

# Classical Coulomb gases and the Renormalized Energy

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# The Hamiltonian

Consider

$$w_n(x_1, \dots, x_n) = - \sum_{i \neq j} \log |x_i - x_j| + n \sum_{i=1}^n V(x_i).$$

and  $x_i \in \mathbb{R}^2$ .  $V$  grows faster than  $\log|x|$  at infinity.

- ▶ Hamiltonian energy for a "Coulomb gas" or "one-component plasma", also related to random matrices for  $V$  quadratic. [book by Forrester](#)
- ▶ Minimizers of  $w_n$  = "weighted Fekete points" (important in interpolation)
- ▶ Analogous problems better studied in dimension 3 (Lieb-Narnhofer, Lieb-Oxford...)
- ▶ In dim 2, physics references ([Alastuey-Jancovici](#), [Jancovici-Leibowitz-Manificat](#))

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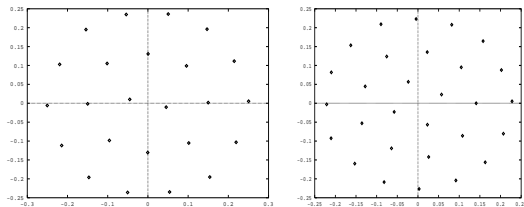
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# Numerical minimization



**Numerical minimization of  $w_n$  by Gueron-Shafir,  $n = 24, 29$**

# Equilibrium measure

Define

$$I(\mu) = \int_{\mathbb{R}^2 \times \mathbb{R}^2} -\log|x-y| d\mu(x) d\mu(y) + \int_{\mathbb{R}^2} V(x) d\mu(x).$$

Easy fact:

$$\frac{w_n}{n^2} \Gamma - \text{converges to } I$$

for the sense of convergence  $\frac{1}{n} \sum_{i=1}^n \delta_{x_i} \rightarrow \mu$ .

$I$  has a unique minimizer among probability measures, called the *equilibrium measure*, denoted  $\mu_0$ .

Denote  $E = \text{Supp}(\mu_0)$  (assumed to be compact).

$$\lim_{n \rightarrow \infty} \frac{\min w_n}{n^2} = I(\mu_0) \quad \lim_{n \rightarrow \infty} \frac{\sum_{i=1}^n \delta_{x_i}}{n} = \mu_0 \quad \text{for a minimizer}$$



## First objective

We know the global distribution of the points and  $\min w_n \sim n^2 I(\mu_0)$ .  
Can we say more about the local distribution of points and the next order terms in  $\min w_n$ ? For that we want to blow up the points at the scale  $\sqrt{n}$  to see them at finite distances from each other.

## Splitting of $w_n$

The idea is to understand the next order behavior by splitting  $w_n$ , writing  $\nu_n := \sum_{i=1}^n \delta_{x_i}$  as  $n\mu_0 + (\nu_n - n\mu_0)$ . We find

$$w_n(x_1, \dots, x_n) = n^2 I(\mu_0) + \frac{1}{\pi} W(\nabla H, \mathbf{1}_{\mathbb{R}^2}) + 2n \sum_{i=1}^n \zeta(x_i)$$

where  $H$  is the solution to

$$H = -2\pi \Delta^{-1} \left( \sum_{i=1}^n \delta_{x_i} - n\mu_0 \right)$$

and

$$\begin{cases} \zeta = \text{cst} + \frac{1}{2} V - \int \log|x-y| d\mu_0(y) \\ \zeta = 0 \\ \zeta > 0 \end{cases} \begin{array}{l} \text{in } E \\ \text{in } \mathbb{R}^2 \setminus E \end{array}$$

and for every function  $\chi$ ,

$$W(\nabla H, \chi) := \lim_{\eta \rightarrow 0} \int_{\mathbb{R}^2 \setminus \cup_{i=1}^n B(x_i, \eta)} \chi |\nabla H|^2 + \pi \log \eta \sum_i \chi(x_i).$$

