Minimization of energy per particle among Bravais lattices in $\mathbb{R}^2$: Lennard-Jones and Thomas-Fermi cases

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Abstract

We prove in this article that the minimizer of Lennard-Jones energy per particle among Bravais lattices is triangular in $\mathbb{R}^2$ for large density of points and the fact that is false for sufficient small density. We show some results about the global minimizer of this energy and finally we prove that the minimizer of the Thomas-Fermi energy per particle in $\mathbb{R}^2$ among Bravais lattices with fixed density is triangular.

1 Introduction

The comprehension of matter’s structure at low temperature is an old challenge. In this case, one of the simplest models is to consider points which represent identical particles such that they interact by pairs only by a Lennard-Jones potential. This model is deterministic and therefore it is not consider entropy or other quantum effects. The problem is to find the configuration of the points which minimizes the total energy of interaction, called Lennard-Jones energy. Radin, in [6], studied this problem in one dimension and showed that, in the case of an infinity of points, the minimizer is periodic. His method is not adaptable in higher dimension and he studied, in [8] and [11], the case of hard-sphere interactions. In other hand, Ventevogel and Nijboer proved in [14], [15] and [16] more general results in one dimension for the Lennard-Jones energy per particle. Indeed, they showed that a unique lattice of the form $a_0^N$ minimizes the Lennard-Jones energy and the fact that all the lattices $a^N$ with $a \leq a_0$ minimizes this energy of the density of point $\rho = a^{-1}$ is fixed. Other results are proved for repulsive potentials, convex or not, with density fixed as necessary condition for the minimality of a lattice. Our article gives some results like in this paper.

After a numerical investigation of Yedder, Blanc, Le Bris, in [19], about the minimization of Lennard-Jones and Thomas-Fermi energy in $\mathbb{R}^2$, it seemed that the triangular lattice is the minimal configuration for the Lennard-Jones problem and the Thomas-Fermi energy with density of nuclei fixed. Some time after, Theil, in [13], gave the first proof of crystallization in two dimensions for a “Lennard-Jones like”, with minimum smaller than one but very close to one, potential very close to the original and showed that the global minimizer of the total energy is the triangular lattice of length one. His method was adapted by E and Li, in [3], for a three-body potential with long range interactions in order to obtain a hexagonal lattice as global minimizer and by Theil and Flatley in three dimensions in [5].

Furthermore Montgomery, in [9], proved that the triangular lattice is the unique minimizer of theta function among Bravais lattices with density fixed and hence the unique minimizer of the Epstein zeta-function by the link between these two functions. As the Lennard-Jones potential is a linear sum of Epstein zeta-functions, it is natural to study the problem of minimization of Lennard-Jones energy among Bravais lattices with and without density fixed.

In this paper we prove that the minimizer of Lennard-Jones energy among Bravais lattices of fixed density is triangular if the density of points is large enough and not triangular if this density is small enough. Moreover we prove that the triangular lattice is the unique minimizer among Bravais lattices with density fixed of the Thomas-Fermi energy of interaction in $\mathbb{R}^2$.

We're proceeding as follows: in the section 2 we give the notations, in the section 3 we show that the triangular lattice is the unique minimizer of the Lennard-Jones energy per particle among Bravais lattices
with density fixed, if the density is sufficiently big and we have arguments in order to explain why the global
minimizer, among Bravais lattices without density fixed, is triangular, in the section 4 we use a proof of
Blanc in [1] to found a lower bound for the interparticle distance of the global minimizer and finally in the
section 5 we study the same kind of problem for the Thomas-Fermi model only when the density is fixed
and we prove that the triangular lattice is the unique minimizer of the Thomas-Fermi energy per particle in
\( \mathbb{R}^2 \) because in this case, \( n = 2 \), the interaction is bipolar.

