{A_3}(s) \) as \( 3 > 8/3 \). This still does not mean that HCP could not prevail for some medium values of \( s \). The values of the third term become equal for \( s \approx 21 \). Hence we performed high precision numerical calculations presented in Figure 3.

We can see that \( \zeta_{A_3}(s) - \zeta_{D_3}(s) \) remains positive for all \( s > 3/2 \), as expected. The apparent non-analyticity at \( s = 3/2 \) is given by the fact, that we subtract another function for \( s < 3/2 \), namely, \( \zeta_{A_3}(s) - \zeta_{D_3}(s) \), to show that A3 does not become the minimizer at any \( s \). Note that the plotted difference is smooth at \( s \to 3 \) although both \( \zeta_{A_3}(s) \) and \( \zeta_{D_3}(s) \) diverge.

Minimization for \( s < 0 \)

Here we use the analytic continuation with respect to \( s \) of the Epstein zeta function. At first let us state that this region is physically not very reasonable, but we can study it nevertheless. As recalled in the introduction, its minimum value is related to the Jellium problem with Riesz interaction. All analytically continued energies include the factor \( 1/\Gamma(s/2) \). It tends to zero at \( s/2 \to 0, -1, -2, \) etc. The case \( s \to 0 \) should be omitted, as we already mentioned that, for all lattice \( L, \zeta_L(s) \to -1/2 \)
in the sense of limit. All the other zeros are present; in the 1D case of Riemann’s zeta function they are called trivial zeros. The energies are analytical functions thus they change signs at these points; they become negative at $-2 < s < 0$, $-6 < s < -4$, etc., and they are positive otherwise. The negativity of energies gives rise to extremely low possible values of energies, say for SH lattice $A_t$ with very large anisotropy parameter $\Delta = d/a$ (where $a$ is the lattice constant and $d$ is the interlayer distance), or for very dilated orthorhombic lattices, and it has no lower bound. In other words for $-4n - 2 < s < -4n$ with $n = 0, 1, 2, \ldots$ there is no lattice the single minimizer as the energies diverge $\zeta_{A_t}(s) \to -\infty$ for $\Delta \to \infty$. Finally for intervals $-4n < s < -4n + 2$ with $n = 1, 2, \ldots$ where the energies are positive we have the minimizer and it is the BCC lattice. This was used in the left part of Figure 3 as well as in Figure 4. One could plot those differences also in the intervals where they are negative and see continuous oscillating functions, but none of the lattices represents the minimizer there.

Concluding, for real $s \neq 3$ we still have two lattices that become minimizers at some intervals of $s$. There is no minimizer for $-4n - 2 < s < -4n$ with $n = 0, 1, 2, \ldots$; the FCC lattice minimizes the Riesz energy for $s > 3/2$ and BCC otherwise. The result for negative $s$ is new.

According to our numerical investigation, we can therefore write the following conjecture for the Riesz energy, completing the one of Sarnak and Strömbergsson in Ref. 23.

**Conjecture 1.** We have the following minimizers in $\widetilde{L}_3(1)$ for the Epstein zeta function $L \mapsto \zeta_L(s)$:
• for all \( n \in \mathbb{N} \) and all \( s \in (-4n, -4n + 2) \), the unique minimizer is \( \mathcal{D}_3^s \);
• for all \( n \in \mathbb{N} \) and all \( s \in (-4n - 2, -4n) \), the lattice energy has no minimizer;
• for all \( s \in (0, 3/2) \), the unique minimizer is \( \mathcal{D}_3^s \);
• for all \( s > 3/2 \), the unique minimizer is \( \mathcal{D}_3^s \).

3 | MINIMIZERS OF THE LENNARD-JONES–TYPE ENERGY

In this section, we numerically investigate the minimizers of the Lennard-Jones–type energy \( L \mapsto E_{n,m}^{\text{LJ}}[L] \) in \( \mathcal{L}_3 \) or \( \mathcal{L}_3(V) \) (i.e., without any constraint on the density) and \( \mathcal{L}_3(V) \) or \( \mathcal{L}_3(V), V > 0 \) (i.e., at fixed density). Using the homogeneity (9) of the Epstein zeta function, we recall that, for all \( V > 0 \) and all \( L \in \mathcal{L}_3(1) \),

\[
E_{n,m}^{\text{LJ}}[V^{1/3}L] = \frac{m}{n-m} \frac{\zeta_L(n)}{V^{n/3}} - \frac{n}{n-m} \frac{\zeta_L(m)}{V^{m/3}}.
\]

For making our plots, we therefore use again the formulas derived in Section 4 evaluated by using the symbolic computer language Mathematica with precision of 16 decimal digits.

Again, only local minimality results for \( E_{n,m}^{\text{LJ}} \) are known. In particular, \( V^{1/3} \mathcal{D}_3 \) and \( V^{1/3} \mathcal{D}_3^* \) have been shown in Ref. 63 to be locally minimal for \( E_{n,m}^{\text{LJ}} \) in \( \mathcal{L}_3(V) \) for all fixed \( V \in (0, V_0) \) where \( V_0 = V_0(n, m) \) is explicit and sharp. Furthermore, the SC lattice \( V^{1/3} \mathbb{Z}^3 \) is also showed in the same work to be locally minimal in a certain interval \((V_1, V_2)\) of volume. The only other known results are the asymptotic global optimality of an FCC lattice for large \( s \) (see Ref. 64) and some other minimality results among lattices with prescribed number of nearest-neighbors in Ref. 58.

The values of the Lennard-Jones exponents \( m \) and \( n \), constrained by \( m < n \), can lie in three distinct regions: \((3, \infty)\), \([0, 3)\) and \((-\infty, 0)\). While the lattice sums are convergent in the region \((3, \infty)\), they diverge (but still individual terms go asymptotically to zero) in the “critical” strip \([0, 3)\) and they diverge (as well as individual terms diverge asymptotically) on the half-line \((-\infty, 0)\). In this paper, we consider only such cases when both Lennard-Jones exponents \( m \) and \( n \) lie in the same region.

