Minimizers of Interaction Energies

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Outline

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Internal Energy

$E\colon \mathcal{P}(\mathbb{R}^d) \to \mathbb{R} \cup \{-\infty, +\infty\}$ by

$$E(\rho) = \begin{cases} \displaystyle\int_{\mathbb{R}^d} U(\rho(x))\,\mathrm{d}x & \text{if } \rho \in \mathcal{P}_{\mathrm{ac},2}(\mathbb{R}^d) \\ +\infty & \text{otherwise} \end{cases},$$

where $U\colon [0,\infty) \to \mathbb{R}$ is the density of *internal energy* satisfying $U(0) = 0$.

Let us consider N particles in $\mathbb{R}^d$ denoted by $x_N := (x_{1,N}, \ldots, x_{N,N}) \in \mathbb{R}^{Nd}$, where N is a positive integer. For all $i \in \{1, \ldots, N\}$, let us write $B_{i,N} := B(x_{i,N}, R_{i,N})$ the open ball of centre $x_{i,N}$ and radius

$$R_{i,N} = \frac{1}{2} \min_{j \neq i} |x_{i,N} - x_{j,N}|.$$

For these N particles consider

$$\rho_N = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{|B_{i,N}|} \chi_{B_{i,N}},$$

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Approximated Internal Energy

Given

$$\mathcal{A}_N(\mathbb{R}^d) = \left\{ \mu \in \mathcal{P}(\mathbb{R}^d) \text{ such that } \exists x_N \in \mathbb{R}^{Nd}, \mu = \delta_{x_N} \right\}.$$

The discrete energy $E_N : \mathcal{A}_N(\mathbb{R}^d) \to \mathbb{R} \cup \{-\infty, +\infty\}$ by

$$E_N(\mu) = \int_{\mathbb{R}^d} H\left(\frac{1}{N} \sum_{i=1}^{N} \frac{1}{|B_{i,N}|} \chi_{B_{i,N}}(x) \right) \mathrm{d}x,$$

where $B_{i,N} = B(x_{i,N}, R_{i,N})$ with x_N satisfying $\mu = \delta_{x_N}$. Note that

$$|B_{i,N}| = C_d R_{i,N}^d = \frac{C_d}{2} \left(\min_{j \neq i} |x_{i,N} - x_{j,N}| \right)^d,$$

where $C_d = |B(0,1)|$ is the volume of the unit ball in dimension d. We clearly have $E(\rho_N) = E_N(\mu)$.

Γ-Convergence Result

- Logarithmic Entropy: Given

$$E_N(\mu) = -\frac{1}{N}\sum_{i=1}^{N} \log\left(\frac{NC_d}{2^d}\left(\min_{j\neq i}|x_{i,N} - x_{j,N}|\right)^d\right),$$

then it Γ-converges in d_2 to the logarithmic entropy $E[\mu]$.

- Nonlinear Entropy: The same holds for

$$E_N(\mu) = \int_{\mathbb{R}^d} \frac{1}{(m-1)N^m}\left(\sum_{i=1}^{N}\frac{1}{|B_{i,N}|}\chi_{B_{i,N}}(x)\right)^m \mathrm{d}x$$

Γ-converging to

$$E(\rho) = \int_{\mathbb{R}^d}\frac{\rho^m(x)}{m-1}\,\mathrm{d}x \quad \text{if } \rho \in \mathcal{P}_{ac,2}(\mathbb{R}^d).$$

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Outline

Discrete JKO scheme

For any N particles in $\mathbb{R}^d$, we denote their weights by $w = (w_1, \ldots, w_N) \in \mathbb{R}^N$, which we assume to satisfy $\sum_{i=1}^N w_i = 1$ and $w_i \geq 0$ for all $i \in \{1, \ldots, N\}$. For any such $w \in \mathbb{R}^N$, define

$$\mathcal{P}_w(\mathbb{R}^d) = \left\{ \rho \in \mathcal{P}(\mathbb{R}^d) \text{ such that } \exists x = (x_1, \ldots, x_N) \in \mathbb{R}^{Nd}, \rho = \sum_{i=1}^N \frac{w_i}{|B(x_i, R_i)|} \chi_{B(x_i, R_i)} \right\},$$

where

$$R_i = \frac{1}{2} \min_{j \neq i} |x_i - x_j|.$$

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Discrete Particle JKO scheme:

$$F(\tilde{\rho}) = \frac{1}{2\Delta t} d_2^2(\rho, \tilde{\rho}) + E(\tilde{\rho}),$$

