# Large deviations for the equilibrium of a Coulomb gas

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# Outline

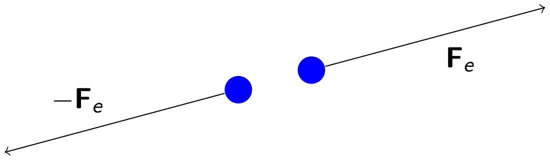
# An Old Problem

# Electric interaction

**Definition (Electr(ostat)ic/Coulomb force)**

*Two particles at $(x, y) \in (\mathbb{R}^3)^2$ with positive charges $q_1$, $q_2$ repulse each other:*

$$\|\mathbf{F}_e\| = \frac{k_e q_1 q_2}{\|\mathbf{r}_{12}\|^2}.$$



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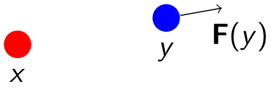
# Potential

Fix a unit charge at $x \in \mathbb{R}^3$. Consider a unit charge at $y$:




**Proposition**

*The Coulomb force is the gradient of a potential:*

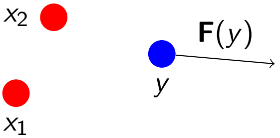
$$\mathbf{F}(y) = -\nabla U^x(y)$$

*where* $$U^x(y) = \frac{1}{\|x - y\|} = W(x, y).$$

$W(x, y)$ *is the interaction potential.*

# Linearity

Electrostatic forces/potentials from different charges add up:




## Definition (Potential field)

*The distribution of charges $\mu = \sum \alpha_i \delta_{x_i}$ creates:*

$$U^{\mu}(y) = \sum \alpha_i U^{x_i}(y) = \sum \alpha_i W(x_i, y) = \int W(x,y)\,d\mu(x).$$

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An additional charge $q$ at position $y$ in this field:

- is subject to a force $-q\nabla U^\mu(y)$;
- has potential energy $qU^\mu(y)$ ($=$ work needed to bring the charge from infinity to $y$).

# Self interaction energy

In $\mu = \sum \alpha_i \delta_{x_i}$, all particles interact. $x_i$ has the potential energy:

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**Definition (Self-interaction energy)**

*The energy of $\mu$ is:*

$$\frac{1}{2} J_f(\mu) = \frac{1}{2} \iint_{x \neq y} W(x, y) d\mu(x) d\mu(y).$$

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- If particles are allowed to move freely (in a conductor) they should "arrange" themselves so as to minimize the energy.
- Without constraints: all particles go to infinity.

# Remarks

- Mathematical inconvenience: $J_f$ is 0 for any Dirac mass. $J(\mu) = \iint W(x,y)d\mu(x)d\mu(y)$ is infinite if $\mu$ has a discrete part.
- Since $-\Delta W(x,\cdot) = \delta_x$, $-\Delta U^\mu = \mu$, so

$$J(\mu) = \int U^\mu(-\Delta U^\mu) = \int |\nabla U^\mu|^2 \, dx.$$

  $\nabla U^\mu$ is the electric field; the energy $J(\mu)$ is the integral of the "carré du champ".

# Constraints

Two factors may prevent degeneracy:

- An external field $V$ that applies to each particle. The total energy is:

$$I(\mu) = \frac{1}{2} J(\mu) + \int V d\mu.$$

- A support constraint: the charged particles may be confined within a conductor.

# The Gauss variational problem (with external field)

## Problem (Gauss variational problem)

*Given a "conductor"* $\Sigma \subset \mathbb{R}^3$, *and an external field* $V$, *minimize*

$$I(\mu) = \frac{1}{2} \iint W(x,y) d\mu(x) d\mu(y) + \int V(x) d\mu(x),$$

*over all* $\mu$ *such that* $\mathrm{supp}(\mu) \subset \Sigma$.

# The Gauss variational problem

- Many known results on existence, uniqueness in a much more general settings (Saff & Totik 1997, Zorii 2003);
- one of the motivations for the development of Potential Theory (capacity, balayage,. . . ) (Landkof 1972);
- Many deep links with probability (Port & Stone 1978), functional inequalities (Maz'ya 2010),. . .

# *Brownian particles in repulsive interaction*

# Charged particles in interaction

$N$ particles, at positions $X_t^1, \ldots X_t^N$, with charge $1/N$.