3.1 | \( 3 < m < n \)

Minimization in \( \mathcal{L}_3 \) and \( \mathcal{L}_3(V) \). Using dimension reduction techniques developed in Ref. 64 for Lennard-Jones–type energies, we investigate the minimum of \( E_{n,m}^{\text{LJ}} \) in \( \mathcal{L}_3 \). As already explained in Ref. 45, only two lattices appear to be global minimizers of this energy: the FCC lattice and the HCP structure (see Figure 5). It seems that a large (resp. narrow) well, that is, when \( n - m \) is small (resp. large) favors the FCC (resp. HCP) lattice as a ground state. It has to be noticed that, whatever \( n \) and \( m \) are, the global minimizer of \( E_{n,m}^{\text{LJ}} \) in \( \mathcal{L}_3 \) is an FCC lattice. This also supports the conjecture that we stated in Ref. 63.

Minimization in \( \mathcal{L}_3(V) \) and \( \mathcal{L}_3(V) \). For the problem of minimizing \( E_{n,m}^{\text{LJ}} \) at fixed density, we have plotted in Figure 6 the phase diagram of \((n, V) \mapsto \arg\min_{L \in \mathcal{L}_3(V)} E_{n,m}^{\text{LJ}}[L] \) where \( m \in \{4, 5, 6\} \).

We observe that there are only three kinds of minimizers in \( \mathcal{L}_3(V) \): the FCC lattice \( V^{1/3} \mathcal{D}_3 \), the SH
FIGURE 5  Global minimizer of $E_{n,m}^{LJ}$ in $\mathcal{L}_3$ with respect to $(n, m)$. The dash line corresponds to $m = n$. The phase diagram for the minimization problem on $\mathcal{L}_3$ is obtained by replacing the HCP phase by an FCC one.

FIGURE 6  Phase diagram of the minimizer of $E_{n,m}^{LJ}$ in $\mathcal{L}_3(V)$ for $m = 4$ (up left) and $m = 5$ (up right) and $m = 6$ (down), $n$ varying. The phase diagram for the minimization problem on $\mathcal{L}_3(V)$ is roughly obtained by replacing the HCP phase by an FCC one.

There exist $V_{n,m}, V'_{n,m} > 0$ such that:

- for all $V \in (0, V_{n,m})$, $V^{1/3}D_3$ is the unique minimizer of $E_{n,m}^{LJ}$ in $\mathcal{L}_3(V)$;
FIGURE 7  Simple hexagonal phase. Plot of $V \rightarrow \arg \min_\Delta E_{12,m}^{LJ} \left( V^\frac{1}{3} A_f(\Delta) \right)$ for $(n, m) \in \{(12, m) : m = 4, 5, 6 \}$

• for all $V \in (V_{n,m}, V'_{n,m})$, $V^\frac{1}{3} A_3$ is the unique minimizer of $E_{12,m}^{LJ}$ in $\widetilde{L}_3(V)$;
• for all $V > V'_{n,m}$, $V^\frac{1}{3} A_f(\Delta)$ is the unique minimizer of $E_{12,m}^{LJ}$ in $\widetilde{L}_3(V)$ for some $\Delta = \Delta(V)$, where the behavior of $\Delta(V)$ is depicted in Figure 7 for $n = 12$ and $m \in \{4, 5, 6\}$.

If we minimize $E_{n,m}^{LJ}$ only in $L_3(V)$, the HCP phase is replaced by an FCC one in such a way that

• for all $V \in (0, V'_{n,m})$, $V^\frac{1}{3} D_3$ is the unique minimizer of $E_{n,m}^{LJ}$ in $L_3(V)$;
• for all $V > V'_{n,m}$, $V^\frac{1}{3} A_f(\Delta)$ is the unique minimizer of $E_{n,m}^{LJ}$ in $L_3(V)$ for some $\Delta = \Delta(V)$ as depicted in Figure 7.

In Ref. 63, the interval of volumes $V$ where the SC lattice is locally minimal for $E_{n,m}^{LJ}$ in $L_3(V)$ has been derived. Here, we have observed that a family of SH lattices have lower energy than the SC one. This is new compared to the two-dimensional case where the square lattice, that has been shown in Ref. 61 to be locally minimal in some interval of volume, is also observed to be minimal in $L_2(V)$ in the same interval. Furthermore, our numerical findings concerning the global minimizer of $E_{n,m}^{LJ}$ in $L_3$ support Ref. 63 and confirm Ref. 45.

3.2 $0 < m < n < 3$

Let us now consider that the Lennard-Jones exponents $n$ and $m$ lie in the critical strip and fix $m = 1$. It turns out that for any value of $1 < n < 3$ the $A_f$ lattice with the extreme value of the anisotropy parameter $\Delta_{opt} \rightarrow \infty$ yields the lowest possible energy per site $E_{A_f} \rightarrow -\infty$. To get nontrivial results at fixed density, we will restrict ourselves to rigid lattices: $Z^3$, $D_3^*$, $D_3$, and $A_3$. One can see in the inset of Figure 8 that for small values of $n$ close to 1 and very small elementary cell volume $V$ up to 0.01, the $D_3^*$ lattice prevails. Note that the phase boundary between $D_3^*$ and $D_3$ lattices ends at $n = 1.5$; this is due to the fact that for an infinitesimal $V$ the $n$ term dominates in the Lennard-Jones energy and it holds that $E_{D_3}(3/2) = E_{D_3^*}(3/2)$ for the Riesz interaction at $\alpha = 3/2$. For larger values of $n$ and $V$, there is a competition between the $D_3$ and $A_3$ lattices as minimizers of the energy. The boundary between the two lattices runs within the interval approximately $1.28 < V < 2.09$. There is numerical evidence that if we chose the exponent $m \geq 1.5$, the $D_3^*$ lattice would disappear from the phase diagram.
3.3 | $-2 < m < n < 0$

Within this interval of the exponents, the $D^*_3$ lattice becomes the minimizer of the energy for any value of $V$. The $A_f$ lattice has its (finite) minimum energy for a finite value of $\Delta_{\text{opt}}$, but its energy is not low enough to become the global minimizer.

3.4 | $-4 < m < n < -2$

Now both $D^*_3$ and $A_f$ lattices are candidates for global minimizers, the latter lattice with a finite parameter $0.6 < \Delta_{\text{opt}} < 0.9$ for the presently calculated data. The typical phase diagram for the Lennard-Jones exponents $m = -3.5$ and $-3.5 < n < -2$ is plotted in Figure 9. The phase curve between the $D^*_3$ and $A_f$ lattices approaches to $n = -3.5$ at asymptotically large $V \rightarrow \infty$. Analogous phase diagrams appear in intervals $-6 < m < n < -4$, etc.