2 Preliminaries

A Bravais lattice (also called a “simple lattice”) of \( \mathbb{R}^2 \) is given by \( L = \mathbb{Z}u \oplus \mathbb{Z}v \) where \( (u, v) \) is a basis of
\( \mathbb{R}^2 \). By Engel’s theorem (see [4]) we can choose \( u \) and \( v \) such that \( \| u \| \leq \| v \| \) and \( (u, v) \in \left[ \frac{\pi}{3}, \frac{\pi}{2} \right] \). We note
\( |L| = \| u \wedge v \| = \| u \| \| v \| \sin(\widehat{u, v}) \) the area of \( L \) which is in fact the area of the primitive cell of the lattice
and \( L^* := L \setminus \{0\} \). The positive definite quadratic form associated to the Bravais lattice
\( L \) is
\[
Q_L(m, n) = \| mu + nv \|^2 = \| u \|^2 m^2 + \| v \|^2 n^2 + 2\| u \|\| v \| \cos(\widehat{u, v}) mn
\]
For a positive definite quadratic form \( q(m, n) = am^2 + bmn + cn^2 \), we define the discriminant \( D = 4ac - b^2 \geq 0 \).
Hence for \( Q_L \): \( D = 4\| u \|^2\| v \|^2 - 4\| u \|^2\| v \|^2 \cos^2(\widehat{u, v}) = 4\| u \|^2\| v \|^2 \sin^2(\widehat{u, v}) = 4|L|^2 \).
In this article, “lattice” means “Bravais lattice” and we define for \( s > 2 \) the Epstein zeta-function on the
lattice \( L \) by \( \zeta_L(s) := \sum_{x \in L^*} \frac{1}{\| x \|^s} = \frac{1}{(m, n) \neq (0, 0)} Q_L(m, n)^{s/2} \).
Let \( A_2 = \mathbb{Z}(1, 0) \oplus \mathbb{Z}(1/2, \sqrt{3}/2) \) be the triangular lattice of length 1, \( \Lambda_1 = \sqrt{\frac{2}{3}} A_2 \) the triangular lattice of
area 1 and \( \Lambda_A \) the triangular lattice of area \( A \). We remark that, for \( s > 2 \), \( \zeta_{A_2}(s) = \left( \frac{\sqrt{3}}{2} \right)^{s/2} \zeta_{A_1}(s) \).
For \( r_0 \geq 0 \), we consider the classical Lennard-Jones potential \( V_{r_0}(r) = \frac{r_0^{12}}{r^{12}} - 2\frac{r_0^6}{r^6} \) with its minimum for
\( r = r_0 \) and for \( L = Zu \oplus Zv \) a Bravais lattice of \( \mathbb{R}^2 \) we let \( E_{r_0}(L) := \sum_{x \in L^*} V_{r_0}(\| x \|) = r_0^{12} \zeta_L(12) - 2r_0^6 \zeta_L(6) \)
be the Lennard-Jones energy of the lattice \( L \).

![Graph of \( V_1 \)](image)

The idea of this article is to study the following two minimization problems :

\[(P_r^A) : \text{Find the minimizer of } E_{r_0} \text{ among lattices } L \text{ such that } |L| = A\]
\[(P_r^r) : \text{Find the minimizer of } E_{r_0} \text{ among lattices}\]
Proposition 2.1. The minimum of $E_{r_0}$ among lattices is achieved.

Proof. We parametrize the lattice with $x = ||u||, y = ||v||$ and $\theta = \langle \widehat{u}, v \rangle$, therefore

$$E_{r_0}(L) = f_{r_0}(x, y, \theta) = \sum_{(m, n) \neq (0, 0)} \left( \frac{r_0^{12}}{(x^2m^2 + y^2n^2 + 2xymn \cos \theta)^6} - \frac{2r_0^6}{(x^2m^2 + y^2n^2 + 2xymn \cos \theta)^3} \right)$$

First case: minimization without fixed area. If $L$ is the solution of $(P_{r_0})$ then $x \neq 0$, else $E_{r_0}(L) = +\infty$ and $y \leq 1$ because if $y > 1$ then a contraction of the line $\mathbb{R}v$ gives a smaller energy. Therefore we have $x, y \in [m, M]$ and $\theta \in [\pi/3, \pi/2]$. The function $(x, y, \theta) \mapsto f_{r_0}(x, y, \theta)$ is continuous on $[m, M] \times [m, M] \times [\pi/3, \pi/2]$ hence its minimum is achieved.

Second case: minimization with fixed area. We can parametrize $L$ with only two variables $x$ and $y$ which are in a compact set by similar argument like in the first case. Therefore its minimum is achieved. \qed

3 Minimization among lattices with fixed area

3.1 Sufficient condition for the minimality of $E_{r_0}$: Montgomery’s method

Here we use the same idea that Sandier and Serfaty used in [12], to prove the minimality of the triangular lattice among periodic lattices for the renormalized energy linked to Ginzburg-Landau theory, based on the paper [9] of Montgomery where he used Epstein zeta-functions in order to prove that the triangular lattice is the unique minimizer of the theta function among lattices of fixed area. An other proof of this result, and the fact that the square lattice is a critical point of the theta function, is given in [10] by Nonnenmacher and Voros.

Theorem 3.1. If $r_0^6 \pi^3 \geq 120A^3$, then $\Lambda_A$ is the unique solution of $(P_{r_0}^A)$.

Proof. We know that $\Lambda_A$ minimizes $\theta_L(\alpha) := \sum_{m,n} e^{-2\pi\alpha Q_L(m,n)} \forall \alpha > 0$ hence we will write $E_{r_0}(L)$ on the form $\int_1^{+\infty} f(\alpha)\theta_L(\alpha) d\alpha$ and study the function $f$. We write $E_{r_0}(L) = r_0^{12} \zeta_L(12) - 2r_0^6 \zeta_L(6) = E_1 - 2E_2$ with $E_1 := r_0^{12} \zeta_L(12)$ and $E_2 := r_0^6 \zeta_L(6)$ and we use the following identity, with the discriminant of the positive definite quadratic form of $L, Q_L$, is $D = 4a_Lc_L - b_L^2 = 1$ : for $Re(z) > 1$,

$$\zeta_L(2s)\Gamma(s)(2\pi)^{-s} = \frac{1}{1 - s} - \frac{1}{s} + \int_1^{\infty} (\theta_L(\alpha) - 1)(\alpha^s + \alpha^{1-s}) \frac{d\alpha}{\alpha}$$

