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Large Systems with Coulomb Interactions : Variational Study and Statistical Mechanics

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Abstract. Systems with Coulomb and logarithmic interactions arise in various settings: an instance is the classical Coulomb gas which in some cases happens to be a random matrix ensemble, another is vortices in the Ginzburg-Landau model of superconductivity, where one observes in certain regimes the emergence of densely packed point vortices forming perfect triangular lattice patterns named Abrikosov lattices, a third is the study of Fekete points which arise in approximation theory. In this review, we describe tools to study such systems and derive a next order (beyond mean field limit) "renormalized energy" that governs microscopic patterns of points. We present the derivation of the limiting problem and the question of its minimization and its link with the Abrikosov lattice and crystallization questions. We also discuss generalizations to Riesz interaction energies and the statistical mechanics of such systems. This is based on joint works with Etienne Sandier, Nicolas Rougerie, Simona Rota Nodari, Mircea Petrache, and Thomas Leblé.

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1. Introduction and motivations

We are interested in the following class of energies

$$H_n(x_1, \ldots, x_n) = \sum_{i \neq j} g(x_i - x_j) + n \sum_{i=1}^{n} V(x_i) \tag{1.1}$$

where $x_1, \ldots, x_n$ are n points in $\mathbb{R}^d$ and the interaction kernel g is given by either

$$g(x) = \frac{1}{|x|^{d-2}} \qquad d \geq 3, \tag{1.2}$$

or

$$g(x) = -\log|x| \quad \text{in dimension } d = 2. \tag{1.3}$$

Later we will also discuss generalizations to

$$g(x) = \frac{1}{|x|^s} \qquad \max(0, d-2) \le s < d, \ d \ge 1, \tag{1.4}$$

or

$$g(x) = -\log|x| \quad \text{in dimension } d = 1, \tag{1.5}$$

that can be treated with slight modifications. We are interested in the asymptotics $n \to \infty$ of the minimum of H_n. One notes that in the cases (1.2)–(1.3), g is a multiple of the Coulomb kernel in dimension d, and there is a constant c_d depending only on d such that

$$-\Delta g = c_d \delta_0, \tag{1.6}$$

where δ_0 is the Dirac mass at the origin.

We now review various motivations for studying such systems.

1.1. Fekete points. Fekete points arise in interpolation theory as the points minimizing interpolation errors for numerical integration [SaTo]. They are often studied on manifolds, such as the d-dimensional sphere, and then correspond to sets of n points which maximize

$$\prod_{i \neq j} |x_i - x_j|.$$

Equivalently they minimize

$$-\sum_{i \neq j} \log|x_i - x_j|.$$

In Euclidean space, one also considers "weighted Fekete points" which maximize

$$\prod_{i \neq j} |x_i - x_j| e^{-n \sum_i V(x_i)}$$

or equivalently minimize

$$-\sum_{i \neq j} \log|x_i - x_j| + n \sum_{i=1}^{n} V(x_i)$$

which in dimension 2 corresponds exactly to the minimization of our Hamiltonian H_n in the particular case (1.3). They also happen to be zeroes of orthogonal polynomials, see [Si].

Since $-\log|x|$ can be obtained as $\lim_{s\to 0}\frac{1}{s}(|x|^{-s}-1)$, there is also interest in studying "Riesz s-energies", i.e. the minimization of

$$\sum_{i\neq j}\frac{1}{|x_i-x_j|^s} \tag{1.7}$$

for all possible s, hence a motivation for (1.4). On all these matters we refer to [SaTo], the review paper [SK, BHS] and the forthcoming monograph [BHS].

1.2. Statistical mechanics. The study of H_n is also interesting for understanding the associated Gibbs measure

$$d\mathbb{P}_{n,\beta}(x_1,\dots,x_n)=\frac{1}{Z_{n,\beta}}e^{-\frac{1}{2}\beta H_n(x_1,\dots,x_n)}\,dx_1\dots,dx_n \tag{1.8}$$

where $\beta>0$ represents an inverse temperature and $Z_{n,\beta}$ is the partition function of the system, i.e. a number that normalizes $\mathbb{P}_{n,\beta}$ to a probability measure on $(\mathbb{R}^d)^n$. This corresponds to the Gibbs measure of a classical "Coulomb gas system" (or a log gas in cases (1.5)–(1.3)) (cf. [Forr]), by extension we can also call it a "Riesz gas" in the case (1.4). Such systems have been studied in the physics literature [SM, JLM, LiLe, LN, PeSm]. They can be considered as a toy model for matter, with classical particles. As always with such statistical mechanics ensembles, one would like to understand the behavior in terms of the temperature: are there critical temperatures corresponding to phase transitions for which the nature of the states changes?

1.3. Random matrix theory. The study of (1.8) has attracted a lot of attention due to its connection with random matrix theory. As first noticed by [Wi, Dy], in the particular cases (1.5)–(1.3) the Gibbs measure (1.8) also corresponds to the law of the eigenvalues (which can be computed algebraically) of some famous random matrix ensembles:

- when (1.3), with $\beta=2$ and $V(x)=|x|^2$, (1.8) is the law of the (complex) eigenvalues of an $n\times n$ matrix where the entries are chosen to be normal Gaussian i.i.d. This is called the *Ginibre ensemble.*
- when (1.5), with $\beta=2$ and $V(x)=x^2/2$, (1.8) is the law of the (real) eigenvalues of an $n\times n$ Hermitian matrix with complex normal Gaussian iid entries. This is called the Gaussian Unitary Ensemble.
- when (1.5), $\beta=1$ and $V(x)=x^2/2$, (1.8) is the law of the (real) eigenvalues of an $n\times n$ real symmetric matrix with normal Gaussian iid entries. This is called the Gaussian Orthogonal Ensemble.
- when (1.5), $\beta=4$ and $V(x)=x^2/2$, (1.8) is the law of the eigenvalues of an $n\times n$ quaternionic symmetric matrix with normal Gaussian iid entries.

One thus observes in these ensembles the phenomenon of "repulsion of eigenvalues": they repel each other logarithmically, i.e. like two-dimensional Coulomb particles.

The particular choice of $\beta = 2$ makes these *determinantal* point processes because then the law can be rewritten

$$\frac{1}{Z_{n,\beta}} \left(\prod_{i<j} |x_i - x_j| \right)^2 e^{-n\sum_{i=1}^n V(x_i)} \, dx_1 \dots dx_n$$

where a square Vandermonde determinant appears. This allows to compute algebraically a lot of quantities in this particular case, such as the partition functions (when V is x^2), the limiting processes at the microscopic scale, etc, and there is a large literature on this. In [BEY1, BEY2], Bourgade-Erdös and Yau manage to understand the case (1.5) for all β and general V, and they show the *universality* (after suitable rescaling) of the microscopic behavior and local statistics of the points, i.e. the fact that they are essentially independent of V.

1.4. Vortices in condensed matter physics. Interaction energies of the form (1.1) in the case (1.3) also arise as effective interaction energies for vortices in models from condensed matter physics: the Ginzburg-Landau model of superconductivity and the Gross-Pitaevskii functionals for superfluids and Bose-Einstein condensates. In this spirit, the mathematical study of such vortices started with Bethuel-Brezis-Hélein [BBH] who studied the simplified functional

$$E_\varepsilon(u) = \frac{1}{2} \int_\Omega |\nabla u|^2 + \frac{(1-|u|^2)^2}{2\varepsilon^2}$$

where u is a function from a two-dimensional (bounded simply connected) domain Ω to the complex plane $\mathbb{C}$, which is prescribed to take boundary values $u = g$ with g a map from $\partial\Omega$ to $\mathbb{S}^1$ of nonzero topological degree n. Bethuel, Brezis and Hélein analyzed minimizers of E_ε under this boundary condition, and showed that they have n zeroes (or *vortices*) of topological degree 1, at locations $x_1^\varepsilon, \dots, x_n^\varepsilon$. These points tend as $\varepsilon \to 0$, to minimize a "renormalized energy"

$$W(x_1, \dots, x_n) = -\sum_{i \neq j} \log |x_i - x_j| + \sum_{i,j} R(x_i, x_j)$$

where R is a regular function depending on the boundary data g. They also proved that

$$\min E_\varepsilon \sim \pi n |\log \varepsilon| + \min W \quad \text{as } \varepsilon \to 0,$$

where the leading order term $\pi n|\log \varepsilon|$ corresponds to the "self-interaction" of all the vortices, and the second order term $\min W$ governs the vortex locations.

