Renormalized Energy Equidistribution and Local Charge Balance in Coulomb Systems

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Framework

Model: n charged particles confined by an external potential in any dimension

$$H_n(x_1,\dots,x_n) = \sum_{i\neq j} g(x_i - x_j) + n \sum_{i=1}^{n} V(x_i) \qquad \text{(H)}$$

Repulsive pair-interaction

Mean-field regime

Confining external potential

Interaction kernel:

$$g(x) = \frac{1}{|x|^s} \qquad \max(0, d-2) \leq s < d,$$

$$g(x) = -\log|x| \qquad d = 1, 2.$$

$\rightsquigarrow$ fundamental solution for $(-\Delta)^{\frac{d-s}{2}}$ on $\mathbb{R}^d$.

Coulomb gases: $s = d-2$ or $g(x) = -\log|x|$ for $d = 2$

External potential V : sufficiently smooth potential such that

$$\lim_{|x|\to+\infty} \frac{V(x)}{2} - \log|x| = +\infty \text{ or } \lim_{|x|\to+\infty} V(x) = +\infty$$

Crystallization Conjecture : appearance of periodic structures for minimizers

Macroscopic behavior of minimizers

Convergence of minimizers: $\{(x_1, \ldots, x_n)\}_n$ minimizer of H_n

$$\underbrace{\frac{1}{n}\sum_{i=1}^{n}\delta_{x_i}}_{\text{empirical measure}} = \frac{1}{n}\nu_n \rightharpoonup \mu_V \quad \text{(in the sense of probability measures)}$$

- μ_V is the unique minimizer over $\mathcal{P}(\mathbb{R}^d)$ of

$$I(\mu) = \iint_{\mathbb{R}^d \times \mathbb{R}^d} g(x-y)\, d\mu(x) d\mu(y) + \int_{\mathbb{R}^d} V(x)\, d\mu(x).$$

First order expansion of H_n: $H_n(x_1, \ldots, x_n) = n^2 I(\mu_V) + o(n^2)$.
Remark :

- existence and characterization of the equilibrium measure μ_V (Frostman, 1935)
- convergence of minimizers and minima of H_n (Choquet, 1959)

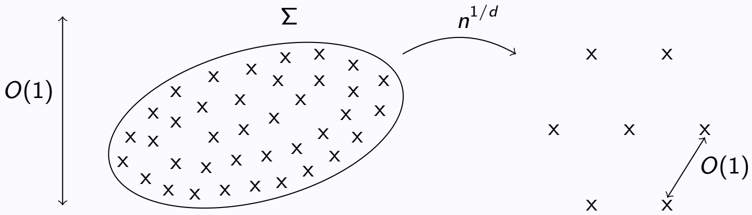
$\rightsquigarrow$ mean-field behavior of ground states: points distribute themselves macroscopically according to the probability law μ_V

Microscopic behavior of minimizers

Goal: understand the optimal microscopic distribution of points

Idea:

1. expand the Hamiltonian to the next order (Coulomb case : done by Sandier-Serfaty ($d = 2$) and Rougerie-Serfaty ($d > 2$), Riesz case: done by Petrache-Serfaty)
2. blow-up the configurations by the factor $n^{1/d}$ (inverse of the typical distance between two points) $\rightsquigarrow$ well-separated point typically with distance $O(1)$



- $\Sigma = \mathrm{supp}(\mu_V)$ compact with $\mathcal{C}^1$ boundary
- m_V density of μ_V bounded and sufficiently regular

Splitting of H_n in the Coulomb case

- Write $\nu_n = \sum_{i=1}^{n} \delta_{x_i}$ as $\nu_n = \underbrace{n\mu_V}_{\text{leading order}} + \underbrace{(\nu_n - n\mu_V)}_{\text{fluctuations}}$
- Insert in the definition of H_n

$$H_n(x_1, \ldots, x_n) = \iint_{\Delta^c} g(x-y)\, d\nu_n(x) d\nu_n(y) + n \int V(x)\, d\nu_n(x)$$
$$= n^2 I(\mu_V) + 2n \sum_{i=1}^{n} \zeta(x_i) + \iint_{\Delta^c} g(x-y)\, d(\nu_n - n\mu_V)(x) d(\nu_n - n\mu_V)(y)$$

with $\zeta = \int g(x-y)\, d\mu_V(x) + \frac{V}{2} - c$, $\zeta = 0$ on Σ and $\zeta > 0$ on Σ^c

- Define $h_n := \int g(x-y)\, d(\nu_n - n\mu_V)(y)$ so that $-\Delta h_n = c_d(\nu_n - n\mu_V)$. Formally

$$\iint_{\Delta^c} g(x-y)\, d(\nu_n - n\mu_V)(x) d(\nu_n - n\mu_V)(y) = \int h_n d(\nu_n - n\mu_V)$$
$$= \int h_n \left(-\frac{1}{c_d} \Delta h_n \right) \approx \frac{1}{c_d} \int |\nabla h_n|^2$$

Problem: $\nabla h_n \notin L^2 \to$ truncation procedure

Truncation procedure

Given $\eta > 0$, define $f_\eta(x) = (g(x) - g(\eta))_+$ and $\delta_0^{(\eta)} := \frac{\Delta f_\eta}{c_d} + \delta_0$.