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$$dX_t^i = \sqrt{2}\beta_N^{-1/2} dB_t^i - \frac{1}{N}\nabla V(X_t^i)dt - \frac{1}{N^2}\sum_{j:j\neq i}\nabla_1 W(X_t^i, X_t^j)dt.$$

Three phenomena:

- Brownian diffusion at "inverse temperature $\beta_N$",

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Three phenomena:

- Brownian diffusion at "inverse temperature $\beta_N$",
- interaction with an external field,
- pair interactions between particles.

# An "inclusion"

The particle systems $(X^1, \dots X^N)$ live in different spaces.
All the configuration spaces $(\mathbb{R}^3)^N$ can be "included" in the common space $\mathcal{M}_1(\mathbb{R}^3)$:

$$\Phi_N : (\mathbb{R}^3)^N \to \mathcal{M}_1(\mathbb{R}^3)$$
$$(x_1, x_2, \dots x_N) \mapsto \frac{1}{N} \sum \delta_{x_i}.$$

# The equilibrium measure

## Proposition (Equilibrium)

*This diffusion on* $(\mathbb{R}^3)^N$ *has an equilibrium (invariant) measure:*

$$dP_N(x_1, \dots x_N) = Z_N^{-1} \exp\left(-\beta_N I_f(\mu_N)\right)$$

where

$$\begin{cases} \mu_N = \Phi_N(x_1, \dots x_N) = \dfrac{1}{N} \sum \delta_{x_i}, \\ I_f(\mu) = \dfrac{1}{2} \displaystyle\iint_{x \neq y} W(x,y) d\mu(x) d\mu(y) + \int V(x) dx, \\ \beta_N = \text{inverse temperature}, \\ Z_N = \text{normalization constant}. \end{cases}$$

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Under $P_N$, $\mu_N$ is a random (point) measure.

## Question

*Asymptotic behaviour of $\mu_N$ when $N \to \infty$ ?*

## Theorem (Large deviations (heuristic))

*Let* $\beta_N = N^2$*. If A is a subset of* $\mathcal{M}_1(\mathbb{R}^d)$ *then:*

$$\mathbf{P}\left[\mu_N \in A\right] \approx \exp\left(-\beta_N \left(\inf_A I - \inf_{\mathcal{M}_1(\mathbb{R}^3)} I\right)\right).$$

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## Theorem (Minimizer, convergence)

*$I$ has a unique minimum $\mu_\star$, computable in simple cases. If the $\mu_N$ are defined on a common probability space,*

$$\mu_N \xrightarrow[N\to\infty]{a.s.} \mu_\star.$$

# Comments

- Valid for $d \geq 3$ and a large class of $V$, $W$.
- $d = 1, 2$ already known (see below).
- Two distinct problems: LDP (probability), minimization (Potential theory).

# *Intermezzo — links and connections*

# Random matrices

## Definition (Complex Ginibre ensemble)

*Set* $M^N = (M^N_{ij})_{i,j\leq N}$ *where* $M^N_{ij}$ *are i.i.d. complex Gaussian:*
$M^N_{i,j} = \frac{1}{\sqrt{2N}}\left(U_{ij} + \sqrt{-1}V_{ij}\right)$.

Let $\mu_N$ be the spectral measure $\mu_N = \sum_k \delta_{\lambda_k}$: $\mu_N$ is a random (point) measure on $\mathbb{C} = \mathbb{R}^2$.

# Random matrices

**Theorem ("Circular law", Mehta, 1967, Ben Arous & Zeitouni, Hiai & Petz 1998)**

*$\mu_N$ has the law of a 2-dimensional Coulomb gas, where*

- $W(x, y) = \log(1/|x - y|)$ *(2d-Coulomb interaction),*
- $V(x) = x^2$.

*The normalized spectral measure converges a.s. to the minimizer of $I$, that is the uniform measure on a ball.*
*Furthermore the corresponding LDP holds.*

# Other links and problems

- Fekete points,
- Calogero–Sutherland gases,
- Simulation problems,
- . . .

Further links and references: see the preprint!

# A rich theory

# The minimizer

For each measure $\mu$:

- a potential $U^{\mu}(x) = \int W(x,y) d\mu(y)$
- an energy $J(\mu) = \int U^{\mu} d\mu = \iint W(x,y) d\mu(x) d\mu(y)$.

$J(\mu)$ is quadratic in $\mu$.

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$J(\mu)$ is quadratic in $\mu$.

