Classical systems with Coulomb/Riesz interactions

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Mean-field and other effective models in mathematical physics

Les Treilles

$\vec{X}_N = (x_1, \dots, x_N)$ **classical** point particles in $\mathbb{R}^{\mathsf{d}}$.

$$\mathcal{H}_N(\vec{X}_N) := \sum_{1 \le i < j \le N} g(x_i - x_j) + \sum_{i=1}^{N} N \cdot V(x_i)$$

Interaction potential

$$g(x-y) = \begin{cases} -\log|x-y| & \text{“log gases”}(\mathsf{d}=1,2) \\ |x-y|^{-\mathsf{s}} & \text{“Riesz gases”}(\mathsf{d} \ge 1) \end{cases}$$

Coulomb: Log for $\mathsf{d} = 2$ and Riesz with $\mathsf{s} = \mathsf{d} - 2$ for $\mathsf{d} \ge 3$.
V “confining” potential, grows fast enough e.g. $V(x) = \|x\|^2$.

Canonical ensemble, inverse temperature $\beta > 0 = \frac{1}{T}$
Gibbs measure

$$d\mathbb{P}_{N,\beta}(\vec{X}_N) = \frac{1}{Z_{N,\beta}} \exp\left(-\beta \mathcal{H}_N(\vec{X}_N)\right) d\vec{X}_N.$$

Volume = Lebesgue measure $d\vec{X}_N = dx_1 \dots dx_N$ on $(\mathbb{R}^{\mathrm{d}})^N$

Motivations?

- Statistical physics
- Random Matrix Theory
- (Appears as square of wavefunction for quantum systems.)

Macroscopic behavior

Empirical measure

$$\mu_N := \frac{1}{N} \sum_{i=1}^{N} \delta_{x_i}.$$

Converges to some compactly supported "equilibrium measure" μ_{eq}, which does not depend on β (only on V).
In general, μ_{eq} minimises the energy functional

$$\mu \mapsto I_V(\mu) := \iint g(x-y) d\mu(x) d\mu(y) + \int V(x) d\mu(x)$$

Examples?
Re-write the energy as

$$\mathcal{H}_N(\vec{X}_N) = N^2 I_V(\mu_{\mathrm{eq}}) + \text{ lower order terms.}$$

Microscopic scale?

Rescale system by $N^{1/\mathsf{d}}$.

- Microscopic point configuration / arrangement

$$\mathcal{C}_N := \sum_{i=1}^{N} \delta_{N^{1/\mathsf{d}} x_i}$$

- Background measure $\tilde{\mu}_{\mathrm{eq}}(x)$

Second-order energy (order N). Sandier-Serfaty.

$$\iint g(x-y)\left(d\mathcal{C}_N(x) - d\tilde{\mu}_{\mathrm{eq}}(x)\right)\left(d\mathcal{C}_N(y) - d\tilde{\mu}_{\mathrm{eq}}(y)\right)$$

"Jellium": positive point charges, negative continuous background.
Drawing?

What happens as $N \to \infty$? Is there a limit object?
Fix z and consider

$$\mathcal{C}_{N,z} := \sum_{i=1}^{N} \delta_{N^{1/\mathrm{d}}(x_i - z)} \longrightarrow_{N \to \infty} \text{“Point process” ?}$$

- Log-gas $\mathrm{d} = 1$, known for $\beta > 0$ (Valkó-Virág)
- Log/Coulomb gas $\mathrm{d} = 2$, known for $\beta = 2$ (Ginibre).
- $\mathrm{d} = 3$???

Empirical field = average of $\mathcal{C}_{N,z}$ over z, “average microscopic behavior”

Theorem (L. - Serfaty)

The law of the empirical field concentrates on minimisers of the "free energy functional" $\mathcal{F}_\beta$.

(Large Deviation Principle at speed N with rate function $\mathcal{F}_\beta$)
P a probability measure on point configurations

$$\boxed{\mathcal{F}_\beta(P) := \beta \mathcal{W}(P) + \mathcal{E}(P)}$$

where $\mathcal{W}$ is the **energy** and $\mathcal{E}$ is the **entropy**.

- $\mathcal{E}(\text{Poisson}) = 0$, $\mathcal{E}(\text{Lattice}) = +\infty$.
- W? minimized by lattice ($\mathrm{d} = 1$ known, $\mathrm{d} = 2$ conjectured, $\mathrm{d} = 3$??)

Valid for Log, Coulomb, Riesz gases. Difficulty?

Morality

Finite object = gas of N particles as $N \to \infty$
$\approx$ (locally, after rescaling and averaging) minimiser of $\mathcal{F}_\beta$ =
infinite object (point process)

Rigidity of the finite object

$$\text{We know: } \frac{1}{N}\sum_{i=1}^{N}\delta_{x_i} \approx \mu_{\mathrm{eq}}.$$

Order of magnitude of $\sum_{i=1}^{N}\delta_{x_i} - N\mu_{\mathrm{eq}}$? Small scales?
Consider fluctuations:

$$\sum_{i=1}^{N}\varphi(x_i) - N\int \varphi(x)d\mu_{\mathrm{eq}}(x), \; \varphi \in C^4$$

d = 1 Log	d = 2 Coulomb	d = 3 Coulomb	Riesz cases
O(1)	O(1)	??	??

