A gradient flow approach to quantization of measures

Mikaela Iacobelli

University of Cambridge

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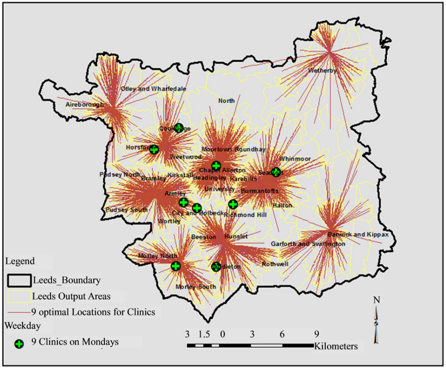
Outline of the talk

1. Introduction to the quantization problem
2. Variational approach and dynamics
3. The 1D case
4. The 2D case
5. Conclusions and future directions

An example of quantization problem

Question: what is the "optimal" way to locate N clinics in a region in order to meet the demand of the population?



- Notion of "optimality"
- Locations $\rightsquigarrow x^i$
- Masses $\rightsquigarrow m_i$

A bit of history

Quantizations occour in various scientific fields, for instance:

- Information theory (signal compression)
- Numerical integration
- Crystallography
- Mathematical models in economics (optimal location of service centers)
- ...

Setup of the problem

Let ρ be a probability density on a domain $\Omega \subset \mathbb{R}^d$.

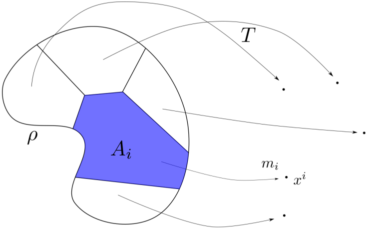
Quantization problem: fixed $N \in \mathbb{N}$, find the best approximation of ρ by an atomic measure $\sum_i m_i \delta_{x^i}$ supported on at most N points in Ω.

Wasserstein distances

Step 1. Fix $r \geq 1$ and consider

$$W_r\Big(\rho, \sum_i m_i \delta_{x^i}\Big)^r := \inf \int_\Omega |y - T(y)|^r \rho(y)\, dy$$

where $T : \Omega \to \Omega$ varies among all maps that transport ρ onto $\sum_i m_i \delta_{x^i}$.



$$A_i = T^{-1}(x^i)$$

$$\int_{A_i} \rho = m_i$$

Voronoi diagrams

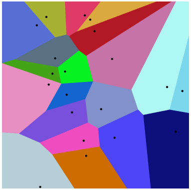
Step 2. Fix N points $x^1, \dots, x^N \in \Omega$, and minimize

$$\inf \left\{ W_r\Big(\rho, \sum_i m_i \delta_{x^i}\Big)^r \;:\; m_1, \dots, m_N \geq 0,\ \sum_i m_i = 1 \right\}.$$

Best choice via the *Voronoi tessellation* of $x^1, \dots, x^N$

$$m_i := \int_{V(x^i)} \rho(y)dy$$

$$V(x^i) := \{ y \in \Omega : |y - x^i| \leq |y - x^j|, \text{for all } j \neq i \}$$



With the optimal choice

$$m_i = \int_{V(x^i)} \rho(y) dy$$

it holds

$$W_r\left(\rho, \sum_i m_i \delta_{x^i}\right)^r = F_{N,r}(x^1, \dots, x^N),$$

where

$$F_{N,r}(x^1, \dots, x^N) := \int_\Omega \min_{1\le i\le N} |x^i - y|^r \, \rho(y)\, dy$$

Step 3. Minimize $F_{N,r}$ to find the optimal configuration for $x^1, \dots, x^N$

Theorem (Bucklew - Wise, 1982; Graf - Luschgy, 2000)

Let $r \geq 1$ and ρ be a probability density on $\mathbb{R}^d$ satisfying

$$\int_{\mathbb{R}^d} |x|^{r+\delta} \rho(x)\, dx < \infty$$

for some $\delta > 0$. Let $x^1, \ldots, x^N$ minimize $F_{N,r} : (\mathbb{R}^d)^N \to \mathbb{R}^+$. Then

$$\frac{1}{N}\sum_{i=1}^{N} \delta_{x^i} \rightharpoonup \frac{\rho^{d/(d+r)}(x)}{\int_\Omega \rho^{d/(d+r)}(y)dy}\, dx \qquad \text{as } N \to \infty.$$

