# Energy approach to Coulomb and log gases

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IAS workshop, April 3, 2014

# The classical Coulomb gas Hamiltonian

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

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

$$-\Delta w = c_d \delta_0 \quad \text{if } d \geq 2$$

$V$ confining potential, sufficiently smooth and growing at infinity

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
- connection to random matrices (first noticed by Wigner, Dyson)
  $d = 1$ 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, Frohlich-Spencer '81, Jancovici-Lebowitz-Manificat '93, Kiessling '93, Kiessling-Spohn '99, Chafai-Gozlan-Zitt '13, Valko-Virag '09, Bourgade-Erdös-Yau '12, Scherbina '14, Beckerman-Figalli-Guionnet '14...
- 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

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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 $\mu_0$ 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 $\mu_0$ among probability measures, called the *equilibrium measure* (Frostman 50's potential theory)

- Denote $\Sigma = Supp(\mu_0)$. We assume $\Sigma$ is compact with $C^1$ boundary and if $d \geq 2$ that $\mu_0$ has a density bounded above and below on $\Sigma$ with is $C^1$ in $\Sigma$.
- With temperature, a corresponding LDP can be proven (Petz-Hiai, Ben Arous-Zeitouni, Ben Arous-Guionnet, Chafai-Gozlan-Zitt)
- We look at next order terms by 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 $H_n$.

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# Approach

- In Sandier-S, we developed an *essentially 2D* approach to the problem, inspired from our work on vortices in Ginzburg-Landau. 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*

$$\begin{cases} \int e^{-\beta_1 V(x)/2}\, dx < \infty \text{ when } d \geq 3 \\ \int e^{-\beta_1 (\frac{V(x)}{2} - \log|x|)}\, dx < \infty \text{ when } d = 1, 2. \end{cases}$$

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

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

$\rightsquigarrow$ transition regime $\beta \gg n^{2/d-1}$ if $d \geq 3$, $\beta \gg 1$ if $d = 1, 2$

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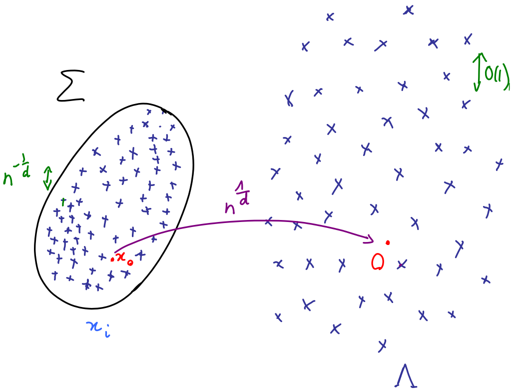
# Blow-up procedure and jellium




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 $\eta$
- **Newton's theorem:** the potentials generated by $\delta_0$ 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

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

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 equilibrium measure $\mu_0$:

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

for some function $\zeta \geq 0$, $\zeta = 0$ in $\Sigma$.
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 $\eta \to 0$.

Dimension 1 is treated in the same way after imbedding the real line into the plane and considering

$$h_n(x', y') = w * \left( \sum_i \delta_{(x_i', 0)} - \mu_0'(x') \delta_{y'=0} \right) \qquad w = -\log |\cdot|$$

equivalent to taking Stieltjes transform

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$$h_n(x', y') = w * \left(\sum_i \delta_{(x'_i, 0)} - \mu'_0(x') \delta_{y'=0}\right) \qquad w = -\log|\cdot|$$

equivalent to taking Stieltjes transform

# 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

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

$\Lambda$ 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 $\nabla h$ such that

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

with $N_p \in \mathbb{N}^*$.

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

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

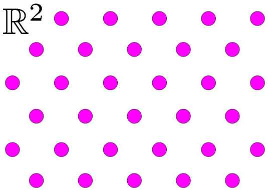
where $G$= Green's function of the torus ($-\Delta G = \delta_0 - 1/|\mathbb{T}|$).