(3.1)

Indeed, as $\Gamma(s)(2\pi)^{-s}Q_L(m, n)^{-s} = \int_0^{\infty} t^{s-1} e^{-t} dt(2\pi)^{-s}Q_L(m, n)^{-s}$ and by $t = 2\pi Q_L(m, n)y$ we obtain

$$\Gamma(s)(2\pi)^{-s}Q_L(m, n)^{-s} = \int_0^{\infty} e^{-2\pi y Q_L(m,n)}y^{s-1}dy$$

by summation over $(m, n) \neq (0, 0)$ and using the identity of Montgomery $\theta_L(1/\alpha) = \alpha \theta_L(\alpha)$ for all $\alpha > 0$, we have :

$$\Gamma(s)(2\pi)^{-s}\zeta_L(2s) = \int_0^{\infty} (\theta_L(y) - 1)y^{s-1}dy = \int_0^{1} (\theta_L(y) - 1)y^{s-1}dy + \int_1^{\infty} (\theta_L(y) - 1)y^{s-1}dy$$

$$= \int_1^{\infty} (\theta_L(1/\alpha) - 1)\alpha^{-s-1}d\alpha + \int_1^{\infty} (\theta_L(\alpha) - 1)\alpha^{s-1}d\alpha$$

$$= \int_1^{\infty} (\alpha \theta_L(\alpha) - 1)\alpha^{-s-1}d\alpha + \int_1^{\infty} (\theta_L(\alpha) - 1)\alpha^{s-1}d\alpha$$

$$= \int_1^{\infty} \theta_L(\alpha)\alpha^{-s}d\alpha - \int_1^{\infty} \alpha^{-1-s}d\alpha + \int_1^{\infty} (\theta_L(\alpha) - 1)\alpha^{s-1}d\alpha$$

$$= \int_1^{\infty} (\theta_L(\alpha) - 1)\alpha^{-s}d\alpha + \int_1^{\infty} (\theta_L(\alpha) - 1)\alpha^{s-1}d\alpha + \int_1^{\infty} \alpha^{-s}d\alpha - \int_1^{\infty} \alpha^{-1-s}d\alpha$$
Thus we have shown that Montgomery proved that for the triangular lattice minimizes the Theta function $r_P^4$. Then the triangular lattice is not the solution of $(P_1)$. Indeed Montgomery proved that for Theta function triangular lattice minimizes $\theta_L(\alpha)$ for all $\alpha \geq 0$. However our bound $r_0^6 \pi^3 = 120 A^3$ is probably not optimal. If it were, by the Proposition 3.3 and its remark, then the triangular lattice is not the solution of $(P_1)$.

Now if $|L| = A$, by the equality $D = (2A)^2$ we have two identities:

$$
r_0^{-12} (2A)^6 \Gamma(6) (2\pi)^{-6} E_1 = \frac{1}{6} - \frac{1}{6} + \int_{1}^{+\infty} (\theta_L(\alpha) - 1) (\alpha^6 + \alpha^{-6}) \frac{d\alpha}{\alpha}
$$

$$
r_0^{-6} (2A)^3 \Gamma(3) (2\pi)^{-3} E_2 = \frac{1}{3} - \frac{1}{3} + \int_{1}^{+\infty} (\theta_L(\alpha) - 1) (\alpha^3 + \alpha^{-3}) \frac{d\alpha}{\alpha}
$$

and we found

$$
E_1 = \frac{\pi^6}{30 (2A)^6 5!} + \int_{1}^{+\infty} (\theta_L(\alpha) - 1) \frac{r_0^{12} (2\pi)^6}{(2A)^6 5!} (\alpha^6 + \alpha^{-5}) \frac{d\alpha}{\alpha}
$$

$$
E_2 = \frac{\pi^3}{6 (2A)^3 2!} + \int_{1}^{+\infty} (\theta_L(\alpha) - 1) \frac{r_0^{6} (2\pi)^3}{(2A)^3 2!} (\alpha^3 + \alpha^{-2}) \frac{d\alpha}{\alpha}
$$

and therefore

$$
E_{r_0}(L) = C_{r_0,A} + \frac{\pi^3}{A^3} \int_{1}^{+\infty} (\theta_L(\alpha) - 1) g_{r_0,A}(\alpha) \frac{d\alpha}{\alpha}
$$

where $g_{r_0,A}(\alpha) := \frac{r_0^6 \pi^3}{A^3 5!} (\alpha^6 + \alpha^{-5}) - (\alpha^3 + \alpha^{-2})$ and $C_{r_0,A}$ is a constant depending on $r_0$ and $A$ but independent of $L$. If we can prove $g_{r_0,A}(\alpha) \geq 0$ for all $\alpha \geq 1$ then $\Lambda_A$ is minimizer among lattices with fixed area. Indeed we have two identities:

\[
E_{r_0}(L) - E_{r_0}(\Lambda_A) = \int_{1}^{+\infty} (\theta_L(\alpha) - \theta_{\Lambda_A}(\alpha)) g_{r_0,A}(\alpha) \frac{d\alpha}{\alpha} \geq 0
\]

hence $\Lambda_A$ is minimizer among lattices of area $A$, and this minimizer is unique.