A dynamical approach

Given N points $x_0^1, \ldots, x_0^N \in \mathbb{R}^d$, consider their evolution under the gradient flow generated by $F_{N,r}$

$$\begin{cases} (\dot{x}^1(t), \ldots, \dot{x}^N(t)) = -\nabla F_{N,r}(x^1(t), \ldots, x^N(t)) \\ (x^1(0), \ldots, x^N(0)) = (x_0^1, \ldots, x_0^N) \end{cases}$$

As $t \to \infty$, $(x^1(t), \ldots, x^N(t))$ should converge to a minimizer $(\bar{x}^1, \ldots, \bar{x}^N)$ of $F_{N,r}$.

Therefore

$$\frac{1}{N} \sum_{i=1}^{N} \delta_{\bar{x}^i} \rightharpoonup \frac{\rho^{d/d+r}(x)}{\int_\Omega \rho^{d/d+r}(y)dy}\, dx \qquad \text{as } N \to \infty.$$

From the discrete to the continuous functional

Bad news: $F_{N,r}$ has many local minima.

Goal: Understand both limits $t \to \infty$ and $N \to \infty$.

Program:

• Isometrically embed every $\mathbb{R}^N$ in $L^2(\mathbb{R}^d; \mathbb{R}^d)$.

• Consider a set of reference points $(\hat{x}^1, \ldots, \hat{x}^N)$ and parameterize a general family of N points x^i as the image of $\hat{x}^i$ via a map $X : \mathbb{R}^d \to \mathbb{R}^d$, that is

$$x^i = X(\hat{x}^i).$$

From the discrete to the continuous functional

• Rewrite the functional $F_{N,r}(x^1, \ldots, x^N)$ in terms of the map X:

$$F_{N,r}(x^1, \ldots, x^N) = F_{N,r}\big(X(\hat{x}^1), \ldots, X(\hat{x}^N)\big)$$

• Show that (a suitable renormalization of) $F_{N,r}$ converges to a nontrivial functional $\mathcal{F}[X]$.

Question: Is the evolution of $x^i(t)$ for N large to be well-approximated by the L^2-gradient flow of $\mathcal{F}$?

Program

• The 1D problem shows already several features of our GF approach. We shall need to understand the dynamics of degenerate parabolic equations and relate them to the discrete dynamics.

• In 2D, the functional $\mathcal{F}$ involves the determinant of ∇X in a singular way. We shall consider perturbations of the regular triangular lattice (which is optimal when $N \to \infty$) and understand the continuous GF in this regime.

THE 1D CASE

Computing $F_{N,r}$ in the 1D Case

$\Omega = [0,1]$, $0 \leq x^1 \leq \ldots \leq x^N \leq 1$.

$$V(x^i) = [x^{i-1/2}, x^{i+1/2}], \qquad x^{i+1/2} := \frac{x^i + x^{i+1}}{2}.$$

Therefore

$$F_{N,r}(x^1, \ldots, x^N) \approx \sum_{i=1}^{N} \int_{x^{i-1/2}}^{x^{i+1/2}} |y - x^i|^r \rho(y) dy.$$

From $F_{N,r}$ to $\mathcal{F}[X]$

Assume

$$x^i = X\left(\frac{i-1/2}{N}\right), \qquad i = 1, \dots, N$$

with $X : [0,1] \to [0,1]$ smooth non-decreasing.

By a Taylor expansion

$$N^r F_{N,r}(x_1, \dots, x_N) \underset{N\to\infty}{\longrightarrow} C_r \int_0^1 \rho(X(\theta))|\partial_\theta X(\theta)|^{r+1} d\theta := \mathcal{F}[X].$$

L^2-GF for $\mathcal{F}[X]$

The L^2-GF for $\mathcal{F}[X]$ is the following parabolic equation

$$\partial_t X(t,\theta) = C_r\Big((r+1)\partial_\theta\big(\rho(X(t,\theta))|\partial_\theta X(t,\theta)|^{r-1}\partial_\theta X(t,\theta)\big) \\ - \rho'(X(t,\theta))|\partial_\theta X(t,\theta)|^{r+1}\Big)$$

with Dirichlet boundary condition

$$X(t,0) = 0, \qquad X(t,1) = 1.$$

Remark: if $\rho \equiv 1$, we get the *p*-Laplacian equation

$$\partial_t X = C_r\,(r+1)\,\partial_\theta\left(|\partial_\theta X|^{r-1}\partial_\theta X\right)$$

with $p - 1 = r$.