According to our numerical study, we can write the following conjecture for the ground state of the Lennard-Jones–type energy.
Conjecture 2. Concerning the global minimizer of $E_{n,m}^{LJ}$, we have:

- for $3 < m < n$, then we have two cases:
  1. in $L_3$, the unique minimizer of $E_{n,m}^{LJ}$ is $D_3$, up to rescaling.
  2. in $\widetilde{L}_3$, there exists $m_0 \approx 5.7$ such that,
     - if $m < m_0$, then there exists $n_m$ such that if $n < n_m$ (resp. $n > n_m$), the unique minimizer of $E_{n,m}^{LJ}$ is $D_3$ (resp. $A_3$), up to rescaling.
     - if $m > m_0$, then the unique minimizer of $E_{n,m}^{LJ}$ is $A_3$.

- for $0 < m < n < 3$, $E_{n,m}^{LJ}$ does not have any minimizer at fixed density.

- for all $k \in \mathbb{N} \cup \{0\}$, for all $-4k - 2 < m < n < -4k$, the unique minimizer of $E_{n,m}^{LJ}$ in $L_3$ is $D_3^*$, up to rescaling;

- for all $k \in \mathbb{N}$, for all $-4k < m < n < -4k + 2$, $D_3^*$ and $A_1$ are both minimizers, up to rescaling, of $E_{n,m}^{LJ}$ in $\widetilde{L}_3$.

4 | EXPLICIT FORMULAS FOR THREE-DIMENSIONAL EPSTEIN ZETA FUNCTIONS

This section is devoted to the construction of explicit formulas for Epstein zeta functions associated to the three-dimensional lattices considered in the present paper. We start with converging sums, that is, the parameter $s$ is larger than dimension 3, and express them as integrals over powers of Jacobi elliptic functions. Then using specific tricks with elliptic functions these integrals are rewritten into the ones which represent an analytic continuation of Epstein zeta functions to the whole complex plane except for $s = 3$.

4.1 | SC lattice

Let particles be localized at sites of the SC lattice with spacing $a$. In this paper, we compare the energy per particle for various 3D lattice structures at a fixed density of particles, say the unit one. The particle density associated with the SC lattice, given by $\rho = 1/a^3$, is equal to one when $a = 1$. Particles interact pairwisely by the Riesz potential $1/r^s$ where $r = |r|$ is the distance between two particles and $s$ is a complex number. The energy per particle is given by the Epstein zeta function associated with the SC lattice

$$\zeta_{\mathbb{Z}^3}(s) = \frac{1}{2} \sum_{(j,k,l) \neq (0,0,0)} \frac{1}{(j^2 + k^2 + l^2)^{s/2}}, \quad (12)$$

where the prefactor $1/2$ is due to the fact that every energy is shared by two particles and the sum converges only if the real part of $s \Re(s) > 3$. Using the $\Gamma$-identity

$$\frac{1}{r^s} = \frac{1}{(r^2)^{s/2}} = \frac{1}{\Gamma(s/2)} \int_0^\infty dt \, t^{s/2 - 1} e^{-r^2t}, \quad (13)$$
the expression (12) can be rewritten as

\[ \zeta_{\mathbb{Z}^3}(s) = \frac{1}{2\Gamma(s/2)} \int_0^\infty \frac{dt}{t^{s/2}} \left[ \sum_{j,k,l=-\infty}^\infty e^{-(j^2+k^2+l^2)t} - 1 \right] \]

\[ = \frac{1}{2\Gamma(s/2)} \int_0^\infty \frac{dt}{t^{s/2}} [\theta_3^3(e^{-t}) - 1] \]

\[ = \frac{\pi^{s/2}}{2\Gamma(s/2)} \int_0^\infty \frac{dt}{t^{s/2}} [\theta_3^3(e^{-\pi t}) - 1], \quad (14) \]

where the Jacobi elliptic function with zero argument \( \theta_3(0,q) \equiv \theta_3(q) = \sum_{j=-\infty}^\infty q^{j^2/2} \) was introduced for \( q = e^{i\tau}, \Im(\tau) > 0 \). Notice that (14) can be obtained from the Mellin transform of the Jacobi theta function (see, e.g., Refs. 73 and 74, Section 1.4.2). With regard to the definition of \( \theta_3(q) \), it holds that \( \theta_3(e^{-\pi t}) \sim t^{-\infty} 1 + 2e^{-\pi t} + \cdots \) and the integral in (14) converges at large \( t \) for any \( s \). Using the Poisson summation formula

\[ \sum_{j=-\infty}^\infty e^{-(j+\phi)^2/2} = \frac{1}{\sqrt{t}} \sum_{j=-\infty}^\infty e^{2\pi i j \phi} e^{-\pi j^2/2t} \]

(15)

it can be shown that

\[ \theta_3(e^{-\pi t}) \sim \frac{1}{\sqrt{t}} (1 + 2e^{-\pi t} + \cdots). \]

(16)

The function under integration in (14) behaves like \( t^{-(s-3)/2} \) for \( t \to 0 \), so the real part of \( s \) must be greater than 3 as was expected.

To derive an analytic continuation of (14) to the complex-\( s \) plane, we follow the derivation presented in Ref. 75 for \( d \)-dimensional hypercubic lattices. In the integral on the rhs of (14), we split the integration over \( t \) into intervals \([0,1]\) and \([1, \infty)\). In the second integral over \( t \in [1, \infty] \), one applies the equality

\[ \theta_3(e^{-\pi t}) = \frac{1}{\sqrt{t}} \theta_3(e^{-\pi/t}), \]

(17)

which follows from (15) and substitutes \( t = 1/t' \) to get

\[ \int_1^\infty \frac{dt}{t^{s/2}} [\theta_3^3(e^{-\pi t}) - 1] = \int_0^1 \frac{dt'}{t'} t'^{(3-s)/2} [\theta_3^3(e^{-\pi t'}) - t'^{-3/2}]. \]

(18)

