

Theta functions, ionic crystals energies and optimal lattices

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Talk based on joint works with

M. Faulhuber (University of Vienna) and **H. Knüpfer** (University of Heidelberg)

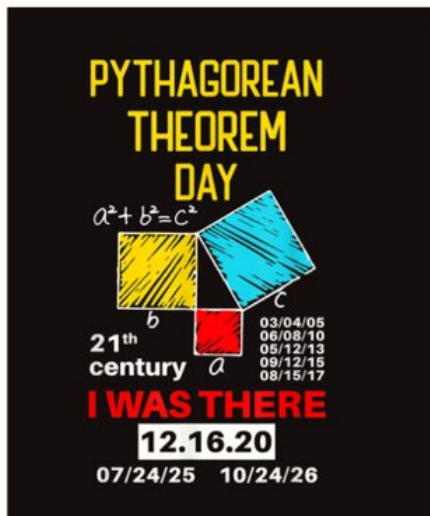
Point Distributions Webinar

December 16, 2020



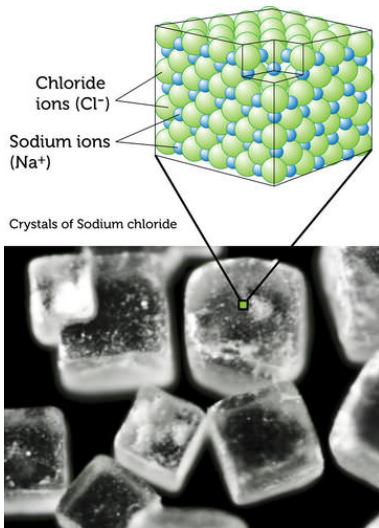
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Before starting...



Motivation from (classical) Physics

- Existence of ionic crystals
- Classical solids (not quantum)
- NaCl structure as ground state
- Pairwise interaction potentials
- Minimal energy approach
- Connection potential \leftrightarrow minimizer

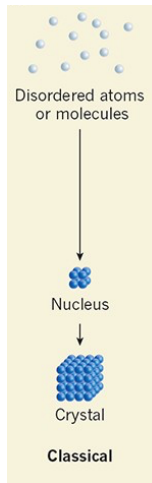


Mathematics of crystallization for pairwise potentials

- **Goal:** Determine the minimizer of the potential energy

$$E_f(X_N) := \sum_{i \neq j} f(|x_i - x_j|) \text{ (possibly in average as } N \rightarrow \infty \text{)}$$

- **Lennard-Jones potential** $f(r) = r^{-12} - r^{-6}$
 \Rightarrow triangular lattice ground state expected (open problem).
- **Few existing results** for identical particles when $d \geq 2$:
 - Triangular lattice: [Heitmann-Radin '80], (...), [Theil '06]
 - Square lattice: [B.-De Luca-Petrache '19]
- **Wigner conjecture** for Jellium (renormalized Coulomb energy)
 - $d = 2$: crystallization on a triangular lattice (GL vortices);
 - $d = 3$: crystallization on a BCC lattice.
 - ($d \in \{8, 24\}$): proved [Cohn et al. / Petrache-Serfaty '19])



Lattice optimality of multi-component systems

Few results. Only in dimensions $d \in \{1, 2\}$!

- **Short-range potentials 2d w.r.t. charges:**
 - [Radin '86] (quasi-periodicity),
 - [Friedrich-Kreutz '19/'20] (honeycomb and square lattices with alternating charges).
- **2d-torus with graph distance:** [Bouman-Draisma-Van Leeuwaarden '13] (square lattice with alternating charges).
- **1d periodic structures/alternation of charges/3 potentials:** [B.-Knüpfer-Nolte '20].
- **Optimality of lattices with alternation of charges:** [Luo-Wei '20] (3-block copolymers, 2-components BEC)
- **Minimization among lattices with prescribed charges:** [B. '20]
- **Numerical investigations:** Many, especially in 2d.

