Energy approach to Coulomb and log gases

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IHP, 21 mars 2014

The classical Coulomb gas

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

$$w(x) = \frac{1}{|x|^{d-2}} \quad \text{if } d \geq 3 \qquad = -\log|x| \quad \text{if } d = 2$$

$$-\Delta w = c_d \delta_0$$

V confining potential, sufficiently smooth and growing at infinity

Can be considered for $d = 1$ and $-\log$, then "log gas"

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

Limit $n \to \infty$?

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Motivations

- statistical mechanics
  $d = 1$ Coulomb kernel: completely solvable Lenard, Aizenman-Martin, Brascamp-Lieb $d = 1$ log gas or $d \geq 2$ Coulomb gas Lieb-Narnhofer '75, Penrose-Smith '72, Sari-Merlini '76, Alastuey-Jancovici '81 , Jancovici-Lebowitz-Manificat '93, Kiessling '93, Kiessling-Spohn '99, Chafai-Gozlan-Zitt '13
- connection to random matrices (first noticed by Wigner, Dyson), Valko-Virag, Bourgade-Erdös-Yau...
- weighted Fekete points, Fekete points on spheres Rakhmanov-Saff-Zhou

$$\min_{x_1,\dots,x_n \in \mathbb{S}^d} -\sum_{i \neq j} \log |x_i - x_j|$$

- Riesz s-energy

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

cf. Smale's 7th problem originating in computational complexity theory

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The mean field limit

- For $(x_1, \ldots, x_n)$ minimizing H_n, one can prove

$$\lim_{n\to\infty} \frac{\sum_{i=1}^n \delta_{x_i}}{n} = \mu_0 \qquad \lim_{n\to\infty} \frac{\min H_n}{n^2} = \mathcal{E}(\mu_0)$$

where μ_0 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_0 among probability measures, called the *equilibrium measure* (Frostman 50's potential theory)

- Denote $\Sigma = Supp(\mu_0)$. We assume Σ is compact with C^1 boundary and μ_0 has a density bounded above and below on Σ with is C^1 in Σ.
- Example: $V(x) = |x|^2$, then $\mu_0 = \frac{1}{c_d} \mathbb{1}_{B_1}$ (circle law).
- With temperature, a corresponding LDP can be proven (Petz-Hiai, Ben Arous-Zeitouni, for $d = 2$)
- Expanding $\sum_{i=1}^n \delta_{x_i}$ as $n\mu_0 + (\sum_{i=1}^n \delta_{x_i} - n\mu_0)$ and inserting into H_n we are able to look into next order terms.

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Approach

- In Sandier-S, we developed an *essentially 2D* approach to the problem, inspired from our work on the Ginzburg-Landau functional of superconductivity. Relies on "ball construction methods", introduced by Jerrard, Sandier in the context of GL. Works for $-\log$ in $d = 1, 2$.
- In Rougerie-S we developed an approach valid for any $d \geq 2$, based instead on Onsager's lemma (smearing out the charges). (Previous related work Rougerie-S-Yngvason)

Next order expansion of $\min H_n$ and $Z_{n,\beta}$

Theorem (ground state energy, Rougerie-S $d \geq 2$, Sandier-S $d = 1, 2$)

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

$$\min H_n =$$
$$\begin{cases} n^2\mathcal{E}(\mu_0) + n^{2-2/d}\left(\frac{\alpha_d}{c_d}\int \mu_0^{2-2/d}(x)dx + o(1)\right) & \text{if } d \geq 3 \\ n^2\mathcal{E}(\mu_0) - \frac{n}{2}\log n + n\left(\frac{\alpha_2}{2\pi} - \frac{1}{2}\int \mu_0(x)\log\mu_0(x)\,dx + o(1)\right) & \text{if } d = 2 \\ n^2\mathcal{E}(\mu_0) - n\log n + n\left(\frac{\alpha_1}{2\pi} - \int \mu_0(x)\log\mu_0(x)\,dx + o(1)\right) & \text{if } d = 1 \end{cases}$$

where $\alpha_d = \min \mathcal{W}$ depends only on d (see later).

