Questions of Crystallization in Systems with Coulomb and Riesz Interactions

Sylvia SERFATY

Université P. et M. Curie Paris 6, Laboratoire Jacques-Louis Lions

AMS-EMS-SPM joint meeting, June 11, 2015

collaborations:
Etienne Sandier
Nicolas Rougerie
Simona Rota Nodari
Mircea Petrache
Thomas Leblé

The question

Several problems coming from physics and approximation theory lead to minimizing, with n large

- $$H_n(x_1, \dots, x_n) = \sum_{i \neq j} w(x_i - x_j) + n \sum_{i=1}^{n} V(x_i) \qquad x_i \in \mathbb{R}^d, d \geq 1$$

- interaction potential

$$w(x) = \frac{1}{|x|^s} \qquad \max(0, d-2) \leq s < d \quad \text{(Riesz)}$$

$$\text{or} \quad w(x) = -\log|x| \quad \text{with } d = 1, 2 \quad \text{(log gas)}$$

- includes Coulomb: $s = d - 2$ for $d \geq 3$, $w(x) = -\log|x|$ for $d = 2$.

- V confining potential, sufficiently smooth and growing at infinity

The question

Several problems coming from physics and approximation theory lead to minimizing, with n large

- $$H_n(x_1, \ldots, x_n) = \sum_{i \neq j} w(x_i - x_j) + n \sum_{i=1}^{n} V(x_i) \qquad x_i \in \mathbb{R}^d, d \geq 1$$

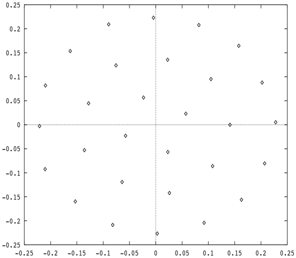
- interaction potential

$$w(x) = \frac{1}{|x|^s} \qquad \max(0, d-2) \leq s < d \quad \text{(Riesz)}$$

$$\text{or} \quad w(x) = -\log|x| \quad \text{with } d = 1, 2 \quad \text{(log gas)}$$

- includes Coulomb: $s = d - 2$ for $d \geq 3$, $w(x) = -\log|x|$ for $d = 2$.

- V confining potential, sufficiently smooth and growing at infinity



Numerical minimization of H_n **for** $w(x) = -\log|x|$**,**
$V(x) = |x|^2$ (Gueron-Shafrir), $n = 29$

Motivation 1: Fekete points

- In logarithmic case minimizers are maximizers of

$$\prod_{i<j} |x_i - x_j| \prod_{i=1}^{n} e^{-n\frac{V}{2}(x_i)}$$

$\rightarrow$ **weighted Fekete sets** (approximation theory) Saff-Totik, Rakhmanov-Saff-Zhou

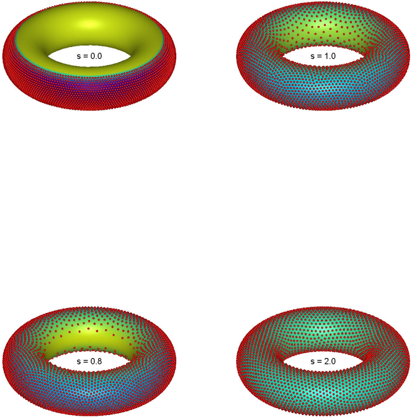
- Fekete points on spheres and other closed manifolds Borodachev-Hardin-Saff, Brauchart-Dragnev-Saff

$$\min_{x_1,\dots,x_n \in \mathcal{M}} -\sum_{i\neq j} \log |x_i - x_j|$$

Smale's 7th problem originating in computational complexity theory

- Riesz s-energy

$$\min_{x_1 \dots x_n \in \mathcal{M}} \sum_{i\neq j} \frac{1}{|x_i - x_j|^s}$$



Minimal *s*-energy points on a torus, $s = 0, 1, 0.8, 2$

(from Rob Womersley's webpage)