In rescaled coordinates  $x' = \sqrt{n}(x - x_0)$  this becomes

$$w_n(x_1, \dots, x_n) = n^2 I(\mu_0) - \frac{n}{2} \log n + \frac{1}{\pi} W(\nabla H', \mathbf{1}_{\mathbb{R}^2}) + 2n \sum_{i=1}^n \zeta(x_i)$$

where  $H'$  is the solution to

$$H'(x') = -2\pi \Delta^{-1} \left( \sum_{i=1}^n \delta_{x'_i} - \mu_0 \left( x_0 + \frac{x'}{\sqrt{n}} \right) \right)$$

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- ▶ remains to understand this  $W(\nabla H', \mathbf{1}_{\mathbb{R}^2})$ , "renormalized" Coulomb interaction between the points in a neutralizing background, of slowly varying density  $\sim \mu_0$
- ▶ difficulties in letting  $n \rightarrow \infty$ , in particular no local "charge neutrality"
- ▶ need to define a total Coulomb interaction for such a system with infinite number of points

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Remark: Using Onsager's lemma, one can quickly obtain a lower bound

$$w_n(x_1, \dots, x_n) \geq n^2 I(\mu_0) - \frac{n}{2} \log n - Cn$$

however the constant  $C$  is not optimal. Moreover, this lower bound cannot be localized due to the absence of local charge balance.

# Complete definition of $W$

Let  $m > 0$  given. Let  $\Lambda$  be a discrete set in  $\mathbb{R}^2$ , and  $j (= \nabla H)$  a vector field such that

$$\operatorname{div} j = 2\pi(\nu - m) \quad \text{and} \quad \operatorname{curl} j = 0, \quad \text{where} \quad \nu = \sum_{p \in \Lambda} \delta_p.$$

We say such a  $j$  belongs to the class  $\mathcal{A}_m$ .

## Definition

For any smooth positive  $\chi$ , let

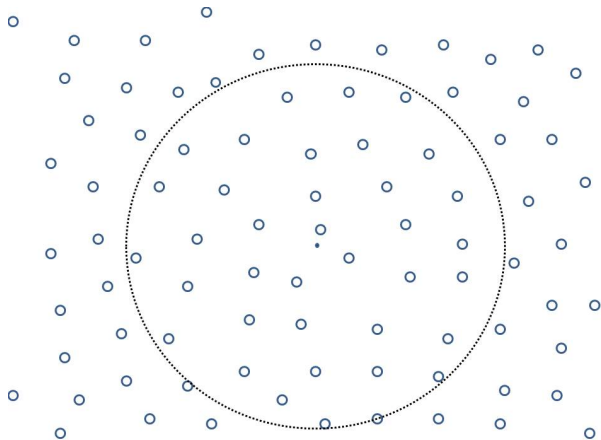
$$W(j, \chi) = \lim_{\eta \rightarrow 0} \left( \frac{1}{2} \int_{\mathbb{R}^2 \setminus \bigcup_{p \in \Lambda} B(p, \eta)} \chi |j|^2 + \pi \log \eta \sum_{p \in \Lambda} \chi(p) \right).$$

We define the **renormalized energy**  $W$  by

$$W(j) = \limsup_{R \rightarrow \infty} \frac{W(j, \chi_{B_R})}{|B_R|},$$

where  $\chi_{B_R}$  is any cutoff function supported in  $B_R$  with  $\chi_{B_R} = 1$  in  $B_{R-1}$  and  $|\nabla \chi_{B_R}| \leq C$ .

# Computing $W$



## The case of the torus

Assume  $\Lambda$  is  $\mathbb{T}$ -periodic. Then  $W$  can be written as a function of  $\Lambda$ . Identify  $\Lambda$  with  $\{a_1, \dots, a_n\} \subset \mathbb{T}$ . Let  $H_{\{a_i\}}$  be a solution of

$$-\Delta H_{\{a_i\}} = 2\pi \left( \sum_{i=1}^n \delta_{a_i} - \frac{n}{|\mathbb{T}|} \right) \quad \text{on } \mathbb{T}.$$

Let  $j_{\{a_i\}} = \nabla H_{\{a_i\}}$ , identified with a periodic vector field on  $\mathbb{R}^2$ .

