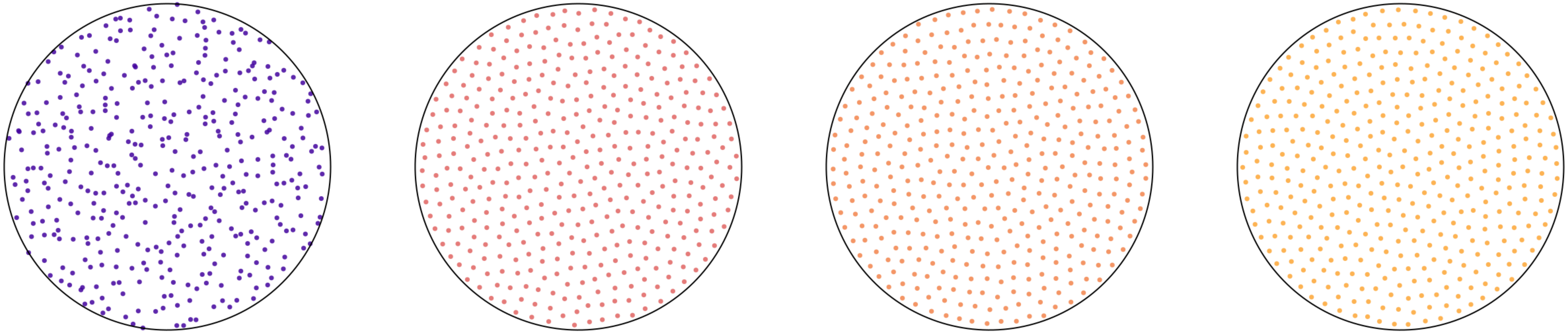


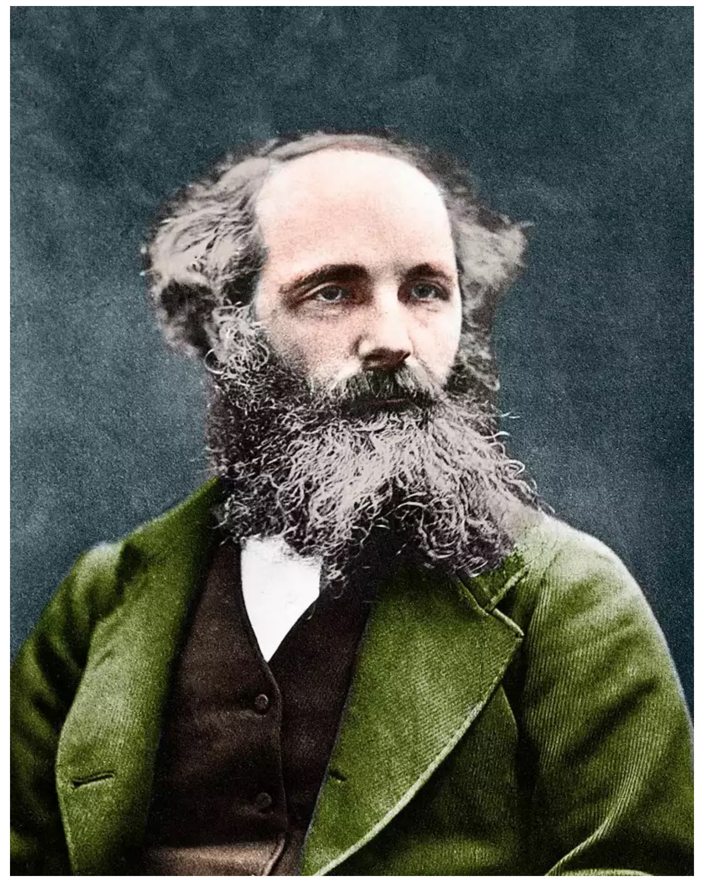
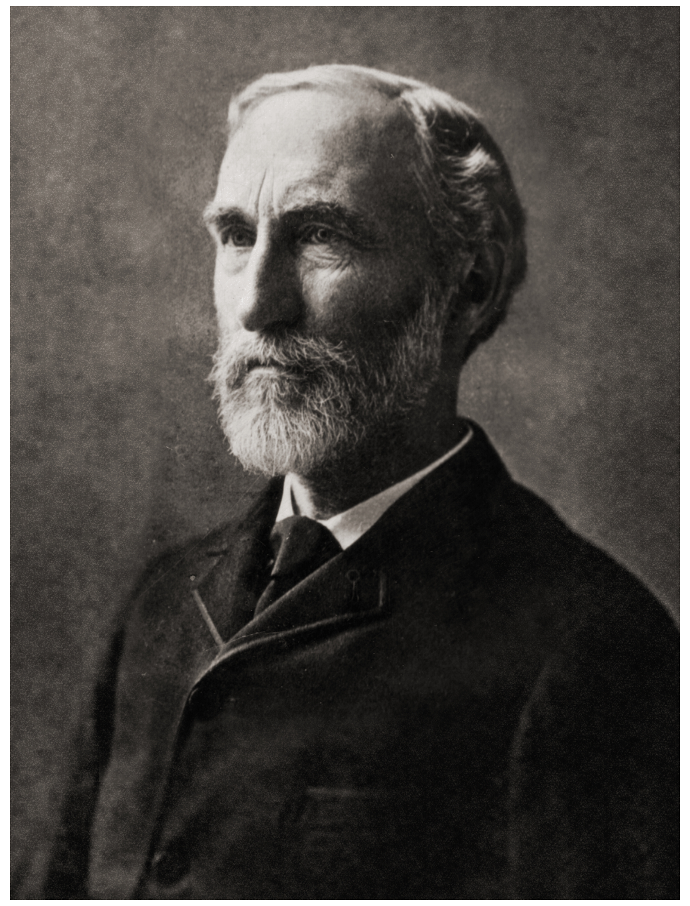
Order and disorder in the 2DOCP

(2-Dimensional One-Component Plasma)

Thomas Leblé, CNRS - Université Paris-Cité

Statistical physics

- Statistical physics = physics of many, *many* elements in interaction
  e.g. H_2O in a pot, molecules in the air of the room…
- Very large number N of elements (1 mole = 10^{23})… almost « infinite » !
- Developed in late 19th / early 20th century (Maxwell, Boltzmann, Gibbs)
- *Thermodynamics* was phenomenological, *statistical mechanics* is reductionist

- The mathematical language of statistical physics is *probability theory*
  (also a lof of analysis, combinatorics, some algebra…)

- Its way of thinking can be applied to other "large interacting systems"
  e.g. people in a big crowd, stock market…

- Emphasis on *microscopic* (one molecule, one human) versus *macroscopic* scales

A reductionist approach?

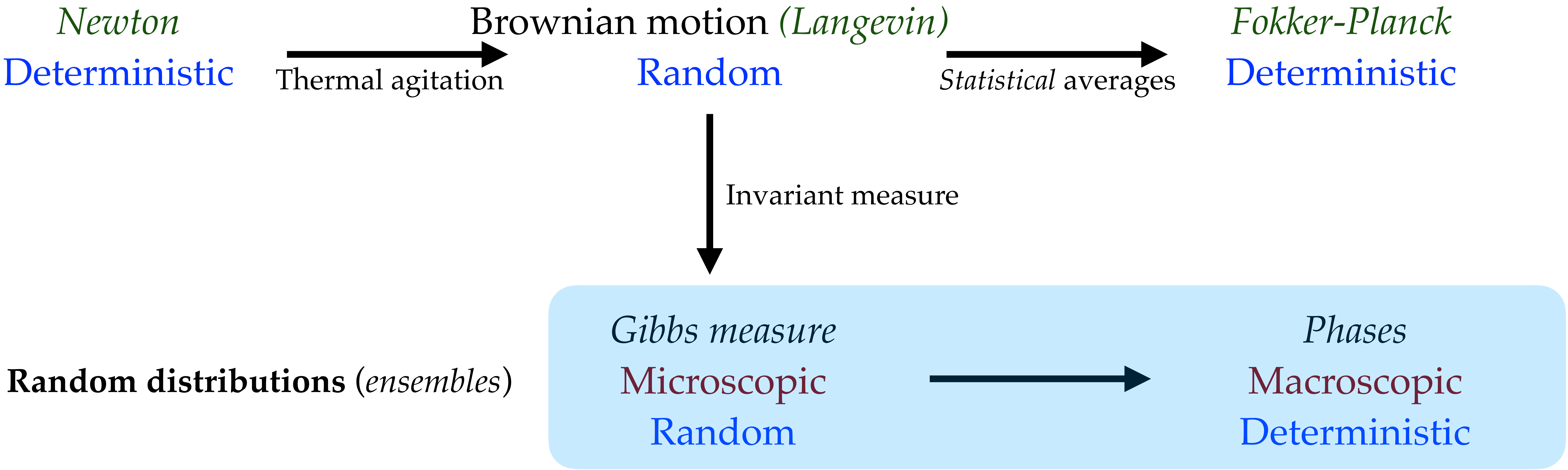
Dynamics: from *microscopic* to *macroscopic*

Laws of motion *(Newton)*
Microscopic

Kinetic theory *(Boltzmann)*
Mesoscopic

Hydrodynamics *(Navier-Stokes, Euler)*
Macroscopic

Dynamics: from *deterministic* to *random*



Newton
Deterministic

Thermal agitation

Brownian motion *(Langevin)*
Random

Statistical averages

Fokker-Planck
Deterministic

Invariant measure

Random distributions (*ensembles*)

Gibbs measure
Microscopic
Random

Phases
Macroscopic
Deterministic

Ingredients of a model

1. *State* space S (all possible states of the system)

   e.g. $S = (\mathbb{R}^d)^N$ for N particles in $\mathbb{R}^d$

2. Reference *measure* μ

   e.g. $\mu =$ Lebesgue

3. *Energy* functional $H : S \to (-\infty, +\infty]$

   e.g. $H =$ sum of all interactions between particles

4. *Inverse temperature* parameter $\beta > 0$

   sets the *strength* of interactions

The basic recipe

The state $\mathbf{X} \in S$ is *random* and distributed as:

$$\mathrm{d}\mathbb{P}(\mathbf{X}) = \frac{1}{\mathrm{Z}} e^{-\beta H(\mathbf{X})} \mathrm{d}\mu(\mathbf{X})$$

Gibbs measure

Boltzmann's factor

Partition function

$$\mathrm{Z} = \int_S e^{-\beta H(\mathbf{X})} \mathrm{d}\mu(\mathbf{X})$$

Microstates, macrostates

- $\mathbf{X} \in S$ a *microstate* = a description of the system at microscopic scale
  e.g. **all** the positions and **all** the velocities of **all** the molecules in the room
  precise but not very *useful*

- *Observable* $\mathcal{O} : S \to Y$ = function of the state, preferably of *macroscopic* nature
  e.g. "the **average** kinetic energy of the molecules in **this corner** of the room"

- *Macrostate* = "all the microstates $\mathbf{X}$ such that $\mathcal{O}(\mathbf{X})$ = a certain value".

- Goal: understand typical values of chosen $\mathcal{O}$, namely *typical macrostates*

Typical ?? Under the Gibbs measure!