First we look for what values of $r_0$ and $A$, $g_{r_0,A}(1) \geq 0$:

$$
g_{r_0,A}(1) \geq 0 \iff \frac{r_0^6 \pi^3}{A^3 5!} - 1 \geq 0 \iff r_0^6 \pi^3 \geq 120 A^3
$$

Secondly we compute $g'_{r_0,A}(\alpha) = \frac{r_0^6 \pi^3}{A^3 5!} (6\alpha^5 - 5\alpha^{-6}) - (3\alpha^2 - 2\alpha^{-3})$ and, if $r_0^6 \pi^3 \geq 120 A^3$ then

$$
g'_{r_0,A}(1) = \frac{r_0^6 \pi^3}{A^3 5!} - 1 \geq 0
$$

Finally we compute $g''_{r_0,A}(\alpha) = \frac{r_0^6 \pi^3}{A^3 5!} (30\alpha^4 + 30\alpha^{-7}) - (6\alpha + 6\alpha^{-4})$. As $\frac{r_0^6 \pi^3}{A^3 5!} \geq 1$ and $\alpha \geq 1$,

$$
\frac{r_0^6 \pi^3}{A^3 5!} (30\alpha^4 + 30\alpha^{-7}) - (6\alpha + 6\alpha^{-4}) \geq 30\alpha^4 + 30\alpha^{-7} - 6\alpha - 6\alpha^{-4} \geq 24\alpha + 30\alpha^{-7} - 6\alpha^{-4} \geq 0
$$

Thus we have shown that $g''_{r_0,A}(\alpha) \geq 0$ for all $\alpha \geq 1$, $g'_{r_0,A}(1) \geq 0$ and $g_{r_0,A}(1) \geq 0$ for any $r_0,A$ such that $r_0^6 \pi^3 \geq 120 A^3$ and $\alpha \geq 1$ hence $g_{r_0,A}(\alpha) \geq 0$ for all $\alpha \geq 1$ and $r_0^6 \pi^3 \geq 120 A^3$. \hfill \Box

Remark 3.2. We prove below (see proposition 3.3) that if $A$ is sufficiently large then $\Lambda_A$ is not longer a solution of $(P_1)$. However our bound $r_0^6 \pi^3 \geq 120 A^3$ is probably not optimal. If it were, by the Proposition 3.3 and its remark, then the triangular lattice is not the solution of $(P_1)$. 

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Remark 3.3. If \( r_0 \geq \frac{2 \times 15^{1/3}}{\pi} \approx 1.57004 \) then \( \Lambda_1 \) is the unique solution of \( (P_{r_0}^1) \).

If \( A \leq \frac{\pi}{2 \times 15^{1/3}} \approx 0.636927 \) then \( \Lambda_A \) is the unique solution of \( (P_A^1) \).

This result explain that the behaviour of the potential is important for the interaction between the first neighbours because in this case the inverse power part \( r^{12} r^{-12} \) is the strongest interaction. This method can be adapted to potentials of the form \( V(r) = \frac{K_1}{r^n} - \frac{K_2}{r^p} \) with \( n > p > 2 \) to obtain similar results.

### 3.2 Necessary condition for the minimality of the triangular lattice for \( E_1 \)

Because \( V_{r_0}(r) = V_1 \left( \frac{r}{r_0} \right) \), we are interested only in the energy \( E_1 \).

**Proposition 3.4.** \( \Lambda_A \) is the solution of \( (P_A^1) \) if and only if \( A \leq \inf_{L \in \Lambda_1} \left( \frac{\zeta_L(12) - \zeta_{\Lambda_1}(12)}{2(\zeta_L(6) - \zeta_{\Lambda_1}(6))} \right)^{1/3} \).

Hence if \( A \) is sufficiently large, \( \Lambda_A \) is not the solution of \( (P_A^1) \).

**Proof.** Suppose that the triangular lattice of area \( A, \Lambda_A = Zu \oplus Zv \) is the minimizer of \( E_1 \) among lattices with fixed area. Hence that is equivalent with the fact that the triangular lattice \( \Lambda_1 = ZA^{-1/2}u \oplus ZA^{-1/2}v \) is the minimizer of \( \bar{E}_1(L) := \sum_{x \in L} (A^{-6}||x||^{-12} - 2A^{-3}||x||^{-6}) \) among lattices of area 1, i.e. \( \Lambda_1 \) is the minimizer of \( \bar{E}_1(L, A) := \sum_{x \in L} (||x||^{-12} - 2A^3||x||^6) \) among lattices with area 1. Therefore \( \bar{E}_1(\Lambda_1, A) \leq \bar{E}_1(L, A) \) for all \( L \) of area 1 and is equivalent with, for all \( L \) of area 1:

\[
\zeta_{\Lambda_1}(12) - 2A^3 \zeta_{\Lambda_1}(6) \leq \zeta_L(12) - 2A^3 \zeta_L(6)
\]

and therefore, as \( \zeta_L(6) > \zeta_{\Lambda_1}(6) \) for all \( L \neq \Lambda_1 \),

\[
A \leq \inf_{L \in \Lambda_1} \left( \frac{\zeta_L(12) - \zeta_{\Lambda_1}(12)}{2(\zeta_L(6) - \zeta_{\Lambda_1}(6))} \right)^{1/3}
\]

\[ \square \]

