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

$$H_N(x_1, \ldots, x_N) = \sum_{i\neq j} w(x_i - x_j) + N \sum_{i=1}^{N} V(x_i) \quad x_i \in \mathbb{R}^d, d \geq 1$$

- interaction potential

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

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

- 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.
The question

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$$H_N(x_1, \ldots, x_N) = \sum_{i \neq j} w(x_i - x_j) + N \sum_{i=1}^{N} V(x_i) \quad x_i \in \mathbb{R}^d, d \geq 1$$

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- $V$ 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

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

→ weighted Fekete sets (approximation theory) Saff-Totik, Rakhmanov-Saff-Zhou...

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

\[ \min_{x_1, \ldots, x_N \in \mathcal{M}} - \sum_{i \neq j} \log |x_i - x_j| \]

▶ 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

\[ \min_{x_1 \ldots x_N \in \mathcal{M}} \sum_{i \neq j} \frac{1}{|x_j - x_j|^s} \]
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

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

\( Z_{N,\beta} \) partition function

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

\[ d\mathbb{P}_{N,\beta}(x_1, \ldots, x_N) = \frac{1}{Z_{N,\beta}} \left( \prod_{i<j} |x_i - x_j| \right)^{\beta} e^{-\frac{N\beta}{2} \sum_{i=1}^N V(x_i)} dx_1 \ldots dx_N \]

\( \beta = 2 \leadsto \) determinantal processes
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\( \beta = 2 \sim \) 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)
  \[ \leftrightarrow d = 2, \beta = 2, V(x) = |x|^2. \]

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 $\infty$ (faster than $\log |x|$ in the log cases).
  For $(x_1, \ldots, x_N)$ minimizing

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

one has (Choquet)

$$\lim_{N \to \infty} \frac{\sum_{i=1}^{N} \delta_{x_i}}{N} = \mu_V \quad \lim_{N \to \infty} \frac{\min H_N}{N^2} = \mathcal{E}(\mu_V)$$

where $\mu_V$ 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 $\mu_V$ among probability measures, called the equilibrium measure (potential theory) Frostman 30’s.
Example: $V(x) = |x|^2$, Coulomb case, then $\mu_V = \frac{1}{cd} 1_{B_1}$ (circle law).

Example $d = 1, w = -\log |x|, V(x) = x^2$ then $\mu_V = \frac{1}{2\pi} \sqrt{4 - x^2} 1_{|x|<2}$ (semi-circle law)

Denote $\Sigma = \text{Supp}(\mu_V)$. We assume $\Sigma$ is compact with $C^1$ boundary and if $d \geq 2$ that $\mu_V$ has a density which is regular enough in $\Sigma$. 
Example: $V(x) = |x|^2$, Coulomb case, then $\mu_V = \frac{1}{c_d} 1_{B_1}$ (circle law).

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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 \( \frac{1}{N} \sum_{i=1}^{N} \delta_{x_i} \approx \mu \nu \)?
- At small scales (\( O(1) \rightarrow O(N^{-1/d+\varepsilon}) \))?
- Deviations bounds?
- Central limit theorem?

Microscopic behavior

Zoom into the system by \( N^{1/d} \rightarrow \) infinite point configuration.
- What does it look like? What quantities can describe the point configurations?
- How does the picture depend on \( \beta \)? On \( \nu \)?
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 $\mu_V$ and $\partial \Sigma$. Let $f \in C^3_\text{c}(\mathbb{R}^2)$. 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

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

where $f^\Sigma = \text{harmonic extension of } f \text{ outside } \Sigma$.