As concerns the first integral over \( t \in [0,1] \), to subtract the singularity of \( \theta_3^3(e^{-\pi t}) \sim t^{-3/2} \) as \( t \to 0 \) one adds the vanishing contribution \( -t^{-3/2} + t^{-3/2} \) and integrates out the remaining terms proportional to \( t^{-3/2} - 1 \), with the result

\[ \frac{\Gamma(s/2)}{\pi^{s/2}} \zeta_{\mathbb{Z}^3}(s) = -\frac{1}{s} - \frac{1}{3-s} + \frac{1}{2} \int_0^1 \frac{dt}{2t} \left[ t^{s/2} + t^{(3-s)/2} \right] [\theta_3^3(e^{-\pi t}) - \frac{1}{t^{3/2}}]. \]

(19)
The difference in the square bracket is proportional to $t^{-3/2}e^{-\pi/\ell t}$ for $t \to 0$ and hence the formula (19) converges for all complex $s$, except for the singular point $s = 3$. The limit $s \to 0$ is not problematic because the singularity $-1/s$ on the rhs of (19) has a counterpart $\Gamma(s/2) \sim 2/s$ on the lhs, so that $\zeta^3(0) = -1/2$. The numerical evaluation of $\zeta^3(s)$ by using (19) at one point $s$ takes around 5 s of CPU time on a standard PC, the achieved accuracy is around 29 decimal digits. Similar characteristics occur in the numerical evaluation of all Epstein functions studied below, except for the HCP structure given by the lattice sum for which the calculation of the Epstein function takes around 1 min.

It is known that the transformation $s \to 3 - s$ connects the lattice sums of dual (reciprocal) lattice structures. The SC lattice is self-dual. The rhs of (19) is invariant with respect to this transformation, hence it holds that

$$\zeta^3(3 - s) = \frac{\pi^{3-3/2} \Gamma\left(\frac{3-s}{2}\right)}{\Gamma\left(\frac{s}{2}\right)} \zeta^3(s).$$

(20)

4.2 | BCC lattice

The BCC lattice is composed of two SC lattices, shifted with respect to one another by half-period along each of the three coordinates. There are two particles per elementary cube of side $a_{BCC}$, that is, $\rho = 2/a_{BCC}^3 = 1$, which implies that the unit density corresponds to $a_{BCC} = 2^{1/3}$. Consequently,

$$\zeta^3_{D_3}(s) = \frac{1}{2^{s/3}} \left[ \zeta^3(s) + \psi(1/2, 1/2, 1/2; s) \right],$$

(21)

where

$$\psi(x_1, x_2, x_3; s) = \frac{1}{2} \sum_{j,k,l=-\infty}^{\infty} \frac{1}{(j-x_1)^2 + (k-x_2)^2 + (l-x_3)^2}$$

$$= \frac{1}{2\Gamma(s/2)} \int_0^{\infty} dt \frac{t^{s/2}}{t} \sum_{j,k,l=-\infty}^{\infty} e^{-[(j-x_1)^2+(k-x_2)^2+(l-x_3)^2]t}$$

(22)

is a sum over a lattice shifted with respect to the original cubic one. Introducing another Jacobi elliptic function $\theta_2(q) = \sum_{j=-\infty}^{\infty} q^{(j+1)^2}$, defined for $q = e^{i\pi \tau}$, $\Im(\tau) > 0$, the BCC energy is expressible as

$$\zeta^3_{D_3}(s) = \frac{1}{2^{s/3}} \left[ \zeta^3(s) + \frac{\pi^{s/2}}{2\Gamma(s/2)} \int_0^{\infty} \frac{dt}{t} \theta_2^3(e^{-\pi t}) \right].$$

(23)

In view of the Poisson summation formula (15), the Jacobi theta function $\theta_4(q) = \sum_{j=-\infty}^{\infty} (-1)^j q^j$ is “dual” to $\theta_2$ in the sense that

$$\theta_2(e^{-\pi t}) = \frac{1}{\sqrt{t}} \theta_4(e^{-\pi t}).$$

(24)
Thus,
\[
\theta_2 \left( e^{-\pi t} \right) \sim \frac{1}{\sqrt{t}} \left( 1 - 2 e^{-\pi / t} + \ldots \right)
\]  
(25)
and the integral in (23) converges at small \( t \) if \( \Re(s) > 3 \) as was expected.

To derive an analytic continuation of (23) we proceed in close analogy with the previous SC lattice. The integration on the rhs of (23) is split into intervals \([0, 1]\) and \([1, \infty)\). The second integral over \( t \in [1, \infty) \) can be transformed by using the relation (24) and the consequent substitution \( t = 1/t' \) to
\[
\int_1^\infty \frac{dt}{t} t^{s/2} \theta_2^3 \left( e^{-\pi t} \right) = \int_0^1 \frac{dt'}{t'} t'^{(1-s)/2} \theta_4^3 \left( e^{-\pi t'} \right).
\]  
(26)
The first integral over \( t \in [0, 1] \) is modified by adding the vanishing contribution \(-t^{-3/2} + t^{-3/2}\); the term \(-t^{-3/2}\) removes the singularity of \( \theta_2^3 \left( e^{-\pi t} \right) \) as \( t \to 0 \) and the term \( t^{-3/2} \) is integrated out. The final formula for the Epstein function associated with the BCC lattice reads as
\[
\frac{2^{s/3} \Gamma(s/2)}{\pi^{s/2}} \xi_{\text{BCC}}^3(s) = \frac{\Gamma(s/2)}{\pi^{s/2}} \xi_{\text{Z}}^3(s) - \frac{1}{3 - s}
\]
\[
+ \int_0^1 \frac{dt}{2t} \left\{ t^{s/2} \left[ \theta_2^3 \left( e^{-\pi t} \right) - \frac{1}{t^{3/2}} \right] + t^{(3-s)/2} \theta_4^3 \left( e^{-\pi t} \right) \right\},
\]  
(27)
where \( \xi_{\text{Z}}^3(s) \) is given by (19). Because
\[
\theta_4 \left( e^{-\pi t} \right) \sim \frac{1}{\sqrt{t}} e^{-\pi / (4t)} + \ldots,
\]  
(28)
the integral in (27) converges for any complex \( s \).