For more references, visit the

Crystallization Page

<https://sites.google.com/site/homepagelaurentbetermin/crystallization-page>

Lattices, Interaction Potentials and Charges

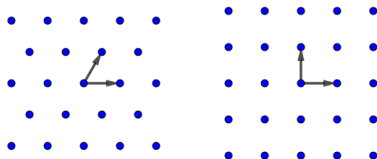
Lattices and two-dimensional examples

We call a lattice $L \subset \mathbb{R}^d$ any discrete set of the form

$$L = \bigoplus_{i=1}^d \mathbb{Z}u_i, \quad \{u_1, \dots, u_d\} \text{ basis of } \mathbb{R}^d.$$

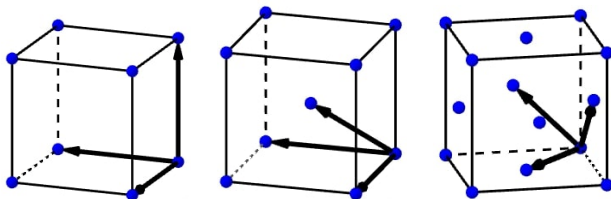
The set of all these lattices is \mathcal{L}_d , and $\mathcal{L}_d(V)$ if the volume of the unit cell is fixed to be $V > 0$. The dual of L is $L^* := \{y \in \mathbb{R}^d : y \cdot p \in \mathbb{Z}, \forall p \in L\}$.

- Square lattice \mathbb{Z}^2 ;
- Triangular lattice $A_2 = \lambda_0 \left[\mathbb{Z}(1, 0) \oplus \mathbb{Z} \left(\frac{1}{2}, \frac{\sqrt{3}}{2} \right) \right]$, λ_0 s.t. $A_2 \in \mathcal{L}_2(1)$.



Lattices in dimension $d \geq 3$

- Orthorhombic lattices: generated by an orthogonal basis (e.g. \mathbb{Z}^d);
- Body-centred-cubic (BCC) and Face-centred-cubic (FCC) lattices;
- E_8 and the Leech lattice Λ_{24} : best packings [\[Viazovska et al. '16\]](#).



Orthorhombic, BCC and FCC lattices

Remark: Orthorh^{*}=Orthorh, Triang^{*}=Triang, BCC^{*}=FCC, $E_8^* = E_8$, $\Lambda_{24}^* = \Lambda_{24}$.

Pairwise interacting potentials

For technical reasons, we sum the energies on the square of distances.

- Laplace transforms of measures, i.e.

$$f(r) = \mathcal{L}[\mu_f](r) = \int_0^\infty e^{-rt} d\mu_f(t).$$

- Particular case: f is completely monotone if, equivalently:

- For all $k \in \mathbb{N}_0$, for all $r > 0$, $(-1)^k f^{(k)}(r) \geq 0$;
- f is the Laplace transform of a positive measure μ_f ;

- Typical example: $f(r) = \frac{1}{r^s}$, where $d\mu_f(t) = \frac{t^{s-1}}{\Gamma(s)} dt$.

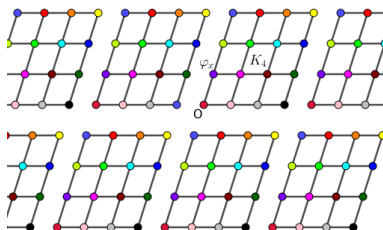
- Strategy: superposition of Gaussians.

$$\bullet \sum_{p \in L \setminus \{0\}} f(|p|^2) = \int_0^\infty \underbrace{\left(\sum_{p \in L \setminus \{0\}} e^{-|p|^2 t} \right)}_{\text{"theta function"}} d\mu_f(t) \text{ for suitable } f.$$

Periodic distribution of charges on a lattice L

- **Distribution of charge** $\varphi : L \rightarrow \mathbb{R}$, s.t. $x \in L$ has charge $\varphi_x = \varphi(x)$.
- **N -periodicity**: $\varphi \in \Lambda_N(L)$, i.e. $\forall x \in L, \forall i, \varphi(x + Nu_i) = \varphi(x)$.
- **The total charge is fixed**: $\sum_{y \in K_N} \varphi_y^2 = N^d$. We assume $\varphi_0 > 0$.
- **Periodicity cube** $K_N := \left\{ x = \sum_{i=1}^d m_i u_i \in L; 0 \leq m_i \leq N-1 \right\}$.