Gibbs measure = distribution of *microstates*

$$\mathrm{d}\mathbb{P}(\mathbf{X}) = \frac{1}{Z} e^{-\beta H(\mathbf{X})} \mathrm{d}\mu(\mathbf{X})$$

Law of *observable*

$$\mathbb{P}\left(\mathcal{O}(\mathbf{X}) = \lambda\right) = \frac{1}{Z} \int_S e^{-\beta H(\mathbf{X})} \mathbf{1}_{\mathcal{O}(\mathbf{X})=\lambda} \mathrm{d}\mu(\mathbf{X})$$

Energy : from "$\mathcal{O}(\mathbf{X}) = \lambda$", can I say that $H(\mathbf{X}) \approx \tilde{H}_\lambda$?

$$\mathbb{P}\left(\mathcal{O}(\mathbf{X}) = \lambda\right) \approx \frac{1}{Z} e^{-\beta \tilde{H}_\lambda} \int_S \mathbf{1}_{\mathcal{O}(\mathbf{X})=\lambda} \mathrm{d}\mu(\mathbf{X})$$

Can I compute the *volume*

$$\int_S \mathbf{1}_{\mathcal{O}(\mathbf{X})=\lambda} \mathrm{d}\mu(\mathbf{X}) = \mu\left(\mathcal{O}(\mathbf{X}) = \lambda\right) \ ?$$

$$\mathbb{P}\left(\mathcal{O}(\mathbf{X}) = \lambda\right) \approx \frac{1}{Z} e^{-\beta \tilde{H}_\lambda} \times \mu\left(\mathcal{O}(\mathbf{X} = \lambda)\right)$$

$$\mathbb{P}\left(\mathcal{O}(\mathbf{X}) = \lambda\right) = \frac{1}{Z} e^{-\beta \tilde{H}_\lambda + \log \mu\left(\mathcal{O}(\mathbf{X}) = \lambda\right)}$$

Free energy

$$\mathbb{P}\left(\mathcal{O}(\mathbf{X}) = \lambda\right) \approx \frac{1}{Z} e^{-\beta \tilde{H}_\lambda + \log \mu\left(\mathcal{O}(\mathbf{X}) = \lambda\right)}$$

Most likely values λ are those for which $\beta \tilde{H}_\lambda - \log \mu\left(\mathcal{O}(\mathbf{X}) = \lambda\right)$ is as **small** as possible

Free energy: “$\beta \times$ Energy – logarithmic volume (Entropy)”

The **minimization** problem clearly depends on β (the inverse temperature)

Do free energy minimizers depend on β in a “dramatic” way? *Phase transition?*

Entropy = logarithmic volume

Entropy

Boltzmann's constant

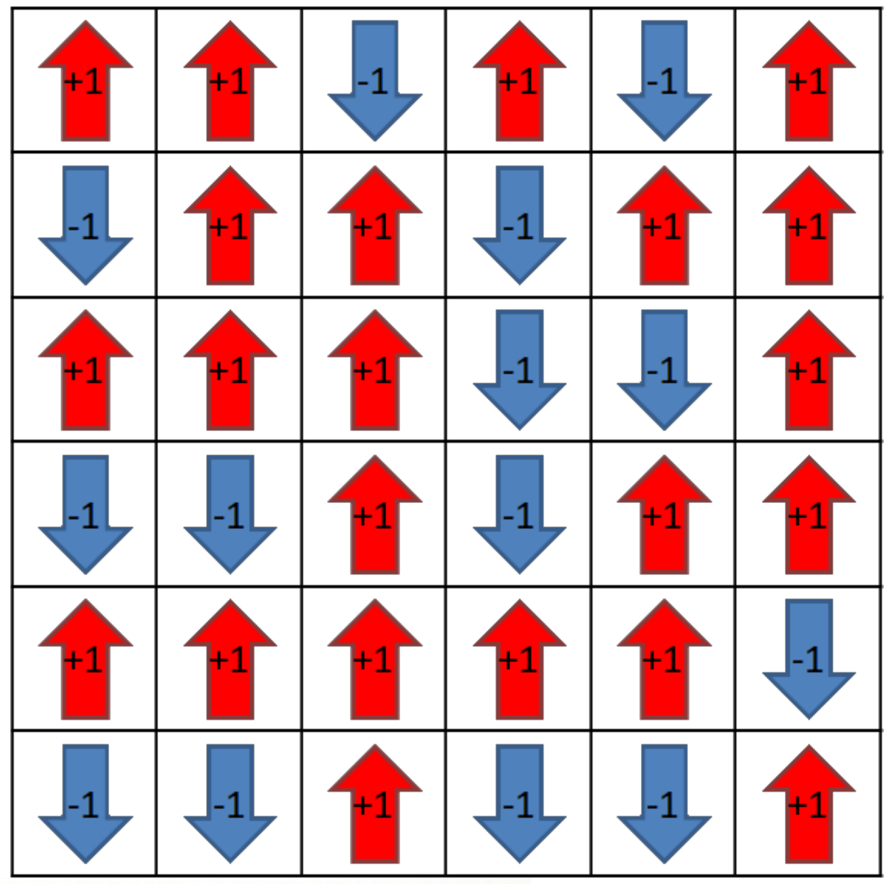
Macrostate volume

Wahrscheinlichkeit

Challenges?

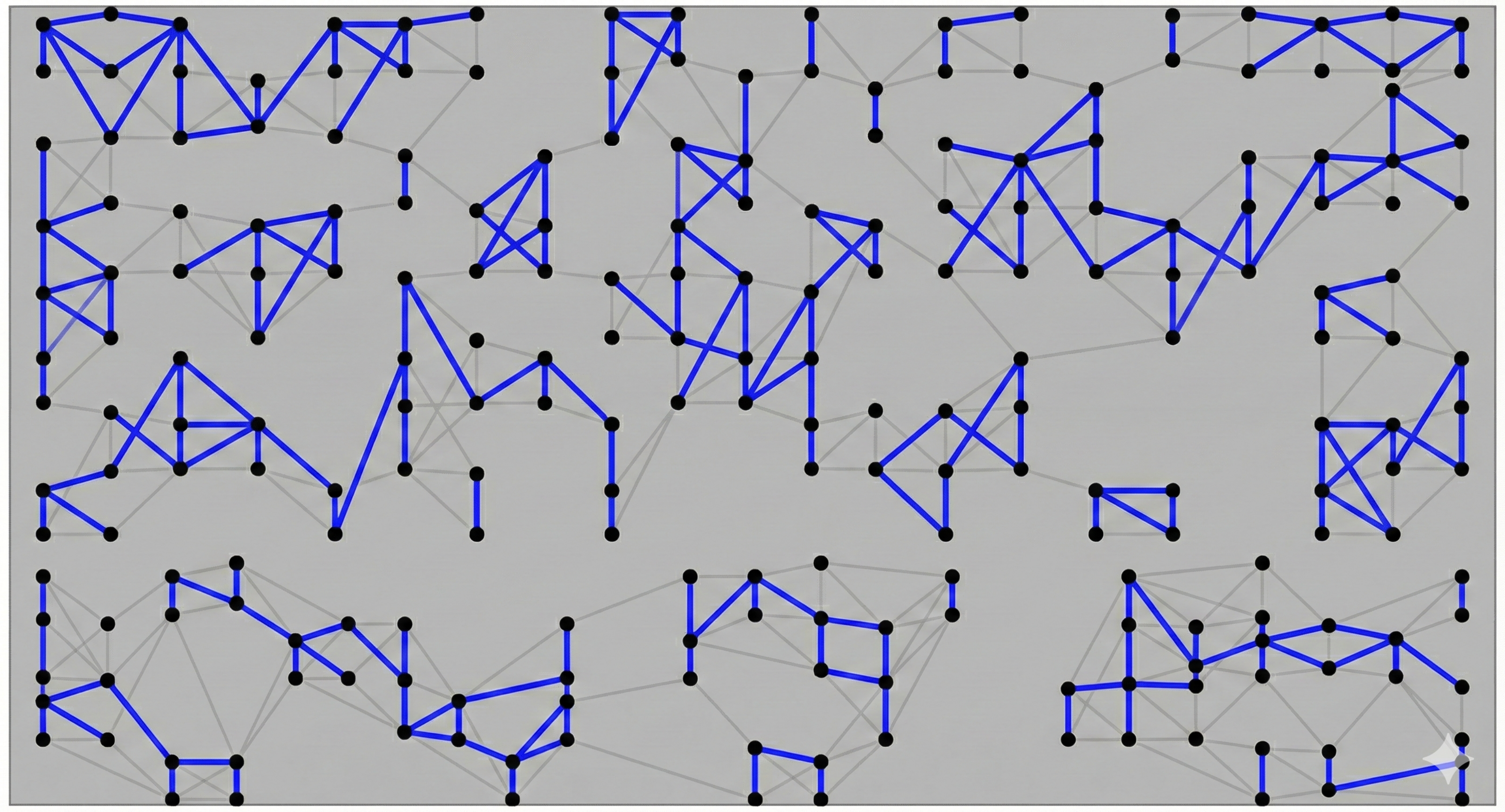
- Finding the right, interesting *observable*
- Saying something about *energy* (= result of a **huge** number of interactions) from this observable
- Computing *volume* in a **huge**-dimensional space
- Minimizing the *free energy* functional over a **huge** space

Some models



+1	+1	-1	+1	-1	+1
-1	+1	+1	-1	+1	+1
+1	+1	+1	-1	-1	+1
-1	-1	+1	-1	+1	+1
+1	+1	+1	+1	+1	-1
-1	-1	+1	-1	-1	+1

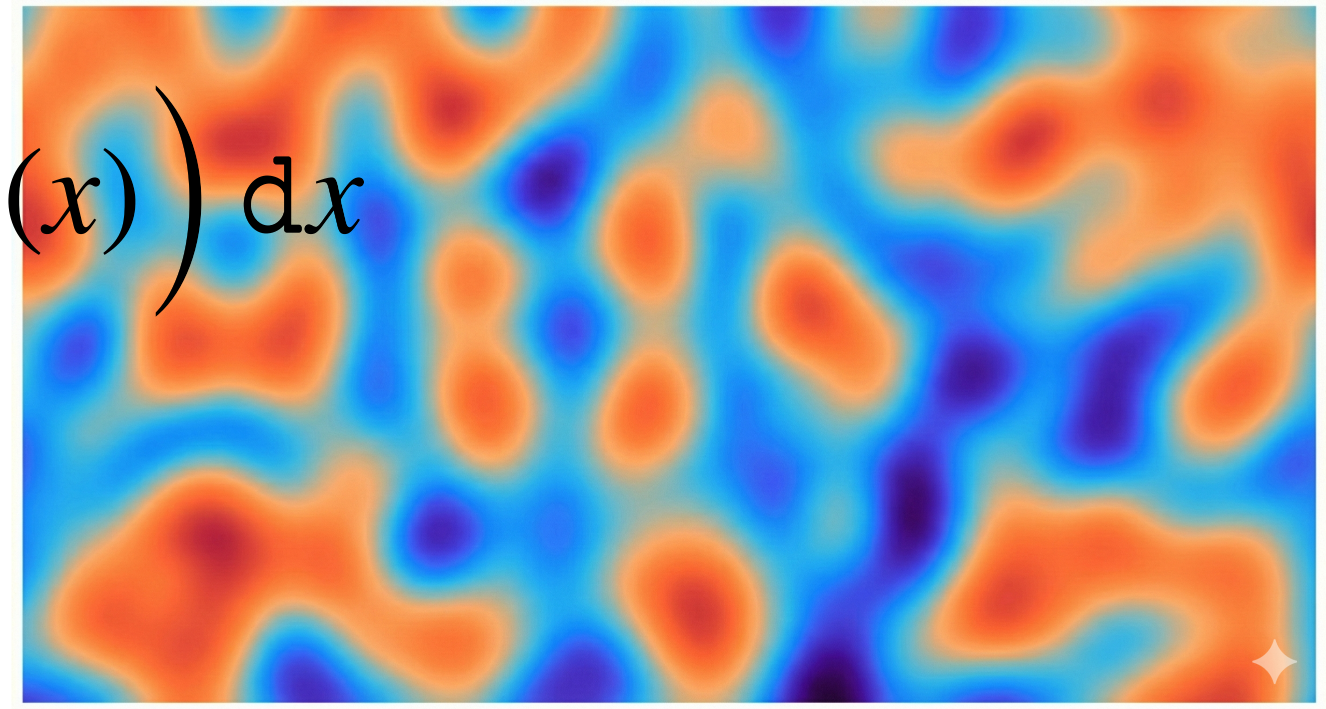
- **Ising model** on a lattice Λ (Ising 1920's, Peierls 30's, Onsager 40's…)
  State space = $\{-1, +1\}^{\Lambda}$ *"spins"*
  Energy = alignement vs. non-alignement of neighboring spins
  Observable = magnetization



- **Percolation** on a graph (V, E)
  State space = $\{\text{open edge, close edge}\}^{E}$
  Energy = number of "open" edges
  Observable = size of largest connected region

- **ϕ^4 field theory**
  State space = "fields" $\phi : \mathbb{R}^d \to \mathbb{R}$
  Energy = "action" of the field
  Observable = correlation $\phi(x)\phi(0)$

$$\int_{\mathbb{R}^d} \Big(|\nabla \phi(x)|^2 + \phi(x)^2 + \phi^4(x) \Big)\, \mathrm{d}x$$



« Phase transitions » ??