Theorem (ctd, free energy expansion)

Assume there exists $\beta_1 > 0$ *such that*

$$\begin{cases} \int e^{-\beta_1 V(x)/2}\,dx < \infty \text{ when } d \geq 3 \\ \int e^{-\beta_1 (\frac{V(x)}{2} - \log|x|)}\,dx < \infty \text{ when } d = 2. \end{cases}$$

Let

$$F_{n,\beta} = -\frac{2}{\beta} \log Z_{n,\beta} \quad \text{free energy.}$$

if $d \geq 3$ *and* $\beta \geq cn^{2/d-1}$ *or* $d = 2$ *and* $\beta \geq c(\log n)^{-1}$

$$|F_{n,\beta} - \min H_n| \leq o(n^{2-2/d}) + C\frac{n}{\beta}.$$

$\rightsquigarrow$ transition regime $\beta \propto n^{2/d-1}$

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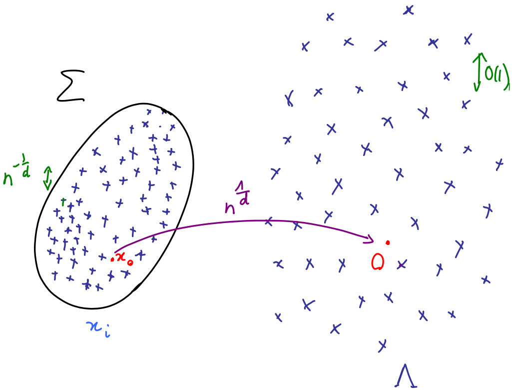
Blow-up procedure and jellium



After blow up the points should interact according to a Coulomb interaction, but screened by a fixed background charge: jellium

Some notation

- Start with the potential generated by $\sum_{i=1}^n \delta_{x_i} - n\mu_0$, and blow up.
- Set $\mu_0'(x') = \mu_0(x' n^{-1/d})$, blown-up background density and for $x_1, \ldots, x_n$, set $x_i' = n^{1/d} x_i$ and

$$h_n(x') = -c_d \Delta^{-1} \Big(\sum_{i=1}^n \delta_{x_i'} - \mu_0' \Big) = w * \Big(\sum_{i=1}^n \delta_{x_i'} - \mu_0' \Big)$$

- For any x, $\eta > 0$, let $\delta_x^{(\eta)} = \frac{1}{|B(0,\eta)|} \mathbb{1}_{B(x,\eta)}$, "smeared out" Dirac mass at scale η
- **Newton's theorem:** the potentials generated by δ_0 and $\delta_0^{(\eta)}$ (i.e. $w * \delta_0 = w$ and $w * \delta_0^{(\eta)}$) coincide outside $B(0,\eta)$, and $w \geq w * \delta_0^{(\eta)}$. Then

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can be defined unambiguously and coincides with h_n outside $\cup_i B(x_i', \eta)$.

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Splitting formula

As in Onsager's lemma (used in "stability of matter", cf Lieb-Oxford, Lieb-Seiringer): from Newton's theorem we have

$$\sum_{i\neq j} w(x_i - x_j) \geq \sum_{i\neq j} \iint w(x-y)\delta_{x_i}^{(\ell)}(x)\delta_{x_j}^{(\ell)}(y)$$

$$= \underbrace{\iint w(x-y)\Big(\sum_{i=1}^n \delta_{x_i}^{(\ell)}\Big)(x)\Big(\sum_{j=1}^n \delta_{x_j}^{(\ell)}\Big)(y)}_{\text{total interaction between smeared-out charges}} - n \underbrace{\iint w(x-y)\delta_0^{(\ell)}(x)\delta_0^{(\ell)}(y)}_{\text{cst self-interaction term}=\kappa_d c_d^{-1} w(\ell)}$$