**Proposition (Pre-Hilbertian structure)**

*$J(\mu,\nu) = \int U^\mu d\nu$ is a scalar product (on a nice space of signed measures).*
*The same is true for more general "Riesz" interactions $W(x,y) = |x-y|^{-\alpha}$.*

# The minimizer

- An idea that goes back to H. Cartan; nice exposition in Landkof (1972);
- provides easy proofs of many "folklore" results:
  1. the uniqueness of the minimizer $\mu_\star$,
  2. a characterization of $\mu_\star$ in terms of its potential $U^{\mu_\star}$.

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  1. the uniqueness of the minimizer $\mu_\star$,
  2. a characterization of $\mu_\star$ in terms of its potential $U^{\mu_\star}$.

Consequence:

**Proposition**

*In the Coulomb case $W(x,y) = 1/\|x-y\|$, if the external field is $V(x) = \|x\|^2$, the equilibrium measure is uniform on a ball.*

# Example

Suppose $\mu_\star$ is the minimizer. For a nice $\nu$ let

$$\phi(t) = I((1-t)\mu_\star + t\nu).$$

Compute $\phi'(0)$ (easy!) to get:

$$\forall \nu, \quad \int (U^{\mu_\star} + V) d\nu \geq C_\star$$

for some explicit $C_\star$. So:

$$U^{\mu_\star} + V \geq C_\star \qquad \text{"quasi-everywhere"}.$$

# *Back to Large Deviations*

# Result

Recall the main result:

$$\mathbf{P}\left[\mu_N \in A\right] \approx \exp\left(-\beta_N\left(\inf_A I - \inf_{\mathcal{M}_1} I\right)\right).$$

i.e.:

**Theorem (Large deviations)**

*For* $I_\star = I - \inf_{\mathcal{M}_1(\mathbb{R}^3)} I$,

$$-\inf_{int(A)} I_\star \leq \liminf \beta_N^{-1} \log \mathbf{P}\left[\mu_N \in A\right]$$
$$\leq \limsup \beta_N^{-1} \log \mathbf{P}\left[\mu_N \in A\right] \leq -\inf_{clo(A)} I_\star.$$

# Difficulties

- The interaction potential $W$ explodes on the diagonal.
- The rate functional $I : \mathcal{M}_1(\mathbb{R}^d) \to \mathbb{R}$ is **not** continuous with respect to the usual (weak) topology.
- If $\mu_n$ is discrete and converges to $\mu$ with finite energy,

$$I(\mu) < \infty = \liminf_n I(\mu_n).$$

- $I$ is lower-semi-continuous: if $\mu_n \to \mu$, $I(\mu) \leq \liminf I(\mu_n)$.

# Upper bound

Bound $\mathbf{P}\left[\mu_N \in A\right]$ from above. Suppose $A$ is a ball $B(\mu, r)$ (in $\mathcal{M}_1(\mathbb{R}^3)$).

$$Z_N \mathbf{P}\left[\mu_N \in A\right] = \int \mathbf{1}_A(\mu_N) \exp(-\beta_N I_f(\mu_N)) dx_1 \cdots dx_N$$

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Bound $I_f$ from below, using

$$I_M(\mu) = \frac{1}{2} \iint (W \wedge M) d\mu d\mu + \int V \wedge M d\mu,$$

to get ($\approx$ 5 lines):

$$Z_N \mathbf{P}[\mu_N \in A] \leq \exp\left(-(\beta_N - N) \inf_A (I_M) + \beta_N M/N\right) \left(\int e^{-V} dx\right)^N.$$

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Take $\limsup_N \beta_N^{-1} \log$ (where $\beta_N = N^2$),

$$\limsup_N \beta_N^{-1} \log Z_N \mathbf{P}\left[\mu_N \in B(\mu, r)\right] \leq -\inf_{B(\mu,r)} I_M$$

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Take $\limsup_N \beta_N^{-1} \log$ (where $\beta_N = N^2$), send $r \to 0$ ($I_M$ is l.s.c.!), then $M$ to infinity:

$$\limsup_N \beta_N^{-1} \log Z_N \mathbf{P}\left[\mu_N \in B(\mu, r)\right] \leq -\inf_{B(\mu,r)} I_M$$

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# Upper bound

For all $\mu$,

$$\lim_{r\to 0} \limsup \beta_N^{-1} \log Z_N \mathbf{P}\left[\mu_N \in B(\mu, r)\right] \leq -I(\mu).$$