The original Ginzburg-Landau model of superconductivity contains a gauge and an applied magnetic field:

$$G_\varepsilon(u, A) = \frac{1}{2} \int_\Omega |\nabla_A u|^2 + |\nabla \times A - h_{ex}|^2 + \frac{(1-|u|^2)^2}{2\varepsilon^2}. \tag{1.9}$$

Here $A : \Omega \to \mathbb{R}^2$ is the gauge of the magnetic field, $\nabla_A = \nabla - iA$ is the covariant derivative, $h := \nabla \times A = \partial_2 A_1 - \partial_1 A_2$ is the induced magnetic field in the sample. The constant parameters are h_{ex}, the intensity of the external magnetic field, and ε a material constant, which is often small. Associated to this functional are the Ginzburg-Landau equations:

$$\text{(GL)} \begin{cases} -(\nabla_A)^2 u = \dfrac{1}{\varepsilon^2} u(1-|u|^2) & \text{in } \Omega \\ -\nabla^{\perp} h = \langle iu, \nabla_A u \rangle & \text{in } \Omega \\ h = h_{ex} & \text{on } \partial\Omega \\ \nabla_A u \cdot \nu = 0 & \text{on } \partial\Omega, \end{cases}$$

where $\nabla^{\perp}$ denotes the operator $(-\partial_2, \partial_1)$, ν is the outer unit normal to $\partial\Omega$ and $\langle a, b \rangle$ is the scalar product in $\mathbb{C}$ as identified with $\mathbb{R}^2$.

The analysis of [BBH] was first generalized to the model with gauge, still with fixed boundary conditions, in [BR]. In the true physics model, vortices arise due to the h_{ex} parameter, with no prescribed boundary data. In the experiments and physics predictions, it is observed that when h_{ex} is above a first critical field H_{c_1} of order $|\log \varepsilon|$, then vortices start to appear. Their number increases as h_{ex} is further increased, and they tend to form perfect triangular *Abrikosov* lattices, named after the physicist Abrikosov who first predicted them.

Several of these features have been proven rigorously in a series of works on the vortices in this Ginzburg-Landau model, which are summarized in [SS1]. (In that reference one can also find a detailed introduction to the functional, as well as references to the mathematics and physics literature.) To analyze the vortices in (1.9) one defines the vorticity of a configuration (u, A) as

$$\mu(u, A) = \nabla \times \langle iu, \nabla_A u \rangle + \nabla \times A.$$

This is the gauge-invariant analogue of the standard vorticity, such as the one defined in fluids. One can show that in the asymptotics $\varepsilon \to 0$, for configurations whose energy is reasonably controlled one has

$$\mu(u, A) \simeq \nabla \times \langle iu, \nabla u \rangle \simeq 2\pi \sum_i d_i \delta_{x_i} \tag{1.10}$$

where x_i are the vortex centers and d_i their integer degrees (all possibly depending on ε). This is not exact, however it can be given some rigorous meaning in some functional space in the asymptotics $\varepsilon \to 0$ (cf. [SS1, Chap. 6]). A more true statement is that the right hand side is a sum of approximate Diracs, smeared out at the scale ε, which we will denote by $\delta_{x_i}^{(\varepsilon)}$. Taking the curl (or the vector product with ∇) of the second equation in (GL) leads to

$$-\Delta h = \nabla \times \langle iu, \nabla_A u \rangle = \mu(u, A) + \nabla \times A$$

or in other terms to what is called the London equation:

$$\begin{cases} -\Delta h + h \simeq 2\pi \sum_i d_i \delta_{x_i}^{(\varepsilon)} & \text{in } \Omega \\ h = h_{ex} & \text{on } \partial\Omega. \end{cases} \tag{1.11}$$

In an electrostatic analogy, h is thus like a Coulomb (or more accurately Yukawa) potential generated by the point vortices, which behave like (smeared out) point charges. Assuming for simplicity that all degrees are $+1$ (which is true for energy minimizers), we may then write with (1.11) that

$$h - h_{ex} = \int_\Omega G_\Omega(x,y)(2\pi \sum_i \delta_{x_i}^{(\varepsilon)} - h_{ex})$$

where G_Ω is the kernel of $-\Delta + I$ with Dirichlet boundary condition i.e.

$$\begin{cases} -\Delta_x G_\Omega + G_\Omega = \delta_y & \text{in } \Omega \\ G_\Omega = 0 & \text{on } \partial\Omega. \end{cases} \tag{1.12}$$

Of course $G_\Omega(x,y) \sim -\log|x-y| + R(x,y)$ where R is some regular remainder, so G_Ω behaves essentially like the two-dimensional Coulomb kernel. One has $|u| \simeq 1$ and $|\nabla_A u|^2 \simeq |\nabla h|^2$ as $\varepsilon \to 0$ by using the second equation in (GL), and then one may formally rewrite (1.9) as

$$\begin{aligned} G_\varepsilon(u,A) &\simeq \frac{1}{2}\int_\Omega |\nabla h|^2 + |h - h_{ex}|^2 \\ &= \frac{1}{2}\iint G_\Omega(x,y)(2\pi \sum_i \delta_{x_i}^{(\varepsilon)} - h_{ex})(x)(2\pi \sum_i \delta_{x_i}^{(\varepsilon)} - h_{ex})(y)\,dx\,dy \\ &\simeq \pi n|\log \varepsilon| - \pi \sum_{i\neq j} \log|x_i - x_j| + \text{remainder terms.} \end{aligned} \tag{1.13}$$

Here the term $\pi n|\log \varepsilon|$ comes from the diagonal terms $i = j$, i.e. the self interaction of the smeared out Dirac masses, the logarithmic terms come from the leading order of G_Ω and the remainder terms from the next order terms of G_Ω, which are regular. We thus see that everything happens formally as if the vortices were a system of points with logarithmic interactions as in (1.3). The works [SS1, SS3] make that analogy rigorous.

2. The leading order behavior of H_n

The leading order behavior of H_n is well understood since [Cho], and the limit (or mean-field limit) is

$$\mathcal{E}(\mu) = \iint_{\mathbb{R}^d \times \mathbb{R}^d} g(x-y)\,d\mu(x)\,d\mu(y) + \int_{\mathbb{R}^d} V(x)\,d\mu(x) \tag{2.1}$$

defined over $\mathcal{P}(\mathbb{R}^d)$, the space of probability measures on $\mathbb{R}^d$. Finding the minimum of $\mathcal{E}$ is also known as the "capacitor problem" in potential theory and was first considered by Gauss and solved by Frostman in the 30's [Fro].

Theorem 2.1 (Frostman)**.** *If V is continuous and $\lim_{|x|\to\infty} V/2+g=+\infty$, then $\mathcal{E}$ has a unique minimizer μ_V among probability measures. Moreover*

- *μ_V has compact support of positive measure*
- *it is uniquely characterized by the fact that there exists a constant c such that*

$$\begin{cases} h^{\mu_V}+\frac{V}{2}\geq c & \text{in } \mathbb{R}^d \\ h^{\mu_V}+\frac{V}{2}=c & \text{q.e. on } Supp(\mu_V) \end{cases} \tag{2.2}$$

where

$$h^{\mu_V}=g*\mu_V. \tag{2.3}$$

This measure μ_V is called the *equilibrium measure*. The uniqueness easily comes from observing that $\mathcal{E}$ is stricly convex on $\mathcal{P}(\mathbb{R}^d)$. The characterization of μ_V comes from making variations of the form $(1-t)\mu_V+t\nu$ with $\nu\in\mathcal{P}(\mathbb{R}^d)$ and letting $t\to 0$. "q.e." means quasi-everywhere or except on a set of capacity 0 (a compact set E is of capacity zero if $\inf_{\mu\in\mathcal{P}(E)}\iint g(x-y)\,d\mu(x)\,d\mu(y)=+\infty$).

Important examples are the case where $V(x)=|x|^2$ with (1.2) or (1.3), then $\mu_V=\frac{1}{|B_1|}\mathbf{1}_{B_1}$. This can be guessed by taking formally the Laplacian of (2.2) on the support of μ_V which yields $-\Delta h^{\mu_V}=\mu_V=\Delta(|x|^2/2)=1$ there. In random matrix theory, in the case (1.3), this corresponds to the so-called *circular law*.

We will always assume that $\Sigma := Supp(\mu_V)$ is compact with a C^1 boundary, and also that μ_V has a density (still denoted $\mu_V(x)$) which is bounded above and C^1 on Σ and behaves like a power of the distance to Σ (cf. [PeSe] for precise assumptions). We will also denote

$$\zeta=h^{\mu_V}+\frac{V}{2}-c \tag{2.4}$$

with c the constant in (2.2). Then $\zeta\geq 0$ in $\mathbb{R}^d$ and $\zeta=0$ in Σ quasi-everywhere (and everywhere as soon as V is regular enough).

Proposition 2.2 (Γ-convergence of H_n)**.** *Assume $(x_1,\dots,x_n)$* [1] *are such that $H_n(x_1,\dots,x_n)\leq Cn^2$, then up to extraction of a subsequence we have $\frac{1}{n}\sum_{i=1}^n\delta_{x_i}\rightharpoonup\mu\in\mathcal{P}(\mathbb{R}^d)$ (for the weak-* topology on probabilities), and*

$$\liminf_{n\to\infty}\frac{H_n(x_1,\dots,x_n)}{n^2}\geq\mathcal{E}(\mu).$$

Conversely, given $\mu\in\mathcal{P}(\mathbb{R}^d)$ with $\mathcal{E}(\mu)<\infty$, there exists a sequence of $(x_1,\dots,x_n)$ such that $\frac{1}{n}\sum_{i=1}^n\delta_{x_i}\rightharpoonup\mu$ and

$$\limsup_{n\to\infty}\frac{H_n(x_1,\dots,x_n)}{n^2}\leq\mathcal{E}(\mu).$$

[1] everywhere we really mean $x_{1,n},\dots,x_{n,n}$ i.e. the whole configuration depends on n

We immediately deduce that if for all n, $(x_1, \dots, x_n)$ minimizes H_n, then $\frac{1}{n}\sum_{i=1}^n \delta_{x_i} \rightharpoonup \mu_V$, where μ_V is the unique minimizer of $\mathcal{E}$ as above, and we must have

$$\lim_{n\to\infty} \frac{\min H_n}{n^2} = \mathcal{E}(\mu_V). \tag{2.5}$$

This settles the leading order behavior of the minimizers of H_n: their macroscopic behavior is to resemble μ_V.