Motivation 2: Statistical mechanics

With temperature: Gibbs measure

$$d\mathbb{P}_{n,\beta}(x_1, \cdots, x_n) = \frac{1}{Z_{n,\beta}} e^{-\frac{\beta}{2} H_n(x_1,\ldots,x_n)} dx_1 \ldots dx_n \qquad x_i \in \mathbb{R}^d$$

$Z_{n,\beta}$ partition function

- $d = 1, 2$, $w = -\log|x|$:

$$d\mathbb{P}_{n,\beta}(x_1, \cdots, x_n) = \frac{1}{Z_{n,\beta}} \left(\prod_{i<j} |x_i - x_j| \right)^{\beta} e^{-\frac{n\beta}{2} \sum_{i=1}^n V(x_i)} dx_1 \ldots dx_n$$

$\beta = 2 \rightsquigarrow$ determinantal processes

Motivation 2: Statistical mechanics

With temperature: Gibbs measure

$$d\mathbb{P}_{n,\beta}(x_1, \cdots, x_n) = \frac{1}{Z_{n,\beta}} e^{-\frac{\beta}{2} H_n(x_1,\dots,x_n)} dx_1 \dots dx_n \qquad x_i \in \mathbb{R}^d$$

$Z_{n,\beta}$ partition function

- $d = 1, 2$, $w = -\log|x|$:

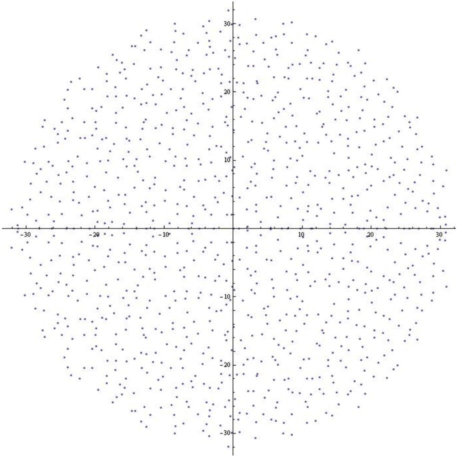
$$d\mathbb{P}_{n,\beta}(x_1, \cdots, x_n) = \frac{1}{Z_{n,\beta}} \Big(\prod_{i<j} |x_i - x_j| \Big)^{\beta} e^{-\frac{n\beta}{2} \sum_{i=1}^n V(x_i)} dx_1 \dots dx_n$$

$\beta = 2 \rightsquigarrow$ determinantal processes

Corresponds to **random matrix models** (first noticed by Wigner, Dyson):

- **GUE** (= law of eigenvalues of Hermitian matrices with complex Gaussian i.i.d. entries)
  $\leftrightarrow d = 1,\ \beta = 2,\ V(x) = x^2/2$.
- **GOE** (real symmetric matrices with Gaussian i.i.d. entries)
  $\leftrightarrow d = 1,\ \beta = 1,\ V(x) = x^2/2$.
- **Ginibre ensemble** (matrices with complex Gaussian i.i.d. entries)
  $\leftrightarrow d = 2,\ \beta = 2,\ V(x) = |x|^2$.

The Ginibre ensemble



Eigenvalues of 1000-by-1000 matrix with i.i.d Gaussian entries ($\beta = 2$, $w(x) = -\log|x|$, $V(x) = |x|^2$) (Borrowed from Benedek Valkó's webpage)

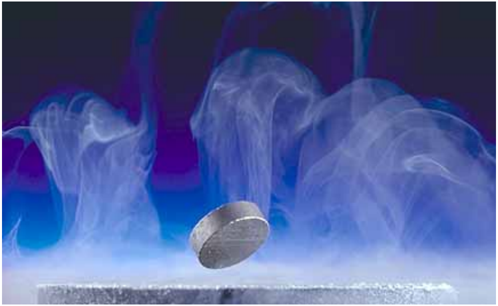
Motivation 3: the Ginzburg-Landau model of superconductivity

- Superconductivity was discovered in 1911 on mercury by H. Kammerling Ohnes. Resistivity vanishes below critical temperature: superconducting currents of superconducting electrons (Cooper pairs)
- Meissner effect