Degeneracy issue: is the condition $\partial_\theta X > 0$ preserved by the flow?

Eulerian Formulation of the Quantization Gradient Flow

Define $f \equiv f(t,x)$ by

$$f(t,x)\,dx = X(t,\cdot)_{\#}d\theta \Leftrightarrow f(t,X(t,\theta)) = \frac{1}{\partial_\theta X(t,\theta)}$$

Then

$$\begin{cases} \partial_t f = -r\,C_r\,\partial_x\left(f\partial_x\left(\frac{\rho}{f^{r+1}}\right)\right), & x \in \mathbb{R} \\ f(t,x+1) = f(t,x) \end{cases}$$

Remark: if $\rho \equiv 1$ the Eulerian equation becomes

$$\partial_t f = -C_r\,(r+1)\,\partial_x^2\left(f^{-r}\right)$$

which is an equation of very fast diffusion type.

Comparison Principle for the Eulerian Equation

Set $m := \rho^{1/(1+r)}$ and $u := f/m$; the Eulerian quantization gradient flow equation becomes

$$\partial_t u = -\frac{(r+1)\,C_r}{m}\partial_x\left(m\,\partial_x\left(\frac{1}{u^r}\right)\right).$$

Note: constants are solutions!

Lemma

If $u > 0$ is a solution and $c > 0$, then

$$\frac{d}{dt}\int_0^1 (u-c)_+(t,x)\, m(x)\, dx \leq 0,$$

$$\frac{d}{dt}\int_0^1 (u-c)_-(t,x)\, m(x)\, dx \leq 0.$$

By the lemma,

$$c_0 \leq u(0,x) \leq C_0 \qquad \Rightarrow \qquad c_0 \leq u(t,x) \leq C_0 \qquad \forall\, t \geq 0.$$

Therefore, if $0 < \lambda \leq \rho \leq 1/\lambda$ and $0 < a_0 \leq \partial_\theta X(0) \leq A_0$,

$$0 < b_0 \leq \partial_\theta X(t) \leq B_0 \qquad \forall\, t \geq 0.$$

Main result

Theorem (Caglioti - Golse - I., M3AS 2015)

Assume $r = 2$, $\|\rho - 1\|_{C^2} \leq \bar{\varepsilon}$, and let $\left(x^1(t), \ldots, x^N(t)\right)$ be the gradient flow of $F_{N,2}$ starting from $\left(x_0^1, \ldots, x_0^N\right)$. Under some suitable assumptions on ρ and the initial data, the continuous and discrete GF remain quantitatively close for all times:

$$\frac{1}{N}\sum_{i=1}^{N}\left|x_i(N^3 t) - X(t, \tfrac{i-1/2}{N})\right|^2 \leq \frac{C'}{N^4}, \quad t \geq 0.$$

In particular

$$W_1\left(\frac{1}{N}\sum_i \delta_{x^i(t)}, \frac{\rho^{1/3}\, d\theta}{\int \rho^{1/3}}\right) \leq \frac{2C'}{N} \qquad \forall\, t \geq \frac{N^3 \log N}{c'}.$$

Strategy of the proof: the case $\rho \equiv 1$

When $\rho \equiv 1$, the L^2-GF of $\mathcal{F}$ depends on $\partial_\theta X$ and $\partial_{\theta\theta} X$, but not on X itself.

By a discrete maximum principle for the incremental quotients, we show that the discrete monotonicity estimate

$$x^{i+1}(t) - x^i(t) \approx \frac{1}{N} \qquad \forall\, i$$

is preserved in time.

This allows us to prove that the discrete and the continuous gradient flows remain uniformly close in L^2 for *all* times by a Gronwall argument.

Strategy of the proof: the case $\rho \not\equiv 1$

The case $\rho \not\equiv 1$ is much more delicate: in this case there is no clear way to show the validity of the discrete monotonicity estimate, and the approach for the case $\rho \equiv 1$ fails.

Strategy: Bootstrap argument via finite-time stability in L^∞ and L^2 exponential convergence.

