Microscopic description of systems of points with Coulomb-type interactions

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collaborations:
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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

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

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

- 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

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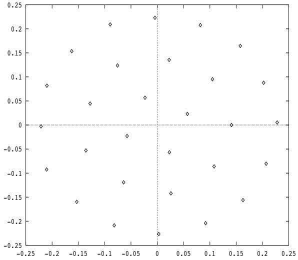


Numerical minimization of H_N for $w(x) = -\log|x|$, $V(x) = |x|^2$ (Gueron-Shafrir), $N = 29$

Motivation 1: Fekete points

- In logarithmic case minimizers are maximizers of

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

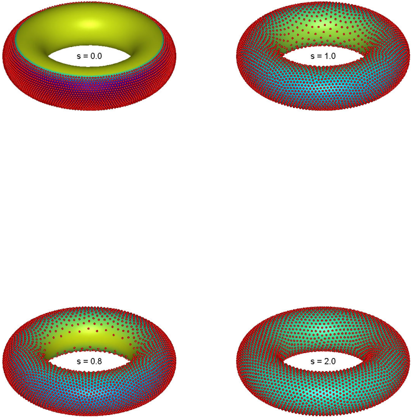
$\rightarrow$ **weighted Fekete sets** (approximation theory) Saff-Totik, Rakhmanov-Saff-Zhou...

- 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 : find an algorithm that computes a minimizer on the sphere up to an error $\log N$, in polynomial time
- 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: Condensed matter physics

Vortices in the Ginzburg-Landau model of superconductivity, in superfluids and Bose-Einstein condensates

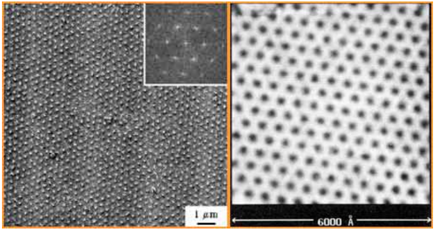


Figure: Abrikosov lattices in superconductors

Motivation 3: Statistical mechanics and Random Matrix Theory

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

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

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$\beta = 2 \rightsquigarrow$ determinantal processes

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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)
  $\leftrightarrow d = 2, \beta = 2, V(x) = |x|^2$.

Also connection with **"two-component plasma"**, **XY model**, **sine-Gordon model** and **Kosterlitz-Thouless** phase transition.

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

- 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)
- 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 regular enough in Σ.

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A 2D log gas for $V(x) = |x|^2$

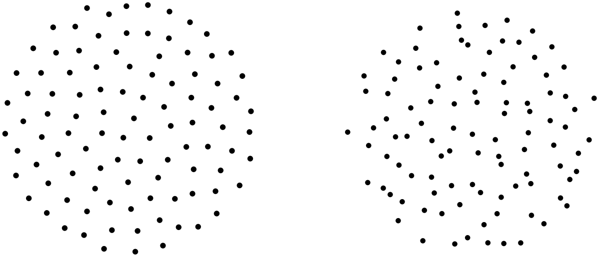

Figure: $\beta = 400$ and $\beta = 5$

Questions

Fluctuations

In what sense does $\frac{1}{N}\sum_{i=1}^N \delta_{x_i} \approx \mu_V$?

- At small scales ($O(1) \to O(N^{-1/d+\varepsilon})$)?
- Deviations bounds?
- Central limit theorem?

Microscopic behavior

Zoom into the system by $N^{1/d}$ $\to$ infinite point configuration.

- What does it look like? What quantities can describe the point configurations?
- How does the picture depend on β? On V?

A CLT for fluctuations (2D Coulomb Gas)

Theorem (Leblé-S)

Assume $d = 2$, $w = -\log$, $\beta > 0$ arbitrary, and the previous assumptions on regularity of μ_V and $\partial\Sigma$. Let $f \in C_c^3(\mathbb{R}^2)$. Then

$$\sum_{i=1}^N f(x_i) - N \int_\Sigma f \, d\mu_V$$

converges in law as $N \to \infty$ to a Gaussian distribution with

$$\textit{mean} = \frac{1}{2\pi}\left(\frac{1}{\beta} - \frac{1}{4}\right) \int \Delta f \, (\mathbb{1}_\Sigma + \log \Delta V)^\Sigma \qquad \textit{var} = \frac{1}{2\pi\beta} \int_\Sigma |\nabla f^\Sigma|^2$$

where $f^\Sigma =$ harmonic extension of f outside Σ.