### Lemma

Take the normalization  $n = |\mathbb{T}|$ . Let  $G$  be the Green function for  $\mathbb{T}$ :

$$-\Delta G(x) = 2\pi \left( \delta_0 - \frac{1}{|\mathbb{T}|} \right) \quad \text{in } \mathbb{T},$$

normalized to have mean zero. Then

$$W(j_{\{a_i\}}) = \frac{\pi}{|\mathbb{T}|} \sum_{i \neq j} G(a_i - a_j) + \pi \lim_{x \rightarrow 0} (G(x) + \log|x|).$$

Moreover,  $j_{\{a_i\}}$  is the minimizer of  $W(j)$  over all  $\mathbb{T}$ -periodic  $j$  satisfying  $\operatorname{div} j = 2\pi(\nu - 1)$  and  $\operatorname{curl} j = 0$ .



## Further expression of $W$ in the square torus case

Let  $\mathbb{T}_N = \mathbb{R}^2 / (N\mathbb{Z})^2$ . By a Fourier series expansion, the Green function of  $\mathbb{T}_N$  is expressed in terms of Eisenstein series. We obtain:

### Proposition

Let  $a_1, \dots, a_n$  be  $n = N^2$  points on  $\mathbb{T}_N$ , we have

$$W(j_{\{a_i\}}) = \frac{1}{2N^2} \sum_{j \neq k} E(a_j - a_k) + \pi \log \frac{N}{2\pi} - 2\pi \log \eta(i).$$

Here  $E(x) = E_{\Re(x/N), \Im(x/N)}(i)$  where  $E_{u,v}(\tau)$  is the Eisenstein series defined for  $\tau \in \mathbb{C}$  and  $u, v \in \mathbb{R}$  by

$$E_{u,v}(\tau) = \sum_{(m,n) \in \mathbb{Z}^2 \setminus \{0\}} e^{2i\pi(mu+nv)} \frac{\Im(\tau)}{|\mathfrak{m}\tau + n|^2}.$$

Finally,  $\eta$  denotes the Dedekind  $\eta$  function, which is given by

$$\eta(\tau) = q^{1/24} \prod_{k=1}^{\infty} (1 - q^k) \quad \text{where } q = e^{2i\pi\tau}.$$

# Minimization of $W$

- ▶  $W$  is unchanged by a compact perturbation of the point configuration.
- ▶ Minimizers of  $W$  exist (requires work)
- ▶ Scaling: call  $\mathcal{A}_m$  the vector fields corresponding to density  $m$ , that is,  $\operatorname{div} j = 2\pi(\nu - m)$  and  $\operatorname{curl} j = 0$ . Then if  $j$  belongs to  $\mathcal{A}_m$ , then  $j' = \frac{1}{\sqrt{m}}j(\cdot/\sqrt{m})$  belongs to  $\mathcal{A}_1$  and

$$W(j) = m \left( W(j') - \frac{\pi}{2} \log m \right)$$

so we can reduce to  $\mathcal{A}_1$ .

- ▶ Proposition:  $\min_{\mathcal{A}_1} W$  is the limit as  $N \rightarrow \infty$  of the min over  $\mathbb{T}_N$ -periodic configurations.

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We can look for minimizers of  $W$  among perfect lattice configurations, i.e.,  $\Lambda = \mathbb{Z}\vec{u} + \mathbb{Z}\vec{v}$ , with unit volume.

