Minimization of lattice energies

From old to new results in dimensions 2 and 3

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OPCOP 2017
19th April 2017, CIEM, Castro Urdiales

Introduction: minimization among Bravais lattices

Definitions

Potential: $f : (0, +\infty) \to \mathbb{R}$ such that $f(r) = O(r^{-\eta})$, $\eta > d/2$

Energy per point of a Bravais lattice $L = \bigoplus_{i=1}^{d} \mathbb{Z}u_i$ is given by

$$E_f[L] := \sum_{p \in L \setminus \{0\}} f\left(|p|^2\right) < +\infty$$

Let V (or A) be the **volume** (area) of L, i.e. the volume of its unit cell.

Problems

Minimizing $L \mapsto E_f[L]$ among all the Bravais lattices L with (or without) a fixed volume V.

Motivation: Crystallization problems; Vortices in superconductors

Main examples

Epstein zeta function

If $f(r) = r^{-s/2}$, $s > d$, then $\zeta_L(s) := \displaystyle\sum_{p\in L\backslash\{0\}} \frac{1}{|p|^s}$.

Theta function

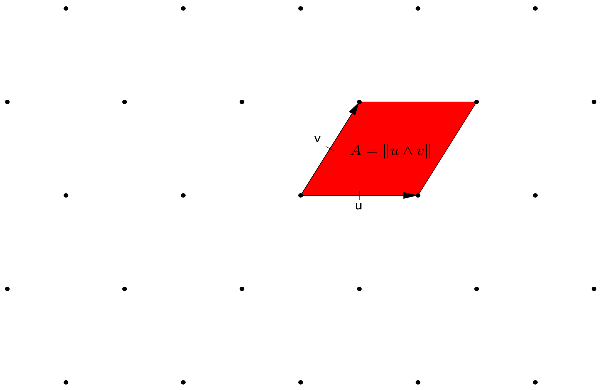
If $f(r) = e^{-\alpha\pi r}$, $\alpha > 0$, then $\theta_L(\alpha) := \displaystyle\sum_{p\in L} e^{-\pi\alpha|p|^2}$.

Lennard-Jones energy

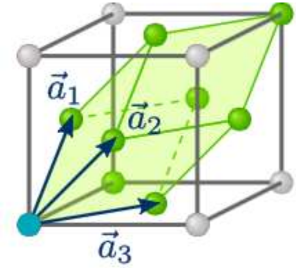
If $f(r) = \dfrac{a_1}{r^{x_1}} - \dfrac{a_2}{r^{x_2}}$, $a_i > 0$, $x_2 > x_1 > d/2$, then

$$E_f[L] = a_2\zeta_L(2x_2) - a_1\zeta_L(2x_1).$$

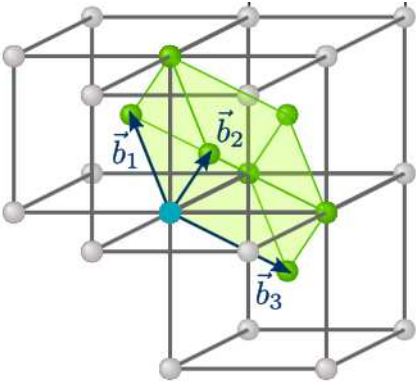
Triangular lattice



FCC and BCC lattices



Face-Centred-Cubic lattice



Body-Centred-Cubic lattice

1. Epstein zeta function and theta function: old results

2. New results for Lennard-Jones energy

3. Theta function in 3d: Local minimality of FCC/BCC lattices

The Epstein zeta function in dimensions 2 and 3

The volume of lattices should be fixed.

- Rankin '53, Cassels '59, Diananda '64, Ennola '64: in **2d**, for any $s > 0$, the minimizer of the Epstein zeta function

$$L \mapsto \zeta_L(s) := \sum_{p \in L \setminus \{0\}} \frac{1}{|p|^s}$$

is a **triangular lattice**, for any fixed area;

- Ennola '64: in **3d**, for any $s > 0$, the **FCC** and the **BCC lattices** are local minimizers of $L \mapsto \zeta_L(s)$, for any fixed volume.