Step 1: Show that

$$\hat{X}(t) := \left(X\left(t, \frac{1/2}{N}\right), \dots, X\left(t, \frac{N-1/2}{N}\right) \right)$$

solves the discrete gradient flow equation up to an error of order $1/N^2$.

Step 2: The discrete and continuous gradient flow stay $1/N^2$-close on a finite interval of time:

$$\left|x^i(N^3t) - X(t, \tfrac{i-1/2}{N})\right| = O\left(\frac{1+T}{N^2}\right) \qquad \forall\, i,\ \forall\, t \in [0,T].$$

Step 3: By Step 2, transfer the discrete monotonicity estimate from $X(t, \frac{i}{N})$ to $x^i(N^3t)$ on $[0, T]$.

Step 4: Perform a Gronwall argument in L^2 to deduce that

$$t \mapsto \frac{1}{N}\sum_{i=1}^{N}\left|x^i(N^3t) - X(t, \tfrac{i-1/2}{N})\right|^2$$

decrease exponentially in time on $[0, T]$.

Step 5: Choosing T carefully, for N large enough, Step 4 allows us to iterate the argument above on all time intervals $[T, 2T]$, $[2T, 3T]$, $[3T, 4T]$, etc. $\square$

Note: The assumptions $\|\rho - 1\|_{C^2} \ll 1$ is necessary to ensure the convexity of $\mathcal{F}$ and perform the L^2-Gronwall argument.

THE 2D CASE

What happens in two dimensions?

Challenges:

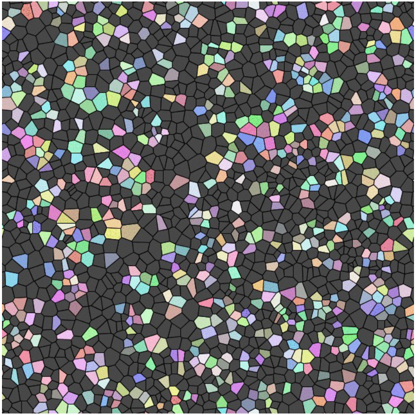
- Difficult to find a nice expression for the functional $F_{N,r}$
- In general, $\mathcal{F}[X]$ depends in a singular way on $\det(\nabla X)$

$\rightsquigarrow \mathcal{F}[X]$ is highly nonconvex

Bad news: no general theory for gradient flows of "highly nonconvex" functionals

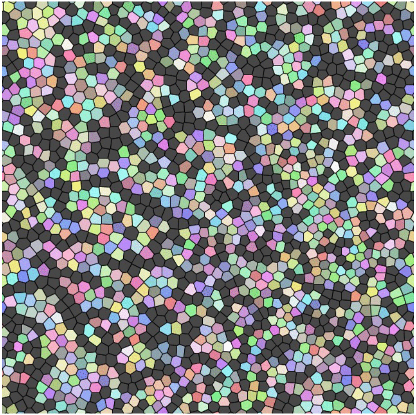
Good news: for $N \to \infty$, Voronoi cells associated to optimal configurations are given by the hexagonal lattice (Fejes Tóth, 1953).

A numerical simulation



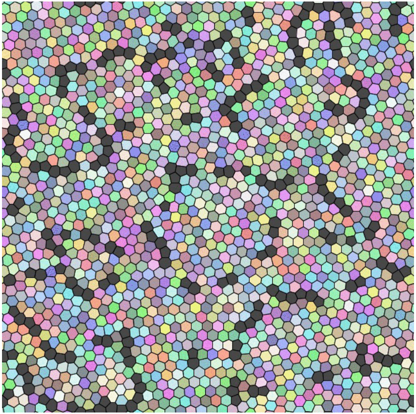
720 points at time 0

A numerical simulation



720 points after 19 iterations

A numerical simulation



720 points after 157 iterations

Weakly Deformed Hexagonal Lattices

Strategy: look at configurations close to the minimal energy state and understand the limit $N \to \infty$.

Consider the triangular regular lattice

$$\mathscr{L} := \mathbb{Z}e_1 \oplus \mathbb{Z}e_2\,, \quad e_1 := (1,0)\,, \quad e_2 := (\tfrac{1}{2}; \tfrac{\sqrt{3}}{2}).$$

We note that the Voronoi cells for the points in $\mathscr{L}$ are regular hexagons.