We note K_N^* the same for the dual lattice L^* .

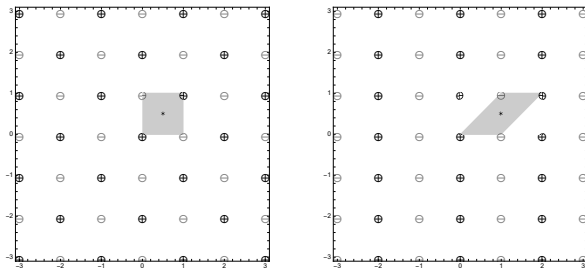


Minkowski reduced basis for center and alternating charges

We choose a reduced basis $\{u_1, \dots, u_d\}$ for all our L in the following sense:

For all $i \in \{1, \dots, d\}$, vector u_i satisfies $|u_i| \leq |u'_i|$ for any lattice vector u'_i such that $\{u_1, \dots, u_{i-1}, u'_i\}$ can be completed to another basis of L .

- \Rightarrow The Minkowski basis of an orthorhombic lattice is the orthogonal one;
- \Rightarrow In dimension 2, $|u_1| \leq |u_2|$ and $(\widehat{u_1, u_2}) \in [\frac{\pi}{3}, \frac{\pi}{2}]$;
- \Rightarrow Good definition of alternating charges distribution and center of the unit cell.



Minkowski basis of \mathbb{Z}^2 vs. another one, with alternation of charges $\varphi_{\pm} \in \{\pm 1\}$.

Theta functions associated to lattices

Translated lattice theta function

For a lattice $L \subset \mathbb{R}^d$, a point $z \in \mathbb{R}^d$ and $\alpha > 0$, we define

$$\theta_{L+z}(\alpha) := \sum_{p \in L} e^{-\pi\alpha|p+z|^2}.$$

We have $\theta_{L+z}(\alpha) = \frac{1}{\alpha^{\frac{d}{2}}} P_L \left(z, \frac{1}{4\pi\alpha} \right)$ where P_L solves the **heat equation**

$$\begin{cases} \partial_t u(z, t) = \Delta_z u & \text{for } (z, t) \in \mathbb{R}^d \times (0, \infty) \\ u(z, 0) = \sum_{p \in L} \delta_p & \text{for } z \in \mathbb{R}^d. \end{cases}$$

Poisson Summation Formula for Gaussians: $\forall \alpha > 0, L \in \mathcal{L}_d(1), z \in \mathbb{R}^d$,

$$\sum_{p \in L} e^{-\pi\alpha|p+z|^2} = \frac{1}{\alpha^{\frac{d}{2}}} \sum_{p \in L^*} \underbrace{e^{2i\pi p \cdot z}}_{\text{"charge"}} e^{-\frac{\pi|p|^2}{\alpha}}.$$

Two types of optimality for the lattice theta functions

$$L \mapsto \theta_L(\alpha) = \sum_{p \in L} e^{-\pi\alpha|p|^2}$$

$$z \mapsto \theta_{L+z}(\alpha) = \sum_{p \in L} e^{-\pi\alpha|p+z|^2}$$

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① Optimality among lattices L when $z = 0$.

- At fixed density 1 - with respect to $\alpha > 0$.
- $d = 1$: [Ventevogel '78], minimality $\forall \alpha > 0$ of \mathbb{Z} .
- $d = 2$: [Montgomery '88], minimality $\forall \alpha > 0$ of \mathbf{A}_2 .
- $d = 3$: [Sarnak-Strombergsson '06], Conjectured only, **BCC** if $\alpha \leq 1$, **FCC** if $\alpha \geq 1$.
- $d \in \{8, 24\}$: [Cohn-Kumar-Miller-Radchenko-Viazovska '19], **E₈** and the Leech Lattice **Λ_{24}** $\forall \alpha > 0$ (among periodic configurations).