[Sarnak-Strömbergsson '06] - Conjecture for $L \mapsto \zeta_L(s)$, $V = 1$

- For any $s > 3/2$, the FCC lattice is the unique minimizer;
- For any $0 < s < 3/2$, the BCC lattice is the unique minimizer.

The theta function in dimensions 2 and 3

The volume of lattices should be fixed.

- Montgomery '88: in **2d**, for any $\alpha > 0$, the minimizer of the theta function
$$L \mapsto \theta_L(\alpha) := \sum_{p\in L} e^{-\pi\alpha|p|^2}$$
is a **triangular lattice**, for any fixed area.

[Sarnak-Strömbergsson '06] - Conjecture for $L \mapsto \theta_L(\alpha)$, $V = 1$

- For any $\alpha > 1$, the FCC lattice is the unique minimizer;
- For any $0 < \alpha < 1$, the BCC lattice is the unique minimizer.

Applications: Heat equation, Ginzburg-Landau Vortices, Bose-Einstein Condensates, Cryptography...

Completely monotone functions and the triangular lattice

By Bernstein Theorem, we get:

Proposition (*Minimality at any fixed volume in 2d*)

Let f be a **completely monotone function** such that $f(r) = O(r^{-p})$, $p > 1$, then for any $A > 0$, the triangular lattice Λ_A is the **unique minimizer** of $L \mapsto E_f[L]$ among Bravais lattices of fixed area A.

Also true for long-range potentials (Ewald summation method).
In particular, the triangular lattice is the minimizer of

$$\sum_{p\in L} e^{-|p|^{2\alpha}}, 0 < \alpha \leq 1; \qquad \sum_{p\in L\backslash\{0\}} K_0(|p|); \qquad \sum_{p\in L\backslash\{0\}} \frac{e^{-a|p|}}{|p|}, a > 0.$$

[Cohn-Kumar '06] - Conjecture

If f is completely monotone, then Λ_A is the unique minimizer of $L \mapsto E_f[L]$ among **periodic lattices** of fixed area A.

Convexity

Proposition [LB '15] (*Example of non optimality of Λ_A*)

Let f be defined by $f(r)=\dfrac{14}{r^2}-\dfrac{40}{r^3}+\dfrac{35}{r^4}$, then

- f is strictly **convex**, strictly **decreasing** and strictly **positive**;
- there exist A_1, A_2 such that Λ_A **is not a minimizer** of E_f among all Bravais lattices of fixed area $A\in(A_1,A_2)$.

Remark: $A_1\approx 2.3152307$ and $A_2\approx 3.759353$.

Lennard-Jones in 2d: results about the global minimizer

For $(a_1, a_2) \in (\mathbb{R}_+^*)^2$ and $1 < x_1 < x_2$, let

$$f_{a,x}^{LJ}(r) := \frac{a_2}{r^{x_2}} - \frac{a_1}{r^{x_1}} \quad \text{and} \quad E_{f_{a,x}^{LJ}}[L] = a_2\zeta_L(2x_2) - a_1\zeta_L(2x_1).$$

Proposition [LB-Zhang '14, LB '15] (*High/low densities*)

• If $A \leq \pi \left(\frac{a_2\Gamma(x_1)}{a_1\Gamma(x_2)}\right)^{\frac{1}{x_2-x_1}}$, then Λ_A is the unique minimizer of $E_{f_{a,x}^{LJ}}$ among Bravais lattices of fixed area A.

• Triangular lattice Λ_A is a minimizer of $E_{f_{a,x}^{LJ}}$ among Bravais lattices of fixed area A if and only if

$$A \leq \inf_{|L|=1, L\neq\Lambda_1} \left(\frac{a_2(\zeta_L(2x_2) - \zeta_{\Lambda_1}(2x_2))}{a_1(\zeta_L(2x_1) - \zeta_{\Lambda_1}(2x_1))}\right)^{\frac{1}{x_2-x_1}},$$

i.e. if A is **sufficiently large**, then Λ_A is **NOT a minimizer**.