Further steps:

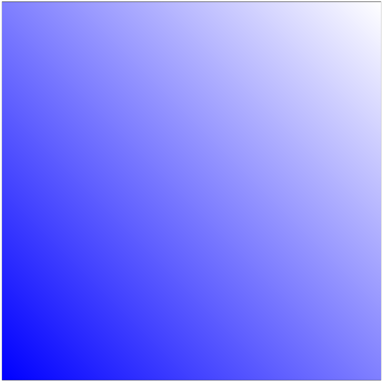
- deal with $Z_N$;
- prove tightness and use standard arguments to deduce the general upper bound.

# Lower bound

Bound $\mathbf{P}\left[\mu_N \in A\right]$ from below.

- (Try to) reduce to the case $A = B(\mu, r)$ for a “nice” measure $\mu$.
- Compute the cost of “forcing” $\mu_N$ to be near $\mu$.

# Lower bound



- $\mu$ with a density;

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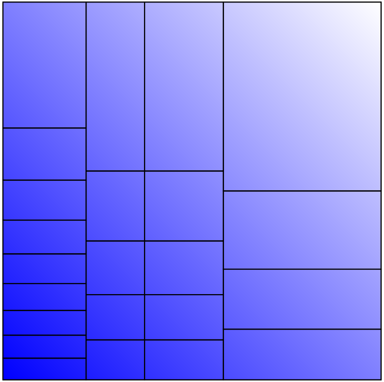

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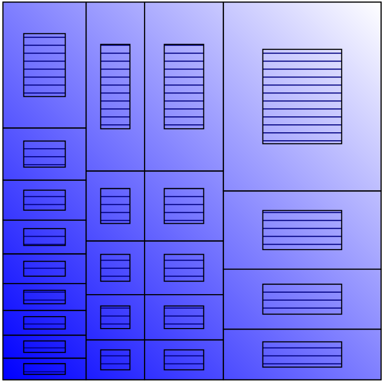

- $\mu$ with a density;
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- draw subboxes;

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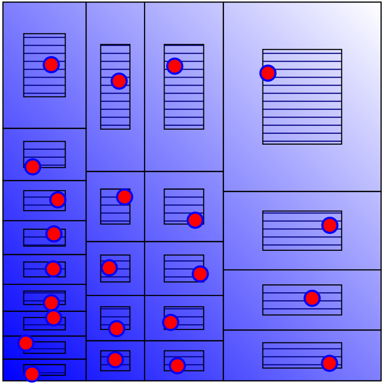

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- force the nice event $\mu_N \in E$: "one particle per small box".

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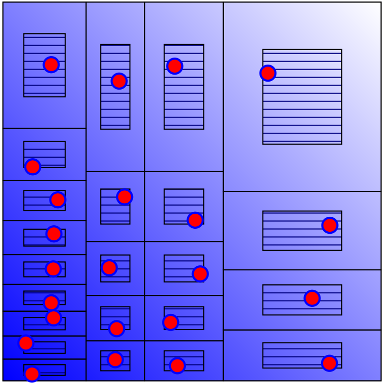

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**Proposition**

*On $E$, $\mu_N \in B(\mu, r)$ and $I(\mu_N) \approx I(\mu)$ ($\approx$ Riemann sum).*

# Lower bound

## Proposition

*On $E$, $\mu_N \in B(\mu, r)$ and $I(\mu_N) \approx I(\mu)$.*

$$\begin{aligned} \mathbf{P}\left[\mu_N \in B(\mu, r)\right] &\geq \mathbf{P}\left[E\right] \\ &= Z_N^{-1} \int \mathbf{1}_E(\mu_N) \exp(-\beta_N I(\mu_N)) \\ &\approx \exp(-\beta_N I(\mu)) \mathbf{Q}\left[\mu_N \in E\right] \end{aligned}$$

where $\mathbf{Q}$ is the law of $N$ uniform points.
The $\mathbf{Q}$ term is handled by the fact that the boxes are balanced.

# Open questions

- Explicit computations of $\mu_\star$: only done in the radial case for $W$ Coulomb. Extension to the Riesz case?
- What happens at other speeds (different $\beta_N$)?
- Does $\max\{\|x\|, x \in \mathrm{supp}(\mu_N)\}$ converge?
- Fluctuations?
- ...