It is difficult to study the minimum of the function \( L \mapsto \frac{\zeta_L(12) - \zeta_{\Lambda_1}(12)}{2(\zeta_L(6) - \zeta_{\Lambda_1}(6))} \) among lattices \( L \neq \Lambda_1 \) such that \( |L| = 1 \), however we could search numerically an upper bound of it.

**Proposition 3.5.** It holds that

\[
\lim_{r \to a} \left( \frac{\zeta_{L_r}(12) - \zeta_{\Lambda_1}(12)}{2(\zeta_{L_r}(6) - \zeta_{\Lambda_1}(6))} \right)^{1/3} = \frac{\sqrt{3}}{2} \left( \frac{\sum_{m,n} 13m^4 + 131m^3n + 270m^2n^2 + 131mn^3 + 13n^4}{(m^4 + mn + n^2)^2} \right)^{1/3}
\]

where \( L_r \) is the lattice such that \( ||u|| = ||v|| = r \) and with area 1 and \( a = \sqrt{2/\sqrt{3}} \) is the length of \( \Lambda_1 \).

**Proof.** Let \( L_r \) the lattice such that \( |L| = 1 \) and \( ||u|| = ||v|| = r \), then \( ||mu + nv||^2 = m^2r^2 + n^2r^2 + 2\sqrt{r^4 - 1}mn \) because \( |L| = \sqrt{D}/2 \). As \( \Lambda_1 \), of length \( a = \sqrt{2/\sqrt{3}} \), is the unique minimizer of \( \zeta_L(12) \) and \( \zeta_L(6) \) among lattices with fixed area, we have

\[
\lim_{L \to \Lambda_1} \left( \frac{\zeta_L(12) - \zeta_{\Lambda_1}(12)}{2(\zeta_L(6) - \zeta_{\Lambda_1}(6))} \right)^{1/3} = \lim_{r \to a} \left( \frac{\zeta_{L_r}(12) - \zeta_{\Lambda_1}(12)}{2(\zeta_{L_r}(6) - \zeta_{\Lambda_1}(6))} \right)^{1/3} = \left( \frac{d^2}{dr} [\zeta_{L_r}(12)]_a}{2(\zeta_{L_r}(6) - \zeta_{\Lambda_1}(6))} \right)^{1/3}
\]

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Now we compute the first and second derivative of $\zeta_L(12)$ and $\zeta_L(6)$, for $r > 1$:

\[
\frac{d}{dr} [\zeta_L(12)]_r = \sum_{(m,n) \neq (0,0)} \frac{-12r((m^2 + n^2)\sqrt{r^4 - 1} + 2mn^2)}{\sqrt{r^4 - 1}(r^2m^2 + r^2n^2 + 2\sqrt{r^4 - 1}mn)^2}
\]

This quantity is equal to 0 for $r = 1$ because $\Lambda_1$ is the minimizer of $\zeta_L(12)$ among lattices with fixed area and

\[
\frac{d^2}{dr^2} [\zeta_L(12)]_a = \sum_{(m,n) \neq (0,0)} \frac{81\sqrt{3}(13m^4 + 131m^3n + 270m^2n^2 + 131mn^3 + 13n^4)}{32(m^2 + mn + n^2)^8}
\]

As far as that goes:

\[
\frac{d}{dr} [\zeta_L(6)]_r = \sum_{(m,n) \neq (0,0)} \frac{-6r((m^2 + n^2)\sqrt{r^4 - 1} + 2mn^2)}{\sqrt{r^4 - 1}(r^2m^2 + r^2n^2 + 2\sqrt{r^4 - 1}mn)^2}
\]

and

\[
\frac{d^2}{dr^2} [\zeta_L(6)]_a = \sum_{(m,n) \neq (0,0)} \frac{27(7m^4 + 83m^3n + 162m^2n^2 + 83mn^3 + 7n^4)}{8(m^2 + mn + n^2)^5}
\]

Now we remark that $\frac{81\sqrt{3}}{2} = \frac{81 \times 8\sqrt{3}}{32 \times 27} = \frac{3\sqrt{3}}{4} = \frac{(\sqrt{3})^3}{2^2}$ and

\[
\left( \frac{d^2}{dr^2} [\zeta_L(12)]_a \right)^{1/3} = \frac{\sqrt{3}}{2} \left( \frac{\sum_{m,n} 13m^4 + 131m^3n + 270m^2n^2 + 131mn^3 + 13n^4}{\left( m^2 + mn + n^2 \right)^8} \right)^{1/3}
\]

Remark 3.6. When we compute this value and obtain $\lim_{L \to \Lambda_1} \left( \frac{\zeta_L(12) - \zeta_L(12)}{2(\zeta_L(6) - \zeta_L(6))} \right)^{1/3} \approx 0.9146906$.