To increase the number of points, we consider its dilations

$$\epsilon\mathscr{L}, \qquad \epsilon > 0.$$

Let

$$\Pi := \{ae_1 + be_2 \,:\, |a| \le 1/2, \, |b| \le 1/2\}$$

be a fundamental domain.

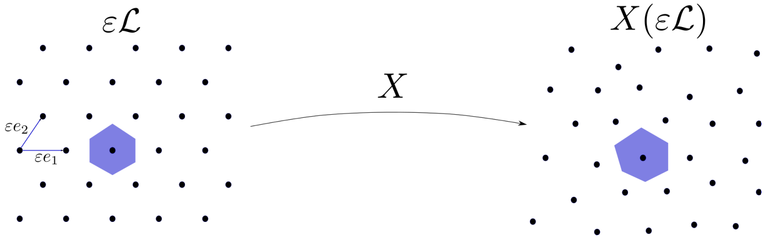
Remark: the periodicity of Π and $\epsilon\mathscr{L}$ are compatible for any $\epsilon = 1/n$.

We look at Π-periodic deformations of these points:

$$X(\epsilon\mathscr{L})\,,\quad \epsilon = 1/n\,,\ n \in \mathbb{N},$$

where $X \in \mathrm{Diff}(\mathbb{R}^2)$ satisfies

$$X \quad \text{is } \Pi\text{-periodic}, \qquad \|X - \mathrm{id}\|_{L^\infty} \ll 1\,.$$



Quantization of $\rho \equiv 1$ with $d = r = 2$ for $N \approx n^2 \to \infty$

Goal: compute the energy $\mathcal{F}$ of X as $\epsilon = 1/n \to 0$, and prove that, under the gradient flow of $\mathcal{F}$, the limit of the near-hexagonal Voronoi tesselation of $X(\mathscr{L}/n)$ converges to the regular hexagonal tesselation.

Let $(x_1^n, \ldots, x_N^n) = X(\mathscr{L}/n) \cap \Pi$ and consider the functional $F_{N,2}(x_1^n, \ldots, x_N^n)$.

We show that

$$F_{N,2}(x_1^n, \ldots, x_N^n) \approx \frac{1}{n^4} \mathcal{F}[X],$$

for some functional $\mathcal{F}[X]$.

The Formula for $\mathcal{F}$

For each $M \in M_2(\mathbb{R})$, define

$$F(M) = \frac{1}{3} \sum_{\omega \in \{e_1, e_2, e_{12}\}} |M \cdot \omega|^4 \Phi(\omega, M) \left(3 + \Phi(\omega, M)^2\right)$$

where

$$\Phi(\omega, M) := \sqrt{\frac{|MR\omega|^2 |MR^T\omega|^2}{\frac{3}{4}\det(M)} - 1}$$

for each $\omega \in \mathbb{S}^2$, with

$$R := \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix},$$

$$e_1 = (1, 0), \quad e_2 = Re_1, \quad e_{12} = R^{-1} e_1 = e_1 - e_2.$$

Then

$$\mathcal{F}[X] = \int_{\Pi} F(\nabla X)\, dx,$$

hence the gradient flow is given by

$$\partial_t X(t,x) = \operatorname{div}\big(\nabla F(\nabla X(t,x))\big)$$

with initial and boundary conditions

$$\begin{cases} X(t) & \text{is } \Pi\text{-periodic,} \\ X(0) = X^{in}. \end{cases}$$

A more manageable formula

$$
\begin{aligned}
F(M) := {} & \frac{1}{16\sqrt{3}} \det(M) \mathrm{tr}[M^T M(2S - I)] \\
& + \frac{1}{64\sqrt{3}} \frac{[\mathrm{tr}(M^T M)]^2 [\mathrm{tr}(M^T MS)]}{\det(M)} \\
& - \frac{1}{192\sqrt{3}} \frac{[\mathrm{tr}(M^T M)]^3 + 4[\mathrm{tr}(M^T MS)]^3}{\det(M)},
\end{aligned}
$$

where

$$
S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
$$

Remark: F depends on $\det(M)$ and blows up as $\det(M) \to 0$.