### 4.3  |  FCC lattice

There are four particles per elementary cube of side \( a_{\text{FCC}} \). thus \( \rho = 4/a_{\text{FCC}}^3 = 1 \), which implies that \( a_{\text{FCC}} = 2^{2/3} \). For \( \Re(s) > 3 \), one gets
\[
\xi_{\text{FCC}}^3(s) = \frac{1}{2^{2s/3}} \left[ \xi_{\text{Z}}^3(s) + \psi \left( 0, 1, \frac{1}{2}; s \right) + \psi \left( 1, 0, \frac{1}{2}; s \right) + \psi \left( 1, \frac{1}{2}, 0; s \right) \right]
\]
\[
= \frac{1}{2^{2s/3}} \left[ \xi_{\text{Z}}^3(s) + \frac{3 \pi^{s/2}}{2 \Gamma(\frac{s}{2})} \int_0^\infty \frac{dt}{t} t^{s/2} \theta_2^2 \left( e^{-\pi t} \right) \theta_3 \left( e^{-\pi t} \right) \right].
\]  
(29)
Splitting the integration into the intervals \([0, 1]\) and \([1, \infty)\) and using the equality
\[
\int_1^\infty \frac{dt}{t} t^{s/2} \theta_2^2 \left( e^{-\pi t} \right) \theta_3 \left( e^{-\pi t} \right) = \int_0^1 \frac{dt}{t} t^{(1-s)/2} \theta_4^2 \left( e^{-\pi t} \right) \theta_3 \left( e^{-\pi t} \right),
\]  
(30)
the analytic continuation of (29) to the whole complex $s$-plane (except for the singular point $s = 3$) takes the form

$$
\frac{2^{2s/3} \Gamma(s/2)}{\pi^{s/2}} \zeta_{D3}(s) = \frac{\Gamma(s/2)}{\pi^{s/2}} \zeta_{Z3}(s) - \frac{3}{3-s} + \frac{3}{2} \int_0^1 \frac{dt}{t} \left\{ t^{s/2} \left[ \theta_2^2(e^{-\pi t}) \theta_3(e^{-\pi t}) - \frac{1}{t^{3/2}} \right] + t^{(3-s)/2} \theta_4^2(e^{-\pi t}) \theta_3(e^{-\pi t}) \right\}.
$$

(31)

The FCC and BCC lattices is a pair of dual structures. Exploring theta-function identities

$$
\vartheta_3(q) = \vartheta_3(q^4) + \vartheta_2(q^4), \quad \vartheta_4(q) = \vartheta_3(q^4) - \vartheta_2(q^4)
$$

(32)
in the representations (27) and (31) it can be shown after some algebra that

$$
\zeta_{D3}^{s/2} = \frac{\pi^{s-3/2} \Gamma(\frac{3-s}{2})}{\Gamma(\frac{s}{2})} \zeta_{D3}(3-s)
$$

(33)
or, vice versa,

$$
\zeta_{D3}(s) = \frac{\pi^{s-3/2} \Gamma(\frac{3-s}{2})}{\Gamma(\frac{s}{2})} \zeta_{D3}^{s/2}(3-s).
$$

(34)
The turning point of these transformations is $s = 3/2$, where $\zeta_{D3}(3/2) = \zeta_{D3}^{s/2}(3/2)$.

## 4.4 SH lattice

The SH lattice is composed of parallel planes composed of the 2D hexagonal lattice with spacing $a_{SH}$, the distance between the nearest-neighbor planes is $d$; the dimensionless parameter $\Delta = d/a_{SH}$. The 2D hexagonal lattice can be considered as the union of two rectangle lattices of sides $a_{SH}$ and $\sqrt{3}a_{SH}$, shifted with respect to one another by a half-period. Thus, the sites of the SH lattice can be parameterized with respect to the reference point $(0,0,0)$ as follows: $a_{SH}(j, \sqrt{3}k, \Delta l)$ with integers $j, k, l$ such that $(j,k,l) \neq (0,0,0)$ and $a_{SH}[(j + \frac{1}{2}, \sqrt{3}(k + \frac{1}{2}), \Delta l]$ with integer $j, k, l$.

There are two particles in the elementary rectangular parallelepiped of volume $\sqrt{3}a_{SH}^2 d$, so the unit density of particles corresponds to $2/(\sqrt{3}a_{SH}^3) = 1$. For $\Re(s) > 3$, the energy per particle for the SH lattice is given by

$$
\zeta_{A_1(\Delta)}(s) = \frac{\pi^{s/2}}{2a_{SH}^3 \Gamma(s/2)} \int_0^\infty \frac{dt}{t} t^{s/2} \left[ \vartheta_3(e^{-\pi t}) \vartheta_3(e^{-3\pi t}) \vartheta_3(e^{-\pi \Delta^2}) - 1 + \vartheta_2(e^{-\pi t}) \vartheta_2(e^{-3\pi t}) \vartheta_3(e^{-\pi \Delta^2}) \right].
$$

(35)
The analytic continuation to the whole complex $s$-plane (except for the point $s = 3$) is obtained in the form

$$
\left( \frac{2}{\sqrt{3}\Delta} \right)^{s/3} \frac{\Gamma(s/2)}{\pi^{s/2}} \zeta_{A_r(\Delta)}(s) = -\frac{1}{s} - \frac{2}{\Delta \sqrt{3}(3 - s)}
$$

$$
+ \int_0^1 \frac{dt}{2t} \left\{ t^{s/2} \left[ \vartheta_3(e^{-\pi t})\vartheta_3(e^{-3\pi t})\vartheta_3(e^{-\pi t\Delta^2}) - \frac{2}{\sqrt{3}\Delta t^{3/2}} \right] + \vartheta_2(e^{-\pi t})\vartheta_2(e^{-3\pi t})\vartheta_3(e^{-\pi t\Delta^2}) \right. \\
+ \left. \frac{t^{(3-s)/2}}{\sqrt{3}\Delta} \vartheta_3(e^{-\pi t})\vartheta_3(e^{-\pi t/3})\vartheta_3(e^{-\pi t/\Delta^2}) - \frac{\sqrt{3}\Delta}{t^{3/2}} + \vartheta_4(e^{-\pi t})\vartheta_4(e^{-\pi t/3})\vartheta_3(e^{-\pi t/\Delta^2}) \right\}. 
$$

(36)

### 4.5 HCP lattice

For very large $s \to \infty$ the Riesz potential $1/r^s$ tends to infinity for $r < 1$ and vanishes for $r > 1$, that is, it approaches the hard-sphere limit. For this case a close-packed structure becomes the minimizer. There are two such lattices in 3D, besides the FCC also the HCP lattice with the same packing ratio. The two lattices have common first-order asymptotic value of the Epstein zeta function—because they have the same nonzero shortest vectors—and it is relatively simple to derive how their difference behaves for large $s$, see the relations (10) and (11).