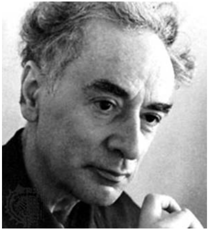
superconductors expell the magnetic field

Motivation 3: the Ginzburg-Landau model of superconductivity

- Superconductivity was discovered in 1911 on mercury by H. Kammerling Ohnes. Resistivity vanishes below critical temperature: superconducting currents of superconducting electrons (Cooper pairs)
- Meissner effect



superconductors expell the magnetic field



Landau
1908-1968 (Nobel 1962)

Ginzburg
1916-2009 (Nobel 2003)

$$G_\varepsilon(\psi, A) = \frac{1}{2}\int_\Omega |\nabla_A \psi|^2 + |\mathrm{curl}\, A - h_{\mathrm{ex}}|^2 + \frac{(1-|\psi|^2)^2}{2\varepsilon^2}$$

superconductors, rotating superfluids and Bose-Einstein condensates

$$G_\varepsilon(\psi, A) = \frac{1}{2}\int_\Omega |\nabla_A \psi|^2 + |\mathrm{curl}\, A - h_{\mathrm{ex}}|^2 + \frac{(1-|\psi|^2)^2}{2\varepsilon^2}$$

- Ω= 2D domain
- A=gauge, ψ= complex-valued “wave function”
- **vortices** = **zeroes of** ψ, with winding number
- h_{ex}=intensity of applied field
- ε= material parameter, taken $\to 0$.

We showed (Sandier-S) that the minimization of G_ε essentially leads to a **Coulomb interaction between the vortices**, acting as quantized charges, like H_n for $d = 2$. Bethuel-Brezis-Hélein in simplified Ginzburg-Landau functional (with fixed bounded number of vortices).

Abrikosov lattice

- H_{c_1} first critical field: the magnetic field penetrates via "vortices" (normal phase regions surrounded by a superconducting current loop). The vortices repell each other and their number increases with increased applied field

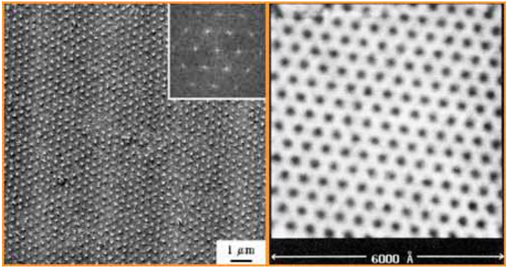
$\rightarrow$ Abrikosov lattices

Abrikosov (Nobel 2003)

Abrikosov lattice

- H_{c_1} first critical field: the magnetic field penetrates via "vortices" (normal phase regions surrounded by a superconducting current loop). The vortices repell each other and their number increases with increased applied field

  $\rightarrow$ Abrikosov lattices



Abrikosov (Nobel 2003)

The leading order to $\min H_n$ (or "mean field limit")

- Assume $V \to \infty$ at ∞ (faster than $\log|x|$ in the log cases). For $(x_1, \dots, x_n)$ minimizing

$$H_n = \sum_{i \neq j} w(x_i - x_j) + n \sum_{i=1}^{n} V(x_i)$$

one has (Choquet)

$$\lim_{n\to\infty} \frac{\sum_{i=1}^n \delta_{x_i}}{n} = \mu_V \qquad \lim_{n\to\infty} \frac{\min H_n}{n^2} = \mathcal{E}(\mu_V)$$

where μ_V is the unique minimizer of

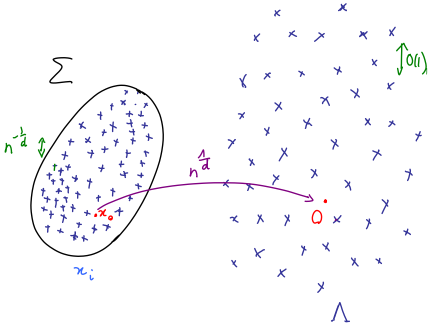
$$\mathcal{E}(\mu) = \int_{\mathbb{R}^d \times \mathbb{R}^d} w(x-y)\, d\mu(x)\, d\mu(y) + \int_{\mathbb{R}^d} V(x)\, d\mu(x).$$

among probability measures.