- $\delta_0^{(\eta)}$ uniform positive measure of mass 1 on $\partial B(0, \eta)$
- $$-\Delta f_\eta = c_d(\delta_0 - \delta_0^{(\eta)})$$

Truncated potential: $h_{n,\eta}(x) = h_n(x) - \sum_{i=1}^{n} f_\eta(x - x_i) \rightsquigarrow$

$$-\Delta h_{n,\eta} = c_d \left(\sum_{i=1}^{n} \delta_{x_i}^{(\eta)} - n\mu_V \right)$$

$\rightarrow$ "smearing out" each Dirac charge uniformly onto the sphere of radius η centered at the charge

Lemma

$$\iint_{\Delta^c} g(x-y)\, d(\nu_n - n\mu_V)(x) d(\nu_n - n\mu_V)(y) = \lim_{\eta \to 0} \left(\frac{1}{c_d} \int_{\mathbb{R}^d} |\nabla h_{n,\eta}|^2 - n g(\eta) \right)$$

Blow-up and splitting formula

Blow-up: $x' := n^{1/d}x,\ m'_V(x') = m_V(x),\ \Sigma' = \mathrm{supp}(\mu'_V) = n^{1/d}\Sigma$

$$-\Delta h'_n = c_d\left(\sum_{i=1}^{n}\delta_{x'_i} - \mu'_V\right) \text{ and } -\Delta h'_{n,\eta} = c_d\left(\sum_{i=1}^{n}\delta^{(\eta)}_{x'_i} - \mu'_V\right)$$

Remark : $h'_n(x') = -\left(\frac{1}{2}\log n\right)\mathbf{1}_{d=2} + n^{2/d-1}h_n(x)$.

Proposition (Splitting formula)

For any $n \geq 1$, for any configuration of distinct points $x_1, \ldots, x_n$ in $\mathbb{R}^d$, $d \geq 2$, the following identity holds :

$$H_n(x_1,\ldots,x_n) = n^2 I(\mu_V) + 2n\sum_{i=1}^{n}\zeta(x_i) - \left(\frac{n}{2}\log n\right)\mathbf{1}_{d=2}$$
$$+\frac{n^{1-2/d}}{c_d}\lim_{\eta\to 0}\left(\int_{\mathbb{R}^d}|\nabla h'_{n,\eta}|^2 - nc_d g(\eta)\right)$$

ζ : effective potential which favors configurations where the points x_i are in $\mathrm{supp}(\mu_V)$

Goal: Analyze the behavior of the last term as n goes to infinity $\rightarrow$ definition of the renormalized energy $\mathcal{W}$

Renormalized energy

Renormalized energy: total Coulomb interaction energy of an infinite configuration of points in the whole space in a constant neutralizing background $\rightarrow$ jellium

Formally,

$$-\Delta h'_n = c_d \left(\sum_{i=1}^{n} \delta_{x'_i} - \mu'_V \right) \xrightarrow[n \to +\infty]{} -\Delta h = c_d \left(\sum_{p \in \Lambda} N_p \delta_p - m \right)$$

with Λ a discrete set of points in $\mathbb{R}^d$, $N_p \in \mathbb{N}^*$, and $m = m_V(0)$ a positive constant (which depends on the center of the blow-up).

Admissible electric fields $\mathcal{A}_m$: $E = \nabla h$ such that

$$-\mathrm{div} E = c_d \left(\sum_{p \in \Lambda} \delta_p - m(x) \right)$$

in $\mathbb{R}^d$ for some discrete set $\Lambda \subset \mathbb{R}^d$ and $m : \mathbb{R}^d \to \mathbb{R}_+$ a nonnegative density function.

Remarks: We take $N_p = 1$ since we are dealing with minimizers

Truncated electric fields: For any $E \in \mathcal{A}_m$ and any $\eta > 0$, let

$$E_\eta = E - \sum_{p \in \Lambda} f_\eta(\cdot - p)$$

Renormalized energy

Renormalized energy: Let $E \in \mathcal{A}_m$ and $\eta > 0$. For any Borel set $A \subset \mathbb{R}^d$, we define

$$\mathcal{W}_\eta(E, A) = \int_A |E_\eta|^2 - c_d g(\eta) \int_A \sum_{p \in \Lambda} \delta_p^{(\eta)}.$$

and

$$\mathcal{W}(E) = \lim_{\eta \to 0} \limsup_{R \to +\infty} \frac{\mathcal{W}_\eta(E, K_R)}{|K_R|}$$

where $K_R = [-R/2, R/2]^d$.