Anyway we can say that if $A > 0.9146907$ then the triangular lattice is not the minimizer of $E_1$ among lattices with fixed area $A$. This correspond to the triangular lattices of length $r > \sqrt{0.9146907 \times \frac{2}{\sqrt{3}}} \approx 1.0277129$.

4 Global minimization of $E_1$ among lattices

4.1 Characterization of the global minimizer

Proposition 4.1. If $L_0$ is the solution of $(P_1)$ then

i) $E_1(L_0) = -\zeta_{L_0}(6) = -\zeta_{L_0}(12) < 0$,

ii) $\|u\| < 1$ and $\|v\| \leq 1$,

iii) $\zeta_{L_0}(6) = \max \{ \zeta_{L_0}(6) : L \text{ s.t. } \zeta_{L}(12) \leq \zeta_{L}(6) \}$.

Proof. i) We consider the function $f(r) = E_1(rL_0) = r^{12}\zeta_{L}(12) - 2r^{-6}\zeta_{L}(6)$. As $L_0$ is a global minimizer of $E_1$, $r = 1$ is a critical point of $f$ and $f'(r) = -12r^{-13}\zeta_{L_0}(12) + 12r^{-7}\zeta_{L_0}(6)$,

\[
f'(1) = 0 \iff \zeta_{L_0}(12) = \zeta_{L_0}(6)
\]

then $E_1(L_0) = \zeta_{L_0}(12) - 2\zeta_{L_0}(6) = -\zeta_{L_0}(6) = -\zeta_{L_0}(12)$.

ii) As $\zeta_{L_0}(12) = \zeta_{L_0}(6)$ it is clear that $\|u\| < 1$ because for all $r > 1$, $r^{-12} < r^{-6}$. If $\|v\| > 1$ a little contraction of $\mathbb{R}v$ gives a new lattice $L_1$ such that $E_1(L_1) < E_1(L_0)$ because some of the distances of the lattice decreases while $\|u\|$ is constant, therefore the energy decreases.

iii) $-\zeta_{L_0}(6) = E_1(L_0) \leq E_1(L) \iff \zeta_{L}(6) - \zeta_{L_0}(6) \leq \zeta_{L}(12) - \zeta_{L}(6)$ and if $L$ is a lattice such that $\zeta_{L}(12) \leq \zeta_{L}(6)$ we obtain $\zeta_{L}(6) \leq \zeta_{L_0}(6)$.

\[ \Box \]
**Corollary 4.2.** $A_2$ cannot be the solution of $(P_1)$ though the minimum of the potential $V_1$ is achieved for $r = 1$.

**Proposition 4.3.** The solution of $(P_1)$ among the dilated of $A_2$ is the triangular lattice $\Lambda_0$ such that

$$
\sigma_0 = \left( \frac{\zeta_{A_2}(12)}{\zeta_{A_2}(6)} \right)^{1/6} \quad \text{and therefore} \quad |\Lambda_0| = \left( \frac{\zeta_{A_2}(12)}{\zeta_{A_1}(6)} \right)^{1/3}.
$$

**Proof.** If $\Lambda_0$ is solution of $(P_1)$ then $\zeta_{A_0}(12) = \zeta_{A_0}(6) \iff \frac{\zeta_{A_2}(12)}{\sigma_0^{12}} = \frac{\zeta_{A_2}(6)}{\sigma_0^{6}} \iff \sigma_0 = \frac{\zeta_{A_2}(12)}{\zeta_{A_2}(6)}$.

Therefore $|\Lambda_0| = \sqrt[3]{\frac{3}{2}} \left( \frac{\zeta_{A_2}(12)}{\zeta_{A_2}(6)} \right)^{1/3} = \left( \frac{(\sqrt{3}/2)^6 \zeta_{A_2}(12)}{(\sqrt{3}/2)^3 \zeta_{A_2}(6)} \right)^{1/3} = \left( \frac{\zeta_{A_1}(12)}{\zeta_{A_1}(6)} \right)^{1/3}. \quad \square$

**Remark 4.4.** By a computation: $\zeta_{A_2}(12) \approx 6.0098139, \, \zeta_{A_2}(6) \approx 6.3758815$, therefore $\sigma_0 \approx 0.9901936$ and $|\Lambda_0| \approx 0.8491236$. We see that it seems be the same case as in Theil’s paper: the length of the triangular lattice which minimizes the energy is a little bit smaller than the distance which minimizes the potential. Moreover $E_1(\Lambda_0) = -\sigma_0^{-6} \zeta_{A_2}(6) = -\frac{\zeta_{A_2}(6)^2}{\zeta_{A_2}(12)} \approx -6.7642484$.