- $\mathcal{E}$ has a unique minimizer μ_V among probability measures, called the *equilibrium measure* (potential theory) Frostman 30's

- Denote $\Sigma = Supp(\mu_V)$. We assume Σ is compact with C^1 boundary and if $d \geq 2$ that μ_V has a density which is $C^{0,\beta}(\Sigma)$, bounded above, and behaves like $c\,\mathrm{dist}(x, \Sigma)^\alpha$ for some $\alpha \geq 0$ near $\partial\Sigma$.
- Example: $V(x) = |x|^2$, Coulomb case, then $\mu_V = \frac{1}{c_d}\mathbb{1}_{B_1}$ (circle law).
- Example $d = 1$, $w = -\log|x|$, $V(x) = x^2$ then $\mu_V = \frac{1}{2\pi}\sqrt{4 - x^2}\mathbb{1}_{|x|<2}$ (semi-circle law)
- Expect n points in region of size $1 \rightsquigarrow$ typical distance $n^{-1/d}$ (macro-micro scale).

Blow-up procedure



- examine next order terms by expanding $\sum_{i=1}^n \delta_{x_i}$ as $n\mu_V + (\sum_{i=1}^n \delta_{x_i} - n\mu_V)$ and inserting into H_n
- blow-up the configurations at scale $(\mu_V(x)n)^{1/d}$
- define interaction energy $\mathbb{W}$ for infinite configurations of points in whole space
- the total energy is the integral or average of $\mathbb{W}$ over all blow-up centers in Σ.

Next order expansion of min H_n

- Sandier-S, Rota Nodari-S: $d = 2$, $w(x) = -\log|x|$
- Sandier-S: $d = 1$, $w(x) = -\log|x|$
- Rougerie-S: Coulomb cases: $d \geq 3$, $w(x) = 1/|x|^{d-2}$ or $d = 2$ and $w(x) = -\log|x|$
- Petrache-S: all previous cases plus Riesz cases $(0, d-2) \leq s < d$

Theorem (ground state energy)

Under suitable assumptions on V, as $n \to \infty$ we have

$$\min H_n =$$

$$\begin{cases} n^2 \mathcal{E}(\mu_V) + n^{1+s/d} \left(\xi_{s,d} \int \mu_V^{1+s/d}(x)dx \right) + o(n^{1+s/d}) \\ n^2 \mathcal{E}(\mu_V) - \frac{n}{d} \log n + n \left(\xi_{0,d} - \frac{1}{d} \int \mu_V(x) \log \mu_V(x)\, dx \right) + o(n) \end{cases}$$

where $\xi_{s,d} = \min \mathbb{W}$ depends only on s, d (see later).

Splitting the energy

From now on let's describe everything in the case where μ_V has density 1 in Σ and the interaction is Coulomb.
The method relies on an explicit splitting formula after expanding the quadratic terms

$$\sum_{i\neq j} w(x_i - x_j) = \iint_{\triangle^c} w(x-y)(\sum_i \delta_{x_i})(x)(\sum_i \delta_{x_i})(y)$$

$$= \int w*(n\mu_V)(n\mu_V) + \int w*(\sum_i \delta_{x_i} - n\mu_V)(\sum_i \delta_{x_i} - n\mu_V) + \text{cross terms}$$

- computing the energy via the potential generated by the distribution $\sum_i \delta_{x_i} - n\mu_V$, i.e.

$$h_n = w * \left(\sum_i \delta_{x_i} - n\mu_V\right).$$

- in the Coulomb case, one can check that

$$-\Delta h_n = c_d \left(\sum_i \delta_{x_i} - n\mu_V \right)$$

  and

$$\int w * (\sum_i \delta_{x_i} - n\mu_V)(\sum_i \delta_{x_i} - n\mu_V) \simeq \frac{1}{c_d} \int |\nabla h_n|^2.$$

- This last integral is really infinite and needs to be "renormalized".