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1D Approximation

$$F(\tilde{\rho}) = \sum_{i=1}^{N} w_i \left(\frac{(x_i - \tilde{x}_i)^2}{2\Delta t} + \frac{(R_i - \tilde{R}_i)^2}{6\Delta t} \right) + E(\tilde{\rho}).$$

where

$$R_i = \begin{cases} \frac{1}{2}|x_2 - x_1| & \text{if } i = 1 \\ \frac{1}{2}\min(x_i - x_{i-1}, x_{i+1} - x_i) & \text{if } 1 < i < N \\ \frac{1}{2}|x_N - x_{N-1}| & \text{if } i = N \end{cases},$$

Assuming that $\tilde{R}_i = R_i + o(1)$, we have

$$\frac{(R_i - \tilde{R}_i)^2}{6\Delta t} \ll \frac{(x_i - \tilde{x}_i)^2}{2\Delta t}.$$

Thus we can approximate the functional F as

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which is the d_2 steepest descent of E_N.

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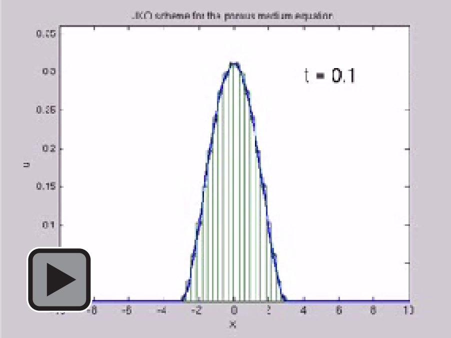
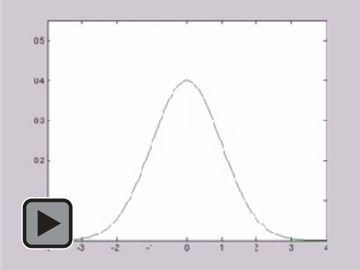
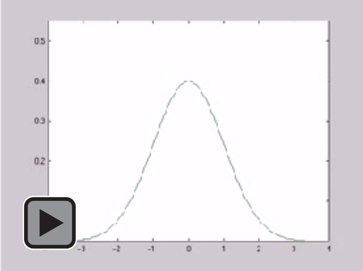
Numerical Simulation: Heat and Fokker-Planck Equations







Outline

Minimization of the Interaction Energy

Minimization Problem

We want to find local minimizers of the total interaction energy

$$\mathcal{F}[\mu] := \frac{1}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} U(x-y)\, d\mu(x) d\mu(y)\,.$$

in some set of probability measures $\mathcal{P}(\mathbb{R}^d)$.

What is the right topology to talk about measures being close?

Recurrent Question in many fields:

- Statistical Mechanics & Crystallization: Typically very singular potentials at zero: Lennard-Jones.
- Semiconductors - Astrophysics - Chemotaxis: Macroscopic model obtained from Vlasov Equation under certain limits. Newtonian Potential.
- Economic Applications: Mean Field Games, Cournot-Nash Equilibria.
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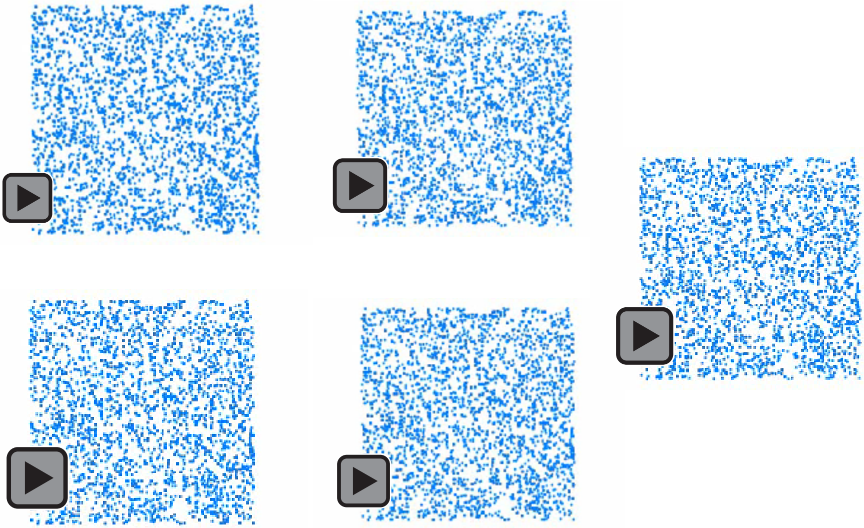
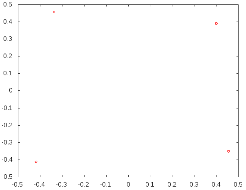
Nontrivial patterns? - Particle Simulations