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

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

Should be generalizable to Coulomb case $d \geq 3$, Riesz cases.
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mean $= \frac{1}{2\pi} \left( \frac{1}{\beta} - \frac{1}{4} \right) \int \Delta f \left( 1 + \log \Delta V \right) \Sigma$ 

var $= \frac{1}{2\pi\beta} \int_{\Sigma} |\nabla f^\Sigma|^2$

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

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**Theorem (Leblé-S)**

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

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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 $N^\varepsilon$, 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 $V, \xi$ 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 $\Sigma$. 
The energy method: expanding the Hamiltonian

Explicit splitting formula

\[ \sum_{i \neq j} w(x_i - x_j) = \int \int_{\Delta_c} w(x - y)(\sum_i \delta_{x_i})(x)(\sum_i \delta_{x_i})(y) \]

\[ = \int w*(N_{\mu_V})(N_{\mu_V}) + \int w*(\sum_i \delta_{x_i} - N\mu_V)(\sum_i \delta_{x_i} - N\mu_V) + \text{cross terms} \]

- 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

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

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

but computed in a “renormalized way”

For point processes (Leblé)

$$<\mathbb{W}> = \liminf_{R \to \infty} \frac{1}{R^d} \int_{K_R \times K_R \setminus \triangle} w(x - y)(\rho_2(x - y) - 1) \, dx \, dy$$
The case of the torus

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

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

where $G =$ Green’s function of the torus ($-\Delta G = \delta_0 - 1/|T|$).

- $G$ can be expressed explicitly via an Eisenstein series and the Dedekind Eta function
Main result on the energy

- Given a configuration $(x_1, \ldots, x_N)$, we examine the blow-up point configurations $\{(\mu_N(x)N^{1/d}(x_i-x))\}$ and their infinite limits $C$. Averaging near the blow-up center $x$ yields a “point process” $P^x = \text{probability law on infinite point configurations}$. $P = \text{“tagged point process”}$, probability on $\Sigma \times \text{configs}$. The limits will all be stationary. We define

\[
\bar{W}(P) := \int_\Sigma \int \bar{W}(C) dP^x(C) dx
\]

- The main result is

\[
H_N(x_1, \ldots, x_N) \sim N^2 \mathcal{E}(\mu_N) - \frac{N}{d} \log N + N^{1 + \frac{s}{d}} \bar{W}(P)
\]

Sandier-S, Rougerie-S, Petrache-S
Main result on the energy

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 \(C\). 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 \(\Sigma \times \text{configs}\). The limits will all be stationary. We define

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\overline{W}(P) := \int_{\Sigma} \int W(C) dP_x(C) dx
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The main result is

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Sandier-S, Rougerie-S, Petrache-S
Consequently, if \((x_1, \ldots, x_N)\) 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 \(W\).

Next order expansion of the minimal energy

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

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 $W$ over all possible configurations is achieved for the lattice $\mathbb{Z}$ ("clock distribution").

- In dimension $d = 2$, the minimum of $W$ over perfect lattice configurations (Bravais lattices) with fixed volume is achieved uniquely, modulo rotations, by the triangular lattice (modulo rotations).
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The proof relies on

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

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

$$
\zeta(s) = \sum_{\substack{p \in \Lambda \backslash \{0\}}} \frac{1}{|p|^s}
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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?
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In dimension 3, does the BCC (body centered cubic) lattice play this role?
Conjecture

In dimension 2, the triangular lattice is a global minimizer of $W$.

- 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 $S^2$.
- link with the Cohn-Kumar conjecture, proved in ’17 for dimensions 8 and 24
- In any case, $W$ can be seen as measuring the disorder of a point configuration / process Borodin-S, Leblé
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- In any case, $W$ can be seen as measuring the disorder of a point configuration / process Borodin-S, Leblé.
Recall

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

- 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 $\mathbb{P}$
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.

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

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

Here,

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

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

and $\Pi$ 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 $\sim$ Poisson process
  - $\beta \propto 1$ intermediate, no crystallization expected

- In 1D log case the limiting process is “sine-$\beta$” (Valko-Virag) and must minimize $\frac{1}{2} W + \frac{1}{\beta} \text{ent}(\cdot | \Pi)$, same for the Ginibre point process in 2D log case $\beta = 2$.

- The crystallization 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:

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

$$C_\beta, \text{ indep of } V$$

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

Riesz cases:

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

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)
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