Continuum models

- Particles $x_1, \ldots, x_N$ in physical space (a domain of $\mathbb{R}^d$, a manifold…)

- Interactions between each pair of particles via a *potential* φ

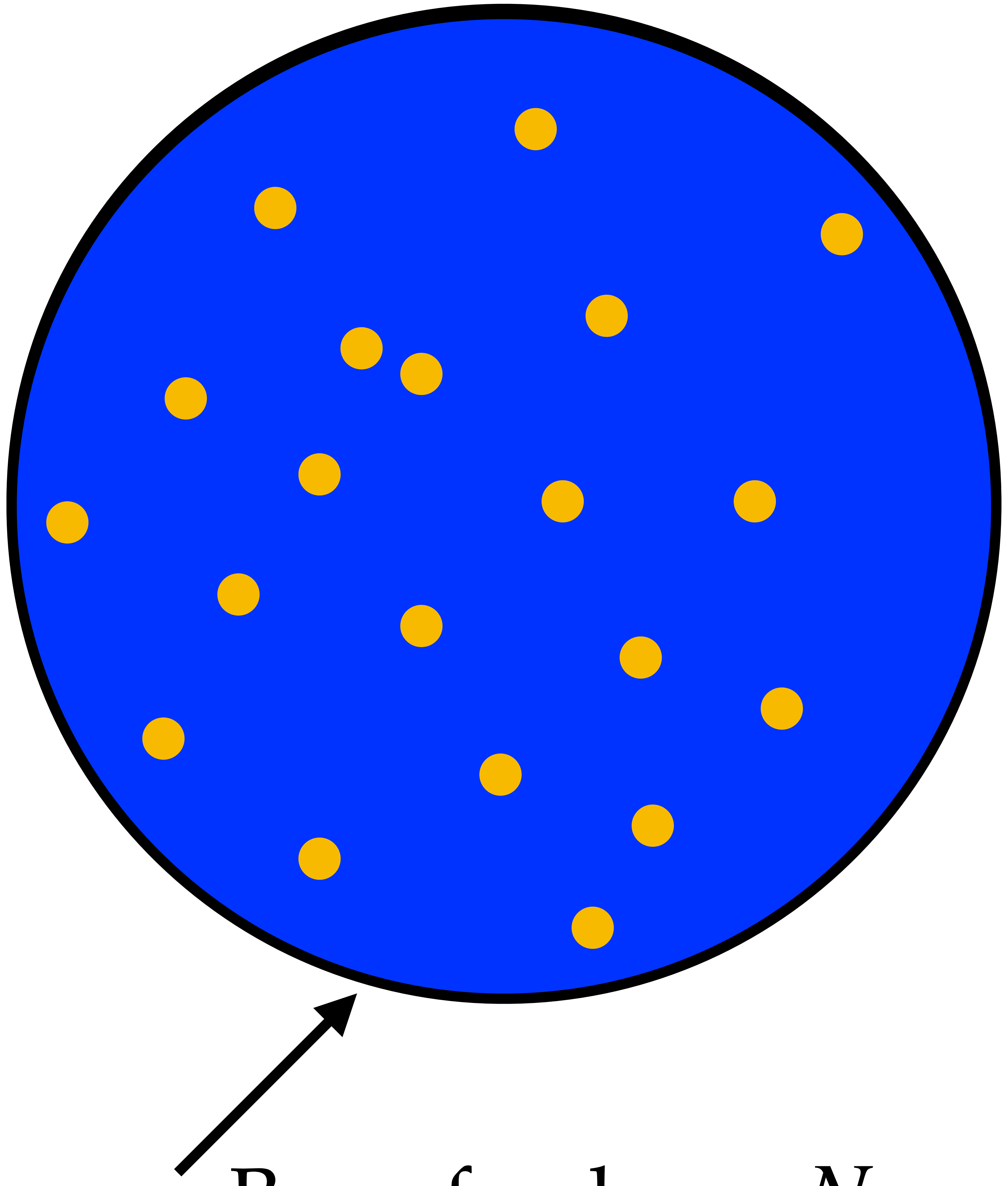
  $$Energy = \sum_{i \neq j} \varphi(x_i - x_j)$$

- Define the Gibbs measure, find a way to characterize "order" or "disorder"

- Derive free energy functional, *find its minimizers* (will **depend on β!**)

- Existence of *phase transitions* between order and disorder in the **continuum** is on B. Simon's 1984 list of « Fifteen problems in mathematical physics »

One-component plasma (OCP)



Box of volume N

N particles $\overrightarrow{X}_N := (x_1, x_2, \ldots, x_N)$

+1 charge

Uniform "neutralizing" background

-1 density

Electrostatics = *Coulomb* potential

$$\varphi(r) = \frac{1}{r} \text{ in dimension 3}$$

$$= -\log r \ \textbf{in dimension 2}$$

Jellium, Coulomb gas, Log-gas

State space and energy

State $\overrightarrow{X}_N = (x_1, x_2, \ldots, x_N)$: a N-tuple of points in the box (particles)

Interaction energy $H_N(\overrightarrow{X}_N)$ in the state $\overrightarrow{X}_N$

$$H_N(\overrightarrow{X}_N) := \frac{1}{2} \iint_{(x,y)\in \mathrm{Box}^2,\ x\neq y} -\log|x-y| \left(\sum_{i=1}^{N} \delta_{x_i} - \mathrm{Leb}\right)(x) \left(\sum_{i=1}^{N} \delta_{x_i} - \mathrm{Leb}\right)(y)$$

No self-interaction

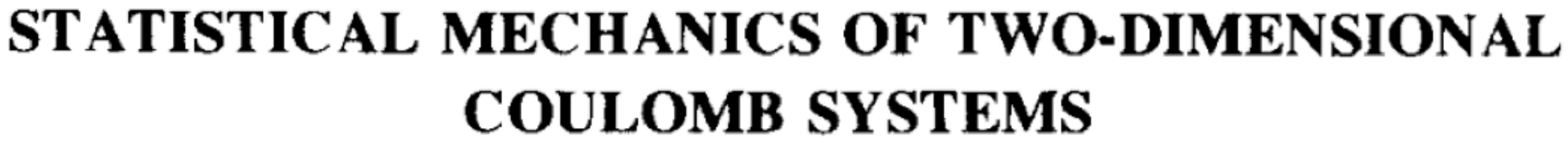
Positive charges

Background

Do physicists care?


On the ground state of the one-component classical plasma

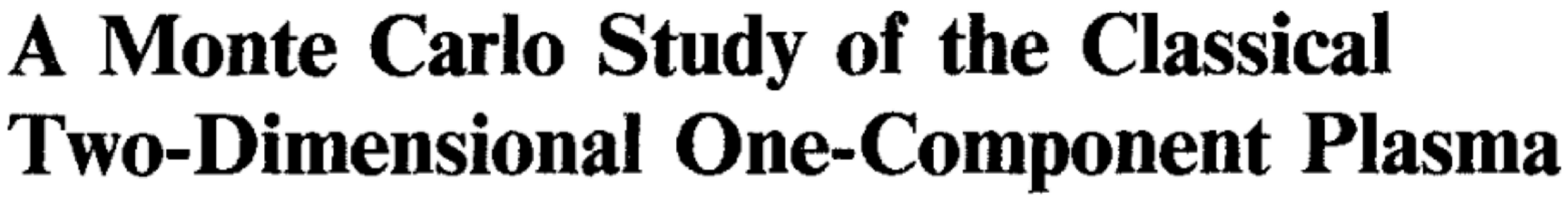

Equilibrium properties of a two-dimensional Coulomb gas

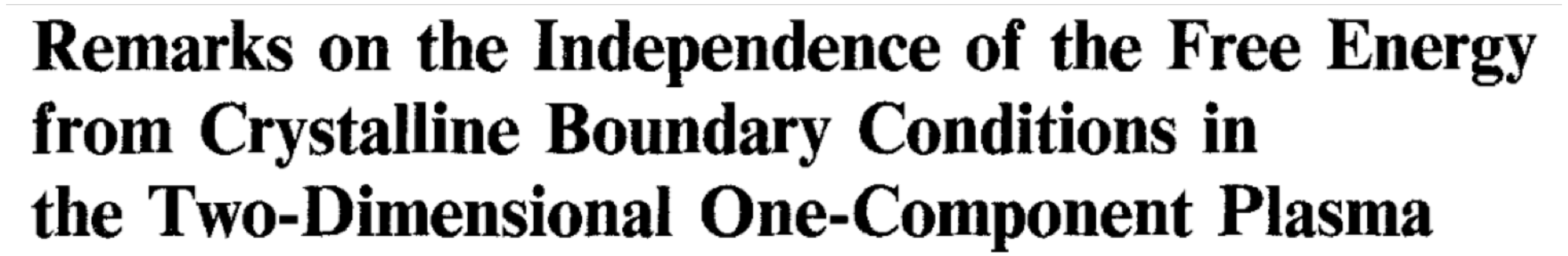

STATISTICAL MECHANICS OF TWO-DIMENSIONAL COULOMB SYSTEMS


Cooperative Phenomena below Melting of the One-Component Two-Dimensional Plasma


On the classical two-dimensional one-component Coulomb plasma


ON "CRITICAL POINTS" IN THE TWO-DIMENSIONAL CLASSICAL JELLIUM


A Monte Carlo Study of the Classical Two-Dimensional One-Component Plasma


Remarks on the Independence of the Free Energy from Crystalline Boundary Conditions in the Two-Dimensional One-Component Plasma

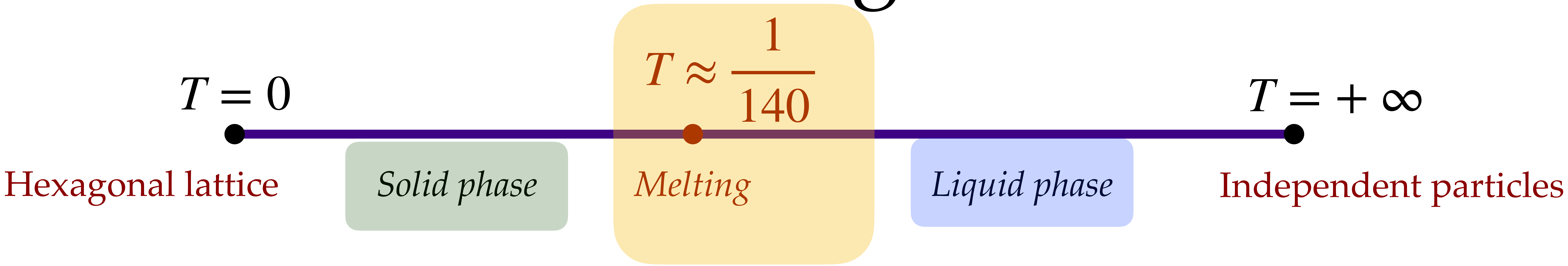
Why do they care?

- One-component plasma as toy model for matter
  small electrons (particles) versus *big protons* (background)

- Strong interest for statistical mechanics in dimension 2
  + *logarithmic interactions* appear elsewhere (vertex systems)

- Singular, long-range (not → 0 fast at infinity) interactions are special
  “classical” theory developed for nice, short-range interactions.