Lennard-Jones in 2d: results about the global minimizer

Theorem [LB '15] (*Global minimizer for LJ type potentials*)

Let $h(t) := \pi^{-t}\Gamma(t)t$. If $h(x_2) \leq h(x_1)$, then the minimizer $L_{a,x}$ of $E_{f_{a,x}^{LJ}}$ **among all Bravais lattices** is unique and **triangular**.
Furthermore, its area is

$$|L_{a,x}| = \left(\frac{a_2 x_2 \zeta_{\Lambda_1}(2x_2)}{a_1 x_1 \zeta_{\Lambda_1}(2x_1)}\right)^{\frac{1}{x_2-x_1}}.$$

Remark: True for $(x_1, x_2) \in \{(1.5, 2); (1.5, 2.5); (1.5, 3); (2, 2.5); (2, 3)\}$.

Cannot be used for the classical Lennard-Jones potential $(x_1, x_2) = (3, 6)$.

Lennard-Jones in 2d: local study

By lattice reduction, $u_1 = \left(\frac{\sqrt{A}}{y}, 0\right)$ and $u_2 = \left(\frac{x\sqrt{A}}{y}, \sqrt{A}\sqrt{y},\right)$, where

$$(x,y) \in \mathcal{D} := \left\{(x,y) \in \mathbb{R}^2; 0 \leq x \leq 1/2, y > 0, x^2 + y^2 \geq 1\right\}.$$

Each (x,y,A) is associated with one Bravais lattice $L = \mathbb{Z}u_1 \oplus \mathbb{Z}u_2$.

Theorem [LB '16] - Local study of $E_{f^{LJ}_{a,x}}$

Given (a,x), there exist $A_0 < A_1 < A_2$ (explicit in terms of infinite sums) such that:

- if $0 < A < A_0$, then Λ_A is a **local minimizer**;
- if $A > A_0$, then Λ_A is a **local maximizer**;
- if $A_1 < A < A_2$, then $\sqrt{A}\mathbb{Z}^2$ is a **local minimizer**;
- if $A \notin [A_1, A_2]$, then $\sqrt{A}\mathbb{Z}^2$ is a **saddle point**.

Degeneracy as $A \to +\infty$

Theorem [LB '16] - Minimizer for large A

Let $f_{a,x}^{LJ}(r^2) = \frac{1}{r^{12}} - \frac{2}{r^6}$, then there exists A_3 such that for any $\boldsymbol{A > A_3}$, the minimizer of $E_{f_{a,x}^{LJ}}$ is a **rectangular lattice**, i.e.

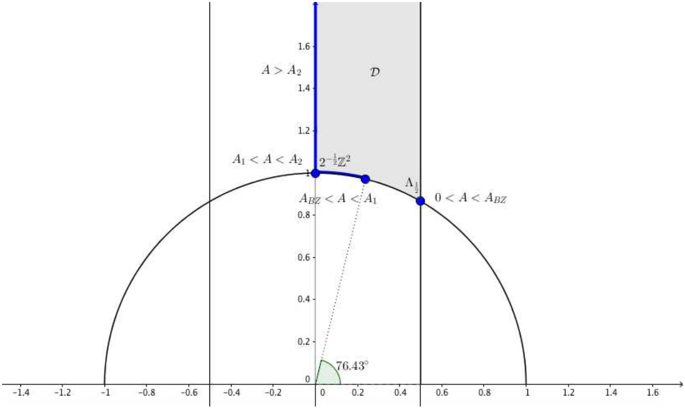
$$(x, y) = (0, y_A) \in \mathcal{D}.$$

Furthermore, $\lim_{A \to +\infty} y_A = +\infty$.

Thanks Doug!