The HCP lattice is pictured in Figure 1; the middle hexagonal layer is shifted by a half-period with respect to the top and bottom hexagonal lattices. Denoting by $a_{\text{HCP}}$ the spacing of the one-layer hexagonal lattice, the distance between top and bottom hexagonal layers is given by $d = \Delta a_{\text{HCP}}$ with $\Delta = \sqrt{8}/3$. As an elementary cell we take the rectangular parallelepiped with sides $a_{\text{HCP}}$ and $\sqrt{3}a_{\text{HCP}}$ on the top and bottom layers and the height $d$, its volume is given by $\sqrt{3}a_{\text{HCP}}^2d = \sqrt{8}a_{\text{HCP}}^3$. There are eight particles on the top and bottom layers each shared by 8 elementary cells, two particles on the top and bottom layers each shared by 2 cells, one particle on the middle layer sitting in the cell interior and two particles on the middle layer sitting on the cell surface (each shared by 2 cells), that is, altogether there are four particles per elementary cell. The density of particles $\rho = 4/(\sqrt{8}a_{\text{HCP}}^3)$ equals to unity when $a_{\text{HCP}} = 2^{1/6}$.

Particle positions on the top and bottom layers can be parameterized with respect to the reference particle at the origin $(0,0,0)$ as follows: $a_{\text{HCP}}(j, \sqrt{3}k, \Delta l)$ with integer $j, k, l$ such that $(j, k, l) \neq (0, 0, 0)$ and $a_{\text{HCP}}[(j + 1/2), \sqrt{3}(k + 1/2), \Delta l]$ with integer $j, k, l$. It can be shown that particle positions on the middle layer can be parameterized as follows: $a_{\text{HCP}}[j, \sqrt{3}(k + 1/3), \Delta (l + 1/2)]$ and $a_{\text{HCP}}[(j + 1/2), \sqrt{3}(k + 1/6), \Delta (l + 1/2)]$ with integer $j, k, l$. The energy per particle of HCP lattice
for $\Re(s) > 3$ thus reads as

$$
\zeta_{A3}(s) = \frac{1}{2^{s/6+1}} \left\{ \sum_{(j,k,l) \neq (0,0,0)} \frac{1}{(j^2 + 3k^2 + \frac{8}{3}l^2)^{s/2}} + \sum_{j,k,l} \frac{1}{[(j + 1/2)^2 + 3(k + 1/2)^2 + \frac{8}{3}(l + 1/2)^2]^{s/2}} \right. \\
+ \sum_{j,k,l} \frac{1}{[(j + 1/2)^2 + 3(k + 2/3)^2 + \frac{8}{3}(l + 1/2)^2]^{s/2}} \\
+ \left. \sum_{j,k,l} \frac{1}{[(j + 1/2)^2 + 3(k + 1/6)^2 + \frac{8}{3}(l + 1/2)^2]^{s/2}} \right\}
$$

(37)

To obtain an analytic continuation of the energy to the whole complex plane $s$, except for the point $s = 3$, all sums over integers $j$ and $l$ can be transformed directly to Jacobi elliptic functions by using the above explained summation techniques. The transformation of the sums over integers $k$ with the shifts of $k$ by $1/6$ and $2/3$ is not so straightforward, but still they are expressible as series of products of Jacobi elliptic functions and the cos-functions. In particular, one gets

$$
\frac{2^{s/6+1}\Gamma(s/2)}{\pi^{s/2}} \zeta_{A3}(s) = \frac{4}{\sqrt{2}(s - 3)} - \frac{2}{s} \\
+ \int_0^1 dt \ t^{s/2-1} \left[ \frac{1}{\sqrt{8}} \theta_3(e^{-\pi t}) \theta_3(e^{-3\pi t/3}) \theta_3(e^{-8\pi t/3}) - \frac{1}{\sqrt{8t^{3/2}}} \right] \\
+ \int_0^1 dt \ t^{(1-s)/2} \left[ \frac{1}{\sqrt{8}} \theta_3(e^{-\pi t}) \theta_3(e^{-3\pi t/3}) \theta_3(e^{-8\pi t/3}) - \frac{1}{t^{3/2}} \right] \\
+ \int_0^1 dt \ t^{s/2-1} \left[ \frac{1}{\sqrt{8}} \theta_3(e^{-\pi t}) \theta_3(e^{-3\pi t/3}) \theta_3(e^{-8\pi t/3}) - \frac{1}{\sqrt{8t^{3/2}}} \right] \\
+ \int_0^1 dt \ t^{(1-s)/2} \theta_4(e^{-\pi t}) \theta_4(e^{-\pi t/3}) \theta_3(e^{-3\pi t/8}) \\
+ \int_0^1 dt \ t^{s/2-1} \left[ \theta_2(e^{-\pi t}) \theta_2(e^{-8\pi t/3}) - \frac{1}{\sqrt{8}/3t} \right] \\
+ 2 \int_0^1 dt \ t^{s/2-1} \theta_2(e^{-\pi t}) \theta_2(e^{-8\pi t/3}) \sum_{j=1}^{\infty} \cos \left( \frac{\pi j}{3} \right) e^{-\pi j^2/(3t)} \\
+ \int_0^1 dt \ t^{(1-s)/2} \theta_4(e^{-\pi t}) \theta_4(e^{-8\pi t/3}) \left[ 1 + 2 \sum_{j=1}^{\infty} \cos \left( \frac{\pi j}{3} \right) e^{-\pi j^2/3} \right]
$$
\[ + \int_{0}^{1} \frac{t^{s/2-1}}{\sqrt{3t}} \left[ \vartheta_3(e^{-\pi t}) \vartheta_2(e^{-8\pi t/3}) - \frac{1}{\sqrt{8/3t}} \right] \]
\[ + 2 \int_{0}^{1} \frac{t^{s/2-1}}{\sqrt{3t}} \vartheta_3(e^{-\pi t}) \vartheta_2(e^{-8\pi t/3}) \sum_{j=1}^{\infty} \cos \left( \frac{4\pi j}{3} \right) e^{-\pi j^2/(3t)} \]
\[ + \int_{0}^{1} \frac{t^{(1-s)/2}}{\sqrt{8}} \vartheta_3(e^{-\pi t}) \vartheta_4(e^{-3\pi t/8}) \left[ 1 + 2 \sum_{j=1}^{\infty} \cos \left( \frac{4\pi j}{3} \right) e^{-\pi j^2/3} \right]. \] (38)

Here, in the numerical computation of infinite sums over cosine functions one has to truncate the sums as follows \( \sum_{j=1}^{K} \) where the upper cut \( K = 1, 2, 3, \ldots \) is a positive integer. It turns out that by increasing \( K \) the convergence of the sums to the exact value \( (K \to \infty) \) is extremely quick. In particular, by using the symbolic computer language Mathematica it was checked for any real value of \( s \) that the \( K = 4 \) energy is determined with precision of 12 decimal digits, for \( K = 5 \) the precision is increased to 16 decimal digits and so on.