### Theorem (Sandier-S. '10)

*The minimum of  $\Lambda \mapsto W(\Lambda)$  over perfect lattice configurations is achieved uniquely, modulo rotations, by the triangular lattice.*

- ▶ in that setting, explicit formula in terms of Eisenstein series
- ▶ by transformations using modular functions or by direct computations, minimizing  $W$  becomes equivalent to minimizing the Epstein zeta function  $\zeta(s) = \sum_{p \in \Lambda} \frac{1}{|p|^s}$ ,  $s > 2$ , over lattices
- ▶ results from number theory (Cassels, Rankin, 60's) say that this is minimized by the triangular lattice

### Conjecture

*The "Abrikosov" triangular lattice is a global minimizer of  $W$ .*

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# $\Gamma$ -convergence of $w_n$ / estimate of ground state energy

## Theorem (Sandier-S)

Fix  $1 < p < 2$  and let  $X = E \times L^p_{loc}(\mathbb{R}^2, \mathbb{R}^2)$ .

**A. Lower bound.** Let  $\nu_n = \sum_{i=1}^n \delta_{x_i}$  be a sequence such that

$$w_n(x_1, \dots, x_n) - n^2 I(\mu_0) + \frac{n}{2} \log n \leq Cn.$$

Let  $P_n$  be the probability on  $X$  which is the push-forward of  $\frac{1}{|E|} dx|_E$  by

$$x \mapsto (x, j_n(\sqrt{n}x + \cdot)), \quad j_n := \nabla H'_n.$$

1. Up to a subsequence,  $P_n$  converges to a probability  $P$  on  $X$ .
2. The first marginal of  $P$  is  $\frac{1}{|E|} dx|_E$ .  $P$  is invariant by  $(x, j) \mapsto (x, j(\lambda + \cdot))$ , for any  $\lambda \in \mathbb{R}^2$ .
3. For  $P$  a.e.  $(x, j)$  we have  $j \in \mathcal{A}_{\mu_0(x)}$ .
- 4.

$$\liminf_{n \rightarrow \infty} \frac{1}{n} \left( w_n(x_1, \dots, x_n) - n^2 I(\mu_0) + \frac{n}{2} \log n \right) \geq \frac{|E|}{\pi} \int W(j) dP(x, j).$$

## Theorem (continued)

**B. Upper bound construction.** Conversely, assume  $P$  is an invariant probability measure on  $X$  whose first marginal is  $\frac{1}{|E|} dx|_E$  and such that for  $P$ -a.e.  $(x, j)$  we have  $j \in \mathcal{A}_{\mu_0(x)}$ . Then there exists a sequence  $\{\nu_n = \sum_{i=1}^n \delta_{x_i}\}_n$  of empirical measures on  $E$  and a sequence  $\{j_n\}_n$  in  $L_{loc}^p(\mathbb{R}^2, \mathbb{R}^2)$  such that  $\operatorname{div} j_n = 2\pi(\nu'_n - \mu'_0)$  and such that the image  $P_n$  of  $\frac{1}{|E|} dx|_E$  by  $x \mapsto (x, j_n(\sqrt{nx} + \cdot))$  converges to  $P$ . Moreover

$$\limsup_{n \rightarrow \infty} \frac{1}{n} \left( w_n(x_1, \dots, x_n) - n^2 I(\mu_0) + \frac{n}{2} \log n \right) \leq \frac{|E|}{\pi} \int W(j) dP(x, j).$$

**C. Consequences for minimizers.** Assume  $(x_1, \dots, x_n)$  minimize  $w_n$  and let  $\nu_n = \sum_{i=1}^n \delta_{x_i}$ . Then  $P_n$  converges to  $P$ , and for  $P$  a.e.  $(x, j)$ ,  $j$  minimizes  $W$  over  $\mathcal{A}_{\mu_0(x)}$ . Moreover,

$$\limsup_{n \rightarrow \infty} \frac{1}{n} \left( w_n(x_1, \dots, x_n) - n^2 I(\mu_0) + \frac{n}{2} \log n \right) = \min \frac{|E|}{\pi} \int W(j) dP(x, j),$$

and  $\lim_{n \rightarrow \infty} \sum_{i=1}^n \operatorname{dist}^2(x_i, E) = 0$ .