Phase diagram



$T = 0$

$T \approx \frac{1}{140}$

$T = +\infty$

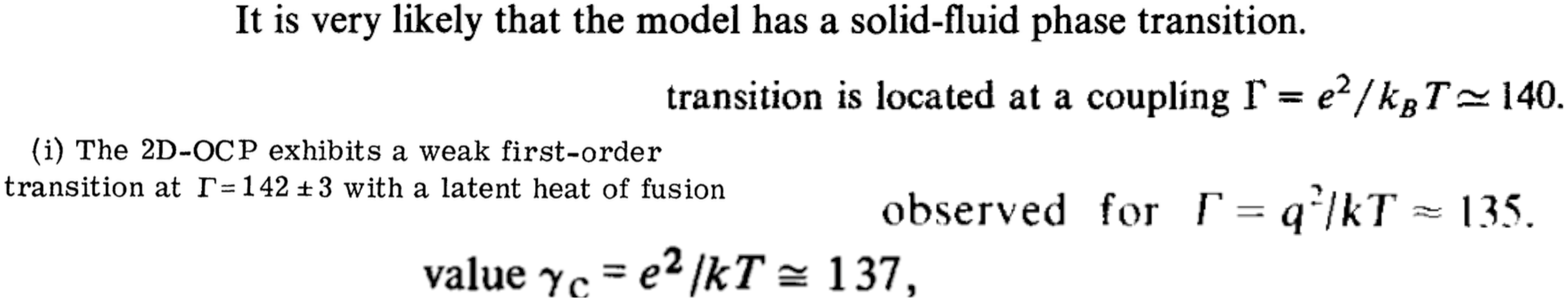
Hexagonal lattice

Solid phase

Melting

Liquid phase

Independent particles



It is very likely that the model has a solid-fluid phase transition.

transition is located at a coupling $\Gamma = e^2/k_B T \simeq 140$.

(i) The 2D-OCP exhibits a weak first-order transition at $\Gamma = 142 \pm 3$ with a latent heat of fusion

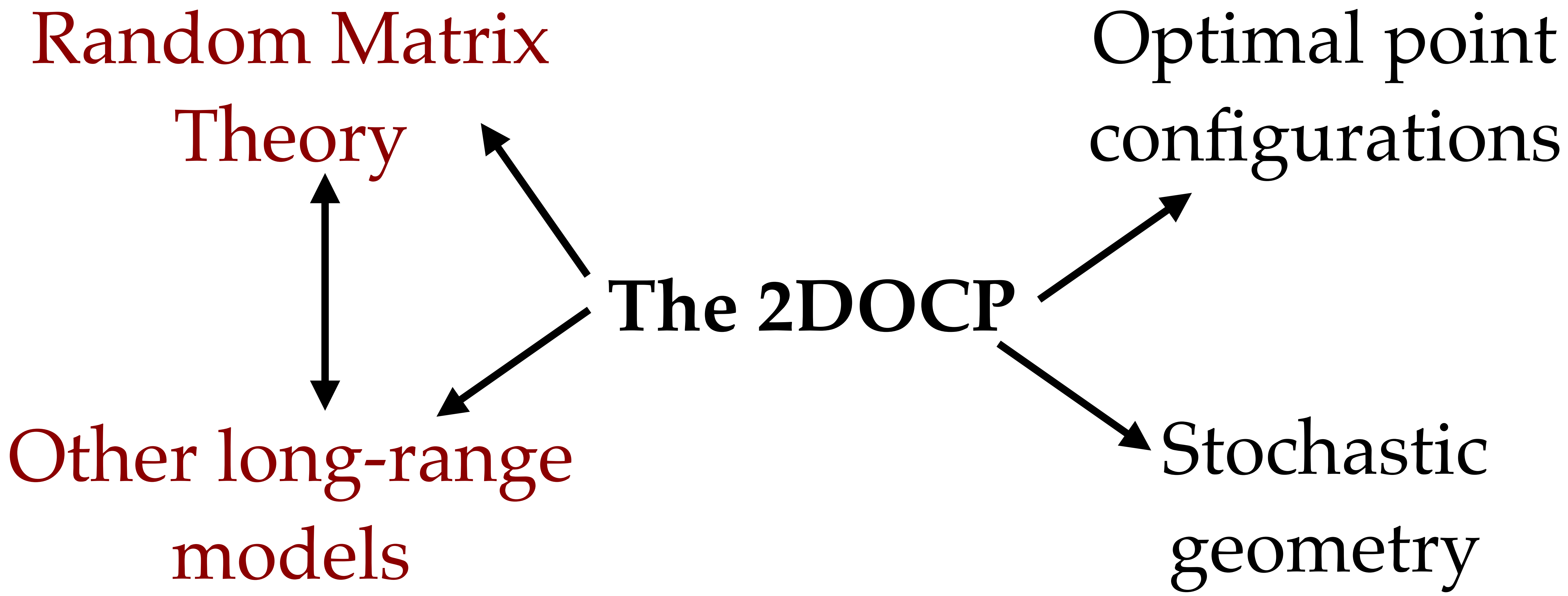
observed for $\Gamma = q^2/kT \approx 135$.

value $\gamma_C = e^2/kT \cong 137$,

Goal: *mathematical confirmation of the physicists' predictions*

Finding an order-disorder transition for the 2DOCP

Other motivations



Random Matrix Theory

Other long-range models

The 2DOCP

Optimal point configurations

Stochastic geometry

A link with RMT: the Ginibre ensemble

Take a $N \times N$ matrix with independent Gaussian coefficients
Joint distribution of eigenvalues is computable: *Ginibre ensemble*

→ Gibbs measure with *logarithmic interaction* at $\beta = 2$ in complex plane
Link between RMT and 2d Coulomb gases

Integrable ("determinantal") case: it "suffices" to do computations
The 2DOCP at $\beta = 2$ *is very well understood*

A close relative: the 1d Log-gas

Take a $N \times N$ Hermitian matrix with Gaussian coefficients

Joint distribution of eigenvalues is computable **Dyson 60's**

→ Gibbs measure with logarithmic interaction… on the line…at $\beta = 2$

Early 2000's: discovery of a « random matrix model » for all $\beta > 0$

Dumitriu-Edelman

RMT and other friends

2DOCP
= Particles + logarithmic interaction in $\mathbb{R}^2$
= Random *complex* eigenvalues ($\beta = 2$)

1d Log-gas
= Particles + logarithmic interaction in $\mathbb{R}$
= Random *real* eigenvalues ($\beta > 0$)

Random polynomials and Gaussian entire functions

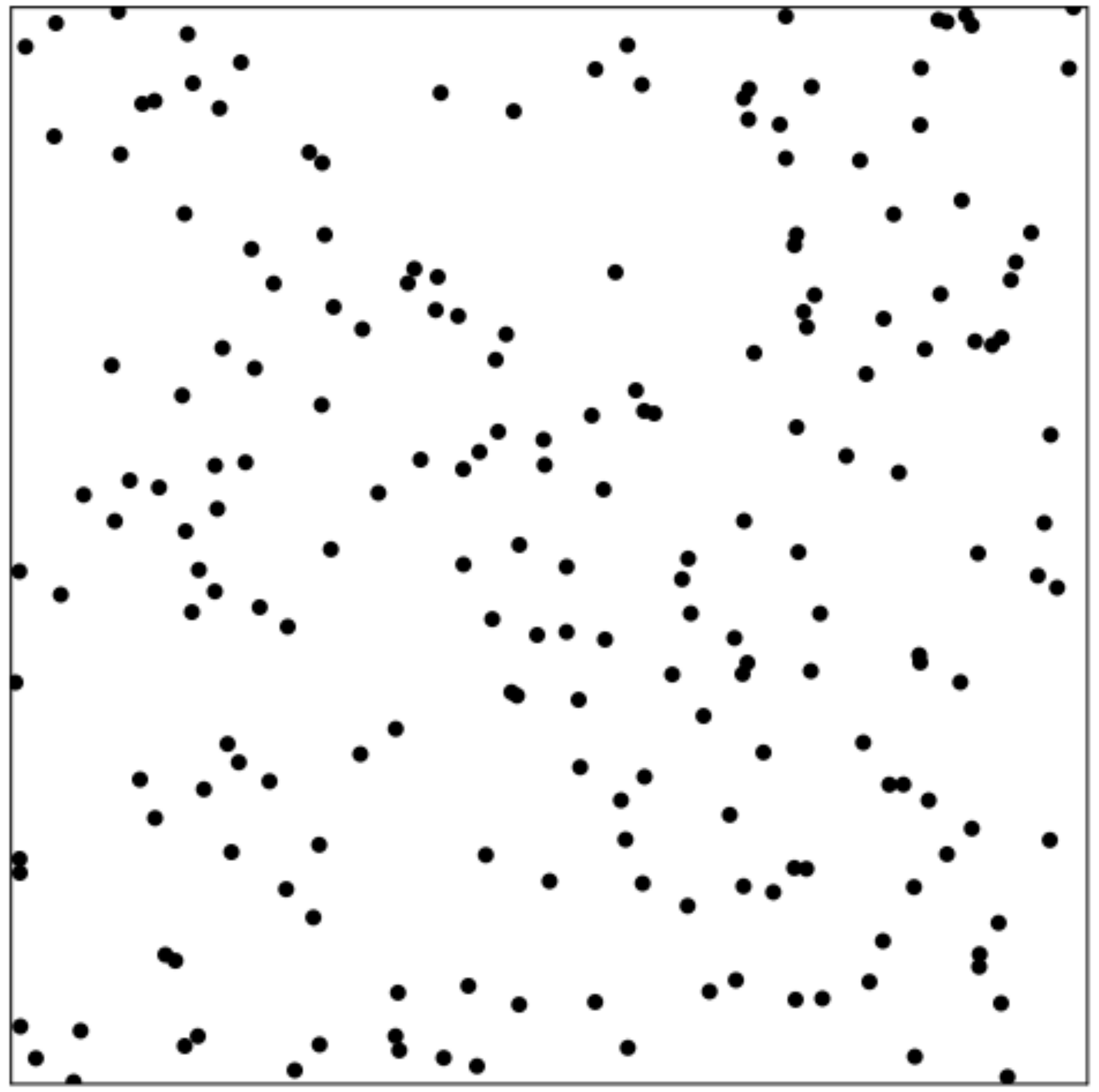
Take $(a_k)_{k\geq 0}$ independent complex Gaussian coefficients, and form:

$$f(z) := \sum_{k\geq 0} \frac{a_k}{\sqrt{k!}} z^k$$

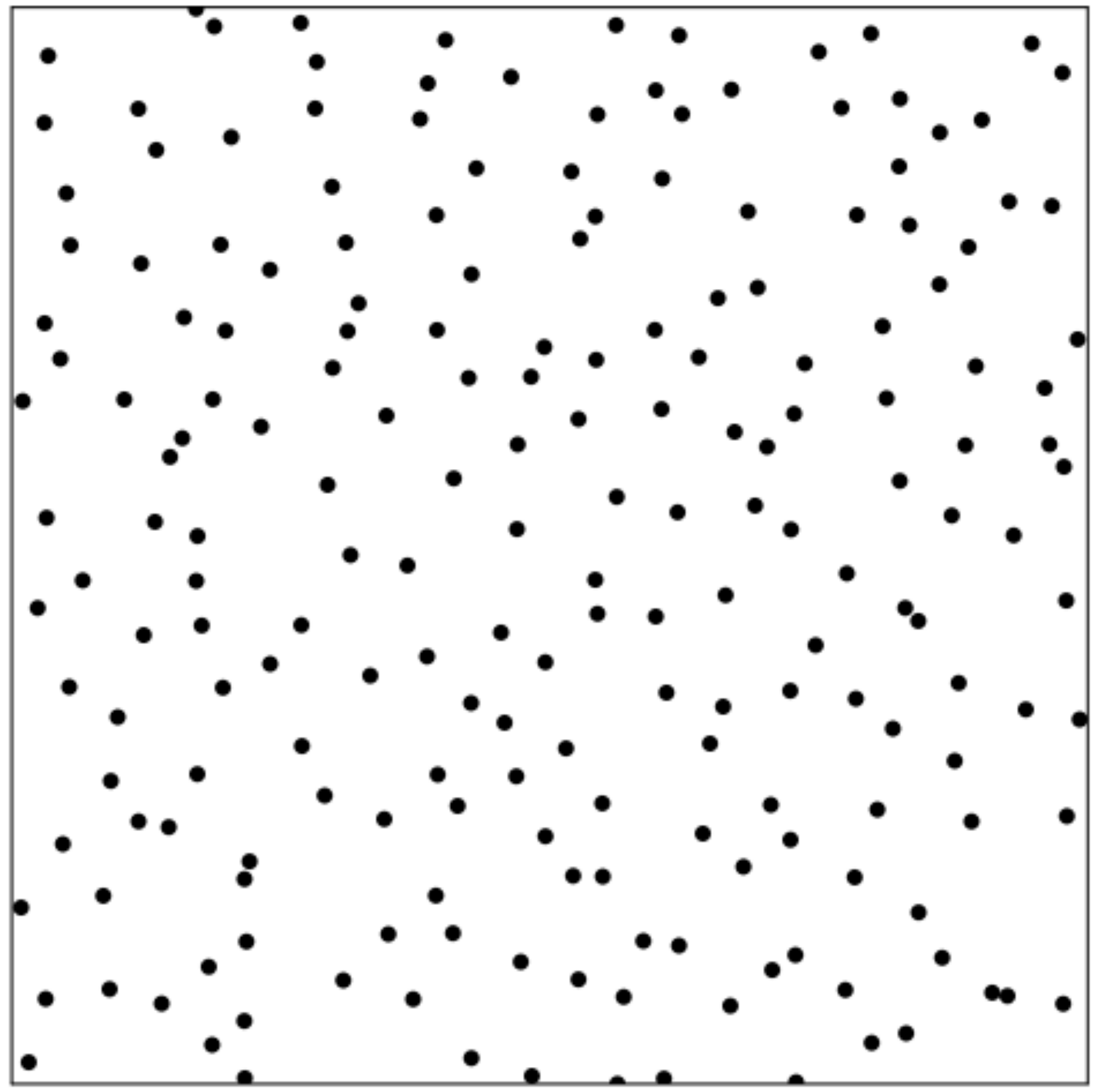
$$P_N(z) := \sum_{k=0}^{N} a_k z^k$$

Gaussian Entire Function (GEF)
Zeroes of f share many similarities
with a 2DOCP

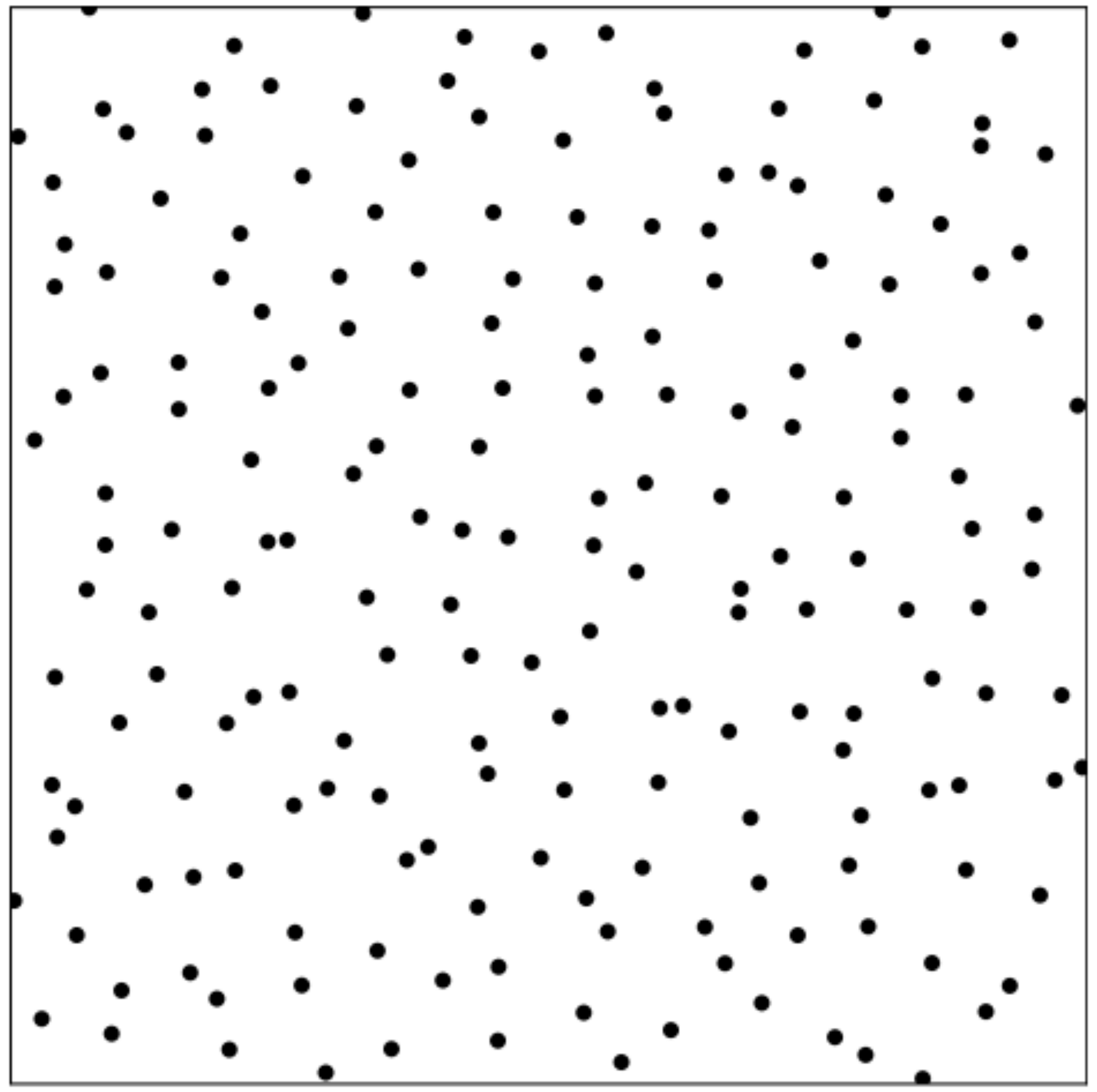
Gaussian Kac Polynomial
Zeroes of P_N share many similarities
with a 1d Log-gas



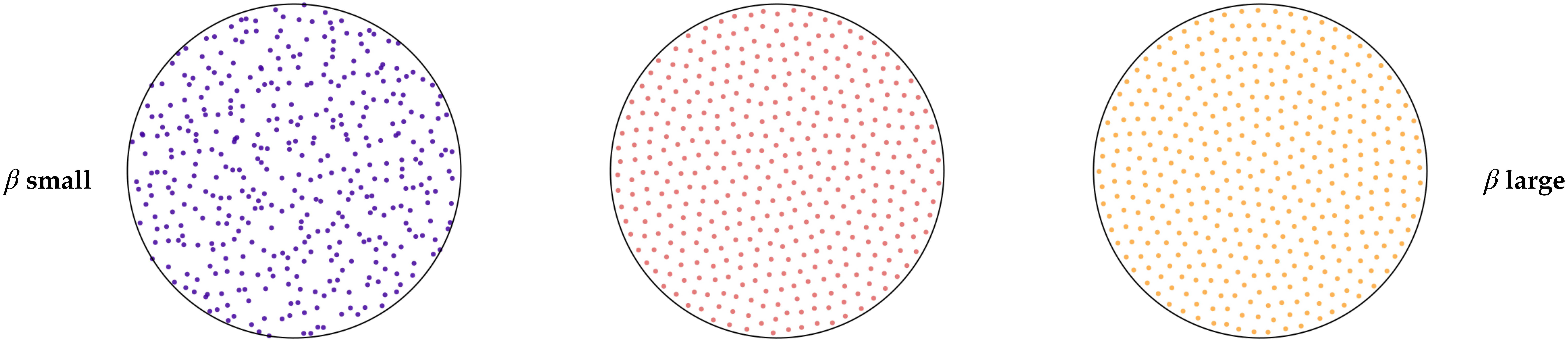
Independent points



Ginibre ensemble (2DOCP)



Zeroes of GEF



Order through correlations

1-point correlation $\rho_1(x)$ = "probability" of having a particle at x
2-point $\rho_2(x, y)$ = "probability" of having a particle at x **and** a particle at y

Decay of correlations ?

$\rho_2(x, y) - \rho_1(x)\rho_1(y) \to 0$ as $|x - y| \to \infty$

Exponential (« fast ») decay = "disorder"
Polynomial (« slow ») decay = "quasi-order"
No decay = "order"

Repulsiveness ?

$\rho_2(x, y) \ll \rho_1(x)\rho_1(y)$ for $|x - y| \ll 1$

But: correlations are hard

- Correlation functions - or simply their decay - are *very hard to compute*

- For the 2DOCP, only known case for 2-point correlation is $\beta = 2$:

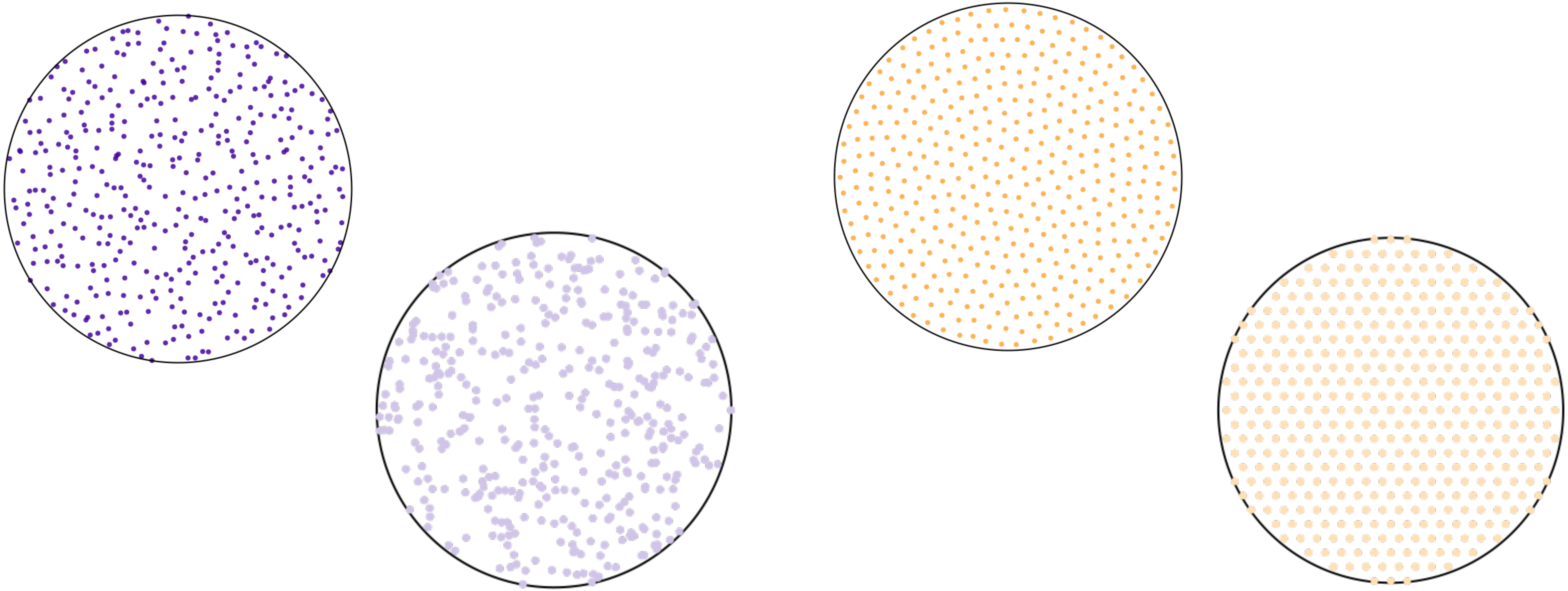
  decay is $e^{-|x-y|^2}$ for $|x-y| \gg 1$ (very fast!)

  vanishes like $|x-y|^2$ for $|x-y| \ll 1$ (*repulsion*)

- Repulsion is well understood, but decay for $\beta \neq 2$ is open

Moreover, some regularity of those systems is **not** captured
by the usual "decay of correlations" criterion
One sometimes speaks of *order within disorder*

Other faces of order



1. Size of fluctuations 2. Rigidity with respect to the exterior 3. Transportation cost

Size of *charge fluctuations*

Take a big disk of radius $R \gg 1$ and count **how many points fall into it**.
What is the ***variance*** of this quantity (measures "*charge fluctuations*") ?
For **independent** points: grows like R^2.
For a **lattice** with independent perturbations, or uniform shift: like R.