In the case with temperature, i.e. (1.8), it is striking that this behavior persists. In fact it was proven in [PH, BZ, BG, CGZ] that $\mathbb{P}_{n,\beta}$ admits a Large Deviation Principle (LDP) at speed n^2 and rate function $\frac{\beta}{2}(\mathcal{E} - \min \mathcal{E})$.

Definition 2.3. One says that a sequence of Borel probability measures $(P_n)_n$ admits an LDP at speed a_n with rate function I if for every Borel set E,

$$-\inf_{\overset{\circ}{E}} I \le \liminf_{n\to\infty} \frac{\log P_n(E)}{a_n} \le \limsup_{n\to\infty} \frac{\log P_n(E)}{a_n} \le -\inf_{\overline{E}} I.$$

In our case, this means roughly that if $\frac{1}{n}\sum_{i=1}^n \delta_{x_i} \rightharpoonup \mu$, then the probability of a neighborhood of that event behaves like

$$e^{-n^2 \frac{\beta}{2}(\mathcal{E}(\mu) - \mathcal{E}(\mu_V))}.$$

Since μ_V is the only minimizer of $\mathcal{E}$, all configurations which converge to $\mu \neq \mu_V$ have exponentially small probability. This means that even with temperature (with the scaling of temperature chosen here), configurations macroscopically resemble μ_V.

For the proof of Proposition 2.2 and of the LDP, we refer to [Ser, Chap. 2].

3. Expanding H_n to next order

The goal is then to understand what governs the next order term in the asymptotics of H_n. This term will at the same time give us information on the microscopic (vs. macroscopic previously) arrangements of the points. We expect that typical configurations of low energy have n points distributed on (or near) the set Σ. Since Σ is a bounded set of dimension d, we can thus expect the typical distance between points to be $n^{-1/d}$: this is the microscopic lengthscale. We will thus blow up configurations at that lengthscale. For simplicity we present the computations in the Coulomb cases.

Here we expand the Hamiltonian by viewing the point distribution $\nu_n := \sum_{i=1}^n \delta_{x_i}$ as a perturbation of $n\mu_V$:

$$\nu_n = n\mu_V + (\nu_n - n\mu_V). \tag{3.1}$$

Inserting the splitting (3.1) into the definition of H_n, one finds that if the points $x_1, \ldots, x_n$ are distinct, and denoting $\triangle$ for the diagonal of $\mathbb{R}^d$,

$$\begin{aligned} H_n(x_1, \ldots, x_n) &= \sum_{i \neq j} g(x_i - x_j) + n \sum_{i=1}^n V(x_i) \\ &= \iint_{\triangle^c} g(x-y) d\nu_n(x) d\nu_n(y) + n \int V d\nu_n \\ &= n^2 \iint_{\triangle^c} g(x-y) d\mu_V(x) d\mu_V(y) + n^2 \int V d\mu_V \\ &+ 2n \iint_{\triangle^c} g(x-y) d\mu_V(x) d(\nu_n - n\mu_V)(y) + n \int V d(\nu_n - n\mu_V) \\ &+ \iint_{\triangle^c} g(x-y) d(\nu_n - n\mu_V)(x) d(\nu_n - n\mu_V)(y). \end{aligned} \tag{3.2}$$

We now recall that ζ was defined in (2.4) so that we may rewrite the middle line in the right-hand side of (3.2) as

$$\begin{aligned} & 2n \iint_{\triangle^c} g(x-y) d\mu_V(x) d(\nu_n - n\mu_V)(y) + n \int V d(\nu_n - n\mu_V) \\ &\qquad = 2n \int (h^{\mu_V} + \frac{V}{2}) d(\nu_n - n\mu_V) = 2n \int (\zeta + c) d(\nu_n - n\mu_V) \\ &\qquad\quad = 2n \int \zeta d\nu_n - 2n^2 \int \zeta d\mu_V + 2nc \int d(\nu_n - n\mu_V) = 2n \int \zeta d\nu_n. \end{aligned}$$

The last equality is due to the facts that $\zeta = 0$ q.e. on the support of μ_V and that ν_n and $n\mu_V$ have the same mass n. We also have to notice that since μ_V has a L^∞ density with respect to the Lebesgue measure, it does not charge the diagonal $\triangle$ (whose Lebesgue measure is zero) and we can include it back in the domain of integration. By that same argument, one may recognize in the first line of the right-hand side of (3.2) the quantity $n^2 \mathcal{E}(\mu_V)$.

We may thus rewrite (3.2) as

$$\begin{aligned} H_n(x_1, \ldots, x_n) = n^2 \mathcal{E}(\mu_V) + 2n \sum_{i=1}^n \zeta(x_i) \\ + \iint_{\triangle^c} g(x-y) d(\nu_n - n\mu_V)(x) d(\nu_n - n\mu_V)(y). \end{aligned} \tag{3.3}$$

Note that this is an exact relation, valid for any configuration of distinct points. The first term in the right-hand side gives the leading order, i.e. the energy of the equilibrium measure. In the second term, ζ plays the role of an effective confining potential, which is active only outside of Σ (recall $\zeta \geq 0$, and $\zeta = 0$ in Σ). The last term in the right-hand side is the most interesting, it measures the discrepancy between the diffuse equilibrium measure μ_V and the discrete empirical measure $\frac{1}{n}\nu_n$. It is an electrostatic (Coulomb) interaction between a "negatively charged background" $-n\mu_V$ and the n positive discrete charges at the points $x_1, \dots, x_n$. In the sequel, we will express this energy term in another fashion, and show that it is indeed a lower-order term.

To go further, we need to introduce h_n, the potential generated by the distribution of charges $\nu_n - n\mu_V$, defined by

$$h_n := g * (\nu_n - n\mu_V) = \int g(\cdot - y) d(\nu_n - n\mu_V)(y). \tag{3.4}$$

Note that h_n decays at infinity, because the charge distribution $\nu_n - n\mu_V$ is compactly supported and has zero total charge, hence, when seen from infinity behaves like a dipole. More precisely, h_n decays like ∇g at infinity, that is $O(\frac{1}{r^{d-1}})$ and its gradient ∇h_n decays like the second derivative $D^2 g$, that is $O(\frac{1}{r^d})$ (in dimension 1, like $1/r$ and $1/r^2$). Formally, using Green's formula (or Stokes' theorem) and the definitions, one would like to say that, at least in dimension $d \geq 2$,

$$\iint_{\triangle^c} g(x-y) d(\nu_n - n\mu_V)(x) d(\nu_n - n\mu_V)(y) = \int h_n d(\nu_n - n\mu_V)$$
$$= \int h_n (-\frac{1}{c_d} \Delta h_n) \approx \frac{1}{c_d} \int |\nabla h_n|^2. \tag{3.5}$$

This is the place where we really use for the first time in a crucial manner the Coulombic nature of the interaction kernel g. Such a computation allows to replace the sum of pairwise interactions of all the charges and "background" by an integral (extensive) quantity, which is easier to handle in some sense. However, (3.5) does not make sense because ∇h_n fails to be in L^2 due to the presence of Dirac masses. Indeed, near each atom x_i of ν_n, the vector-field ∇h_n behaves like ∇g and the integrals $\int_{B(0,\eta)} |\nabla g|^2$ are divergent in all dimensions. Another way to see this is that the Dirac masses charge the diagonal $\triangle$ and so $\triangle^c$ cannot be reduced to the full space.

To remedy this, we introduce truncated potentials, and a "renormalized" way of computing the integral. Given $\eta > 0$, set

$$f_\eta(x) = (g(x) - g(\eta))_+ \tag{3.6}$$

and observe that f_η solves

$$-\Delta f_\eta = c_d (\delta_0 - \delta_0^{(\eta)})$$

where $\delta_0^{(\eta)}$ denotes the uniform measure of mass 1 on $\partial B(0, \eta)$. For h_n as in (3.4), we then define the truncated potential

$$h_{n,\eta}(x) = h_n(x) - \sum_{i=1}^n f_\eta(x - x_i) \tag{3.7}$$

and note that it solves

$$-\Delta h_{n,\eta} = c_d(\sum_{i=1}^n \delta_{x_i}^{(\eta)} - n\mu_V). \tag{3.8}$$

We then have the following

Lemma 3.1.