The renormalized energy (Coulomb case)

Definition

Let $\mathcal{C} = \sum_{p\in\Lambda} N_p \delta_p \in \mathcal{X} :=$ discrete infinite point configurations (with multiplicity). We let

$$\mathbb{W}(\mathcal{C}) := \inf\{\mathcal{W}(\nabla h) \mid -\Delta h = c_d(\mathcal{C} - 1)\}$$

$$\mathcal{W}(\nabla h) = \lim_{\eta\to 0}\left(\limsup_{R\to\infty} \fint_{[-R/2,R/2]} |\nabla h_\eta|^2 - m c_d w(\eta)\right).$$

- 1 = average density of points = uniform background charge density
- h_η is similar to $\min(h, w(\eta)) \leftrightarrow$ replacing δ_p by $\delta_p^{(\eta)}$ uniform measure of mass 1 on $\partial B(p,\eta)$
- $\mathbb{W}$ is bounded below, and has a minimizer. Its minimum can be achieved as the limit of energies of periodic configurations (with larger and larger period)

The case of the torus

- Assume Λ is $\mathbb{T}$-periodic. Then $\mathbb{W}$ is $+\infty$ unless all $N_p = 1$, and can be written as a function of $\Lambda " = " \{a_1, \ldots, a_M\}$, $M = |\mathbb{T}|$.

$$\mathbb{W}(a_1, \cdots, a_M) = \frac{c_d^2}{|\mathbb{T}|} \sum_{j \neq k} G(a_j - a_k) + cst,$$

where $G=$ Green's function of the torus $(-\Delta G = \delta_0 - 1/|\mathbb{T}|)$.
- G can be expressed explicitly via an Eisenstein series and the Dedekind Eta function

Results

- Let $x_1, \dots, x_n$ be a minimizer of H_n. Then, after blow-up at scale $(\mu_V(x)n)^{1/d}$ around a point $x \in \Sigma$, for a.e. $x \in \Sigma$, the limiting infinite configuration as $n \to \infty$ minimizes $\mathbb{W}$. Sandier-S, Rougerie-S, Petrache-S
- For minimizers, points are separated by $\frac{C}{(n\|\mu_V\|_\infty)^{1/d}}$ and there is uniform distribution of points and energy (rigidity result) Petrache-S, Rota Nodari-S
- Let $(\psi_\varepsilon, A_\varepsilon)$ minimize the Ginzburg-Landau energy G_ε. In the suitable regime of (ε, h_{ex}), after blow-up at scale $\sqrt{h_{ex}}$ near x in the sample, the limit as $\varepsilon \to 0$ of the point vortices is an infinite point configuration which for a.e. x, minimizes $\mathbb{W}$. Sandier-S
- Similar result for the "Ohta-Kawasaki model" of diblock copolymers Goldman-Muratov-S.
- Next order expansion of the minimal energy in all instances

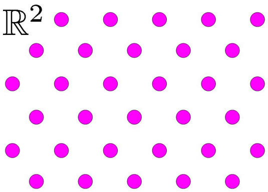
$\rightsquigarrow$ understand minimizers of $\mathbb{W}$?

Partial minimization results

- In dimension $d = 1$, the minimum of $\mathbb{W}$ over all possible configurations is achieved for the lattice $\mathbb{Z}$ ("clock distribution").
- In dimension $d = 2$, the minimum of $\mathbb{W}$ over perfect lattice configurations (Bravais lattices) with fixed volume is achieved uniquely, modulo rotations, by the triangular (Abrikosov) lattice.

Partial minimization results

- In dimension $d = 1$, the minimum of $\mathbb{W}$ over all possible configurations is achieved for the lattice $\mathbb{Z}$ ("clock distribution").
- In dimension $d = 2$, the minimum of $\mathbb{W}$ over perfect lattice configurations (Bravais lattices) with fixed volume is achieved uniquely, modulo rotations, by the triangular (Abrikosov) lattice.