Physics literature: **Anything with variance $o(R^2)$ is interesting**.
Hyperuniform or *super-homogenous* systems.

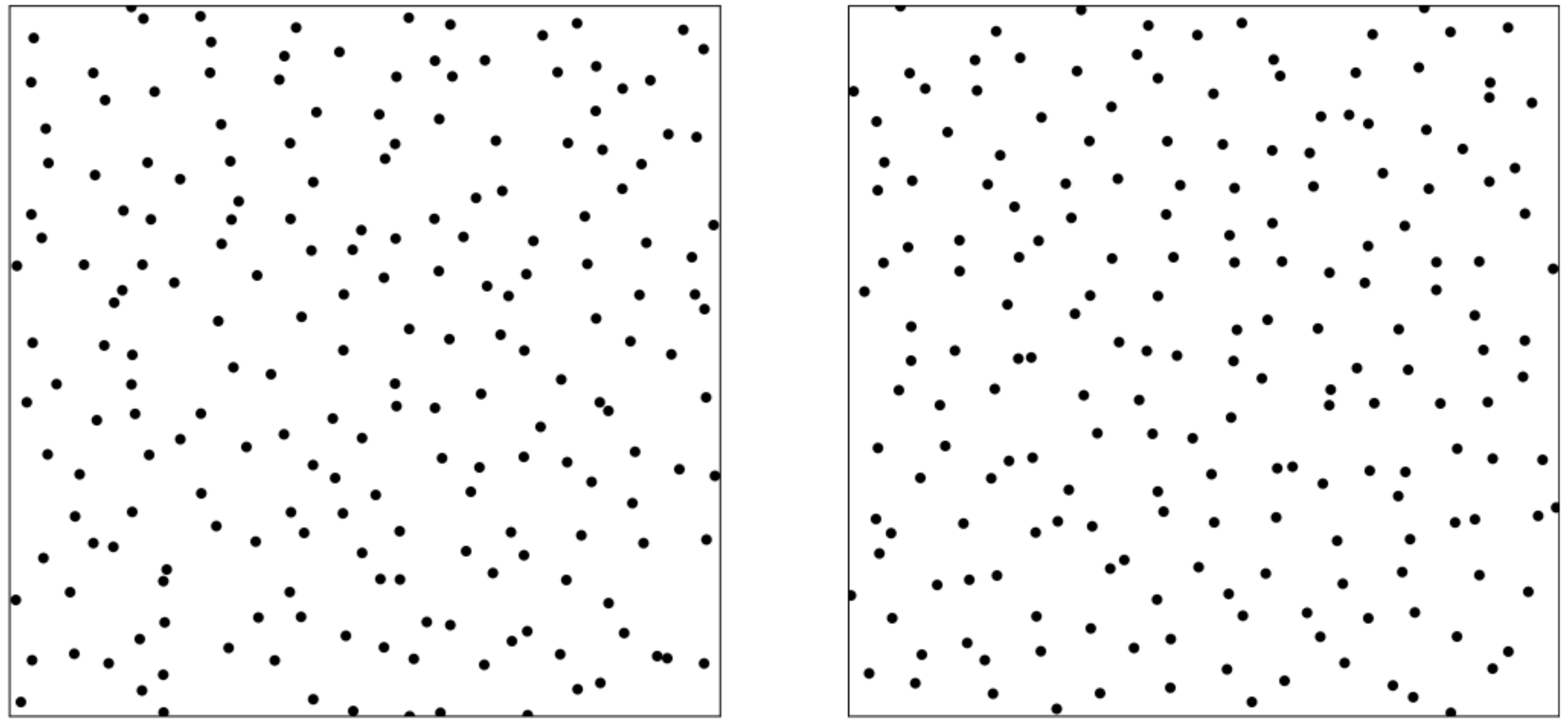
Also physics literature: **the 2DOCP is** *hyperuniform at all temperatures.*
Even in the « liquid » (disordered) phase !

Cancellation of charge fluctuations

For $\beta = 2$, the variance of the number of points scales like R… (*Order*)
yet the correlations have a super fast decay! (*Disorder*)

L. '23 For all $\beta > 0$, the variance is $\mathcal{O}\left(\frac{R^2}{(\log R)^c}\right)$ (sharp bound should be R…)

Sharp bound is true for
zeroes of the Gaussian Entire Function



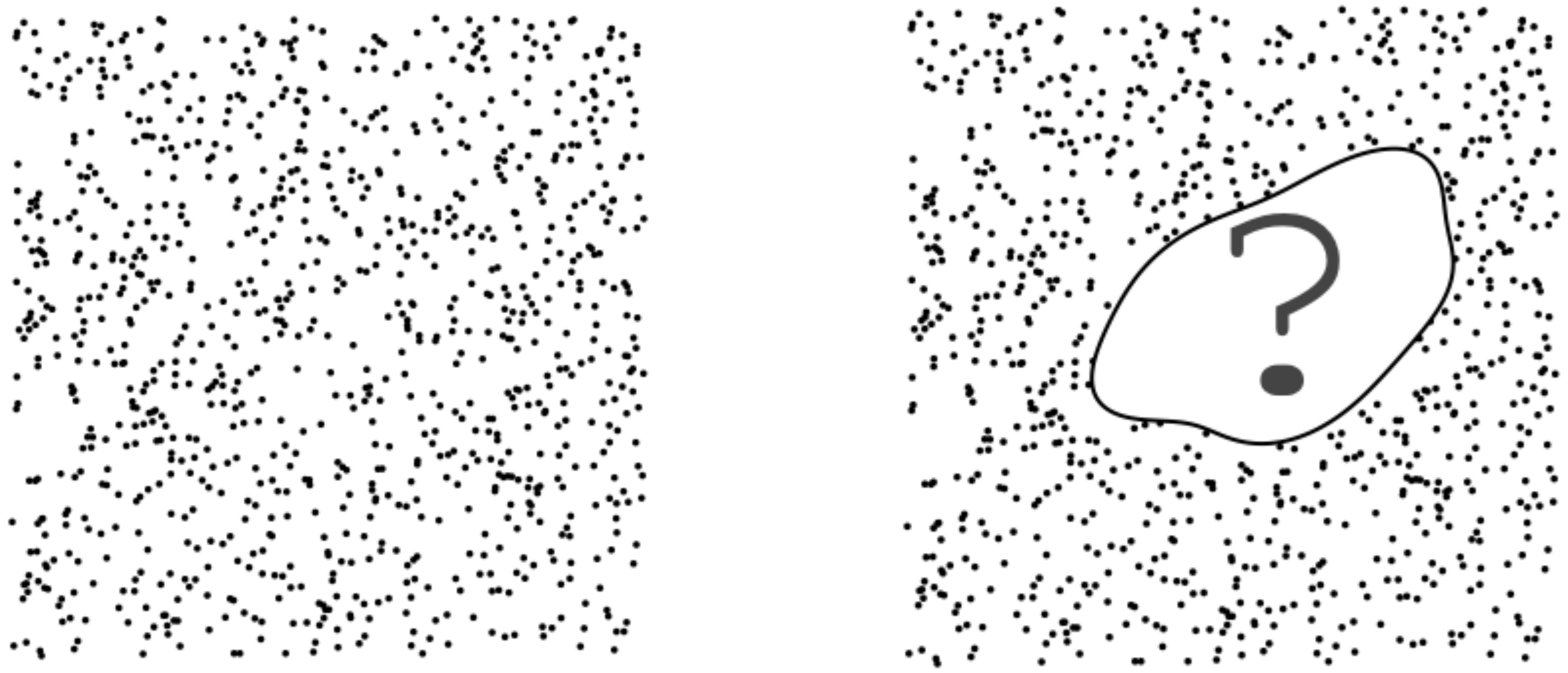
Rigidity properties

Ghosh-Peres '12

What can we say about
the *inside* region
from looking *outside*?

- (Almost surely) guess the **number** of points? *Number-rigid.*
- (Almost surely) guess the **center of mass**? *Barycenter-rigid*.
- (Almost surely) guess the full **configuration**? *Fully-rigid.*

Who is rigid?



- A Poisson point process (independent points)
  No rigidity
- A lattice (perfectly ordered)
  Fully-rigid

What about lattice + i.i.d. perturbations? The 2DOCP? Our friends?

Surprisingly subtle question
Answer depends on dimension
+ on the *size of perturbations*

Peres-Sly '14

Number-rigid $\forall \beta > 0$….
even in *liquid phase*!