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

Proof. Let us compute the right-hand side of this relation. Let us choose R so that all the points are in $B(0, R-1)$ in $\mathbb{R}^d$, and η small enough that $2\eta < \min_{i\neq j} |x_i - x_j|$. Since $h_{n,\eta} = h_n$ (defined in (3.4)) at distance $\geq \eta$ from the points, by Green's formula and (3.7), we have

$$\begin{aligned}\int_{B_R} |\nabla h_{n,\eta}|^2 &= \int_{\partial B_R} h_n \frac{\partial h_n}{\partial \nu} - \int_{B_R} h_{n,\eta}\Delta h_{n,\eta} \\ &= \int_{\partial B_R} h_n \frac{\partial h_n}{\partial \nu} + c_d \int_{B_R} h_{n,\eta}\left(\sum_i \delta_{x_i}^{(\eta)} - n\mu_V\right). \end{aligned} \tag{3.9}$$

In view of the decay of h_n at infinity mentioned above, the boundary integral tends to 0 as $R \to \infty$. We thus find

$$\begin{aligned}\int_{\mathbb{R}^d} |\nabla h_{n,\eta}|^2 &= c_d \int_{\mathbb{R}^d} h_{n,\eta}\left(\sum_{i=1}^n \delta_{x_i}^{(\eta)} - n\mu_V\right) \\ &= c_d \int_{\mathbb{R}^d}\left(h_n - \sum_{i=1}^n f_\eta(\cdot - x_i)\right)\left(\sum_{i=1}^n \delta_{x_i}^{(\eta)} - n\mu_V\right). \end{aligned} \tag{3.10}$$

Since $f_\eta(\cdot - x_i) = 0$ on $\partial B(x_i, \eta) = \mathrm{Supp}(\delta_{x_i}^{(\eta)})$ and outside of $B(x_i,\eta)$, and since the balls $B(x_i,\eta)$ are disjoint, we may write

$$\int_{\mathbb{R}^d} |\nabla h_{n,\eta}|^2 = c_d \int_{\mathbb{R}^d} h_n \left(\sum_{i=1}^n \delta_{x_i}^{(\eta)} - n\mu_V\right) - nc_d \int_{\mathbb{R}^d} \sum_{i=1}^n f_\eta(\cdot - x_i)\mu_V.$$

Let us now use (temporarily) the notation $h_n^i(x) = h_n(x) - g(x - x_i)$ (for the potential generated by the distribution bereft of the point x_i). The function h_n^i is regular near x_i, hence $\int h_n^i \delta_{x_i}^{(\eta)} \to h_n^i(x_i)$ as $\eta \to 0$. It follows that

$$\begin{aligned} &c_d \int_{\mathbb{R}^d} h_n \left(\sum_{i=1}^n \delta_{x_i}^{(\eta)} - n\mu_V\right) - nc_d \int_{\mathbb{R}^d} \sum_{i=1}^n f_\eta(x - x_i)\mu_V \\ &= nc_d g(\eta) + c_d \sum_{i=1}^n h_n^i(x_i) - nc_d \int_{\mathbb{R}^d} h_n\mu_V + O(n^2\|\mu_V\|_{L^\infty})\int_{B(0,\eta)} |f_\eta| + o(1). \end{aligned} \tag{3.11}$$

We can check that $\int_{B(0,\eta)}|f_\eta|\to 0$ as $\eta\to 0$, so

$$\lim_{\eta\to 0}\frac{1}{c_d}\int_{\mathbb{R}^d}|\nabla h_{n,\eta}|^2-ng(\eta)=\sum_{i=1}^n h_n^i(x_i)-n\int_{\mathbb{R}^d}h_n\mu_V. \tag{3.12}$$

Now, from the definitions it is easily seen that

$$h_n^i(x_i)=\int_{\mathbb{R}^d\setminus\{x_i\}}g(x_i-y)d(\nu_n-n\mu_V)(y), \tag{3.13}$$

from which it follows that

$$\iint_{\triangle^c}g(x-y)d(\nu_n-n\mu_V)(x)d(\nu_n-n\mu_V)(y)$$
$$=\sum_{i=1}^n\int_{\mathbb{R}^d\setminus\{x_i\}}g(x_i-y)d(\nu_n-n\mu_V)(y)-n\int_{\mathbb{R}^d}h_n\,\mu_V=\sum_{i=1}^n h_n^i(x_i)-n\int_{\mathbb{R}^d}h_n\mu_V.$$

In view of (3.12), we conclude that the formula holds. □

Combining (3.3) and Lemma 3.1, we obtain

$$H_n(x_1,\dots,x_n)=n^2\mathcal{E}(\mu_V)+2n\sum_{i=1}^n\zeta(x_i)+\lim_{\eta\to 0}\left(\frac{1}{c_d}\int_{\mathbb{R}^d}|\nabla h_{n,\eta}|^2-ng(\eta)\right). \tag{3.14}$$

The final step consists in rescaling this quantity, as announced, by changing x into $x'=n^{1/d}x$. We let $\mu'_V(x')=\mu_V(x)$ be the blown-up density of the equilibrium measure, $\Sigma'=n^{1/d}\Sigma$ and set

$$h'_n=g*\Big(\sum_{i=1}^n\delta_{x'_i}-\mu'_V\Big) \tag{3.15}$$

and as above

$$h'_{n,\eta}=g*\Big(\sum_{i=1}^n\delta_{x'_i}^{(\eta)}-\mu'_V\Big),$$

which of course satisfy

$$-\Delta h'_n=c_d\Big(\sum_{i=1}^n\delta_{x'_i}-\mu'_V\Big)\quad\text{and}\quad-\Delta h'_{n,\eta}=c_d\Big(\sum_{i=1}^n\delta_{x'_i}^{(\eta)}-\mu'_V\Big). \tag{3.16}$$

Changing variables in (3.14) yields

Proposition 3.2. *For any n, any $(x_1,\dots,x_n)$, we have*

$$H_n(x_1,\dots,x_n)=n^2\mathcal{E}(\mu_V)+2n\sum_{i=1}^n\zeta(x_i)+(-\frac{n}{2}\log n)\mathbf{1}_{d=2}$$
$$+\frac{n^{2-2/d}}{c_d}\lim_{\eta\to 0}\left(\frac{1}{n}\int_{\mathbb{R}^d}|\nabla h'_{n,\eta}|^2-c_dg(\eta)\right). \tag{3.17}$$

We have thus obtained a completely algebraic splitting of the energy, valid for all configurations for fixed n, which separates the leading order term $n^2\mathcal{E}(\mu_V)$ from terms which are expected to be of next order. This result was obtained in [SS4, SS5, RouSe], and its analogue for (1.4) in [PeSe]. We will now focus on studying the asymptotics of

$$F_n(x_1,\ldots,x_n) = \lim_{\eta\to 0}\left(\frac{1}{n}\int_{\mathbb{R}^d}|\nabla h'_{n,\eta}|^2 - c_d g(\eta)\right). \tag{3.18}$$

A nice feature of the quantity defining F_n is its almost monotonicity:

Lemma 3.3. *If $\alpha < \eta$, we have*

$$\frac{1}{n}\int_{\mathbb{R}^d}|\nabla h'_{n,\eta}|^2 - c_d g(\eta) \le \frac{1}{n}\int_{\mathbb{R}^d}|\nabla h'_{n,\alpha}|^2 - c_d g(\alpha) + o_\eta(1),$$

where the $o_\eta(1)$ depends only on d and $\|\mu_V\|_{L^\infty}$.

The proof is based on integration by parts similarly as in Lemma 3.1. It can be found in [Ser, Chap. 3].

4. The renormalized energy

When taking limits in (3.16), if the blow-up was centered at a point x_0, we are led to solutions of relations of the form

$$-\Delta h = c_d\Big(\sum_{p\in\Lambda} N_p\delta_p - m\Big) \quad \text{in } \mathbb{R}^d \tag{4.1}$$

where $N_p \in \mathbb{N}^*$ and Λ is a discrete (infinite) set of points. Here m is a constant, equal to $\mu_V(x_0)$ (indeed, when centered around x_0, the density μ'_V converges to the constant $\mu_V(x_0)$) since μ_V was assumed to be a continuous density. We call $\mathcal{A}_m$ the class of vector fields $E = \nabla h$ with h satisfying a relation of the form (4.1). To each such h naturally corresponds as in (3.7) a truncated potential

$$h_\eta := h - \sum_{p\in\Lambda} N_p f_\eta(x-p),$$

which satisfies

$$-\Delta h_\eta = c_d\left(\sum_{p\in\Lambda} N_p\delta_p^{(\eta)} - m\right). \tag{4.2}$$

In view of (3.18), it is then quite natural to define

Definition 4.1 (Renormalized energy)**.** For $\nabla h \in \mathcal{A}_m$ and $0 < \eta < 1$, we define

$$\mathcal{W}_\eta(\nabla h) = \limsup_{R\to\infty}\left(\frac{1}{|K_R|}\int_{K_R}|\nabla h_\eta|^2 - mc_d g(\eta)\right) \tag{4.3}$$

with $K_R = [-R, R]^d$, and

$$\mathcal{W}(\nabla h) = \lim_{\eta \to 0} \mathcal{W}_\eta(\nabla h). \tag{4.4}$$

We note that $\mathcal{W}_\eta$ is in fact monotone (nonincreasing) in η just as in Lemma 3.3, so that the limit exists, thus $\mathcal{W}_\eta \ge \mathcal{W}_1$ for any $\eta \le 1$, while $\mathcal{W}_1$ is easily seen to be bounded below by $-mc_d g(1)$. Therefore $\mathcal{W}$ is bounded below on $\mathcal{A}_m$ by a constant depending only on m and d.