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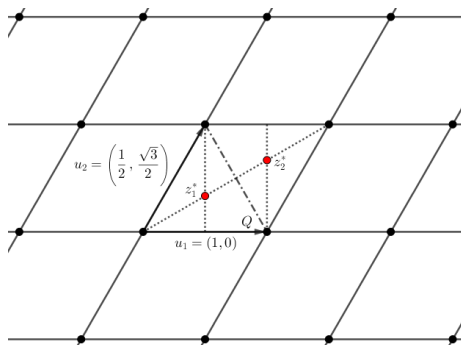
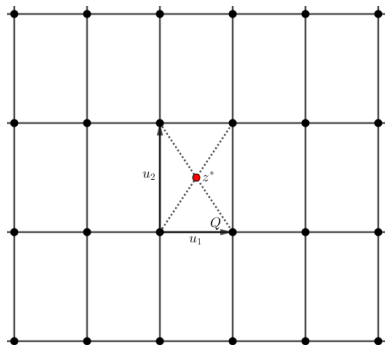
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② Optimality among vectors z when L is fixed (up to periodicity.).

- $d = 1$: $L = \mathbb{Z}$ - Minimum at the center of an interval $z_0 = 1/2$.
- Orthorhombic lattices: [B.-Petrache '17] - Center of the cell z_0 .
- Triangular lattice: [Baernstein II '97] - Barycenter of a triangle z_0 .

Optimality among vectors z when L is fixed

Minimizer of $z \mapsto \theta_{L+z}(\alpha) = \sum_{p \in L} e^{-\pi\alpha|p+z|^2} \quad \forall \alpha > 0.$



Proof of Born's Conjecture

L. Bétermin and H. Knüpfer, **On Born's conjecture about optimal distribution of charges for an infinite ionic crystal**, *Journal of Nonlinear Science* 28, 2018.

Born's problem for the electrostatic energy (1921)



Max Born (1882-1970)

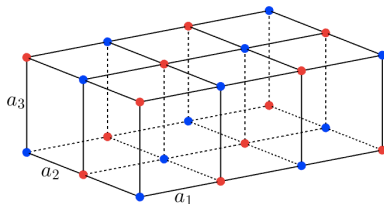
*"How to arrange positive and negative charges
on a simple cubic lattice
so that the electrostatic energy is minimal?"*

Über elektrostatische Gitterpotentiale,
Zeitschrift für Physik, 7:124-140, 1921

Born's Conjecture (1921) for Coulomb potential

Conjecture [Born '21]

The alternate distribution of charges $\varphi_{\pm} = \pm 1$ (NaCl) is the unique solution among all periodic distributions of charges $\varphi \in \bigcup_N \Lambda_N(\mathbb{Z}^3)$.



The total amount of charge is fixed and the **neutrality** has to be assumed (the Coulomb potential is not summable on \mathbb{Z}^3).

Born's proofs: 1d and local minimality in 3d for Coulomb interaction.

Energy in terms of translated theta function

If $r \mapsto f(r^2) \in \ell^1(L \setminus \{0\})$ and $\mu_f \geq 0$, then, using the Discrete Fourier Transform,

$$\begin{aligned}\mathcal{E}_{L,f}[\varphi] &= \lim_{\eta \rightarrow 0} \left(\frac{1}{2N^d} \sum_{p \in L \setminus \{0\}} \sum_{y \in K_N} \varphi_y \varphi_{p+y} f(|p|^2) e^{-\eta|p|^2} \right) \\ &= \frac{1}{2N^d} \sum_{k \in K_N^*} \xi_k E[k], \quad \xi_k := N^{-\frac{d}{2}} \widehat{\varphi * \varphi}(k) \geq 0\end{aligned}$$

where, using $f(r) = \mathcal{L}[\mu_f](r)$ and the Poisson Summation Formula,

$$E[k] = \sum_{p \in L \setminus \{0\}} e^{-\frac{2\pi i}{N} p \cdot k} f(|p|^2) = \int_0^\infty \left(\pi^{\frac{d}{2}} t^{-\frac{d}{2}} \theta_{L^* + \frac{k}{N}} \left(\frac{\pi}{t} \right) - 1 \right) d\mu_f(t).$$