Insert splitting $\sum_{i=1}^n \delta_{x_i}^{(\ell)} = n\mu_0 + \left(\sum_{i=i}^n \delta_{x_i}^{(\ell)} - n\mu_0\right)$ and characterization of μ_0:

$$w * \mu_0 + \frac{1}{2}V = \zeta + \left(\frac{1}{2}\mathcal{E}(\mu_0) + \iint w(x-y)\, d\mu_0(x) d\mu_0(y)\right)$$

for some function $\zeta \geq 0$, $\zeta = 0$ in Σ.
Then choose $\ell = \eta n^{-1/d}$ and blow-up everything by $n^{1/d}$.

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Proposition (Splitting formula)

For $d \geq 2$, *for any* n, $(x_1, \ldots, x_n)$, $\eta > 0$,

$$H_n(x_1, \ldots, x_n) \geq n^2 \mathcal{E}(\mu_0) - \left(\frac{n}{2} \log n\right) \mathbb{1}_{d=2}$$

$$+ n^{1-2/d} \left[\frac{1}{c_d} \left(\int_{\mathbb{R}^d} |\nabla h_{n,\eta}|^2 - n\kappa_d w(\eta) \right) - C\eta^2 \right] + \underbrace{2n \sum_{i=1}^{n} \zeta(x_i)}_{\geq 0}.$$

The next step is to study the term in brackets and take its limit $n \to \infty$, then $\eta \to 0$.

The renormalized energy

Recall

$$-\Delta h_n = c_d(\sum_{i=1}^{n} \delta_{x_i'} - \mu_0').$$

Centering the blow-up around a point $x_0 \in \Sigma$, in the limit $n \to \infty$ we get solutions to

$$-\Delta h = c_d\Big(\sum_{p\in\Lambda} N_p\delta_p - \mu_0(x_0)\Big) \longleftrightarrow -\Delta h_\eta = c_d\Big(\sum_{p\in\Lambda} N_p\delta_p^{(\eta)} - \mu_0(x_0)\Big)$$

Λ infinite discrete set of points in $\mathbb{R}^d$, $N_p \in \mathbb{N}^*$.

Definition

Let $m > 0$. Call $\overline{\mathcal{A}}_m$ the class of ∇h such that

$$-\Delta h = c_d \Big(\sum_{p \in \Lambda} N_p \delta_p - m \Big)$$

with $N_p \in \mathbb{N}^*$ and $\mathcal{A}_m$ the class of ∇h such that all $N_p = 1$.

Definition (Rougerie-S)

Set $K_R = [-R, R]^d$. For $\nabla h \in \overline{\mathcal{A}}_m$ we let

$$\mathcal{W}(\nabla h) = \liminf_{\eta \to 0} \left(\limsup_{R \to \infty} \fint_{K_R} |\nabla h_\eta|^2 - \kappa_d m w(\eta) \right).$$

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- If $\mathcal{W}(\nabla h) < +\infty$ then $\lim_{R\to\infty} \fint_{K_R} (\sum_p N_p \delta_p) = m$.
- By scaling, one can reduce to $\overline{\mathcal{A}}_1$, with

$$\inf_{\overline{\mathcal{A}}_m} \mathcal{W} = m^{2-2/d} \inf_{\overline{\mathcal{A}}_1} \mathcal{W} \qquad d \geq 3$$

$$= m \left(\inf_{\overline{\mathcal{A}}_1} \mathcal{W} - \pi \log m \right) \qquad d = 2$$

- $\mathcal{W}$ is bounded below, and has minimizers over $\overline{\mathcal{A}}_1$, even sequences of periodic minimizers (with larger and larger period)

The case of the torus

Assume Λ is $\mathbb{T}$-periodic. Then W is $+\infty$ unless all $N_p = 1$, and can be written as a function of $\Lambda \text{``}=\text{''} \{a_1, \ldots, a_M\}$, $M = |\mathbb{T}|$.