The constant m is acting like a uniform negative background charge which neutralizes the points, and also corresponds to the average density of points. In fact we can prove that if $\mathcal{W}(\nabla h) < \infty$ then

$$\lim_{R \to \infty} \frac{\sum_{p \in \Lambda \cap K_R} N_p}{|K_R|} = m. \tag{4.5}$$

This follows from the fact that a relation of the form (4.1) allows to estimate the discrepancy between the number of points and the volume via the energy itself: one integrates (4.2) (applied for some $\eta < 1$ small but fixed) against a cut-off function χ_R equal to 1 in K_R and vanishing outside K_{R+1}. Green's theorem then allows to find

$$\int \chi_R \left(\sum_{p \in \Lambda} N_p \delta_p^{(\eta)} - m \right) = \frac{1}{c_d} \int \nabla \chi_R \cdot \nabla h_\eta \tag{4.6}$$

which is $o(R^d)$ as $R \to \infty$. Using the Cauchy-Schwarz inequality, the right-hand side can be bounded above by

$$C \sqrt{R^{d-1} |K_R| (\mathcal{W}_\eta(\nabla h) + mc_d g(\eta))}$$

which is $o(R^d)$ as $R \to \infty$. On the other hand, since $\eta < 1$,

$$\sum_{p \in \Lambda \cap K_{R-2}} N_p \le \int \chi_R \sum_{p \in \Lambda} N_p \delta_p^{(\eta)} \le \sum_{p \in \Lambda \cap K_{R+2}} N_p$$

hence the left-hand side of (4.6) is easily seen to be equivalent to $\sum_{p \in \Lambda \cap K_R} N_p - m|K_R|$, and we conclude that (4.5) holds.

We also have the following scaling property of W: if $E \in \mathcal{A}_m$ then $\hat{E} := m^{1/d-1} E(\frac{\cdot}{m^{1/d}}) \in \mathcal{A}_1$ and

$$\mathcal{W}(E) = m^{2-2/d} \mathcal{W}(\hat{E}) - (2\pi m \log m) \mathbf{1}_{d=2}. \tag{4.7}$$

Thus it suffices to study $\mathcal{W}$ on $\mathcal{A}_1$. On this class we can show (as seen just above) that it is bounded below, and also that it has a minimizer. The big open question is to identify the minimum and the minimizers.

If the configuration Λ is periodic, or equivalently if it lives on a torus $\mathbb{T}$ of volume N and if

$$-\Delta h = c_d(\sum_{i=1}^n \delta_{a_i} - 1) \quad \text{in } \mathbb{T} \tag{4.8}$$

with possible repetitions in the a_i, then we can compute $\mathcal{W}$ in a more explicit form:

Lemma 4.2. *Assume* (4.8) *holds. If some a_i is repeated then $\mathcal{W}(E) = +\infty$, otherwise*

$$\mathcal{W}(\nabla h) = \frac{c_d^2}{N}\sum_{i\neq j} G(a_i - a_j) + c_d^2 \lim_{x\to 0}\left(G - \frac{g}{c_d}\right) \tag{4.9}$$

where G is the solution on the torus of

$$-\Delta G = \delta_0 - \frac{1}{N}.$$

The function G is the Green function of the torus, and behaves like $\frac{g}{c_d}$ near the origin. Up to a constant, the value of $\mathcal{W}$ just consists of a sum of pairwise interactions, but now computed with a periodic Green's function, which naturally includes a neutralizing background.

Proof. We may write $h(x) = c_d \sum_{i=1}^n G(x - a_i)$. Then

$$\mathcal{W}(\nabla h) = \lim_{\eta\to 0}\limsup_{R\to\infty} \fint_{K_R} |\nabla h_\eta|^2 - c_d g(\eta) = \lim_{\eta\to 0}\fint_{\mathbb{T}} |\nabla h_\eta|^2 - c_d g(\eta)$$

by periodicity. We then write

$$\int_{\mathbb{T}} |\nabla h_\eta|^2 = -\int_{\mathbb{T}} h_\eta \Delta h_\eta.$$

We may then insert that $h_\eta(x) = c_d \sum_{i=1}^n G(x-a_i) - \sum_{i=1}^n f_\eta(x-x_i)$ and $-\Delta h_\eta = c_d(\sum_{i=1}^n \delta_{x_i}^{(\eta)} - 1)$ and expand exactly as in the proof of Lemma 3.1, to obtain the result. □

The particular case where $N=1$, i.e. there is only one point per period, corresponds to a configuration which is exactly a (Bravais) lattice Λ (with fundamental cell normalized to 1). Then the formula above reduces to

$$\mathcal{W} = c_d^2 \lim_{x\to 0}\left(G - \frac{g}{c_d}\right)$$

and this can be computed by expanding G in Fourier series. One finds that

$$G(x) = \sum_{k\in\Lambda^*\setminus\{0\}} \frac{e^{2i\pi k\cdot x}}{4\pi^2|k|^2}.$$

The right-hand side is an Eisenstein series. Using this formula one can prove (cf. [SS3]) that in dimension 2, if Λ_1 and Λ_2 are two lattices of unit volume, then

$$\mathcal{W}(\Lambda_1) - \mathcal{W}(\Lambda_2) = \lim_{s\to 0} \sum_{p\in\Lambda_1^*\setminus\{0\}} \frac{1}{|p|^{2+s}} - \sum_{p\in\Lambda_2^*\setminus\{0\}} \frac{1}{|p|^{2+s}} = \lim_{s\to 0} \zeta_{\Lambda_1^*}(s) - \zeta_{\Lambda_2^*}(s), \tag{4.10}$$

where $\zeta_\Lambda(s)$ is called the Epstein zeta function of the lattice Λ. The minimization of $\mathcal{W}$ among lattices is then solved via the following result due to Cassels, Rankin, Ennola, Diananda, Montgomery (for a nice proof see [Mon]):

Theorem 4.3. *Assume $d = 2$ and $s > 0$. Then $\Lambda \mapsto \zeta_\Lambda(s)$ is uniquely minimized among lattices of volume 1 by the triangular lattice (i.e. the one based on $e^{i\pi/3}$).*

It follows from (4.10) that in dimension 2, $\mathcal{W}$ is uniquely minimized among volume 1 lattices, by the triangular lattice. This reconnects to the Abrikosov lattice that was observed in superconductivity, and leads us to conjecture that the triangular lattice achieves a global minimum of $\mathcal{W}$. Note that [BS] showed that this conjecture is equivalent to a conjecture of [BHS].

In dimensions larger than 2, the minimization of the ζ function is not understood, and so even the minimization of $\mathcal{W}$ among lattices is not sorted out. It is for example reasonable to believe that in dimension 3, the minimum is achieved by the BCC (body-centered cubic) lattice, see [SaSt]. For this, and more generally all questions on crystallization, we also refer to the recent review [BL].

5. The screening result and analysis of minimizers of H_n

5.1. Screening. The screening procedure is a way to localize the energy, which is by nature nonlocal in the point configuration: the electric potential h at any point depends a priori on the configuration everywhere. The idea is to cut the domain into cubes, and modify the configurations near the boundary of each such cubes in such a way that the energy becomes equal to the sum of the energies on the subcubes. For that we need to relax the problem and instead of working with electric potentials h satisfying (4.1), work with electric fields $E = \nabla h$, which then satisfy

$$-\mathrm{div}\ E = c_d\Big(\sum_{p\in\Lambda} N_p\delta_p - m\Big) \quad \text{in } \mathbb{R}^d, \tag{5.1}$$

(this idea originates in [ACO]). Relaxing the constraint that E has to be a gradient, it is then possible to glue together two electric fields on adjacent cubes keeping a relation of the form (5.1), *provided* that their normal components coincide on the common boundary (then no divergence is created across the interface). The goal is thus to modify electric fields in such a way that their normal components always coincide, by making them vanish on the boundaries. The energy of a vector field constructed by such a pasting becomes additive in the pasted pieces, i.e. essentially local. At the end one may recover a gradient vector field by L^2 projection onto gradients, which naturally only decreases the energy.