L. '24

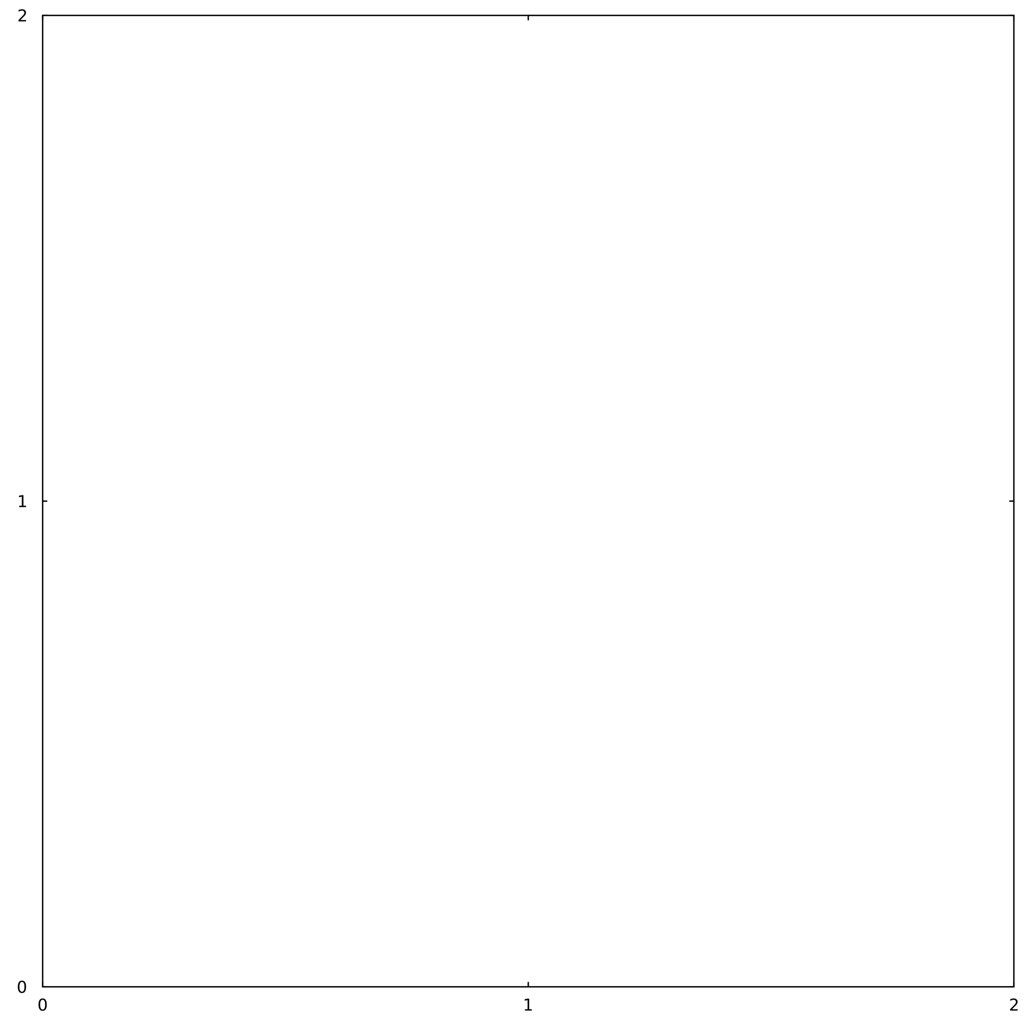
Chhaibi-Najnudel '15

1d Log-gas is
Number-rigid $\forall \beta > 0$

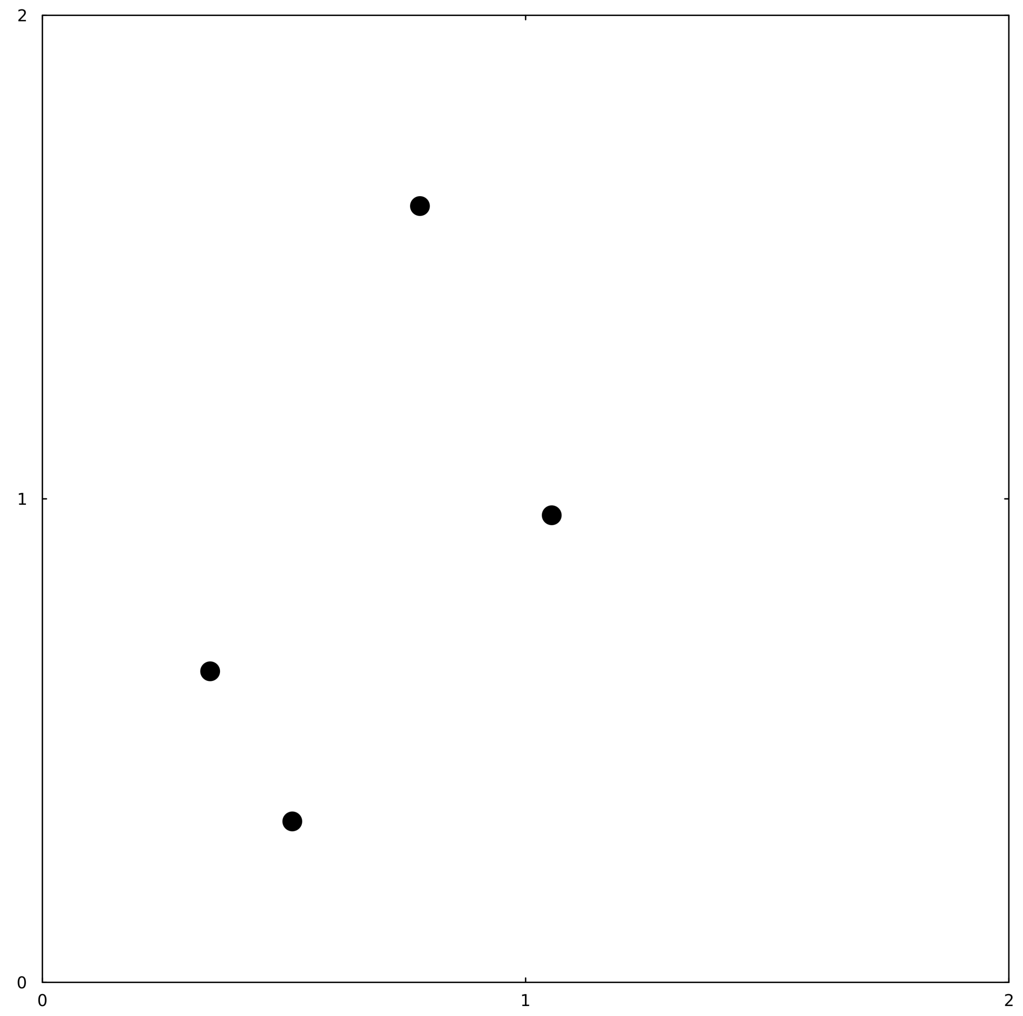
Zeroes of GEF are
number-rigid **and**
barycenter-rigid

Ghosh-Peres '12

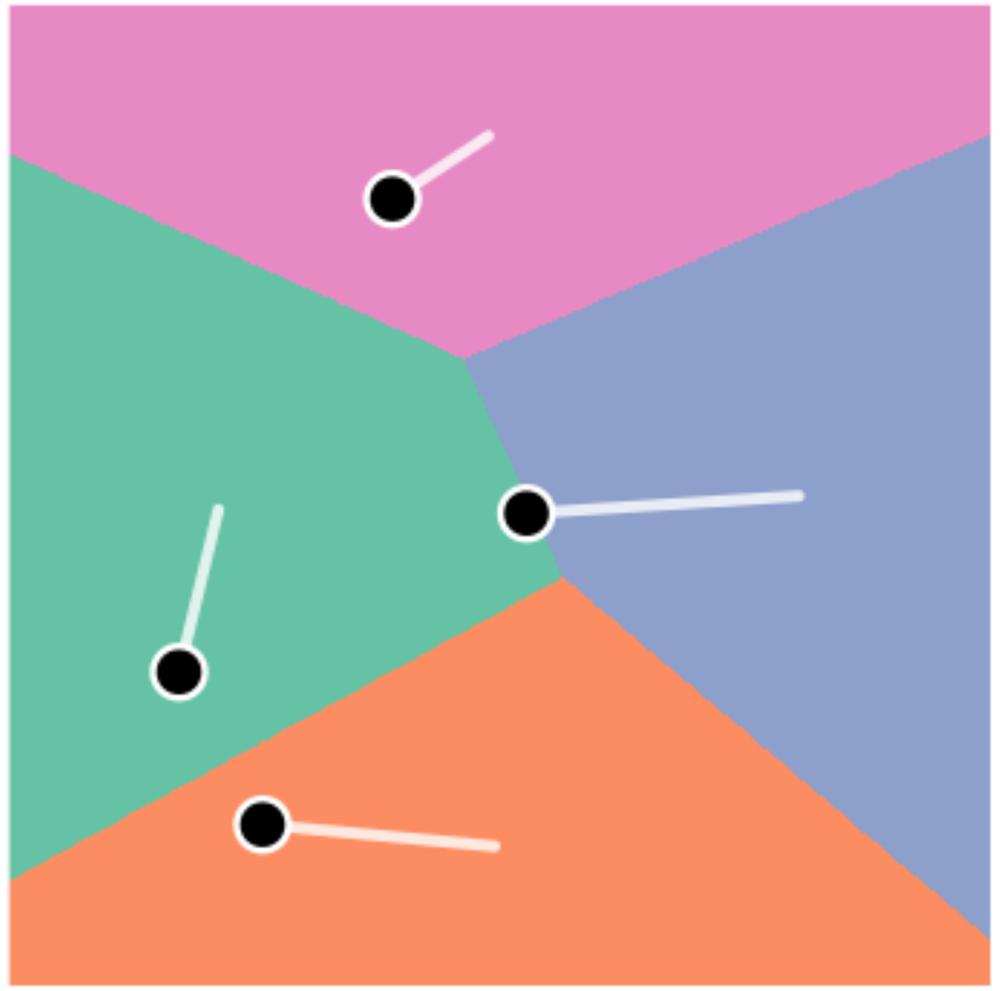
Transportation cost



Take a $L \times L$ square



Place L^2 points



Associate to each point x
a **cell** C_x of area 1

Quadratic transportation cost

for the x-cell: $\int_{C_x} |x-t|^2 \,\mathrm{d}t$

Transportation cost

$$\sum_x \int_{C_x} |x-t|^2 \,\mathrm{d}t$$

What is the *minimal* cost?

Two extreme cases

If the points are on a grid (*order*)
the cost (per point) is **bounded**

For 2DOCP at all $\beta > 0$
average cost is bounded.

L.-Huesmann '24 In fact:
Finite Coulomb energy
$\Longrightarrow$ bounded average cost

Ajtai-Komlos-Tusnady '84

If points are drawn i.i.d. at random (*disorder*)
average cost **diverges as** $L \to +\infty$ in $d = 2$.

Same for zeroes of the GEF.

Can we construct a "good"
transportation map?

Nazarov
Sodin
Volberg

Gravitational allocation

Given a family of points $\mathbf{X} = \{x_i\}$ in $\mathbb{R}^2$
pretend they are "stars" with mass 1,
and the rest of $\mathbb{R}^2$ is dust

The dust feels the attraction of the stars

Where does each grain fall?

Fun fact:

Each star should receive exactly a unit mass of dust.

Gravitational allocation studied for independent points, for GEF, but not for 2DOCP.

What happens?

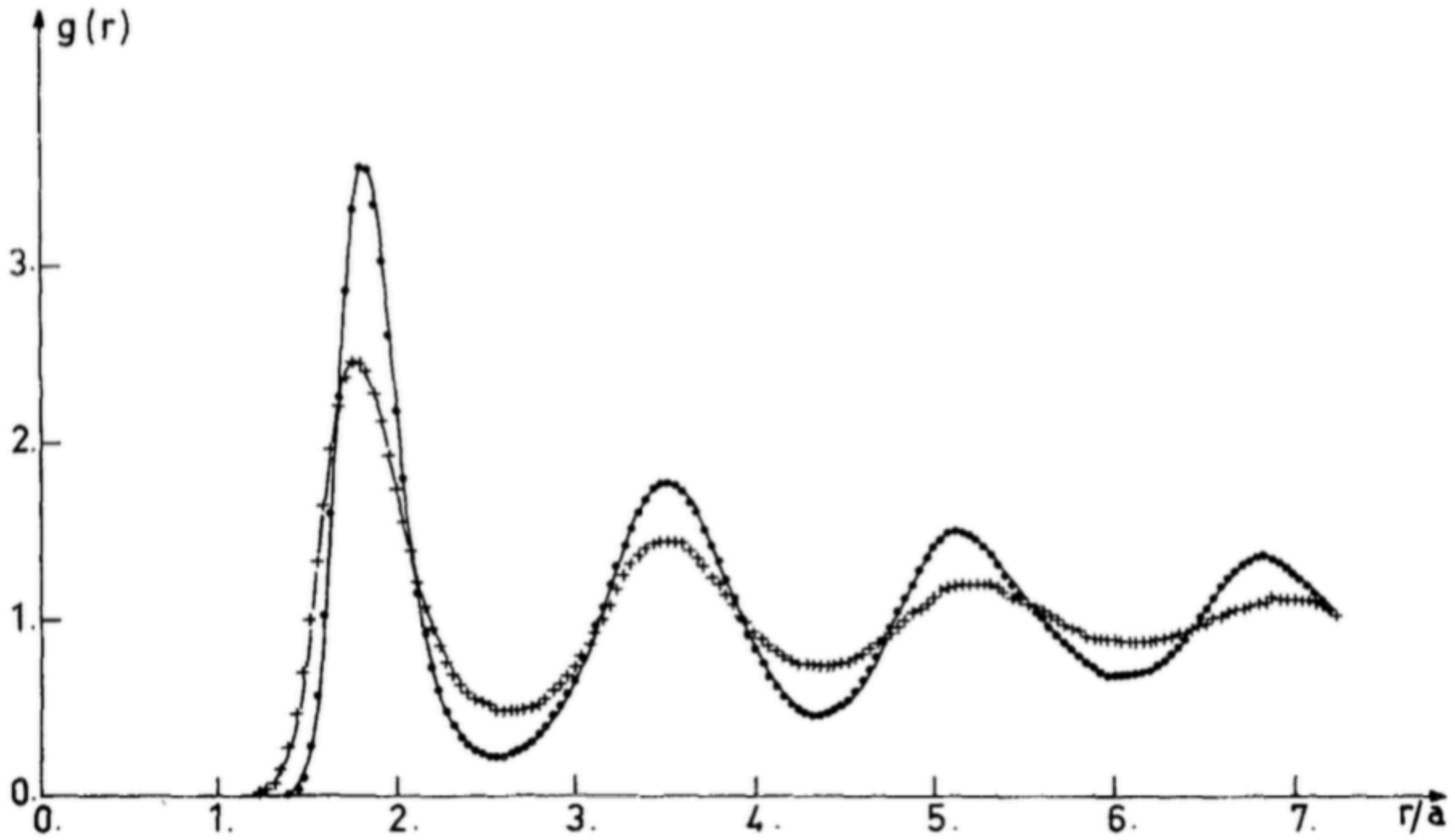
- We are looking for a transition between *order* and *disorder* within the 2DOCP
- But every property seems to place it strongly on the “order” side at all $\beta > 0$
- Yet we know that for $\beta = 2$ it looks quite disordered, and correlations decay
- Apparently: *the long-range nature of the potential creates strong, subtle correlations*

Nature of the melting?