# Method of the proof

- ▶  $\Gamma$ -convergence: prove general (ansatz-free) lower bounds and upper bounds which match
- ▶ Introduce a new general method for lower bound on two-scale energies (after splitting + blow-up, the domain becomes of infinite size, so it is difficult to localize energy lower bounds). A probability measure approach allows to do this via the use of the ergodic theorem (idea of **Varadhan**)
- ▶ That method applies well to positive (or bounded below) energy densities, but those associated to  $W(\nabla H, \chi)$  are not!
- ▶ Start by modifying the energy density to make it bounded below: method of mass transport, using sharp energy lower bounds by "ball construction" methods (à la **Jerrard / Sandier**)

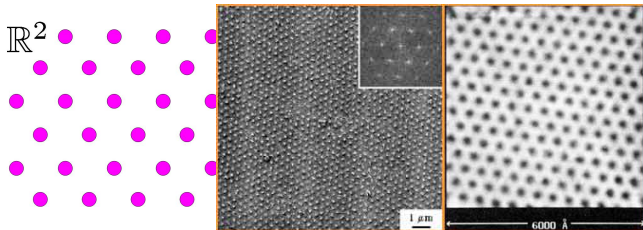
# Original motivation: the Ginzburg-Landau model

$W$  is derived as a limit problem for the minimization of the  $2D$  Ginzburg-Landau functional of superconductivity:

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

(motivations: superconductivity, rotating superfluids and Bose-Einstein condensates) in the asymptotic limit  $\varepsilon \rightarrow 0$  and  $|\log \varepsilon| \leq h_{\text{ex}} \ll \frac{1}{\varepsilon^2}$ .

Minimizers  $(\psi, A)$  of  $G_\varepsilon$  have "vortices" (= zeros of the complex-valued function  $\psi$ ) which are densely-packed in the domain.



**Abrikosov lattice**

## From Ginzburg-Landau to $W$

### Theorem (Sandier-S. '10)

*Consider minimizers  $(\psi_\varepsilon, A_\varepsilon)$  of the Ginzburg-Landau energy. After blow-up around a randomly chosen point, the vortices converge to configurations of points in the plane whose associated currents  $(= \lim_{\varepsilon \rightarrow 0} \nabla \text{curl } A_\varepsilon)$ , almost surely, minimize  $W$ .*

- ▶  $W$  is like an analogue for an infinite number of points of the renormalized energy **Bethuel-Brezis-Hélein** derived for a finite number of vortices (for a simplified energy), or of the Kirchhof-Onsager function.
- ▶ Method: same as for Coulomb gases, but complicated by the presence of vortices of arbitrary signs and degrees

# The statistical mechanics of Coulomb gases

Probability law (=Gibbs measure)

$$d\mathbb{P}_n^\beta(x_1, \dots, x_n) = \frac{1}{Z_n^\beta} e^{-\frac{\beta}{2} w_n(x_1, \dots, x_n)} dx_1 \cdots dx_n$$

where  $Z_n^\beta$  is the associated partition function, and

$$w_n(x_1, \dots, x_n) = - \sum_{i \neq j} \log |x_i - x_j| + n \sum_{i=1}^n V(x_i).$$

and  $x_i \in \mathbb{R}^d$ .

For general  $\beta$  and  $V$ , these ensembles are called Coulomb gases, or sometimes  $\beta$ -ensembles.

# Important examples

- ▶ For  $d = 1$ ,  $\beta = 2$ ,  $V(x) = x^2/2 \rightsquigarrow$  **GUE** (= law of eigenvalues of Hermitian matrices with complex Gaussian i.i.d. entries).
- ▶ For  $d = 1$ ,  $\beta = 1$ ,  $V(x) = x^2/2 \rightsquigarrow$  **GOE** (real symmetric matrices with Gaussian i.i.d. entries).
- ▶ For  $d = 2$ ,  $\beta = 2$  and  $V(x) = |x|^2 \rightsquigarrow$  **Ginibre ensemble** (matrices with complex Gaussian i.i.d. entries).