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Strategy (general): Finding the minimizer z_0 of $z \mapsto \theta_{L^* + z}(\alpha)$ for all $\alpha > 0$ and such that $\exists N_0 > 0$ where $z_0 \in N_0^{-1}L^*$ gives the solution (ξ and then φ).

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Remark: Also true for non-summable $f(r^2)$ if $\sum_{y \in K_N} \varphi_y = 0$ (Ewald Summation Method).

Proof of Born's Conjecture

Our general result works for any completely monotone potential f .

- If L^* is orthorhombic, then $z_0 = \frac{1}{2} \sum_{i=1}^d u_i^*$ is the center and $N_0 \in 2\mathbb{N}$.
- If $L^* = A_2^* = A_2$, then z_0 is a barycenter of a triangle and $N_0 \in 3\mathbb{N}$.

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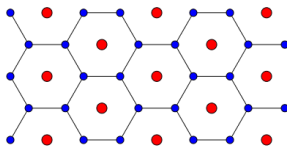
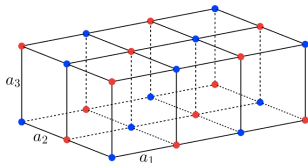
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Theorem - Solution of Born's problem [B.-Knüpfer '17]

The unique minimizer of $\varphi \mapsto \mathcal{E}_{L,f}[\varphi]$ in $\bigcup_N \Lambda_N(L)$ is:

- The alternate distribution φ_{\pm} of charges -1 and $+1$ if L is orthorhombic;
- The honeycomb-like distributions of charges $\left\{ -\frac{\sqrt{2}}{2}, +\sqrt{2} \right\}$ if $L = A_2$.



Rock-Salt (NaCl) structure and Sodium Sulfide (Na_2S) layer

Maximal Theta Function among alternated lattices

L. Bétermin and M. Faulhuber, **Maximal Theta Functions - Universal Optimality of the Hexagonal Lattice for Madelung-Like Lattice Energies**, arXiv:2004.04553, 2020.

Alternate and centred lattice theta functions

- We choose φ to be the alternate distribution $\varphi_{\pm} := \pm 1$.

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- There is no minimizer for $L \mapsto \mathcal{E}_{L,f}[\varphi_{\pm}]$ if $\mu_f \geq 0$.
- **Problem:** Finding the maximizer in $\mathcal{L}_d(1)$, for fixed $\alpha > 0$, of the alternate lattice theta function,

$$L \mapsto \theta_L^{\pm}(\alpha) := \sum_{p \in L} \varphi_{\pm}(p) e^{-\pi \alpha |p|^2}.$$

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- Equivalently, by Poisson Summation Formula, we want to maximize in $\mathcal{L}_d(1)$, for fixed $\alpha > 0$, the centred lattice theta function

$$L \mapsto \theta_L^c(\alpha) = \sum_{p \in L} e^{-\pi \alpha |p + c_L|^2}, \quad c_L := \frac{1}{2} \sum_{i=1}^d u_i.$$

A new universal optimality result

$$\theta_L^\pm(\alpha) := \sum_{p \in L} \varphi_\pm(p) e^{-\pi\alpha|p|^2}, \quad \theta_L^c(\alpha) = \sum_{p \in L} e^{-\pi\alpha|p+c_L|^2}.$$

Theorem - Maximality of the triangular lattice [B.-Faulhuber '20]

For any $\alpha > 0$, A_2 is the unique maximizer of $\theta_L^\pm(\alpha)$ and $\theta_L^c(\alpha)$ in $\mathcal{L}_2(1)$.