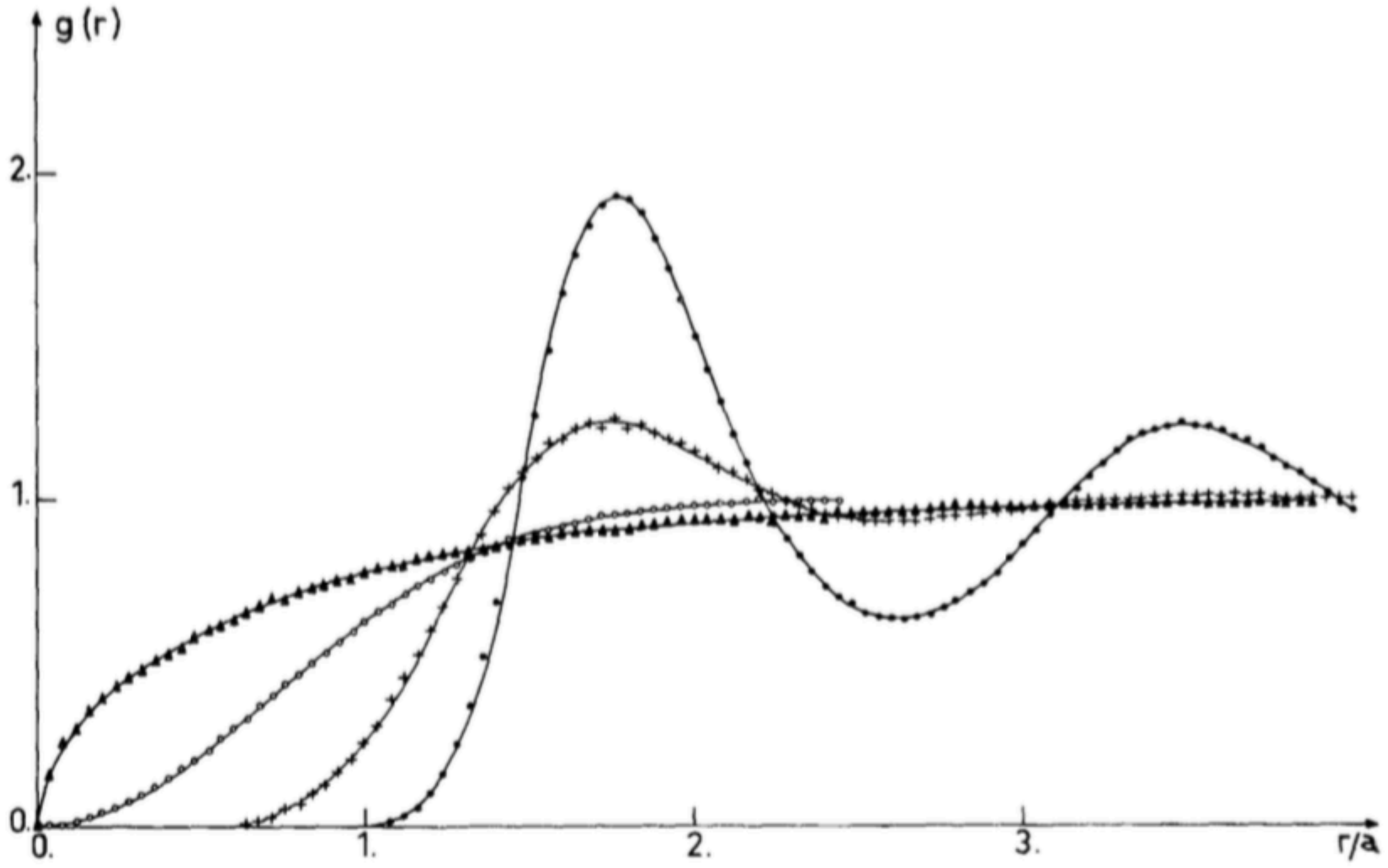
- One would first need to understand the *ground state* $(T = 0,\ \beta = +\infty)$: which configurations minimize the energy?

- « Abrikosov » conjecture : energy is minimized for an hexagonal **lattice** related to “universal optimality” questions

- What happens once we start warming up?



Caillol
Levesque
Weis
Hansen
‘82



Long-range orientational order

- The radial correlations of the lattice disappear slowly

- **Angular** correlations seem to disappear **suddenly**

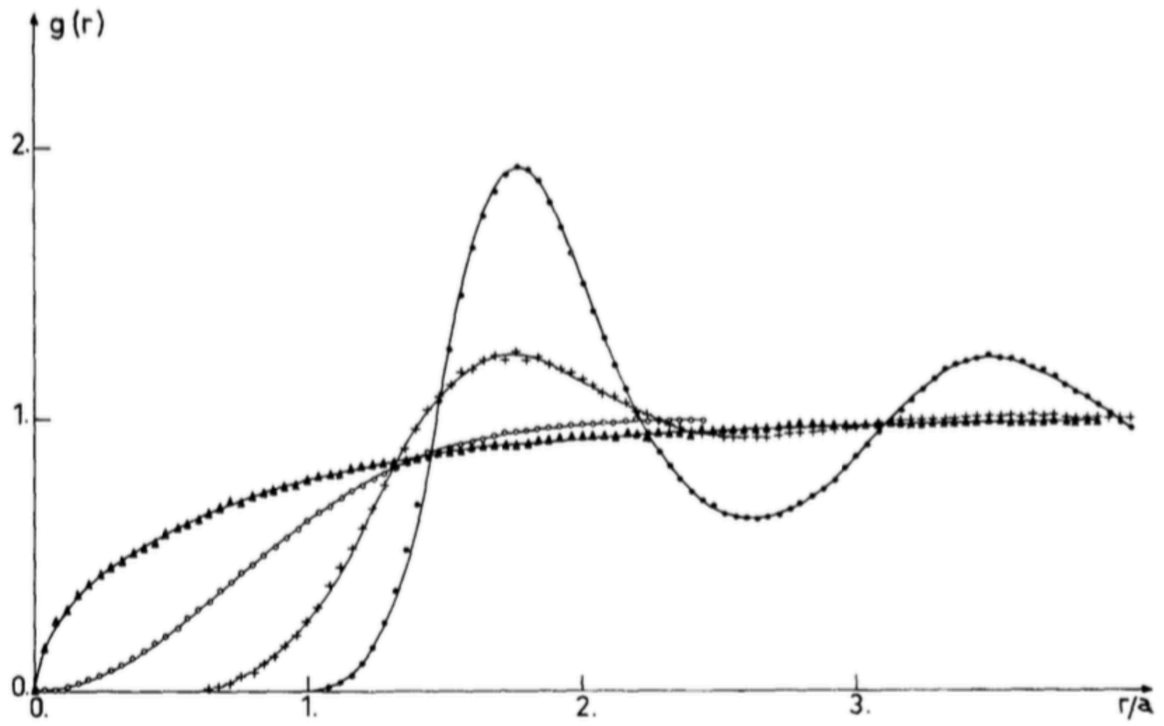
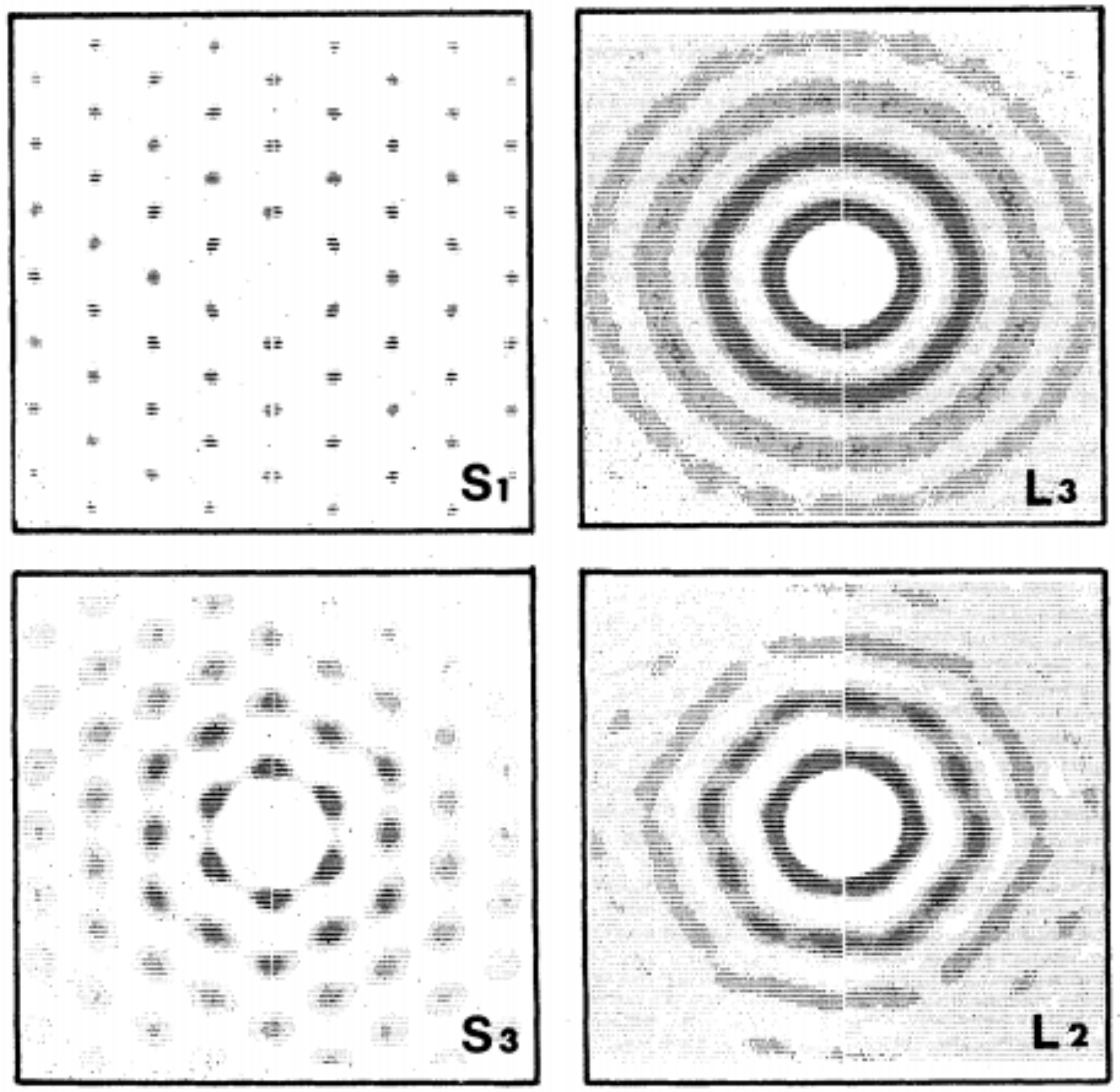


Fig. 1. Pair distribution function $g(r)$ versus $x = r/a$, from the Monte Carlo simulations on a sphere at $\Gamma = 0.5$ (triangles), $\Gamma = 2$ (circles), $\Gamma = 10$ (crosses), and $\Gamma = 40$ (dots).



Choquard-Clérouin ’83

Characterizing this order *mathematically* is one of the next challenges!

Thank you for your attention

And friendly thoughts
from Paris!