Reference texts:

- ▶ Anderson-Guionnet-Zeitouni, Deift, Forrester, Mehta.

# Next-order expansion of the partition function

## Theorem (Sandier-S.)

$$n\beta f_1(\beta) \leq \log Z_n^\beta - (-\beta n^2 I(\mu_0) + \frac{\beta n}{2} \log n) \leq n\beta f_2(\beta),$$

where  $f_1(\beta)$  and  $f_2(\beta)$  are independent of  $n$ , bounded, and

$$\lim_{\beta \rightarrow \infty} f_1(\beta) = \lim_{\beta \rightarrow \infty} f_2(\beta) = \alpha_0,$$

where

$$\alpha_0 = \frac{1}{\pi} \min_{\mathcal{A}_1} W - \frac{1}{2} \int \mu_0 \log \mu_0 dx.$$



# Estimates for the probability of some rare events

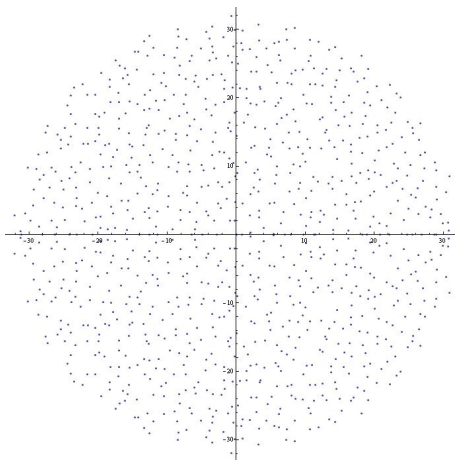
## Theorem (Sandier-S.)

Let  $\nu = \sum_{i=1}^n \delta_{x_i}$ . There exist universal  $C > 0, R_0 > 0$ , such that for any  $\beta_0 > 0$ ,  $n$  large enough depending on  $\beta_0$  and any  $\beta > \beta_0$ , any  $R > R_0$  and any  $\eta > 0$ , for any ball  $B = B_{Rn^{-1/2}}(x_0)$  we have

$$\mathbb{P}_n^\beta (|\nu(B) - n\mu_0(B)| \geq \eta R^2) \leq \exp(-c\beta \min(\eta^2, \eta^3)R^4 + C\beta(R^2 + n) + Cn),$$

$$\mathbb{P}_n^\beta \left( \left(1 + \frac{R^2}{n}\right)^{-\frac{1}{2}} \|\nu - n\mu_0\|_{\text{Lip}^*(B)} \geq \eta\sqrt{n} \right) \leq \exp(-Cn\beta\eta^2 + Cn(\beta+1)),$$

$$\mathbb{P}_n^\beta \left( \int \text{dist}(x, \text{supp}(\mu_0))^2 \nu \geq \eta \right) \leq \exp\left(-\frac{1}{2}n\beta\eta + Cn(\beta+1)\right).$$



**Eigenvalues of 1000-by-1000 matrix with i.i.d Gaussian entries**

(Stolen from Benedek Valkó's webpage)

# Large deviations type result

## Theorem (Sandier-S.)

Let  $A_n \subset (\mathbb{R}^2)^n$ . Then

$$\limsup_{n \rightarrow \infty} \frac{1}{n} \log \mathbb{P}_n^\beta(A_n) \leq -\beta \left( \frac{|E|}{\pi} \inf_{P \in A} \int W(j) dP(x, j) - \alpha_0 + \frac{C}{\beta} \right),$$

and  $A$  is the set of probability measures which are limits of blow-ups at rate  $n^{1/2}$  around a point  $x$  of the current  $j$  associated to  $\nu = \sum_{i=1}^n \delta_{x_i}$  with  $(x_i) \in A_n$ .

Improves on large deviations results of **Ben Arous-Guionnet, Ben Arous-Zeitouni**.