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- It is a new type of universal optimality among lattices, i.e. true for any completely monotone potential (see [Cohn-Kumar '07]).

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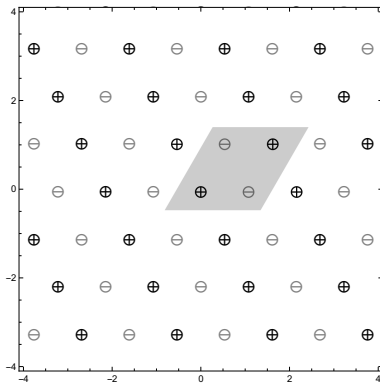
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- Conjectured to be true in dimensions $d \in \{8, 24\}$ for E_8 and Λ_{24} .

The maximal structure (A_2, φ_{\pm}) amongst (L, φ_{\pm})

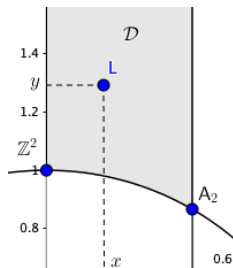


Maximality of A_2 - Idea of the proof

- 1 We parametrize L by a point (x, y) in the half-elliptic domain

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

- 2 We show that $x \mapsto \theta_L^\pm(\alpha)$ is increasing on $[0, 1/2]$;
- 3 Fixing $x = 1/2$, we show that $y \mapsto \theta_L^\pm(\alpha)$ is decreasing on $\left[\frac{\sqrt{3}}{2}, \infty\right)$.
- 4 Use of estimates comparable to the one of [\[Montgomery '88\]](#).



Optimality of the rock-salt structure among lattices and charges

L. Bétermin, M. Faulhuber and H. Knüpfer, **On the optimality of the rock-salt structure among lattices with charge distributions**, accepted in *Mathematical Models and Methods in Applied Sciences*, arXiv:2004.04553, 2020.

A new energy E_{f_1, f_2} with repulsion at 0

- We remark that, if $\mu_f \geq 0$, then $\min_{L, \varphi} \mathcal{E}_{L, f}[\varphi] = -\infty$.
- We add a completely monotone repulsive part f_1 , defining a new f :

$$f(|x - y|^2) = \underbrace{f_1(|x - y|^2)}_{\text{Repulsion at the origin}} + \underbrace{\varphi_x \varphi_y f_2(|x - y|^2)}_{\text{Tail - Charges interaction}}.$$

- Chosen potentials: $f_1(r) = r^{-p}$, $f_2(r) = r^{-q}$, such that $p > q > d/2$.
- New total energy per point:

$$E_{f_1, f_2}[L, \varphi] := \underbrace{\sum_{p \in L \setminus \{0\}} f_1(|p|^2)}_{E_{f_1}[L]} + \underbrace{\frac{1}{N_d} \sum_{p \in L \setminus \{0\}} \sum_{y \in K_N} \varphi_y \varphi_{p+y} f_2(|p|^2)}_{2\mathcal{E}_{L, f_2}[\varphi]}.$$

- **Problem:** Find the minimizer of E_{f_1, f_2} in $\mathcal{L}_d \times \bigcup_N \Lambda_N(\mathcal{L}_d)$.
Is it a rock-salt structure $(\lambda \mathbb{Z}^d, \pm 1)$? (for some $\lambda > 0$)

The two competitive energies

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- If $\mu_{f_1} \geq 0$, E_{f_1} has a **minimizer** in $\mathcal{L}_d(V)$ for fixed $V > 0$ (not in \mathcal{L}_d):
 - $d = 2$: A_2 for all $V > 0$.
 - $d = 3$: BCC or FCC (conjecture), probably changing with V .
 - $d \in \{8, 24\}$: E_8 and the Leech lattice Λ_{24} .
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- If $\mu_{f_2} \geq 0$, $(L, \varphi) \mapsto \mathcal{E}_{L, f_2}[\varphi]$ does not have any minimizer, only **maximizers**.
 - If L is fixed, possibility to find the optimal φ (Born's problem).
 - If $\varphi = 1$, then $\mathcal{E}_{L, f_2}[\varphi] = E_{f_2}[L]$ (see above), but not optimal.
 - Among all lattices of $\mathcal{L}_2(V)$ with φ_{\pm} , A_2 is the unique maximizer.
 - **Among orthorhombic lattices with φ_{\pm}** , $V^{\frac{1}{d}}\mathbb{Z}^d$ is the unique maximizer in $\mathcal{L}_d(V)$ [Faulhuber-Steinerberger '17].