$\rightsquigarrow \Delta^{-1}\left(\sum_{i=1}^N \delta_{x_i} - N\mu_V\right)$ *converges to the Gaussian Free Field.*

The result can be localized with f supported on any mesoscale $N^{-\alpha}$, $\alpha < \frac{1}{2}$.

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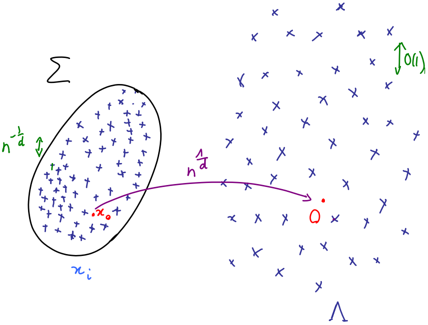
Previous results

- 2D log case
  - Rider-Virag same result for $\beta = 2$, $V(x) = |x|^2$
  - Ameur-Hedenmalm-Makarov same result for $\beta = 2$, $V \in C^\infty$ and analyticity in case the support of f intersects $\partial\Sigma$
  - suboptimal bounds (in N^ε, but with quantified error in probability), including at mesoscale, on $\|\sum_{i=1}^N \delta_{x_i} - N\mu_V\|$ Sandier-S, Leblé, Bauerschmidt-Bourgade-Nikkula-Yau
  - simultaneous result by Bauerschmidt-Bourgade-Nikkula-Yau for $f \in C^4_c(\Sigma)$
- 1D log case
  - Johansson 1-cut, V polynomial
  - Borot-Guionnet, Shcherbina 1-cut and V, ξ locally analytic, multi-cut and V analytic
  - Bekerman-Leblé-S with weaker assumptions
  - new proof Lambert-Ledoux-Webb for 1-cut, mesoscopic result Bekerman-Lodhia

Blow-up procedure



- 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.

The energy method: expanding the Hamiltonian

Explicit splitting formula

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

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

- compute the energy via the potential

$$h_N = w * \left(\sum_i \delta_{x_i} - N\mu_V\right)$$

$$-\Delta h_N = \left(\sum_i \delta_{x_i} - N\mu_V\right)$$

The renormalized energy

Sandier-S, Rougerie-S, Petrache-S

At the limit $N \to \infty$ and after blow-up, in Coulomb cases

$$-\Delta h = (\mathcal{C} - 1) \qquad \mathcal{C} = \sum_{p \in \mathcal{C}} \delta_p$$

$$\mathbb{W}(\mathcal{C}) := \liminf_{R \to \infty} \frac{1}{R^d} \int_{K_R} |\nabla h|^2$$

but computed in a "renormalized way"

For point processes (Leblé)

$$< \mathbb{W} > = \liminf_{R \to \infty} \frac{1}{R^d} \iint_{K_R \times K_R \setminus \triangle} w(x-y)(\rho_2(x-y) - 1) dx dy$$

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 Λ“ = ”$\{a_1, \dots, a_M\}$, $M = |\mathbb{T}|$.

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

  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

Main result on the energy

- 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. P = "tagged point process", probability on $\Sigma \times$ *configs*. The limits will all be *stationary*. We define

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

- The main result is

$$H_N(x_1, \dots, x_N) \sim N^2 \mathcal{E}(\mu_V) - \frac{N}{d} \log N + N^{1+\frac{s}{d}} \overline{\mathbb{W}}(P)$$

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- Consequently, if $(x_1, \dots, x_N)$ is a minimizer of H_N, 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 $\mathbb{W}$
- Next order expansion of the minimal energy

$$\min H_N \sim N^2 \mathcal{E}(\mu_V) - \frac{N}{d} \log N + \begin{cases} N \left(C_{d,0} - \frac{1}{2d} \int \mu_V(x) \log \mu_V(x) \right) \\ C_{d,s} \int \mu_V^{1+s/d}(x)\, dx. \end{cases}$$

- Expansion to order N for minimal logarithmic energy on the sphere Bétermin-Sandier
- 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
- Similar results for the Ginzburg-Landau model of superconductivity Sandier-S

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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 lattice (modulo rotations).