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**REFERENCES**

1. Huygens C. *Traité de la lumière*. Chez Pierre vander Aa, marchand libraire, A Leide, 1690, 1690.
2. Blanc X, Lewin M. The crystallization conjecture: a review. *EMS Surv Math Sci.* 2015;2:255-306.
3. Ventoegel WJ, Nijboer BRA. On the configuration of systems of interacting particle with minimum potential energy per particle. *Physica A-Statist Mech Its Appl.* 1979;98A:274-288.
4. Blanc X, Le Bris C. Periodicity of the infinite-volume ground state of a one-dimensional quantum model. *Nonlin Anal T.M.A.* 2002;48(6):791-803.
5. Cohn H, Kumar A. Universally optimal distribution of points on spheres. *J Amer Math Soc.* 2007;20(1):99-148.
6. Sandier E, Serfaty S. 1d log gases and the renormalized energy: crystallization at vanishing temperature. *Prob Theory and Rel Fields.* 2015;162(3-4):795-846.
7. Bétermin L, Knüpfer H, Nolte F. Note on crystallization for alternating particle chains. *J Stat Phys.* 2020;181(3):803-815.
8. Heitmann RC, Radin C. The ground state for sticky disks. *J Stat Phys.* 1980;22:281-287.
9. Theil F. A proof of crystallization in two dimensions. *Comm Math Phys.* 2006;262(1):209-236.
10. Süto A. Crystalline ground states for classical particles. *Phys Rev Lett.* 2005;95:265501.
11. E W, Li D. On the crystallization of 2D hexagonal lattices. *Comm Math Phys.* 2009;286:1099-1140.
12. Mainini E, Piovano P, Stefanelli U. Finite crystallization in the square lattice. *Nonlin.* 2014;27:717-737.
13. Mainini E, Stefanelli U. Crystallization in carbon nanostructures. *Comm Math Phys.* 2014;328:545-571.
14. Bétermin L, De Luca L, Petricek M. Crystallization to the square lattice for a two-body potential. *Arch Ration Mech Anal.* 2021;240:987-1053.
15. De Luca L, Friesecke G. Crystallization in two dimensions and a discrete Gauss-bonnet theorem. *J Nonlin Sci.* 2018;28(1):69-90.
16. Flatley L, Theil F. Face-centred cubic crystallization of atomistic configurations. *Arch Ration Mech Anal.* 2015;219(1):363-416.
17. Cohn H, Elkies N. New upper bounds on sphere packings I. *Ann Math.* 2003;157:689-714.
18. Viazovska M. The sphere packing problem in dimension 8. *Ann Math.* 2017;185(3):991-1015.
19. Cohn H, Kumar A, Miller SD, Radchenko D, Viazovska M. The sphere packing problem in dimension 24. *Ann Math.* 2017;185(3):1017-1033.
20. Cohn H, Kumar A, Miller SD, Radchenko D, Viazovska M. Universal optimality of the $E_8$ and Leech lattices and interpolation formulas. *to appear in Annals of Math*. 2019. arXiv:1902.05438.

21. Petrache M, Serfaty S. Crystallization for Coulomb and Riesz interactions as a consequence of the Cohn-Kumar conjecture. *Proc Amer Math Soc*. 2020;148:3047-3057.

22. Bétermin L. Effect of periodic arrays of defects on lattice energy minimizers. *Annales Henri Poincaré*. 2021;22:2995-3023.

23. Sarnak P, Strömbergsson A. Minima of Epstein’s zeta function and heights of flat tori. *Invent Math*. 2006;165:115-151.

24. Wigner E. On the interaction of electrons in metals. *Phys Rev*. 1934;46(11):1002-1011.

25. Lewin M. Coulomb and Riesz gases: the known and the unknown. *J Math Phys*. 2022;63:061101.

26. Abrikosov A. The magnetic properties of superconducting alloys. *J Phys Chem Solids*. 1957;2:199-208.

27. Sandier E, Serfaty S. From the Ginzburg-Landau model to vortex lattice problems. *Comm Math Phys*. 2012;313(3):635-743.

28. Rougerie N, Serfaty S. Higher dimensional coulomb gases and renormalized energy functionals. *Commun Pure Appl Math*. 2016;69(3):519-605.

29. Petrache M, Serfaty S. Next order asymptotics and renormalized energy for riesz interactions. *J Institute Math Jussieu*. 2017;16(3):501-569.

30. Cotar C, Petrache M. Equality of the Jellium and Uniform Electron Gas next-order asymptotic terms for Riesz potentials. *Preprint*. arXiv:1707.07664, 2017.

31. Lewin M, Lieb EH, Seiringer R. Floating Wigner crystal with no boundary charge fluctuations. *Phys Rev B*. 2019;100(3):035127.

32. Lauritzen AB. Floating wigner crystal and periodic Jellium configurations. *J Math Phys*. 2021;62:083305.

33. Ghosh S, Miyoshi N, Shirai T. Disordered complex networks: energy optimal lattices and persistent homology. *IEEE Trans Inf Theory*. 2022;68(8):5513-5534.

34. Sobolev SL, Vaskevitch V. The Theory of Cubature Formulas. Springer; 1997.

35. Osgood B, Phillips R, Sarnak P. Extremals of determinants of Laplacians. *J Func Anal*. 1988;80:148-211.

36. Coulangeon R, Lazzarini G. Spherical designs and heights of Euclidean lattices. *J Number Theor*. 2014;141:288-315.

37. Jones JE. On the determination of molecular fields II. From the equation of state of a gas. *Proc R Soc London Ser A*. 1924;106:463-477.