The modification of the configuration in each cube is achieved through the following screening proposition:

Proposition 5.1. *Given $E \in \mathcal{A}_1$ with $\mathcal{W}(E) < \infty$, satisfying*

$$-\text{div } E = c_d(\sum_{p\in\Lambda} N_p\delta_p - 1).$$

Given R such that $|K_R| \in \mathbb{N}$, and given $\varepsilon > 0, \eta > 0$ there exists $\hat{\Lambda}$ a configuration of points and $\hat{E}$ a vector field (both possibly also depending on η) defined in K_R and satisfying $\hat{E} = E$ in $K_{R(1-\varepsilon)}$ (hence $\hat{\Lambda} = \Lambda$ there too)

$$\begin{cases} -\text{div } \hat{E} = c_d\Big(\sum_{p\in\hat{\Lambda}} \delta_p - 1\Big) & \text{in } K_R \\ \hat{E}\cdot\nu = 0 & \text{on } \partial K_R \end{cases} \tag{5.2}$$

and

$$\int_{K_R} |\hat{E}_\eta|^2 \le \int_{K_R} |E_\eta|^2 + \varepsilon g(\eta) R^d. \tag{5.3}$$

The way to understand this is that given $E \in \mathcal{A}_1$ and K_R, we keep E preserved in a large subcube, and use the thin layer near the boundary to completely modify the configuration and place points "by hand" in such a way that they cancel the effect of what is happening inside (hence the name "screening"), and a negligible energy is added. The points in the layer compensate the oscillation of E on the boundary of the subcube and also make the whole configuration globally neutral. Indeed, the boundary condition $\hat{E}\cdot\nu = 0$ implies by integrating (5.2) over K_R and using Green's theorem, that the number of points in K_R must equal $|K_R|$.

This screening allows to efficiently obtain upper bounds on the minimal energy by constructing vector fields by truncating vector fields on cubes K_R, applying Proposition 5.1 and pasting together the results.

The screening result has several consequences, that were explored in [RNSe] in the case (1.3). Since it allows to modify boundary traces of vector fields without changing the energy too much, it proves that $\min_{\mathcal{A}_1} \mathcal{W}$ is also equal to the limit as $R \to \infty$ of the minimum of $\mathcal{W}$ over K_R-periodic configurations, and also to

$$\lim_{\eta\to 0}\lim_{R\to\infty} \min\left\{ \fint_{K_R} |\nabla h_\eta|^2 - c_d g(\eta), -\Delta h = c_d\left(\sum_p N_p\delta_p - 1\right) \text{ in } K_R \right. \\ \left. \text{and } \partial_\nu h = \varphi \text{ on } \partial K_R \right\} \tag{5.4}$$

for reasonable given boundary data φ.

In other words, boundary effects are negligible in the overall energy, and to compute $\min \mathcal{W}$, it would suffice to compute the minimum over periodic configurations, for which the formula (4.9) is available, and then take the limit of large period.

5.2. Minimizers of H_n in the case (1.3)**.** The screening also allows to get the following result of equidistributions of points and energy (it was written in the case (1.3) but should work in all Coulomb cases):

Theorem 5.2 ([RNSe])**.** *Assume* (1.3)*. Let* $(x_1, \dots, x_n) \subset (\mathbb{R}^2)^n$ *minimize* H_n*, then*

- *for all* i*,* $x_i \in \Sigma$
- *we have rigidity of the number of points: letting* $x'_i = n^{1/d} x_i$ *and* $K_\ell(a) = [a-\ell, a+\ell]^d$*, if* $\ell \ge c > 0$ *and* $dist(K_\ell(a), \partial\Sigma') \ge n^{\beta/2}$ $(\beta < 1)$*, we have*

$$\limsup_{n\to\infty} \left| \#\{x'_i \in K_\ell(a)\} - \int_{K_\ell(a)} \mu'_V(x)\, dx \right| \le C\ell. \tag{5.5}$$

- *we have equidistribution of energy*

$$\limsup_{n\to\infty} \left| \lim_{\eta\to 0} \int_{K_\ell(a)} |\nabla h'_{n,\eta}|^2 - c_d \#\{x'_i \in K_\ell(a)\} g(\eta) \; - \int_{K_\ell(a)} \Big(\min_{\mathcal{A}_{\mu'_V(x)}} \mathcal{W} \Big)\, dx \right| \le o_\ell(\ell^2). \tag{5.6}$$

This result is based on a comparison argument. Let $(x_1, \dots, x_n)$ be a minimizer, let us blow up (at scale $n^{1/d}$) and consider $E_n = \nabla h'_n$ the electric field that it generates. If one examines a microscopic box $K_\ell(a) = [a-\ell, a+\ell]^d \subset \Sigma'$, one can delete E_n in that box, and replace it by a vector field of choice, obtained by applying Proposition 5.1 to a minimizer of $\mathcal{W}$ (with the right density i.e $\mu_V(x)$), thus making a new point configuration. By comparison, the energy of the new total vector field should be larger than the original one (since it was a minimizer), and this should say that the energy of the original E_n in the box is (5.6). In order to make this reasoning rigorous one has to use Proposition 5.1 to glue together the old and new vector fields. One also has to find, by a mean value argument, a good boundary of the cube on which E_n is well behaved. This cannot be done at small scales a priori but the reasoning has to be applied iteratively at smaller and smaller scales and bootstrapped until one gets to scale $\ell = O(1)$. Gluing together the old vector field E_n outside $K_\ell(a)$ and the new one inside $K_\ell(a)$ will not produce a gradient vector field, but as above, we may project it later onto gradients (in L^2) while decreasing the energy. Once (5.6) is proven, (5.5) follows essentially by integrating (3.16) over the given cube, integrating by parts and using the control of (5.6) to control the boundary terms.

A result analogous to (5.5) is proven in [AOC] by very different methods, but there is no result of the type (5.6).

Theorem 5.2 naturally implies an asymptotic expansion to next order of the minimum of H_n. However we will present that result below in the more general setting of all dimensions.

6. Gamma-convergence approach

The approach outlined for Theorem 5.2 works for true minimizers of H_n, but it is also of interest (in particular for studying the case with temperature) to obtain information for generic configurations. This is done via a Γ-convergence approach: in this section, we will describe how to obtain lower bounds for generic configurations. In view of (3.17), it suffices to study F_n given by (3.18). We note that the integral defining F_n is given in a large (even infinite) domain. To bound it from below we introduced [SS3, SS4] a general abstract method which allows to get "lower bounds for 2-scale energies", and was inspired by Varadhan. In the present context, given a configuration $(x_1, \ldots, x_n)$ (or really a sequence of configurations depending on n), we let P_n be the 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 given by (3.15). This defines a probability measure on the set of (points in Σ, vector fields) which can be thought of as a "tagged electric field process", where for each vector field, we keep as a tag the memory of the point where it was blown-up. We let i_n be the map $(x_1, \ldots, x_n) \mapsto P_n$, which embeds $(\mathbb{R}^d)^n$ into this space of probability measures. To obtain a lower bound for F_n, we may naturally assume that $F_n \le C$ along the sequence, where C is independent of n. It is then not too difficult to show that, F_n being coercive enough, this implies that the sequence $(P_n)_n$ is tight, and thus up to extraction it converges to some probability measure P. We may also check that P satisfies by construction of P_n the following properties:

- the first marginal of P is the normalized Lebesgue measure
- the second marginal of P is translation-invariant
- for P-a.e. (x, E) we have $E \in \mathcal{A}_{\mu'_V(x)}$.

We say such probability measures are *admissible*. Defining then for any E in some $\mathcal{A}_m$

$$\mathbf{f}_\eta(x, E) = \fint_{B(0,1)} |E_\eta|^2 - c_d \mu_V(x) g(\eta)$$

where to each $E \in \mathcal{A}_m$ we may naturally associate an E_η via

$$E_\eta = E - \sum_p N_p \nabla f_\eta(\cdot - p).$$

We may compute that by definition of the push-forward, the fact that the first marginal of P_n is the normalized Lebesgue measure on Σ, and that $\int \mu_V = 1$,

$$\begin{aligned}\int \mathbf{f}_\eta(x, E)\, dP_n(x, E) &= \fint_\Sigma \frac{1}{|B(0,1)|} \mathbf{1}_{y \in B_1} |\nabla h'_{n,\eta}|^2 (n^{1/d}x + y)\, dy\, dx - \frac{c_d}{|\Sigma|} g(\eta) \\ &\le \frac{1}{|\Sigma'|} \int_{\{\mathrm{dist}(z, \Sigma') \le 1\}} |\nabla h'_{n,\eta}|^2(z)\, dz - \frac{c_d}{|\Sigma|} g(\eta)\end{aligned}$$

where we used the change of variables $z = n^{1/d}x + y$ and Fubini's theorem. Since $|\Sigma'| = n|\Sigma|$ we deduce that

$$\int \mathbf{f}_\eta(x,E)\,dP_n(x,E) \le \frac{1}{|\Sigma|} F_n(x_1,\dots,x_n).$$

The weak convergence of P_n to P and the continuity of $\mathbf{f}_\eta$ allows to take the limit $n \to \infty$ in this expression and obtain

$$\liminf_{n\to\infty} F_n(x_1,\dots,x_n) \ge |\Sigma| \int \mathbf{f}_\eta(x,E)\,dP(x,E).$$

Next, we exploit the fact that P is translation-invariant in its second variable. The multi-parameter ergodic theorem (cf. [Bec]) states that it implies that

$$\int \mathbf{f}_\eta(x,E)\,dP(x,E) = \int \mathbf{f}^*_\eta(x,E)\,dP(x,E)$$

where

$$\mathbf{f}^*_\eta(x,E) := \fint_{K_R} \mathbf{f}_\eta(x, E(\lambda+\cdot))\,d\lambda.$$