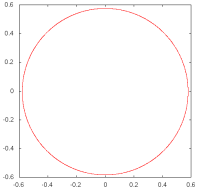


Summary: Particle Simulations $d = 2$

Potential $a = 4$, $b = 2.1$



Potential $a = 4$, $b = 1.85$



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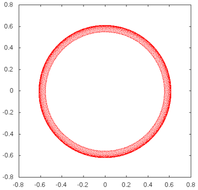
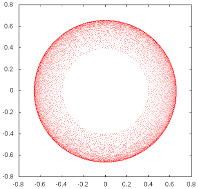
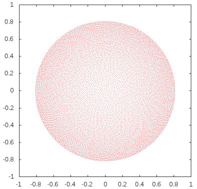


Potential $a = 4$, $b = 0.85$



Potential $a = 4$, $b = 0.05$



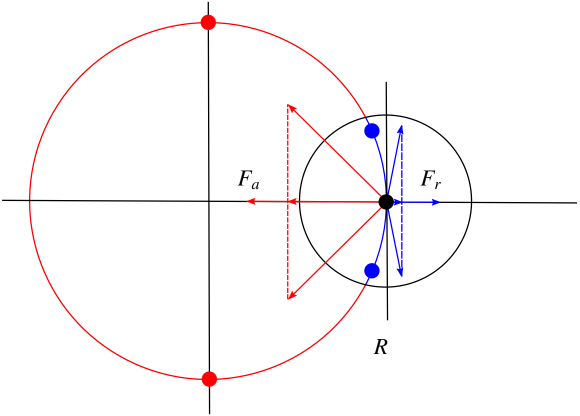
$$\dot{X}_i = -\sum_{j \neq i} m_j \, \nabla U(X_i - X_j)$$

$$U(x) = \frac{|x|^a}{a} - \frac{|x|^b}{b}$$

$$2 - d \leq b < a$$

Spherical shell

A spherical shell for some radius R is a stationary state for the aggregation equation for radial potentials.

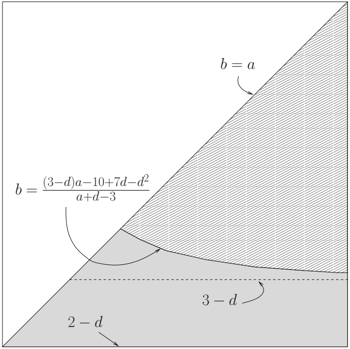


Power-Law Case

$$U(x) = \frac{|x|^a}{a} - \frac{|x|^b}{b} \qquad 2-d < b < a$$

Theorem: Ins/Stability of Delta Rings with respect to radial perturbations.

- There is a computable value of R such that the uniform distribution on the sphere of radius R, δ_R is an steady state.
- If the velocity field generated by δ_R is strictly increasing at R then it is unstable.
- If the velocity field generated by δ_R is strictly decreasing at R then it is locally asymptotically stable.



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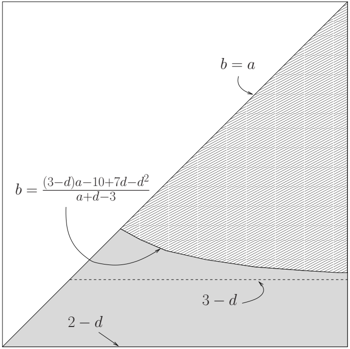

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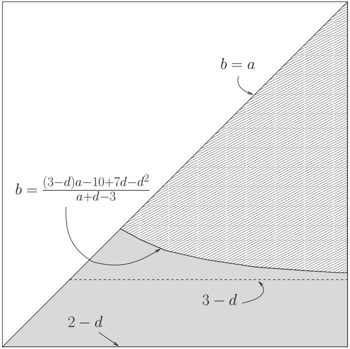

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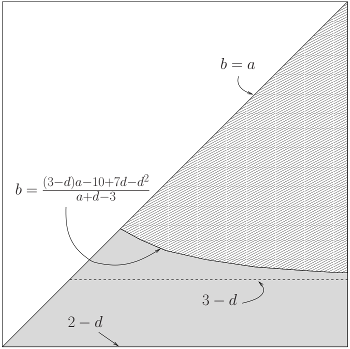

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W_∞-Topology

The W_∞-distance is defined as the optimal maximal mass displacement given by

$$W_\infty(\mu,\nu) = \inf_{\pi\in\Pi(\mu,\nu)} \sup_{(x,y)\in \mathrm{supp}(\pi)} |x-y|\,,$$

- It is a good topology since it is closer to linearization around equilibrium of dynamical systems.
- It is the coarser topology among Wasserstein distances since all of them are ordered.
- Then, a local minimizer in W_2 is a local minimizer in W_∞ but not viceversa.

Basic Hypotheses:
(H1) U is a bounded from below lower semi-continuous function in $L^1_{loc}(\mathbb{R}^d)$.

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(H1) U is a bounded from below lower semi-continuous function in $L^1_{loc}(\mathbb{R}^d)$.