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

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

Minimization among lattices

We can look for minimizers of $\mathcal{W}$ among perfect lattice configurations (Bravais lattices) with unit volume.

Theorem (Sandier-S.)

In dimension $d = 1$ ($w = -\log$), the minimum of $\mathcal{W}$ over all possible configurations is achieved for the lattice $\mathbb{Z}$.
In dimension $d = 2$, the minimum of $\mathcal{W}$ over perfect lattice configurations is achieved uniquely, modulo rotations, by the triangular lattice.

Relies on a number theory result of Cassels, Rankin, Ennola, Diananda, 50's, on the minimization of $\zeta(s) = \sum_{p \in \Lambda} \frac{1}{|p|^s}$.

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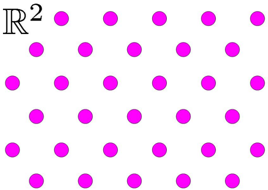
There is no corresponding result in higher dimension! In dimension 3, does the FCC (face centered cubic) lattice play this role?

Conjecture

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



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 $\mathbb{S}^2$.

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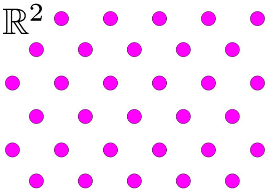

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Equidistribution of points and energy in dimension 2

Theorem (Rota Nodari-S)

Let $(x_1, \ldots, x_n) \subset (\mathbb{R}^2)^n$ *minimize* H_n*, and assume the equilibrium measure* $\mu_0 \in L^\infty$*, then*

- for all i, $x_i \in \Sigma$

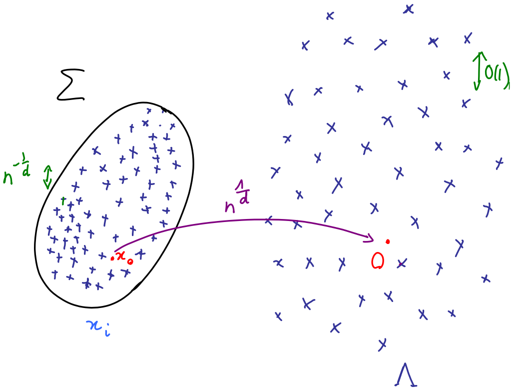
- letting $\nu_n' = \sum_i \delta_{x_i'}$*, if* $\ell \geq c > 0$ *and* $dist(K_\ell(a), \partial\Sigma') \geq n^{\beta/2}$ $(\beta < 1)$*, we have*

$$\limsup_{n\to\infty} \left| \nu_n'(K_\ell(a)) - \int_{K_\ell(a)} \mu_0'(x)\,dx \right| \leq C\ell.$$

- equidistribution of energy

$$\limsup_{n\to\infty,\eta\to 0} \left| \int_{K_\ell(a)} |\nabla h_{n,\eta}'|^2 - \kappa_d \nu_n'(K_\ell(a)) w(\eta) - \int_{K_\ell(a)} \big(\min_{\overline{\mathcal{A}}_{\mu_0'(x)}} \mathcal{W}\big)\,dx \right| \leq o_\ell(\ell^2).$$

- Method inspired by Alberti-Choksi-Otto
- We prove the same for minimizers of $\mathcal{W}$ themselves
- Should work also in $d \geq 3$
- Compare to Ameur- Ortega Cerda: only first result, with $o(\ell^2)$ error.