(It is part of the theorem that the limit exists). Computing and using Fubini's theorem again easily gives that

$$\mathbf{f}^*_\eta(x,E) = \lim_{R\to\infty} \fint_{K_R} |E_\eta|^2 - c_d \mu_V(x) g(\eta) = \mathcal{W}_\eta(E)$$

for $E \in \mathcal{A}_{\mu_V(x)}$. We have thus obtained that

$$\liminf_{n\to\infty} F_n(x_1,\dots,x_n) \ge |\Sigma| \int \mathcal{W}_\eta(E)\,dP(x,E).$$

We may then use Fatou's theorem to take the $\eta \to 0$ limit and obtain

$$\liminf_{n\to\infty} F_n(x_1,\dots,x_n) \ge |\Sigma| \int \mathcal{W}(E)\,dP(x,E) := \widetilde{\mathcal{W}}(P). \tag{6.1}$$

Combining with (3.17), we have obtained a general lower bound for H_n. This lower bound is expressed as an average of $\mathcal{W}$ over all blown-up centers, and an average over all blown-up profiles of the configuration (like a Young measure). Using the third property of admissible measures, we may easily compute that

$$\min_{P \text{ admissible}} \widetilde{\mathcal{W}}(P) = \int_\Sigma \min_{\mathcal{A}_{\mu_V(x)}} \mathcal{W}\,dx.$$

Also by scaling (4.7) we deduce that

$$\min_{P \text{ admissible}} \widetilde{\mathcal{W}}(P) = \min_{\mathcal{A}_1} \mathcal{W} \int \mu_V(x)^{2-2/d}\,dx + \left(\int \mu_V(x) \log \mu_V(x)\,dx \right) \mathbf{1}_{d=2}. \tag{6.2}$$

The final step consists in showing that this minimum can be asymptotically achieved by some sequence of n-point configurations. To prove that, we split Σ' (the blow-up of Σ) into cubes of size R on which $\int \mu'_V$ is integer. We paste in each cube a minimizer of $\mathcal{W}$ which has first been truncated and screened via Proposition 5.1 and then rescaled so as to make it have the right density μ'_V. As mentioned above, once such screened vector fields have been pasted together, one may estimate the energy of the underlying point configuration by projecting the global vector field onto gradients. This can only decrease the energy, and we conclude that the desired minimum can be achieved. The final result is

Theorem 6.1 ([SS4, RouSe]). *Assume we are in the cases* (1.2) *or* (1.3). *As* $n \to \infty$ *we have*

$$\min H_n = n^2 \mathcal{E}(\mu_V) - \left(\frac{n}{2}\log n\right)\mathbf{1}_{d=2} + n^{2-2/d} \min_{P \ admissible} \widetilde{\mathcal{W}} + o(n^{2-2/d}), \quad (6.3)$$

with $\min \widetilde{\mathcal{W}}$ *given by* (6.2). *In addition, if* $(x_1, \dots, x_n) \in (\mathbb{R}^d)^n$ *minimize* H_n, *letting* $P_n = i_n(x_1, \dots, x_n)$, *up to extraction* $P_n \rightharpoonup P$ *with* P *a minimizer* $\widetilde{\mathcal{W}}$, *i.e.* P*-a.e.* (x, E), E *minimizes* $\mathcal{W}$ *over* $\mathcal{A}_{\mu_V(x)}$.

7. Generalization to the Riesz case

As mentioned at the beginning, the approach we described can be extended beyond the Coulomb case to the case of Riesz interaction potentials as in (1.4) and to the case of one-dimensional logarithmic interactions as in (1.5). This was done in [SS5] for the case (1.5) and in [PeSe] for the case (1.4). It was a crucial ingredient in the Coulomb case that the sum of pairwise interaction could be transformed via (3.17) into a quantity which is extensive in space and local in h_n. This relied on the Coulomb nature of the potential, more precisely the fact that g was the kernel of a local operator. This is no longer the case for (1.4) and (1.5), however these kernels can be seen as the kernels of local operators via the Caffarelli-Silvestre extension formula for fractional Laplacians. In that procedure one embeds the space $\mathbb{R}^d$ into $\mathbb{R}^{d+1}$ by writing

$$\mathbb{R}^{d+1} = \{X = (x, y), x \in \mathbb{R}^d, y \in \mathbb{R}\}.$$

One then considers the local operator $-\mathrm{div}\,(|y|^\gamma \nabla \cdot)$ (which is elliptic, thus with a good regularity theory) when the space $\mathbb{R}^d$ is extended by one dimension to

$$\mathbb{R}^{d+1} = \{X = (x, y), x \in \mathbb{R}^d, y \in \mathbb{R}\},$$

and div and ∇ act on $\mathbb{R}^{d+1}$. Let g be as in (1.4). Then one has that given a measure μ on $\mathbb{R}^d$ and denoting by $\delta_{\mathbb{R}^d}$ the uniform measure on $\mathbb{R}^d$ seen as a subspace of $\mathbb{R}^{d+1}$, the potential

$$h := g * (\mu \delta_{\mathbb{R}^d}) = \int_{\mathbb{R}^{d+k}} g(X - X')\, (\mu \delta_{\mathbb{R}^d})(X')$$

is the solution in $\mathbb{R}^{d+1}$ of

$$-\text{div }(|y|^\gamma \nabla h) = c_{d,s}\mu\delta_{\mathbb{R}^d}$$

for

$$\gamma = s - d + 1 \tag{7.1}$$

and $c_{d,s}$ a constant depending only on d and s. The same is true in the case (1.5) by taking $s = 0$ in the formula (7.1). In that case $\gamma = 0$ and h is really the harmonic extension to the plane of the potential defined on the line. One may then write in all cases (1.4) or (1.5)

$$\int_{\mathbb{R}^d} (g * \mu)\mu = c_{d,s} \int_{\mathbb{R}^{d+1}} |y|^\gamma |\nabla h|^2.$$

One still defines $f_\eta = (g - g(\eta))_+$ which makes sense in $\mathbb{R}^{d+1}$ and one sets

$$\delta_0^{(\eta)} := \text{div }(|y|^\gamma \nabla f_\eta) + \delta_0.$$

With the help of this formula, the whole approach described in the previous sections then works identically, replacing the Laplacians by the operators $-\text{div }(|y|^\gamma \nabla \cdot)$ and the integrals over $\mathbb{R}^d$ by integrals over $\mathbb{R}^{d+1}$ with weight $|y|^\gamma$. For example the class $\mathcal{A}_m$ is defined as the set of gradient vector fields E over $\mathbb{R}^{d+1}$ such that

$$-\text{div }(|y|^\gamma E) = c_{d,s}\left(\sum_{p\in\Lambda} N_p\delta_p - m\delta_{\mathbb{R}^d}\right) \quad \text{in } \mathbb{R}^{d+1}$$

where Λ is a discrete subset of $\mathbb{R}^{d+1}$. The renormalized energy is then defined as

$$\mathcal{W}(E) = \lim_{\eta\to 0} \limsup_{R\to\infty} \frac{1}{|K_R|}\int_{K_R\times\mathbb{R}} |y|^\gamma |E_\eta|^2 - c_{d,s} m g(\eta).$$

The analogue of Theorem 6.1 is then the following (in which one should understand s as being 0 in the case (1.5)):

Theorem 7.1 ([SS5],[PeSe])**.** *Assume we are in the cases* (1.5) *or* (1.4). *As $n \to \infty$ we have*

$$\min H_n = n^2\mathcal{E}(\mu_V) - \Big(n\log n\Big)\mathbf{1}_{d=1,g=-\log} + n^{1+s/d} \min_{P \text{ admissible}} \widetilde{\mathcal{W}} + o(n^{1+s/d}), \tag{7.2}$$

with

$$\mathcal{W}(P) = \int_\Sigma \min_{\mathcal{A}_{\mu_V(x)}} \mathcal{W}\, dx$$

and

$$\min_{P \text{ admissible}} \widetilde{\mathcal{W}}(P) = \min_{\mathcal{A}_1} \mathcal{W} \int \mu_V(x)^{1+s/d}\, dx + \left(\int \mu_V(x)\log\mu_V(x)\, dx\right)\mathbf{1}_{d=1,g=-\log}.$$

In addition, if $(x_1,\dots,x_n) \in (\mathbb{R}^d)^n$ minimize H_n, letting $P_n = i_n(x_1,\dots,x_n)$, up to extraction $P_n \rightharpoonup P$ with P a minimizer $\widetilde{\mathcal{W}}$, i.e. P-a.e. (x,E), E minimizes $\mathcal{W}$ over $\mathcal{A}_{\mu_V(x)}$.