$O(1)$ surprising, different from i.i.d. Valid at small scales.

d = 1 Johansson "very effective cancellations"

d = 2 Bauerschmidt-Bourgade-Nikula-Yau, L.-Serfaty

Questions

- Why?
- Can be rephrased as the convergence of

$$\phi_N(z) := z \mapsto \sum_{i=1}^{N} \log |z - x_i|$$

to a Gaussian Free Field. What about $\max \phi_N$?
- What is the minimal regularity on φ?
- For φ indicator function, Jancovici-Lebowitz-Manificat conjecture on the speed of deviations for the number of points in boxes (Coulomb, $\mathrm{d} = 2, 3$).

Phase portrait

Infinite object: translation-invariant minimiser of $\mathcal{F}_\beta := \beta\mathcal{W} + \mathcal{E}$.
Dependency on β? Phase transition?

- Dimension 1 (log-gas) the partition function is known explicitly (Selberg's integral) and analytic in β

Theorem (Erbar-Huesmann-L.)

1d log-gas: uniqueness of minimisers of $\mathcal{F}_\beta$ for $\beta > 0$.

(probably also true for Riesz cases, $d = 1$).

Usual argument: strict convexity. Here, the functional $P \mapsto \mathcal{F}_\beta(P)$ is **affine** in P for the usual linear interpolation, so no strict convexity.
Idea (A. Guionnet): show that it is strictly *displacement* convex.

Displacement interpolation ?

Let μ_0, μ_1 be two measures on $\mathbb{R}^n$ (+ some regularity). What is the midpoint between μ_0 and μ_1?
Usual answer: $\frac{1}{2}(\mu_0 + \mu_1)$.
Another option:

1. Consider a transport map $T : \mathbb{R}^n \to \mathbb{R}^n$ that (optimally) pushes μ_0 onto μ_1.
2. Define $T_{1/2} := \frac{\mathrm{id}+T}{2}$
3. Define the "half displacement interpolate" $\mathrm{M}_{1/2}$ as the push-forward of μ_0 by T.

Example: $\mu_0 = \delta_0$, $\mu_1 = \delta_1$, get $\boxed{\delta_{1/2}}$ instead of $\frac{1}{2}(\delta_0 + \delta_1)$

Consider certain functionals depending on a probability measure μ.

$$\mu \mapsto \begin{cases} \int V d\mu \\ \iint g(x-y) d\mu(x) d\mu(y) \\ \int F(d\mu) d\mu \end{cases}$$

Consider certain functionals depending on a probability measure μ.

Usual interpolation

$$\mu \mapsto \begin{cases} \int V d\mu & \text{linear} \\ \iint g(x-y) d\mu d\mu & \text{not necessarily convex even if } g \text{ convex} \\ \int F(d\mu) d\mu & \text{depends. Entropy is convex} \end{cases}$$

Consider certain functionals depending on a probability measure μ.

Displacement interpolation

$$\mu \mapsto \begin{cases} \int V d\mu & \text{convex if } V \text{ convex} \\ \iint g(x-y) d\mu(x) d\mu(y) & \text{convex if } g \text{ convex} \\ \int F(d\mu) d\mu & \text{depends, but entropy is convex} \end{cases}$$

(McCann, 1997)

(Specific relative) Entropy

$$\mathcal{E}(P) = \lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} \int \rho_\Lambda \log \rho_\Lambda$$

$\rho =$ density of P w.r.t. Poisson

Energy

$$\mathcal{W}(P) := \lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} \mathbf{E}_P \left[\iint_{\Lambda\times\Lambda} -\log|x-y|(d\mathcal{C}(x)-dx)(d\mathcal{C}(y)-dy) \right]$$

Difficulty: transportation of measure is well-defined on $\mathbb{R}^n$. Here, we work with infinite point configurations, so more like $\mathbb{R}^{\mathbb{Z}}$. Also need **strict** convexity, in the thermoynamic limit.

Phase portrait (bis)

In higher dimensions? Conjecture (numerical simulations Alastuey-Jancovici, Caillol-Levesque-Weis-Hansen, Choquard-Clerouin early 80's): **phase transition at $\beta \approx 140$.** For d $= 2$, but similar results for d $= 3$. "Crystallization"? Nature, even conjectural, is not well-understood.

In d $= 1$ we have DLR equations to describe the infinite object. Not in higher dimensions (for now). (Non-)uniqueness of solutions?

Two-point correlations? For Ginibre ($\beta = 2$, $2d$ Coulomb case) decays as $\exp(-r^2)$...

2D2CP

Two-component system: d $= 2$, positive charges $\vec{X}_N$ and negative charges $\vec{Y}_N$, in a box $\Lambda = [0,1]^2$. Classical point particles, no short-range repulsion, no hardcore "protection".

$$\mathcal{H}_N(\vec{X}_N, \vec{Y}_N) = \sum_{i<j} -\log|x_i - x_j| + \sum_{i<j} -\log|y_i - y_j| + \sum_{i \leq j} -\log|x_i - y_j|$$

System is well-defined for $\beta < 2$ (partition function is finite). [L. - Serfaty - Zeitouni] free energy functional (similar to the one-component case).

- Fluctuations?

$$\sum_i \varphi(x_i) - \varphi(y_i) \text{ small ?}, \quad \sum_i \varphi(x_i) + \varphi(y_i) \text{ big ?}$$

- Two-point correlations?
- BKT transition? Define the model...

Thank you for your attention.