38. Frenkel D, Smit B. *Understanding Molecular Simulation: From Algorithms to Applications*, 2nd ed. Academic Press; 2002.

39. Kaplan IG. *Intermolecular Interactions: Physical Picture, Computational Methods, Model Potentials*. John Wiley and Sons Ltd, 2006.

40. Wang X, Ramirez-Hinestrosa S, Dobnikae J, Frenkel D. The Lennard-Jones potential: when (not) to use it. *Phys Chem Chem Phys*. 2020;22:10624-10633.

41. Mogilner A, Edelstein-Keshet L, Bent I, Spiros A. Mutual interactions, potentials, and individual distance in a social aggregation. *J Math Biol*. 2003;47(4):353-389.

42. Vojcicki P, Zientarski T. Application of the Lennard-Jones potential in modelling robot motion. *Informatyka, Automatyka, Pomiary W Gospodarce I Ochronie Srodowiska*. 2019;9(4):14-17.

43. Blanc X, Le Bris C, Yedder BH. A numerical investigation of the 2-dimensional crystal problem. *Preprint du laboratoire J.-L. Lions, Université de Paris 6*, 2003.

44. Zschorlnak M, Leisegang T, Meutzner F et al. Harmonic principles of elemental crystals—from atomic interaction to fundamental symmetry. *Symmetry*. 2018;10(6):228.

45. Partay LB, Ortner C, Bartok AP, Pickard CJ, Csanyi G. Polytypism in the ground state structure of the Lennard-Jonesium. *Phys Chem Chem Phys*. 2017;19:19369.

46. Bétermin L, Friedrich M, Stefanelli U. Lattice ground states for embedded-atom models in 2D and 3D. *Lett Math Phys*. 2021;111:107.

47. Epstein P. Zur Theorie allgemeiner Zetafunctionen. *Mathematische Annalen*. 1903;56(4):615-644.

48. Elizalde E, Romeo A. Regularization of general multidimensional Epstein Zeta-functions. *Rev Math Phys*. 1989;1(1):113-128.

49. Rankin RA. A minimum problem for the Epstein zeta-function. *Proc Glasgow Math Assoc*. 1953;1:149-158.
51. Ennola V. A Lemma about the Epstein zeta-function. *Proc Glasgow Math Assoc.* 1964;6:198-201.
52. Cassels JWS. On a problem of rankin about the Epstein zeta-function. *Proc Glasgow Math Assoc.* 1959;4:73-80.
53. Diananda PH. Notes on two lemmas concerning the Epstein zeta-function. *Proc Glasgow Math Assoc.* 1964;6:202-204.
54. Montgomery HL. Minimal theta functions. *Glasg Math J.* 1988;30(1):75-85.
55. Ennola V. On a problem about the Epstein zeta-function. *Math Proc Cambridge Philos Soc.* 1964;60:855-875.
56. Delone BN, Ryshkov SS. A contribution to the theory of the extrema of a multidimensional zeta-function. *Dokl Akad Nauk SSSR.* 1967;175(4):991-994.
57. Gruber PM. Application of an idea of Voronoï to lattice zeta functions. *Proc Steklov Inst Math.* 2012;276:103-124.
58. Bétermin L. On energy ground states among crystal lattice structures with prescribed bonds. *J Phys A.* 2021;54(24):245202.
59. Bétermin L. Two-dimensional theta functions and crystallization among bravais lattices. *SIAM J Math Anal.* 2016;48(5):3236-3269.
60. Bétermin L. Optimality of the triangular lattice for Lennard-Jones type lattice energies: a computer-assisted method. *Preprint. arXiv:2104.09795*, 2021.
61. Bétermin L. Local variational study of 2d lattice energies and application to Lennard-Jones type interactions. *Nonlin.* 2018;31(9):3973-4005.
62. Travêne I, Šamaj L. Two-dimensional Wigner crystals of classical Lennard-Jones particles. *J Phys A: Math Theor.* 2019;52(20):205002.
63. Bétermin L. Local optimality of cubic lattices for interaction energies. *Anal Math Phys.* 2019;9(1):403-426.
64. Bétermin L, Petracek M. Optimal and non-optimal lattices for non-completely monotone interaction potentials. *Anal Math Phys.* 2019;9(4):2033-2073.
65. Bétermin L, Faulhuber M, Knüpfer H. On the optimality of the rock-salt structure among lattices with charge distributions. *Math Model Meth Appl Sci.* 2021;31(2):293-325.
66. Bétermin L, Faulhuber M. Maximal theta functions - universal optimality of the hexagonal lattice for Madelung-like lattice energies. *Journal d'Analyse Mathématique (to appear), arXiv:2007.15977*, 2020.
67. Bétermin L, Faulhuber M, Steinerberger S. A variational principle for Gaussian lattice sums. *Preprint. arXiv:2110.06008*, 2021.
68. Mehl MJ, Hicks D, Toher C, Levy O, Hanson RM, Hart GLW, Curtarolo S. *Encyclopedia of Crystallographic Prototypes.*
69. Terras A. *Harmonic Analysis on Symmetric Spaces and Applications II.* Springer; 1988.
70. Ren X, Wei J. The BCC lattice in a long range interaction system. *Preprint. arXiv:2208.00528*, 2022.
71. Chiu P. Height of flat tori. *Proc Amer Math Soc.* 1997;125(3):723-730.
72. Gradshteyn IS, Ryzhik IM. *Table of Integrals, Series, and Products.* 6th ed. Academic Press; 2000.
73. Jorgenson J, Lang S. The Ubiquitous Heat Kernel. In: Enqist B and Schmid W, eds. *Mathematics Unlimited - 2001 and Beyond.* Springer; 2001.
74. Terras A. *Harmonic Analysis on Symmetric Spaces and Applications I.* Springer; 1985.
75. Travêne I, Šamaj L. Generation of off-critical zeros for hypercubic Epstein zeta-functions. *Appl Math Comput.* 2022;413:126611.
76. Borwein JM, McPhedran ML, Wan RC, Zucker IJ. *Lattice sums: then and now.* volume 150 of Encyclopedia of Mathematics, 2013.
77. Whittaker ET, Watson GN. *A Course of Modern Analysis.* Reprinted edition. Cambridge University Press; 1969.

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