8. Application to the statistical mechanics

The analysis described in the last sections allows to get without much more work some information on the case with temperature, this is what was done in [SS4, SS5, RouSe, PeSe]. Indeed, combining (3.17) with (6.1) we obtain a general lower bound on H_n which we may then insert into (1.8) to get

$$Z_{n,\beta} \le \exp\left(n^2 \frac{\beta}{2}\mathcal{E}(\mu_V) + \frac{\beta}{2}\left(\frac{n}{d}\log n\right)\mathbf{1}_{d=1,2,g=-\log} + \frac{\beta}{2} n^{1+s/d}\min \widetilde{\mathcal{W}}\right) \int_{(\mathbb{R}^d)^n} e^{-\beta n \sum_{i=1}^n \zeta(x_i)} dx_1 \dots dx_n$$

and since $\zeta \to \mathbf{1}_\Sigma$ this can be written

$$\log Z_{n,\beta} \le n^2 \frac{\beta}{2}\mathcal{E}(\mu_V) + \frac{\beta}{2}\left(\frac{n}{d}\log n\right)\mathbf{1}_{d=1,2,g=-\log} + \frac{\beta}{2} n^{1+s/d}\min \widetilde{\mathcal{W}} + o(\beta n^{1+s/d}) + O(n). \tag{8.1}$$

This is already a nontrivial bound (new in many cases), which can be complemented without too much effort with a bound from below. However, it does not give an optimal estimate up to $o(n)$. Such an estimate can be provided by a stronger result, obtained with Thomas Leblé: in [LS], we obtained a full Large Deviations Principle which characterizes the behavior of the system at the microscopic scale for all β. To obtain a nontrivial result, it is better to rescale temperature in (1.8) and consider instead

$$d\mathbb{P}_{n,\beta}(x_1, \cdots, x_n) = \frac{1}{Z_{n,\beta}} e^{-\frac{\beta}{2} n^{-\frac{s}{d}} H_n(x_1,\dots,x_n)} dx_1 \dots dx_n \qquad x_i \in \mathbb{R}^d. \tag{8.2}$$

Our result is expressed in terms of tagged point processes instead of tagged electric field processes as in Section 6. First, for a given infinite configuration of points $\mathcal{C}$ and a given $m > 0$ we may define a renormalized energy on points via

$$\mathbb{W}_m(\mathcal{C}) = \inf\left\{\mathcal{W}(E), E \in \mathcal{A}_m, -\mathrm{div}\ E = c_d\Big(\sum_{p\in\mathcal{C}} \delta_p - m\Big)\right\}.$$

(This can be done in cases (1.5)–(1.4) as well). For each $(x_1, \dots, x_n)$, we then consider $\bar{P}_n$ the push-forward of the normalized Lebesgue measure on Σ by

$$x \mapsto (x, \theta_{n^{1/d}x}(x_1', \dots, x_n'))$$

where θ_λ represents the action of translating by λ a configuration. Such measures are again tight under good energy bounds, and converge up to extraction. As in Section 6, the first marginal of $\bar{P}$ is the normalized Lebesgue measure on Σ, and the second marginal of $\bar{P}$ is translation invariant. The measure $\bar{P}$ can also be disintegrated (i.e. sliced) into $\frac{1}{|\Sigma|}dx_{|\Sigma} \otimes \bar{P}^x$. We then define

$$\mathcal{F}_\beta(\bar{P}) = \frac{\beta}{c_{d,s}} \int_\Sigma \int \mathbb{W}_{\mu_V(x)}\, d\bar{P}^x\, dx + \int_\Sigma \mathsf{ent}[\bar{P}^x|\text{Poisson}]\, dx$$

where $\mathsf{ent}[P|\text{Poisson}]$ is the specific relative entropy of the point process P with respect to the Poisson point process of intensity 1 (it is a large volume limit analogue of the usual relative entropy).

The main result is

Theorem 8.1 ([LS])**.** *The push forward of* $\mathbb{P}_{n,\beta}$ *by* $j_n : (x_1, \dots, x_n) \mapsto \bar{P}_n$ *satisfies an LDP with speed* n *and rate function* $\mathcal{F}_\beta - \inf \mathcal{F}_\beta$*.*

Roughly speaking this means that

$$\mathbb{P}_{n,\beta}(\bar{P}_n \simeq \bar{P}) \simeq e^{-n(\mathcal{F}_\beta(\bar{P}) - \inf \mathcal{F}_\beta)}$$

hence the Gibbs measure $\mathbb{P}_{n,\beta}$ concentrates on minimizers of $\mathcal{F}_\beta$. This minimization problem corresponds to some balancing (depending on β) between a term based on $\mathbb{W}$, which prefers order of the configurations (and expectedly crystallization), and an entropy term which measures the distance to the Poisson process, thus prefers microscopic disorder and decorrelation between the points. As $\beta \to 0$, or temperature gets very large, the entropy term dominates and one can prove [Le2] that the minimizer of $\mathcal{F}_\beta$ converges to the Poisson process. On the contrary, when $\beta \to \infty$, the $\mathbb{W}$ term dominates, and prefers regular configurations (conjecturally, lattices). In dimension 1 where the minimum of $\mathbb{W}$ is known to be achieved by the lattice, this can be made into a complete proof of crystallization as $\beta \to \infty$ (cf. [Le1, Le2]). When β is intermediate then both terms are important and one does not expect crystallization nor complete decorrelation.

This result has several consequences. The first one is that the limiting point processes obtained in random matrix models: the sine-beta and Ginibre point processes, can be characterized as minimizing $\frac{\beta}{c_d}\mathbb{W}_1 + \mathsf{ent}(\cdot|\text{Poisson})$ (defined for the logarithmic interaction) among stationary point processes of intensity 1.

The second is the existence of a thermodynamic limit, i.e. an order n expansion of $\log Z_{n,\beta}$.

Corollary 8.2 (Thermodynamic limit, [LS])**.**

$$\log Z_{n,\beta} = -\frac{\beta n^{2-\frac{s}{d}}}{2}\mathcal{E}(\mu_V) - n\beta \min \mathcal{F}_\beta + o((\beta+1)n) \tag{8.3}$$

in the cases (1.4)*; and in the cases* (1.5)–(1.3)

$$\log Z_{n,\beta} = -\frac{\beta n^2}{2}\mathcal{E}(\mu_V) + \frac{\beta n}{2d}\log n - n\beta \min \mathcal{F}_\beta + o((\beta+1)n)$$

or more explicitly

$$\log Z_{n,\beta} = -\frac{\beta n^2}{2}\mathcal{E}(\mu_V) + \frac{\beta n}{2d}\log n - n\beta \min\left(\frac{1}{2}\mathbb{W}_1 + \frac{1}{\beta}\mathsf{ent}[\cdot|\text{Poisson}]\right) - n\beta\left(\frac{1}{\beta} - \frac{1}{2d}\right)\int_\Sigma \mu_V(x)\log\mu_V(x)\,dx + o((\beta+1)n). \quad (8.4)$$

Here the $o(1)$ *tend to zero as* $n \to \infty$ *independently of* β.

This provides an asymptotic expansion of the free energy (i.e. $-\frac{1}{\beta}\log Z_{n,\beta}$) up to order n, where the order n term itself has the structure of a free energy. This formulae are to be compared with the recent results of [Shc13, BG13b, BG13a, BFG13] in the dimension 1 logarithmic case. In both logarithmic cases, we also recover in (8.4) the cancellation of the order n term when $\beta = 4$ in dimension 2 and $\beta = 2$ in dimension 1 that was first observed in [Dy, Part II, section II] and [ZW06]. Such an expansion is completely new in the case (1.4).

The proof of Theorem 8.1 requires a thorough reworking of the problem, but still relies on the two crucial ingredients described above: the asymptotic expansion of H_n and the screening result. To prove an LDP, one needs to obtain an upper bound and a lower bound for $\mathbb{P}_{n,\beta}(j_n(x_1,\dots,x_n) \in B(\bar{P},\varepsilon))$. By classical large deviations theorems (à la Sanov), one has

$$\lim_{\varepsilon\to 0}\lim_{n\to\infty}\frac{1}{n}\log\left(|\{(x_1,\dots,x_n)\in\Sigma^n, j_n(x_1,\dots,x_N)\in B(\bar{P},\varepsilon)\}|\right) = -\int_\Sigma \mathsf{ent}(\bar{P}|\text{Poisson})\,dx. \quad (8.5)$$

In other words, the specific relative entropy corresponds to the (logarithm of the) volume in phase-space occupied by configurations whose $\bar{P}_n = j_n(x_1,\dots,x_n)$ is close to $\bar{P}$. One then wishes to insert the splitting (3.17)–(3.18) into the explicit form for $\mathbb{P}_{n,\beta}(j_n(x_1,\dots,x_n) \in B(\bar{P},\varepsilon))$. The lower bound (6.1) combined with (8.5) then allows to obtain an upper bound for $\mathbb{P}_{n,\beta}(j_n(x_1,\dots,x_n) \in B(\bar{P},\varepsilon))$. To obtain a lower bound is much more delicate, due to the need to take the $n\to\infty$ limit in F_n and the lack of continuity of $\mathcal{W}$. In order to achieve it, we examine configurations of n points that are drawn at random according to a Bernoulli process in Σ (and by (8.5) we know how to evaluate the volume in phase-space that they occupy), and we show that we may modify each of them, using the screening result, and a procedure for separating pairs of points that are too close to each other, so that the resulting set of configurations still occupies enough logarithmic volume in phase space (we lose volume, but not too much) and so that their F_n is close to $\mathbb{W}(\bar{P})$. For details, as well as open questions and perspectives, we refer to [LS].

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