Orthorhombic lattices with φ_{\pm} at fixed density

$$E_{f_1, f_2}^{\pm}[L] := E_{f_1, f_2}[L, \varphi_{\pm}] = \sum_{p \in L \setminus \{0\}} f_1(|p|^2) + \sum_{p \in L \setminus \{0\}} \varphi_{\pm}(p) f_2(|p|^2)$$

Born: Restricted to orthorhombic lattices, $E_{f_1, f_2}^{\pm}[L] \leq E_{f_1, f_2}[L, \varphi] \quad \forall N, \forall \varphi \in \Lambda_N(L)$.

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Theorem - Optimality of the rock-salt structure [B.-Faulhuber-Knüpfer '20]

Let $f_1(r) = r^{-p}$ and $f_2(r) = r^{-q}$, $p > q > d/2$.

- $\forall d \geq 1$, $V^{\frac{1}{d}}\mathbb{Z}^d$ is a critical point of E_{f_1, f_2}^{\pm} in $\mathcal{L}_d(V)$.
- $\forall d \geq 1$, there exists V_0 such that for all $V \in (0, V_0)$, $V^{\frac{1}{d}}\mathbb{Z}^d$ is the **unique minimizer** of E_{f_1, f_2}^{\pm} among orthorhombic lattices with fixed volume $V > 0$.
- $\forall d \geq 1$, there exists V_1 such that for all $V \in (V_1, \infty)$, $V^{\frac{1}{d}}\mathbb{Z}^d$ is **not a minimizer** of E_{f_1, f_2}^{\pm} among orthorhombic lattices with fixed volume $V > 0$.

In particular, restricted to orthorhombic lattices, the rock-salt structure is globally optimal among charges and lattices at high density.

Global optimality of the rock-salt structure

We define the alternate Epstein zeta function by

$$\zeta_L^\pm(s) := \sum_{p \in L \setminus \{0\}} \frac{\varphi_\pm(p)}{|p|^s}, \quad s > d.$$

We already know that $\zeta_L^\pm(s) < \zeta_{A_2}^\pm(s) < 0$ for all $L \in \mathcal{L}_2(1)$ by [\[B.-Faulhuber '20\]](#). This is expected to be true for all $d \geq 1$.

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Theorem - Minimal energy among dilated [B.-Faulhuber-Knüpfer '20]

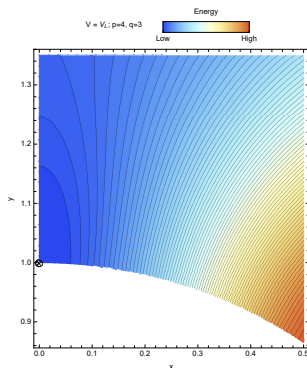
Let $d \geq 1$, $f_1(r) = r^{-p}$ and $f_2(r) = r^{-q}$, $p > q > d/2$. For $L \in \mathcal{L}_d(1)$, if $\zeta_L^\pm(2q) < 0$, then

$$\mathcal{E}_L^\pm := \min_{V > 0} E_{f_1, f_2}^\pm[V^{\frac{1}{d}}L] = \frac{(q-p)(-q\zeta_L^\pm(2q))^{\frac{p}{p-q}}}{qp(p\zeta_L(2p))^{\frac{q}{p-q}}} < 0.$$

Problem: What is the minimizer of $L \mapsto \mathcal{E}_L^\pm$ in $\mathcal{L}_d(1)$? (shape of the global min)

Numerics in dimension 2 for $f_1(r^2) = r^{-8}$, $f_2(r^2) = r^{-6}$.