Σ
$n^{-\frac{1}{d}}$
x_0
x_i
$n^{\frac{1}{d}}$
$O(1)$
0
Λ

The averaged formulation

- Let $(x_1, \ldots, x_n) \in (\mathbb{R}^d)^n$. We denote P_n the probability, push-forward of the normalized Lebesgue measure on Σ by

$$x \mapsto (x, \nabla h_n(n^{1/d} x + \cdot))$$

  where h_n is the potential generated by $\sum_{i=1}^n \delta_{x_i'} - \mu_0'$.
- If the next order terms in H_n are bounded by $Cn^{2-2/d}$, then P_n is tight and up to a subsequence converges to some probability P
- P belongs to the class $\mathcal{C}$ of probabilities on $(x, \nabla h)$'s such that
  1. The first marginal of P is the normalized Lebesgue measure on Σ, and P is translation-invariant
  2. For $P-$a.e. $(x, \nabla h)$, we have $\nabla h \in \overline{\mathcal{A}}_{\mu_0(x)}$.
- Define then $\widetilde{\mathcal{W}}(P) = \frac{|\Sigma|}{c_d} \int \mathcal{W}(\nabla h)\, dP(x, \nabla h)$

$$\min_{\mathcal{C}} \widetilde{\mathcal{W}} = \frac{1}{c_d} \int_\Sigma \min_{\overline{\mathcal{A}}_{\mu_0(x)}} \mathcal{W}\, dx.$$

Theorem (Rougerie-S)

Let $d \geq 2$, $(x_1, \ldots, x_n) \in (\mathbb{R}^d)^n$ and P_n be as above. Up to extraction of a subsequence, we have $P_n \to P \in \mathcal{C}$ and

$$\liminf_{n\to\infty} n^{2/d-2}\left(H_n(x_1,\ldots,x_n) - n^2\mathcal{E}(\mu_0) + (\frac{n}{2}\log n)\mathbb{1}_{d=2}\right) \geq \widetilde{\mathcal{W}}(P).$$

This lower bound is sharp, thus for minimizers of H_n

$$\liminf_{n\to\infty} n^{2/d-2}\left(\min H_n - n^2\mathcal{E}(\mu_0) + (\frac{n}{2}\log n)\mathbb{1}_{d=2}\right) = \min_{\mathcal{C}} \widetilde{\mathcal{W}}$$

and P minimizes $\widetilde{\mathcal{W}}$ over $\mathcal{C}$ (i.e. P-a.e. $(x, \nabla h)$ we have ∇h minimizes $\mathcal{W}$ over $\overline{\mathcal{A}}_{\mu_0(x)}$).

Informally: for minimizers, after blow-up around "almost every point in Σ", we get in the limit $n \to \infty$ an infinite configuration of points minimizing $\mathcal{W}$ in the corresponding class.

Microscopic behavior of thermal states

Theorem (Rougerie-S $d \geq 3$, Sandier-S $d = 2$)

Let $\bar{\beta} = \limsup_{n \to +\infty} \beta n^{1-2/d}$*, assume* $\bar{\beta} > 0$*. Then, there exists* $C_{\bar{\beta}}$ *such that* $\lim_{\bar{\beta} \to \infty} C_{\bar{\beta}} = 0$*, and if* $A_n \subset (\mathbb{R}^d)^n$

$$\limsup_{n \to \infty} \frac{\log \mathbb{P}_{n,\beta}(A_n)}{n^{2-2/d}} \leq -\frac{\beta}{2} \left(\inf_{P \in A_\infty} \widetilde{\mathcal{W}} - \xi_d - C_{\bar{\beta}} \right)$$

where

$$A_\infty = \{P : \exists (x_1, \ldots, x_n) \in A_n, \, P_n \to P \text{ up to a subsequence}\}.$$

Extensions (ongoing)

- With T. Leblé, full LDP at speed $n^{2-2/d}$ with rate function

$$\frac{\beta}{2}\widetilde{\mathcal{W}}(P) + Ent(P)$$

  where Ent is a specific relative entropy with respect to a Poisson-type process.

- With M. Petrache, case of Riesz kernel interaction potential:

$$H_n(x_1,\dots,x_n) = \sum_{i\neq j} \frac{1}{|x_i - x_j|^s} + n\sum_{i=1}^n V(x_i) \quad d-2<s<d$$

  similar “renormalized energy" derived for minimizers

Thank you for your attention!