Because $|\Lambda_0| > 0.636927$, our theorem 3.1 is not sufficient to prove that $\Lambda_0$ is the solution of $(P_1)$. Therefore if the lower bound of

$$
\left( \frac{\zeta_L(12) - \zeta_{A_1}(12)}{2(\zeta_L(6) - \zeta_{A_1}(6))} \right)^{1/3}
$$

among lattices $L$ of area 1 is bigger than $\left( \frac{\zeta_{A_1}(12)}{\zeta_{A_1}(6)} \right)^{1/3}$ the solution of $(P_1)$ is the triangular lattice $\Lambda_0$, which is equivalent to

$$
\zeta_L(12) - \frac{\zeta_{A_1}(12)}{\zeta_{A_1}(6)} \zeta_L(6) \geq -\zeta_{A_1}(12) \quad \text{for all lattice } L \quad \text{such that} \quad |L| = 1
$$

We remark that is exactly equivalent to $\Lambda_1$ is the solution of $(P_1^*)$ with $a = \left( \frac{\zeta_{A_1}(6)}{\zeta_{A_1}(12)} \right)^{1/6} \approx 1.0852119$, but our method using the result of Montgomery is not sufficient to answer this question. We remark that this problem is equivalent to find the maximum of $Z(X,Y) = \frac{2}{\zeta_{A_1}(6)} \zeta_{L_{X,Y}} (6) - \frac{1}{\zeta_{A_1}(12)} \zeta_{L_{X,Y}} (12)$ where $L_{X,Y}$ the lattice of area 1, $X = \|u\|$ and $Y = \|v\|$. The following graphs show us that the maximum of $Z(X,Y)$ is achieved for $X = Y = \sqrt{\frac{2}{\sqrt{3}}} \approx 1.0745699$ is probably true.

Graph of $(X,Y) \mapsto Z(X,Y) = \frac{2}{\zeta_{A_1}(6)} \zeta_{L_{X,Y}} (6) - \frac{1}{\zeta_{A_1}(12)} \zeta_{L_{X,Y}} (12)$ with $(X,Y) \in [1,2]^2$ on the left side and $(X,Y) \in [1,1.1]^2$ on the right side.
4.2 Minimal distance of the lattice for the global minimizer

Because our method does not show that the triangular lattice of length $\sigma_0$ is the global minimizer of the Lennard-Jones energy among lattices, we used a proof of Blanc, in [1], in order to find a lower bound for the minimal distance in the globally minimizing lattice. His result was for the Lennard-Jones interaction of $N$ points in $\mathbb{R}^2$ and $\mathbb{R}^3$. Xue in [20] and Schachinger, Addis, Bomze and Schoen in [2] improved this one. We use Blanc’s method because it is well suited to our problem.

**Proposition 4.5.** If $L_0 = \mathbb{Z}u \oplus \mathbb{Z}v$ is the solution of $(P_1)$, then the minimal distance is greater than an explicit constant $c$ such that $c > 0.7403477$.

**Proof.** In his paper, Blanc proved that $E_1(L_0) \geq V_1(\|u\|), 23 + \frac{1}{\|u\|^{12}} \sum_{k \geq 2} \frac{16k + 8}{k^{12}} \frac{1}{\|u\|^{6}} \sum_{k \geq 2} \frac{32k + 16}{k^{6}}$. As we have $E(L_0) \leq E(A_0) = -\frac{\zeta A_2(6)^2}{\zeta A_2(12)}$, we obtain, with $P := \sum_{k \geq 2} \frac{16k + 8}{k^{12}}$ and $Q := \sum_{k \geq 2} \frac{32k + 16}{k^{6}}$,

$$33 - \frac{\zeta A_2(6)^2}{\zeta A_2(12)} \geq \frac{P + 1}{\|u\|^{12}} \frac{Q + 2}{\|u\|^{6}}$$

Now, setting $t = \|u\|^{-6}$, we have $(P + 1)t^2 - (Q + 2)t - 23 + \frac{\zeta A_2(6)^2}{\zeta A_2(12)} \leq 0$ which implies

$$t \leq \frac{Q + 2 + \sqrt{(Q + 2)^2 + 4 \left( 23 - \frac{\zeta A_2(6)^2}{\zeta A_2(12)} \right) (P + 1) }}{2P + 2}$$

and we obtain

$$\|u\| \geq \left( \frac{2P + 2}{Q + 2 + \sqrt{(Q + 2)^2 + 4 \left( 23 - \frac{\zeta A_2(6)^2}{\zeta A_2(12)} \right) (P + 1) }} \right)^{1/6} =: c$$

Because $P \approx 0.0098757$ and $Q \approx 1.4591772$, we obtain $c \approx 0.7403478$.