# Partial minimization results

**Theorem (Sandier-S.)**

*In dimension $d = 1$ ($w = -\log$), the minimum of $\mathcal{W}$ over all possible configurations is achieved for the lattice $\mathbb{Z}$ ("clock distribution"). In dimension $d = 2$, the minimum of $\mathcal{W}$ over perfect lattice configurations (Bravais lattices) with fixed volume 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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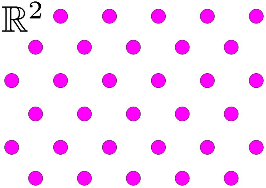

There is no corresponding result in higher dimension! In dimension 3, does the FCC (face centered cubic) lattice play this role?

## Conjecture

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

- 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 $\mathbb{S}^2$.
- by our result, solving the conjecture (or identifying $\min \mathcal{W}$) is equivalent to computing the $\lim_{\beta\to\infty}$ of the order $n$ term in $\log Z_{n,\beta}$
- $\mathcal{W}$ is a measure of disorder of a given point configuration
- it allows to control things such as fluctuations of number of points

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# Equidistribution of points and energy in dimension 2

## Theorem (Rota Nodari-S)

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

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

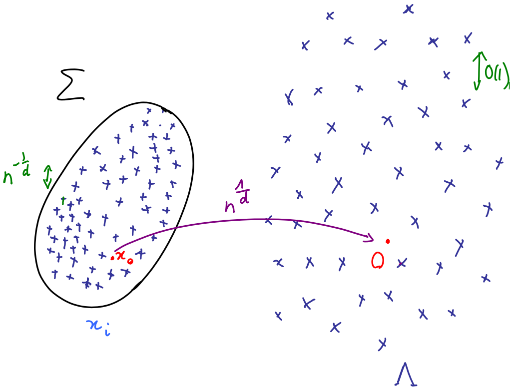
*- letting* $\nu_n'=\sum_i\delta_{x_i'}$*, if* $\ell\ge c>0$ *and* $dist(K_\ell(a),\partial\Sigma')\ge n^{\beta/2}$ $(\beta<1)$*, we have*

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

*- equidistribution of energy*

$$\limsup_{n\to\infty,\eta\to0}\left|\int_{K_\ell(a)}|\nabla h_{n,\eta}'|^2-\kappa_d\nu_n'(K_\ell(a))w(\eta)\right.$$
$$\left.-\int_{K_\ell(a)}(\min_{\mathcal{A}_{\mu_0'(x)}}\mathcal{W})\,dx\right|\le o_\ell(\ell^2).$$

- 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
$n^{-\frac{1}{d}}$
$x_0$
$x_i$
$n^{\frac{1}{d}}$
0
O(1)
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 $\Sigma$ 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 $\Sigma$, 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 $\nabla h$ minimizes $\mathcal{W}$ over $\overline{\mathcal{A}}_{\mu_0(x)}$).*

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

# Microscopic behavior with temperature (LDP style)

**Theorem (Rougerie-S $d \geq 3$, Sandier-S $d = 1, 2$)**

*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*

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

# 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 the specific relative entropy with respect to a Poisson process (cf. Rassoul Agha - Seppalainen)

- gives the existence of a thermodynamic limit or order $n$ term in $\log Z_{n,\beta}$ expansion
- shows crystallization happens for $\beta \gg n^{2/d-1}$ but not before

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

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

similar “renormalized energy" derived for minimizers
Use extension to one more space dimension to replace $\Delta^\alpha$ by a local operator (Caffarelli-Silvestre)

- E. Sandier, S.S. 2D Coulomb Gases and the Renormalized Energy, to appear in *Annals of Proba*.
- E. Sandier, S.S. 1D Log Gases and the Renormalized Energy: Crystallization at Vanishing Temperature, `arXiv`
- S. Rota Nodari, S.S. Renormalized Energy Equidistribution and Local Charge Balance in 2D Coulomb Systems, to appear in *IMRN*
- N. Rougerie, S. S. Higher Dimensional Coulomb Gases and Renormalized Energy Functionals, `arXiv`


Thank you for your attention!