The proof relies on

Theorem (Cassels, Rankin, Ennola, Diananda, 50's)

For $s > 2$, the Epstein zeta function of a lattice Λ in $\mathbb{R}^2$:

$$\zeta(s) = \sum_{p \in \Lambda \setminus \{0\}} \frac{1}{|p|^s}$$

is uniquely minimized among lattices of volume one, by the triangular lattice (modulo rotations).

There is no corresponding result in higher dimension except for dimensions 8 and 24 (E_8 and Leech lattices)

In dimension 3, does the BCC (body centered cubic) lattice play this role?

The proof relies on

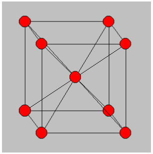
Theorem (Cassels, Rankin, Ennola, Diananda, 50's)

For $s > 2$, the Epstein zeta function of a lattice Λ in $\mathbb{R}^2$:

$$\zeta(s) = \sum_{p \in \Lambda \setminus \{0\}} \frac{1}{|p|^s}$$

is uniquely minimized among lattices of volume one, by the triangular lattice (modulo rotations).

There is no corresponding result in higher dimension except for dimensions 8 and 24 (E_8 and Leech lattices)
In dimension 3, does the BCC (body centered cubic) lattice play this role?



Conjecture

In dimension 2, the "Abrikosov" triangular lattice is a global minimizer of $\mathbb{W}$.

- this conjecture was made in the context of vortices in the GL model, which form Abrikosov lattices
- Bétermin shows that this conjecture is equivalent to a conjecture of Brauchart-Hardin-Saff on the order n term in the expansion of the minimal logarithmic energy on $\mathbb{S}^2$.
- $\mathbb{W}$ is a measure of disorder of a given point configuration

Crystallization questions : many ramifications

- more general family of crystallization problems: given V, minimize
$$\sum_{i\neq j} V(x_i - x_j)$$
(+some kind of boundary condition needed)? Or rather
$$\lim_{R\to\infty} \frac{1}{|B_R|} \sum_{i\neq j, x_i, x_j \in B_R} V(x_i - x_j)?$$
Is the min achieved for lattices?
- important scientific question: cristalline structure of matter
- cf the Cohn-Kumar conjecture: if $V(x) = f(|x|^2)$ with f completely monotonic, i.e. $(-1)^k f^{(k)}(x) \geq 0$, then the minimum is achieved by the triangular lattice for $d = 2$, (the E_8 root lattice in dimension $d = 8$, the Leech lattice in dimension $d = 24$).
- in $d = 2$, the Abrikosov lattice is expected to have some universal minimizing property

Crystallization questions : many ramifications

- more general family of crystallization problems: given V, minimize
$$\sum_{i\neq j} V(x_i - x_j)$$
(+some kind of boundary condition needed)? Or rather
$$\lim_{R\to\infty} \frac{1}{|B_R|} \sum_{i\neq j, x_i, x_j \in B_R} V(x_i - x_j)?$$
Is the min achieved for lattices?
- important scientific question: cristalline structure of matter
- cf the Cohn-Kumar conjecture: if $V(x) = f(|x|^2)$ with f completely monotonic, i.e. $(-1)^k f^{(k)}(x) \geq 0$, then the minimum is achieved by the triangular lattice for $d = 2$, (the E_8 root lattice in dimension $d = 8$, the Leech lattice in dimension $d = 24$).
- in $d = 2$, the Abrikosov lattice is expected to have some universal minimizing property

Crystallization questions : many ramifications

- more general family of crystallization problems: given V, minimize
$$\sum_{i \neq j} V(x_i - x_j)$$
(+some kind of boundary condition needed)? Or rather
$$\lim_{R \to \infty} \frac{1}{|B_R|} \sum_{i \neq j, x_i, x_j \in B_R} V(x_i - x_j)?$$
Is the min achieved for lattices?
- important scientific question: cristalline structure of matter
- cf the Cohn-Kumar conjecture: if $V(x) = f(|x|^2)$ with f completely monotonic, i.e. $(-1)^k f^{(k)}(x) \geq 0$, then the minimum is achieved by the triangular lattice for $d = 2$, (the E_8 root lattice in dimension $d = 8$, the Leech lattice in dimension $d = 24$).
- in $d = 2$, the Abrikosov lattice is expected to have some universal minimizing property