5 Thomas-Fermi model in $\mathbb{R}^2$

In the model of Thomas-Fermi for interactions in a solid we consider $N$ nuclei at position $X_N = (x_1, x_2, ..., x_N)$, where $x_i \in \mathbb{R}^2$ for all $1 \leq i \leq N$, associated to $N$ electrons with total density $\rho \geq 0$. Then the Thomas-Fermi energy is given by

$$E_{TF}(\rho, X_N) = \int_{\mathbb{R}^2} \rho^2(x)dx - \frac{1}{2} \int \int_{\mathbb{R}^2 \times \mathbb{R}^2} \log \|x - y\| \rho(x) \rho(y) dx dy + \sum_{j=1}^{N} \int_{\mathbb{R}^2} \log \|x - x_j\| \rho(x) dx - \frac{1}{2} \sum_{j \neq k} \log \|x_j - x_k\|$$

Because the system is neutral, the number of electrons is exactly equal to $N$ and we study the minimization problem $I_{N}^{TF} = \inf_{X_N} \{ E_{TF}(X_N) \}$, where

$$E_{TF}(X_N) := \inf \left\{ E_{TF}(\rho, X_N), \rho \geq 0, \rho \in L^1(\mathbb{R}^2) \cap L^2(\mathbb{R}^2), \int_{\mathbb{R}^2} \rho = N \right\}$$

Now we write the Euler-Lagrange equation of this minimization problem and obtain, for the minimizer $\tilde{\rho}$:

$$2\rho - \tilde{\rho} \ast \log \|x\| + \sum_{j=1}^{N} \log \|x - x_j\| = \theta$$
where $\theta$ is the Lagrange multiplier associated to the constraint $\int \rho = N$. If we take the Laplacian of this equation, we have

$$-\Delta \tilde{\rho} + \pi \tilde{\rho} = \pi \sum_{j=1}^{N} \delta_{x_j}$$

We know that the Yukawa potential $W_{TF}$ is the solution of $-\Delta W_{TF} + \pi W_{TF} = \delta_0$ and its integral formula is $W_{TF}(x) = W_{TF}(|x|) = \frac{1}{2} K_0(\sqrt{\pi} |x|)$ where $K_0$ is the modified Bessel function of the second kind given by $K_0(r) = \int_{0}^{\infty} e^{-r \cosh(t)} dt$ (see [7] and [17] for details).

Hence we have $\tilde{\rho}(x) = \pi \sum_{j=1}^{N} W_{TF}(|x - x_j|)$ and when one replaces in the total energy, we obtain

$$E^{TF}(X_N, \tilde{\rho}) = \sum_{i \neq j} W_{TF}(|x_i - x_j|) + N \lim_{x \to 0} \left( W_{TF}(|x|) + \frac{1}{2} \log |x| \right)$$

and therefore $E^{TF}(X_N) = \sum_{i \neq j} W_{TF}(|x_i - x_j|) + N A$, where $A$ is a constant independent of $N$ and $X_N$. For more details, see [19] and [18].

Now, if we consider that the nuclei are in a lattice $L$, we can study, by mean, the energy per point

$$E_{TF}(L) = \sum_{x \in \Lambda^*} W_{TF}(|x|)$$

The Yukawa potential is strictly decreasing, therefore it is an evidence that the good problem is the minimization of this energy among lattices only with fixed area.

**Theorem 5.1.** $\Lambda_A$ is the unique minimizer of $E_{TF}$ among lattices of fixed area $A$.

**Proof.** This problem is equivalent to find the minimizer of $\sum_{x \in \Lambda^*} K_0(|x|)$ among lattices with fixed area. We put $y = \frac{1}{2} |x| e^1$ for $x \neq 0$ in the integral formula for $K_0(|x|)$:

$$K_0(|x|) = \frac{1}{2} \int_{-\infty}^{+\infty} e^{-|x| \cosh(t)} dt = \frac{1}{2} \int_{0}^{+\infty} e^{-|x| \cosh(t)} \cosh(t) y^{-1} dt$$

$$= \frac{1}{2} \int_{0}^{+\infty} e^{-|x| y^{-1}} y^{-1} dy$$

and

$$= \frac{1}{2} \int_{0}^{+\infty} e^{-|x| y^{-1}} e^{-y^{-1}} dy$$

Now, for all $y > 0$ and any lattice $L$ of area $A$ we have

$$\sum_{x \in \Lambda^*} e^{-\frac{|x|^2}{4y}} = \theta_L \left( \frac{1}{8\pi y} \right) - 1$$

hence by the Montgomery theorem the triangular lattice $\Lambda_A$ minimizes $\theta_L(\alpha)$ for all $\alpha > 0$ and it is the unique minimizer of $L \mapsto \theta_L(\alpha)$ for all $\alpha > 0$ among Bravais lattices with fixed area $A$.

Therefore $\Lambda_A$ is the unique minimizer of the energy $E_y(L) := \sum_{x \in \Lambda^*} e^{-\frac{|x|^2}{4y}}$ among lattices with fixed area $A$. Now it is clear, as $E_y(\Lambda_A) \leq E_y(L)$ for all $y > 0$ and for any lattice $L$ with area $A$, that

$$\frac{1}{2} \int_{0}^{+\infty} E_y(\Lambda_A) e^{-y} y^{-1} dy \leq \frac{1}{2} \int_{0}^{+\infty} E_y(L) e^{-y} y^{-1} dy$$

therefore, for all $L$ of fixed area $A$ : $E_{TF}(\Lambda_A) = \sum_{x \in \Lambda_A^*} W_{TF}(|x|) \leq \sum_{x \in \Lambda^*} W_{TF}(|x|) = E_{TF}(L).$ \hfill \square

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