The Small Deformation Regime

Write $X = \mathrm{id} + \tau Y$. Then

$$3\sqrt{3}\, F(\mathrm{Id} + \tau \nabla Y) = 10 + 20\, \tau\, \mathrm{div}(Y) + \tau^2 (14\, \det(\nabla Y) + 10\, \mathrm{div}(Y)^2 + 3\, |\nabla Y|^2) + O(\tau^3).$$

Crucial facts:

(1)

$$\int_\Pi \mathrm{div}(Y) = \int_\Pi \det(\nabla Y) = 0.$$

(2) For $A \in M_2(\mathbb{R})$, define

$$F_0(A) = F(A) - \frac{20}{3\sqrt{3}} \mathrm{Tr}(A - \mathrm{Id}) - \frac{14}{3\sqrt{3}} \det(A - \mathrm{Id}).$$

Then F_0 is uniformly convex if $|A - \mathrm{Id}| \leq \eta \ll 1$.

Thus,

$$\mathcal{F}[X] = \int_{\Pi} F_0(\nabla X)\, dx,$$

and $\mathcal{F}$ is uniformly convex on functions that are sufficiently close to the identity in C^1.

Therefore, if

$$\|\nabla X(t) - \mathrm{Id}\|_\infty \le \eta \qquad \forall\, t \ge 0, \tag{1}$$

$X(t) \to \mathrm{id}$ exponentially fast in L^2 by the theory of gradient flows for convex functionals.

So, the main issue is to obtain (1). For this, we combine results from parabolic regularity theory for systems.

Main result: The hexagonal lattice is asymptotically optimal and dynamically stable

Theorem (E. Caglioti, F. Golse, M. I., 2016)

Assume that $X^{in} \in Diff(\mathbb{R}^2)$ satisfies

$$X^{in} \text{ is } \Pi\text{-periodic and } \int_\Pi X^{in}(x)dx = 0,$$

and

$$\|X^{in} - \mathrm{id}\|_{W^{s,p}(\Pi)} \leq \eta/2 \ll 1$$

for some $p > 2$ and $s > 1 + 2/p$.
Then the Cauchy problem for the L^2-gradient flow of $\mathcal{F}$ has a unique solution X with initial data X^{in}, and

$$\|X(t) - \mathrm{id}\|_{L^2(\Pi)} \leq \|X^{in} - \mathrm{id}\|_{L^2(\Pi)} e^{-\mu t}, \quad \mu > 0.$$

Strategy of the proof

Step 1: Construct an auxiliary convex functional $\mathcal{G}$ that coincides with $\mathcal{F}$ on maps that are C^1-close to the identity.

Step 2: Denote by $Y(t)$ the GF of $\mathcal{G}$. Then $Y(t)$ converges exponentially fast in L^2 to id.

Goal: Prove that the GF of $\mathcal{G}$ satisfies

$$\|\nabla Y(t) - \mathrm{Id}\|_\infty \leq \eta \qquad \forall\, t \geq 0$$

with η small enough. This will imply that $\mathcal{G} = \mathcal{F}$ nearby $Y(t)$ for all $t \geq 0$, hence $Y(t)$ is also the GF for $\mathcal{F}$.

Step 3: By the Sobolev regularity on the initial datum and propagation of regularity for short times, we get

$$\|\nabla Y(t) - \mathrm{Id}\|_\infty \leq \eta \qquad \forall\, t \in [0, t_0]$$

for some $t_0 > 0$ small.

Step 4: Combine the L^2 exponential convergence of $Y(t)$ to id with an ϵ-regularity theorems for parabolic systems to show that

$$\|\nabla Y(t) - \mathrm{Id}\|_\infty \leq \eta \qquad \forall\, t \geq t_0.$$

$\square$

Conclusions

• Our result in 1D shows that the discrete evolution is well approximated by the continuous GF, uniformly in time. One needs to understand the dynamics of a parabolic (possibly degenerate) equation, and relate it to the discrete dynamics. The lack of convexity of the discrete functional is a source of challenges.

• The 2D result gives a new mathematical justification of the asymptotic optimality of the hexagonal lattice among its nearby configurations

Future directions

• Prove the convergence of the discrete GF to the continuous one, at least in the perturbative regime

• Understand if there is an Eulerian formulation, and what happens when $\rho \not\equiv 1$

• Go out of the perturbative regime

• Understand minimal configurations in higher dimensions and develop analogous programs

Thanks for your attention