Corollary: crystallisation as  $\beta \rightarrow \infty$ :  $\rightsquigarrow$  after blowing up around a point  $x$  in the support of  $\mu_0$ , at the scale of  $(n\mu_0(x))^{1/2}$ , we see (almost surely) a configuration which minimizes  $W$ .

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# Definition of $\mathcal{W}$ for arbitrary point processes (with Borodin)

By analogy with the  $\mathbb{T}_N$ -periodic case, we define for any point process the random variable

$$\mathcal{W}_N = -\frac{1}{N} \sum_{i \neq j, a_i, a_j \in [0, N]} \log \left| 2 \sin \frac{\pi(a_i - a_j)}{N} \right| + \log N \quad \text{in dimension 1,}$$

and

$$\mathcal{W}_N = \frac{1}{2\pi N^2} \sum_{i \neq j, a_i, a_j \in [0, N]^2} E(a_i - a_j) + \log \frac{N}{2\pi \eta(i)^2} \quad \text{in dimension 2.}$$

For stationary processes, we give conditions for  $\mathbb{E}\mathcal{W}_N$  to have a limit as  $N \rightarrow \infty$  as well as for  $\text{Var}\mathcal{W}_N$ .

# Characterization of the expectation of $W$

## Theorem (Borodin-S.)

Let a random point process in  $\mathbb{R}^d$  ( $d = 1$  or  $2$ ) have two-point correlation function  $\rho_2(x, y) = 1 - T_2(x - y)$ . If  $\int T_2 = 1$  and  $T_2$  satisfies some decay conditions, then

$$\lim_{N \rightarrow \infty} \mathbb{E} \mathcal{W}_N = \int_{\mathbb{R}^d} \log |2\pi v| T_2(v) dv.$$

Moreover, under additional decay conditions,  $\lim_{N \rightarrow \infty} \text{Var} \mathcal{W}_N = 0$ .

## Examples

- ▶ Poisson process in dimensions  $d = 1, 2$ :  $\lim_{N \rightarrow \infty} \mathbb{E}W_N = +\infty$ .
- ▶ perfect lattice  $\mathbb{Z}$  in dimension  $d = 1$ :  $\lim_{N \rightarrow \infty} \mathbb{E}W_N = \mathbb{E}W_N = 0$ .
- ▶ sine-beta process in dimension  $d = 1$ :

$$\left\{ \begin{array}{ll} \lim_{N \rightarrow \infty} \mathbb{E}W_N = 2 - \gamma - \log 2 & \beta = 1, \\ \lim_{N \rightarrow \infty} \mathbb{E}W_N = 1 - \gamma & \beta = 2, \\ \lim_{N \rightarrow \infty} \mathbb{E}W_N = \frac{3}{2} - \gamma - \log 2 & \beta = 4, \end{array} \right.$$

Directly related to the "thermodynamic energy per particle" for the log gas found in [Dyson '62](#), [Dyson-Mehta '63](#),  $\mathcal{W}$  provides the rigorous quantity.

- ▶ The determinantal process ( $d = 2$ ) with kernel  $e^{-\frac{\pi}{2}|x-y|^2}$ :

$$\lim_{N \rightarrow \infty} \mathbb{E}W_N = \frac{1}{2}(\gamma - \log \pi).$$

- ▶ Zeros of Gaussian Analytic Functions:

$$\lim_{N \rightarrow \infty} \mathbb{E}W_N = -\frac{1}{2}(1 + \log \pi)$$

# Extensions

- ▶ extension of the definition of  $W$  to 1D and analogous results (with E. Sandier).  
In 1D,  $\min W$  is achieved by the perfect lattice  $\mathbb{Z}$ , and the crystallisation result is complete.
- ▶ study usual Fekete points on a compact set (with E. Sandier)
- ▶ study quantum Coulomb gases in 2D (with M. Lewin and P. T. Nam). There the  $-\frac{1}{2}n \log n$  term is absent.
- ▶ higher dimensions.