Lennard-Jones in 2d: numerical investigation

We consider the classic case $f_{a,x}^{LJ}(r^2) = \frac{1}{r^{12}} - \frac{2}{r^6}$.



$$A_{BZ} = \inf_{\substack{|L|=1 \\ L \neq \Lambda_1}} \left(\frac{\zeta_L(12) - \zeta_{\Lambda_1}(12)}{2(\zeta_L(6) - \zeta_{\Lambda_1}(6))} \right)^{1/3} \approx 1.138, \; A_1 \approx 1.143, \; A_2 \approx 1.268.$$

Lennard-Jones in 3d: local study

By lattice reduction, $L = \mathbb{Z}u_1 \oplus \mathbb{Z}u_2 \oplus \mathbb{Z}u_3$ of volume V is such that

$$u_1 = \sqrt{C}\left(\frac{1}{\sqrt{u}}, 0, 0\right), u_2 = \sqrt{C}\left(\frac{x}{\sqrt{u}}, \frac{v}{\sqrt{u}}, 0\right), u_3 = \sqrt{C}\left(\frac{y}{\sqrt{u}}, \frac{vz}{\sqrt{u}}, \frac{u}{v\sqrt{2}}\right)$$

where $C = V^{2/3}2^{1/3}$. We have 5 parameters (u, v, x, y, z).

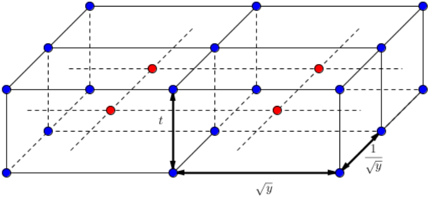
Theorem [LB '16] - Local optimality of BCC and FCC

For any f, BCC and FCC lattices are **critical points** of $L \mapsto E_f[L]$.
Given (a, x), there exist $V_0 < V_1$ (explicit) such that

- if $0 < V < V_0$, then BCC and FCC are **local minimizers** of $E_{f_{a,x}^{LJ}}$;
- if $V_0 < V < V_1$, then BCC and FCC are **saddle points** of $E_{f_{a,x}^{LJ}}$;
- if $V > V_1$, then BCC and FCC are **local maximizers** of $E_{f_{a,x}^{LJ}}$.

Proof: following Ennola's proof for $L \mapsto \zeta_L(s)$.

$L \mapsto \theta_L(\alpha)$ in 3d: minimality of BCC among BCO lattices



Body-Centred-Orthorhombic (BCO) lattice L_y, $t = 1$, $y \geq 1$.

Theorem [LB-Petrache '16] - Optimality of BCC/FCC

- There exists α_0 such that, for any $\alpha > \alpha_0$, $y = 1$ is **not** a minimizer of $y \mapsto \theta_{L_y}(\alpha)$.
- If $\alpha \in \{0.001k; k \in \mathbb{N}, 1 \leq k \leq 1000\}$, then the BCC lattice is the **unique minimizer** of $y \mapsto \theta_{L_y}(\alpha)$.

Proof: Asymptotics of the energy + Computer assistant.

Consequence for the local minimality of BCC/FCC

Using the previous result and

[Baernstein '97] - Optimality of the barycenter in the triangular lattice case

For any $\alpha > 0$, the minimizer of $z \mapsto \theta_{\Lambda_1+z}(\alpha)$ is, up to symmetry, the **barycenter** of a primitive triangle.

we get

Theorem [LB-Petrache '16] - Local minimality for some α

There exists $\alpha_0 > 0$ such that

- for any $\alpha > \alpha_0$, the BCC lattice is **not** a local minimizer;
- for any $0 < \alpha < 1/\alpha_0$, the FCC lattice is **not** a local minimizer.

If $\alpha \in \{0.001k; k \in \mathbb{N}, 1 \leq k \leq 1000\}$, then the BCC lattice is a **local minimizer**.
The same holds for the FCC lattice if $\alpha \in \{k; k \in \mathbb{N}, 1 \leq k \leq 1000\}$.

$L \mapsto \theta_L(\alpha)$ in 3d: local minimality of FCC/BCC, $V = 1$

Using Ennola's method, we get:

Theorem [LB '16] - Local minimality of BCC/FCC for α small/large

There exists $\alpha_1 < \alpha_2$ such that

- for any $0 < \alpha < \alpha_1$ (resp. $\alpha > 1/\alpha_1$), the FCC (resp. BCC) lattice is a **saddle point**;
- for any $\alpha > \alpha_2$ (resp. $0 < \alpha < 1/\alpha_2$), the FCC (resp. BCC) lattice is a **local minimizer**.

Thank you for your attention!

Simon Beck, Brean Beach (UK) , 2014

Constructed with a rake and a compass...