We plot $L \mapsto \mathcal{E}_L^\pm$ in the fundamental domain \mathcal{D} of 2d lattices.



Numerically, the global minimum of E_{f_1, f_2}^\pm in \mathcal{L}_2 is a square lattice.

The same is expected in dimensions $d \in \{3, 8, 24\}$ for \mathbb{Z}^3 , \mathbb{Z}^8 and \mathbb{Z}^{24} . We have compared different values of \mathcal{E}_L^\pm .

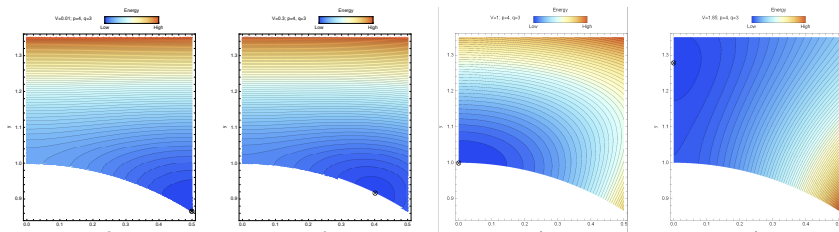
Other numerical observations

- We have compared $\mathcal{E}_{\mathbb{Z}^d}^{\pm}$ with other optimal charge distributions, without finding any better candidate for being a minimizer of $(L, \varphi) \mapsto E_{f_1, f_2}[L, \varphi]$.

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- As V increases, $\operatorname{argmin}_{L \in \mathcal{L}_2(V)} E_{f_1, f_2}^\pm$ exhibits a phase transition of type:

Triangular - Rhombic - Square - Rectangular.

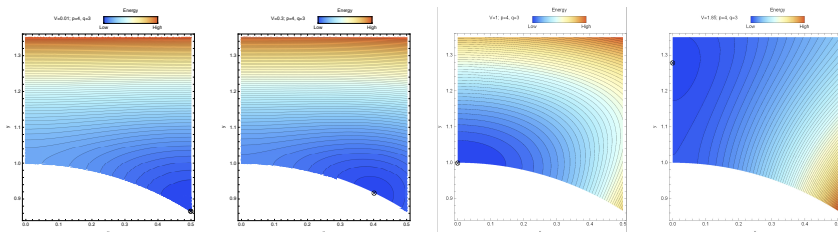


Already observed for Lennard-Jones/Morse potentials, 3-block copolymers, two-components Bose-Einstein-Condensates.

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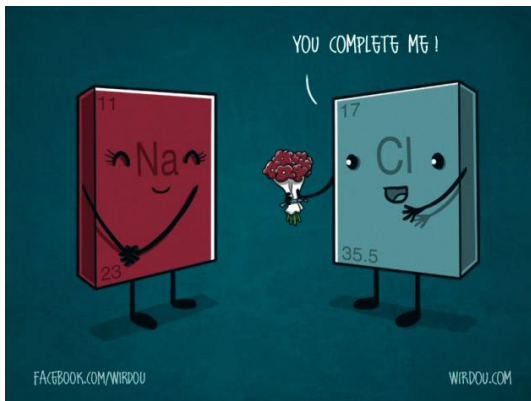


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- If $p - q$ is small enough, the minimizer of E_{f_1, f_2}^\pm in \mathcal{L}_2 is not a square lattice.

Conclusion

- New general strategy to optimize energies among charges on a lattice.
 - Key point: minimization of $z \mapsto \theta_{L^*+z}(\alpha)$ for all $\alpha > 0$.
- New universal optimality property for the triangular lattice.
 - Key point: minimization of $L \mapsto \theta_L^\pm(\alpha)$ for all $\alpha > 0$.
- New type of minimization problem for \mathbb{Z}^d - NaCl ground state.
 - Similar to minimizing $L \mapsto \theta_L(\beta) + \theta_L^\pm(\alpha)$, $\beta > \alpha$.



Thank you for your attention!