Microscopic description of Coulomb-type systems

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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

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

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

- 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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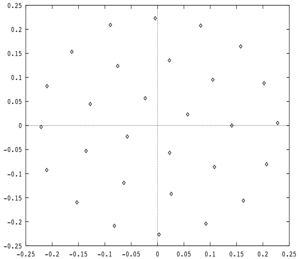


Numerical minimization of H_N for $w(x) = -\log|x|$,
$V(x) = |x|^2$ (Gueron-Shafrir), $N = 29$

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

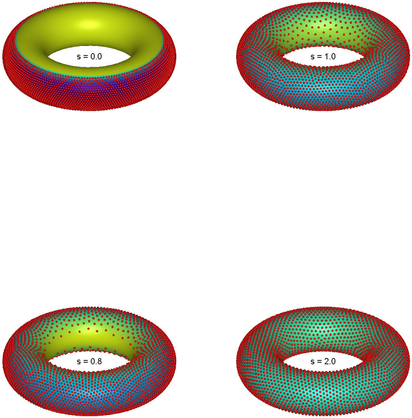
- Fekete points on spheres and other closed manifolds Borodachev-Hardin-Saff, Brauchart-Dragnev-Saff

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

Smale's 7th problem originating in computational complexity theory

- Riesz s-energy

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



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
- Ohta-Kawasaki model of diblock copolymers

Figure: The Meissner effect in superconductors

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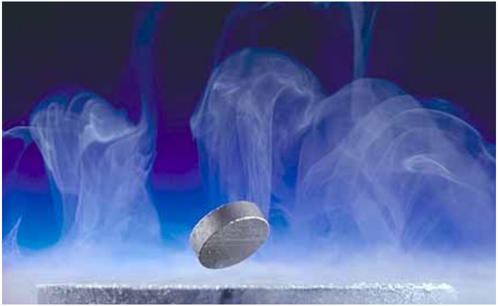

Figure: The Meissner effect in superconductors

Patterns

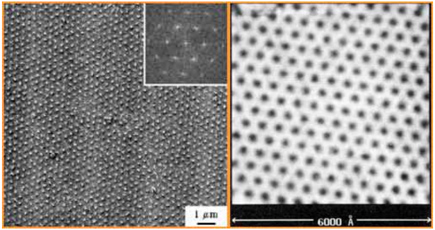

Figure: Abrikosov lattices in superconductors

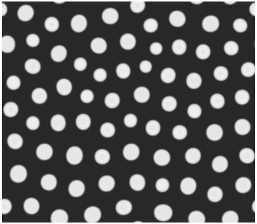

Figure: Simulation of the Ohta-Kawasaki energy

The Ginzburg-Landau model

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

- 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 $d = 2$.
Cf. Bethuel-Brezis-Hélein in simplified Ginzburg-Landau functional (with fixed bounded number of vortices).

Motivation 3: 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

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

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

- 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)

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

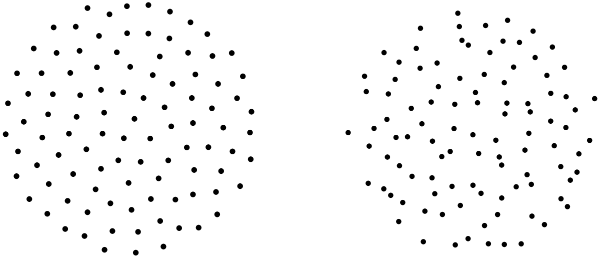


Figure: $\beta = 400$ and $\beta = 5$

Leading order LDP

Theorem

The push-forward of $\mathbb{P}_{n,\beta}$ *by* $(x_1, \ldots, x_N) \mapsto \frac{1}{N}\sum_{i=1}^{N} \delta_{x_i}$ *satisfies a Large Deviation Principle at speed* N^2 *and good rate function*

$$\frac{\beta}{2}(\mathcal{E} - \mathcal{E}(\mu_V)).$$

In other words

$$\mathbb{P}_{n,\beta}\left(\frac{1}{N}\sum_{i=1}^{N} \delta_{x_i} \in A\right) \simeq e^{-\beta N^2(\inf_A \mathcal{E} - \min \mathcal{E}))}.$$

$\rightsquigarrow$ the Gibbs measure concentrates near μ_V

Petz-Hiai, Ben Arous - Guionnet, Ben Arous - Zeitouni, Chafai-Gozlan-Zitt...

Questions

Fluctuations

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

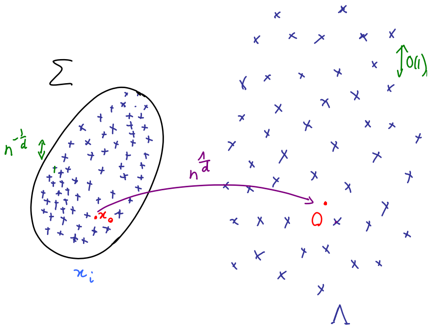
- At small scales ($O(1) \to O(N^{-1/d+\varepsilon})$)?
- Deviations bounds?
- Central limit theorem?

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?

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

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

The renormalized energy

Sandier-S, Rougerie-S, Petrache-S

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

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

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

Roughly

$$\mathbb{W}(\mathcal{C}) \simeq \liminf_{R \to \infty} \frac{1}{R^d} \left[\iint_{K_R \times K_R \setminus \triangle} w(x-y)\,(d\mathcal{C}(x) - dx)\,(d\mathcal{C}(y) - dy) \right]$$

Borodin-S, Leblé

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

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

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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.
- 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.

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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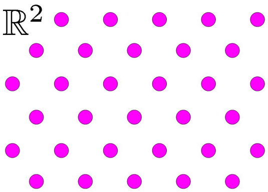

The proof relies on

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)

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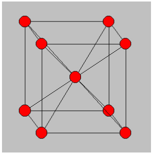

Conjecture

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 $\mathbb{S}^2$.

Large deviations principle

Recall

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

- 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*.*

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 $\frac{1}{2}\mathbb{W} + \frac{1}{\beta}\mathrm{ent}(\cdot|\Pi)$, 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

A CLT for fluctuations of the 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* $f \in C_c^{3,1}(\mathbb{R}^2)$. *The law of*

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

converges as $N \to \infty$ *to a Gaussian distribution with*

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

where $f^\Sigma =$ *harmonic extension of* f *outside* Σ.
$\rightsquigarrow \sum_{i=1}^N \delta_{x_i} - N\mu_V$ *converges to the Gaussian Free Field.*
The result can be localized with f *supported on any mesoscale* $N^{-\alpha}$, $\alpha < \frac{1}{2}$.

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 $f \in C_c^4(\Sigma)$
- 1D log case
  - Johansson 1-cut, V polynomial
  - Borot-Guionnet, Shcherbina 1-cut and V, ξ locally analytic, multi-cut and V analytic
  - universality in V of local statistics Bourgade-Erdös-Yau

Questions

- Crystallization: identify minimizers of $\mathbb{W}$ or of other interesting interaction energies
- Crystallization: understand rate of decay of ρ_2
- Universality in V of local statistics, as in 1D
- Extend the CLT to higher dimensions and Riesz cases
- Prove more results on the two-component case: CLT? Kosterlitz-Thouless phase transition?

THANK YOU FOR YOUR ATTENTION!