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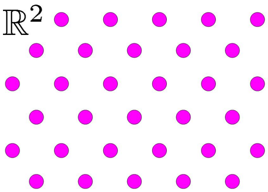

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Theorem (Cassels, Rankin, Ennola, Diananda, 50's)

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)

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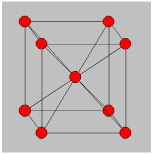

Conjecture

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

- this conjecture was made in the context of vortices in the GL model, which form triangular Abrikosov lattices
- Bétermin-Sandier show 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 $\mathbb{S}^2$.
- link with the Cohn-Kumar conjecture, proved in '17 for dimensions 8 and 24
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Large deviations principle

Recall

$$d\mathbb{P}_{N,\beta}(x_1, \cdots, x_N) = \frac{1}{Z_{N,\beta}} e^{-\frac{\beta}{2} N^{-\frac{s}{d}} H_N(x_1,\ldots,x_N)} dx_1 \ldots dx_N \qquad x_i \in \mathbb{R}^d$$

- insert next-order expansion of H_N and combine it with an estimate for the volume in phase-space occupied by a neighborhood of a given limiting tagged point process P

Theorem (Leblé-S, '15)

We have a Large Deviation Principle at speed N with good rate function $\beta(\mathcal{F}_\beta - \inf \mathcal{F}_\beta)$, i.e.

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

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

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

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

and Π is the Poisson point process of intensity 1.

For specific relative entropy see Rassoul-Agha - Seppäläinen

Interpretation

- Three regimes
  - $\beta \gg 1$ crystallization expected
  - $\beta \ll 1$ entropy dominates $\rightsquigarrow$ Poisson process
  - $\beta \propto 1$ intermediate, no crystallization expected
- In 1D log case the limiting process is "sine-β" (Valko-Virag) and must minimize $\frac{1}{2}\mathbb{W} + \frac{1}{\beta}\mathsf{ent}(\cdot|\Pi)$, same for the Ginibre point process in 2D log case $\beta = 2$.
- The **cristallization** result is **complete** in 1D (uses uniqueness result of Leblé).
- In 2D log case: local version of the result at any mesoscale Leblé
- Generalization to the 2D "two component plasma" Leblé-S-Zeitouni

Expansion of $\log Z_{N,\beta}$

1D and 2D Log gas case:

$$\log Z_{N,\beta} = -\frac{\beta N^2}{2}\mathcal{E}(\mu_V) + \frac{\beta N}{2d}\log N - \beta N \underbrace{\min\left(\frac{1}{2\pi}\mathbb{W} + \frac{1}{\beta}\mathrm{ent}[\cdot|\Pi^1]\right)}_{C_\beta,\ \text{indep of } V}$$

$$-\beta N\left(\frac{1}{\beta} - \frac{1}{2d}\right)\int_\Sigma \mu_V(x)\log\mu_V(x)\,dx + o(N).$$

Riesz cases:

$$\log Z_{N,\beta} = -\frac{\beta N^{2-\frac{s}{d}}}{2}\mathcal{E}(\mu_V) - \beta N \min \mathcal{F}_\beta + o(N).$$

To be compared with Borot-Guionnet, Shcherbina, $d = 1$ log case (expansions to larger order in N under stronger assumptions on V), Wiegmann-Zabrodin, $d = 2$ log case (semi-formal)

THANK YOU FOR YOUR ATTENTION!

and some advertising:
ICERM Semester Program on "Point Configurations in Geometry, Physics and Computer Science" February 1, May 4, 2018
https://icerm.brown.edu/programs/sp-s18/