Known results: minimizers of H_n tend to minimize $\mathcal{W}$ after blow-up at scale $n^{1/d}$ around almost every point in Σ (Sandier-Serfaty, Rougerie-Serfaty and Petrache-Serfaty)

Goal: understand the behavior of minimizers of $\mathcal{W}$

Remarks:

- if m is constant $\min_{\mathcal{A}_m} \mathcal{W}$ is finite and achieved for any $d \geq 2$
- for $d = 2$ the triangular lattice is the minimizer over lattices

Equidistribution of the renormalized energy for Coulomb gases

Theorem ((RN, Serfaty 2015, Petrache, RN 2018))

Let $(x_1, \dots, x_n)$ be a minimizer of H_n and $E_n' = \nabla h_n'$ be the vector fields expressed as the gradient of the potentials of blow-up configurations corresponding to these minimizer. There exists $q \in]0,1[$ such that for $a_n \in \Sigma'$, if $K_\ell = a_n + [-\ell/2, \ell/2]^d \subset \mathbb{R}^d$ and in the regime where $\mathrm{dist}(K_\ell(a_n), \partial\Sigma') \geq n^{q/d}$, we have

$$\lim_{\eta\to 0} \limsup_{\ell\to\infty} \limsup_{n\to\infty} \left| \frac{\mathcal{W}_\eta(E_n', K_\ell(a_n))}{|K_\ell|} - \frac{1}{|K_\ell|} \int_{K_\ell(a_n)} \min_{\mathcal{A}_{m_V'(x')}} \mathcal{W} \, dx' \right| = 0 \qquad (1)$$

- minimizers of H_n tend to minimize $\mathcal{W}$ after blow-up at scale $n^{1/d}$ around any point in Σ (sufficiently far from $\partial\Sigma$)
- for minimizers of H_n, renormalized energy $\mathcal{W}_\eta$ is equidistributed at the microscopic scale in an arbitrary hypercube provided that the hypercube is chosen sufficiently far away from $\partial\Sigma$

Question: Can we interchange the renormalization limit $\eta \to 0$ with the other ones ? Not easy because of the lack of control on the support of the smeared charges $\delta_p^{(\eta)}$

Equidistribution of the renormalized energy for Coulomb gases

Idea of the proof:

- screening procedure + bootstrap argument
- select hypercubes K with good boundaries $\rightsquigarrow \int_K |E_\eta|^2 \leq C|K|$

Problem: Error terms are multiplied by $g(\eta)$

Solution: Allow perturbations of the boundary of $K_\ell(a_n)$ and use charge separation result for minimizers

Theorem ((Petrache, RN 2018))

Let $(x_1, \ldots, x_n)$ be a minimizer of H_n and $E_n' = \nabla h_n'$ as before.
There exists $q \in]0,1[$ such that for $a_n \in \Sigma'$, if $K_\ell = a_n + [-\ell/2, \ell/2]^d \subset \mathbb{R}^d$ and in the regime where $\mathrm{dist}(K_\ell(a_n), \partial\Sigma') \geq n^{q/d}$, there exist sets Γ_n which can be expressed as bi-Lipschitz deformations $f_n : K_\ell(a_n) \to \Gamma_n$ such that $\|f_n - \mathrm{Id}\|_{L^\infty} \leq 1$ and such that we have

$$\limsup_{\ell\to\infty} \limsup_{n\to\infty} \left| \frac{\mathcal{W}(E_n', \Gamma_n)}{|\Gamma_n|} - \frac{1}{|\Gamma_n|} \int_{\Gamma_n} \min_{\mathcal{A}_{m_V'(x')}} \mathcal{W}\, dx' \right| = 0. \tag{2}$$

Moreover, we may assume that Γ_n is a hyperrectangle.

Remark: This result has been recently improved by Armstrong-Serfaty.

Bound on charge discrepancy for Coulomb gases

Theorem ((RN, Serfaty 2015, Petrache, RN 2018))

Under the same hypotheses as before, consider a regime in which (1) holds. Then letting

$$\nu_n' = \sum_{i=1}^{n} \delta_{x_i'},$$

we have a finite asymptotic bound of the discrepancy of the ν_n' with respect to μ_V' as follows:

$$\limsup_{\ell\to\infty}\limsup_{n\to\infty}\frac{1}{\ell^{d-1}}\left|\nu_n'(K_\ell(a)) - \int_{K_\ell(a)} m_V'(x)\,dx\right| < \infty$$

Remarks: Ameur, Ortega-Cerdà prove that $\left|\nu_n'(K_\ell(a)) - \int_{K_\ell(a)} m_V'(x)\,dx\right| = o(\ell^d)$

Perspective: Extend the results to Riesz gases (without 'too strong' additional conditions)