Large deviations principle

Recall

$$d\mathbb{P}_{n,\beta}(x_1,\cdots,x_n) = \frac{1}{Z_{n,\beta}} e^{-\frac{\beta}{2} n^{-\frac{s}{d}} H_n(x_1,\dots,x_n)} dx_1 \dots dx_n \qquad x_i \in \mathbb{R}^d$$

- Given a configuration $(x_1,\dots,x_n)$, we examine the blow-up point configurations $\{(\mu_V(x)n)^{1/d}(x_i - x)\}$ and their infinite limits $\mathcal{C}$. Averaging near the blow-up center x yields a "point process" P^x = probability law on infinite point configurations. We can define

$$\overline{\mathbb{W}}(P) := \int_\Sigma \int \mathbb{W}(\mathcal{C}) dP^x(\mathcal{C}) dx$$

Large deviations principle

Recall

$$d\mathbb{P}_{n,\beta}(x_1, \cdots, x_n) = \frac{1}{Z_{n,\beta}} e^{-\frac{\beta}{2} n^{-\frac{s}{d}} H_n(x_1,\ldots,x_n)} dx_1 \ldots dx_n \qquad x_i \in \mathbb{R}^d$$

- Given a configuration $(x_1, \ldots, x_n)$, we examine the blow-up point configurations $\{(\mu_V(x)n)^{1/d}(x_i - x)\}$ and their infinite limits $\mathcal{C}$. Averaging near the blow-up center x yields a "point process" P^x = probability law on infinite point configurations. We can define

$$\overline{\mathbb{W}}(P) := \int_\Sigma \int \mathbb{W}(\mathcal{C}) dP^x(\mathcal{C}) dx$$

Theorem (Leblé-S, '15)

We have a Large Deviation Principle at speed n with good rate function $\beta(\mathcal{F}_\beta - \inf \mathcal{F}_\beta)$ where

$$\mathcal{F}_\beta(P) := \frac{1}{2}\overline{\mathbb{W}}(P) + \frac{1}{\beta}\int_\Sigma \mathrm{ent}[P^x|\Pi]\, dx,$$

$$\mathrm{ent}[P|\Pi] := \lim_{N\to\infty} \frac{1}{|K_N|}\mathrm{Ent}\left(P_{K_N}|\Pi_{K_N}\right) \quad \textbf{specific relative entropy}$$

and Π is the Poisson point process of intensity 1.

In other words

$$\mathbb{P}_{n,\beta}(P) \simeq \exp\left(-\beta n\left(\mathcal{F}_\beta(P) - \inf \mathcal{F}_\beta\right)\right)$$

$\rightsquigarrow$ the Gibbs measure concentrates on minimizers of $\mathcal{F}_\beta$

Interpretation

- Three regimes: $\beta \gg 1$ crystallization expected, $\beta \ll 1$ entropy dominates $\rightsquigarrow$ Poisson process, $\beta \propto 1$ intermediate, no crystallization expected
- This includes the minimization of H_n (formally $\beta = \infty$) = the previous result.
- In 1D log case the limiting process is "sine-β" (Valko-Virag) and must minimize $\frac{1}{2}\mathbb{W} + \frac{1}{\beta}\mathrm{ent}(\cdot|\Pi)$, same for the Ginibre process in 2D log case $\beta = 2$.
- The **cristallization** result is **complete** in 1D (uses uniqueness result of Leblé)
- Next order expansion of the partition function ("thermodynamic limit"), to be compared with results of Bourgade-Erdös-Yau, Borot-Guionnet, Shcherbina which treat $d = 1$, $w = -\log$

Further questions

- cristallization: identify minimizers of $\mathbb{W}$ or other interactions
- understanding behavior with temperature in terms of decay of two-point correlation functions: is there a critical temperature?
- study systems with oppositely charged particles ("two-component plasma"), with Leblé, Zeitouni
- extend to more general Riesz interactions ($s \leq d-2$, $s \geq d$), with Hardin, Leblé, Saff