W_∞-Topology

The W_∞-distance is defined as the optimal maximal mass displacement given by

$$W_\infty(\mu,\nu) = \inf_{\pi\in\Pi(\mu,\nu)} \sup_{(x,y)\in \mathrm{supp}(\pi)} |x-y|\,,$$

- It is a good topology since it is closer to linearization around equilibrium of dynamical systems.
- It is the coarser topology among Wasserstein distances since all of them are ordered.
- Then, a local minimizer in W_2 is a local minimizer in W_∞ but not viceversa.

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Euler-Lagrange Conditions

W_∞ EL-Conditions

Assume that U satisfies (H1) and let μ be a local compactly supported minimizer of the energy $\mathcal{F}[\mu]$ in the W_∞ ball or radius ε. Then any point $x_0 \in \text{supp}(\mu)$ is a local minimimum of $\psi = U * \mu$ in the sense that

$$\psi(x_0) \le \psi(x) \text{ for a.e. } x \in B_\varepsilon(x_0).$$

Note that ε is uniform on the support of μ.

W_2 EL-Conditions

Under the same assumptions, if μ is a W_2-local minimizer of the energy, then the potential ψ satisfy

(i) $\psi(x) = (U * \mu)(x) = 2\mathcal{F}[\mu]$ μ-a.e.

(ii) $\psi(x) = (U * \mu)(x) \ge 2\mathcal{F}[\mu]$ for a.e. $x \in \mathbb{R}^d$.

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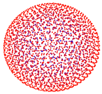
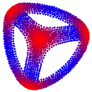
Regularity??

Dimensionality of the support

Some simulations with power law potentials of the form

$$U(x) = \frac{|x|^a}{a} - \frac{|x|^b}{b}, \qquad 2 - d < b < a$$

dim=3	dim=2	dim=2	dim=0
			
$b = -0.5$ $a = 5$	$b = 0.5$ $a = 23$	$b = 1.25$ $a = 15$	$b = 2.5$ $a = 5$

Local minimizers in 3D for different parameters when $b > -1$ increases. The computations were done with $n = 2,500$ particles.

Mild versus Strong Repulsive potentials

Support is essentially 0-dimensional for $b > 2$.

Let $U \in C^2(\mathbb{R}^N)$ be a radially symmetric potential which behaves like $-|x|^b/b$ in a neighborhood of the origin with $b > 2$.

Then a local minimizer of the interaction energy $\mathcal{F}$ with respect to W_∞ cannot have a s-dimensional smooth components for any $1 \leq s \leq d$.

Dimension of the Support depends on $2 - d < b < 2$.

Assume that μ is a local minimizer of the interaction energy $\mathcal{F}$ with respect to W_∞ such that U is radial with $U(x) \sim -|x|^b$ near zero and $2 - d < b < 2$. If μ contains s-Haussdorff dimensional connected components in its support, then $s > 2 - b$.

(Balagué, C., Laurent, Raoul; ARMA 2013)

Strategy: Pure variational approach: by contradiction we build better competitors.

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Outline

Existence Global Minimizers

Non-HStable: Energy at infinity cost more than near the origin, i.e., the potential U satisfies

(H2) There exists $\mu \in \mathcal{P}(\mathbb{R}^d)$ compactly supported such that $\mathcal{F}[\mu] < 0$.

(H2) $\lim_{|x|\to\infty} U(x) \geq 0$.

Main Theorem

Assume that the radial potential U satisfies Hypotheses (H1), (H2), and is increasing outside a large ball. Then there exists a global minimiser for the energy $\mathcal{F}$. Furthermore, any such global minimiser has compact support.

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Main ideas: Uniform repartition of the mass over the support.

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Key Estimate

By (H1) for R large enough:

$$E_R := \min \left\{ \mathcal{F}[\mu] \mid \mu \in \mathcal{P}_R(\mathbb{R}^d) \right\} \leq E_* < 0$$

Euler-Lagrange: for ρ_R-almost all $z \in \operatorname{supp}\rho_R$ we have

$$\frac{1}{2} \int_{\mathbb{R}^d} U(z-x)\, \mathrm{d}\rho_R(x) = E_R.$$

Choose $A \in \mathbb{R}$ with $\frac{1}{2} U_{\min} \leq E_* < A < 0$ and $r' > 0$ with $U(x) \geq 2A$ for $|x| \geq r'$. Then for ρ_R-almost every z we have

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Examples

Power-laws & Morse Potentials

Consider the following potentials for all $x \in \mathbb{R}^d$ and $C_A, C_R, \ell_A, \ell_R > 0$:

(i) *(Power-law potential)* $U(x) = \frac{|x|^a}{a} - \frac{|x|^b}{b}$ with $-d < b < a$,

(ii) *(Morse potential)* $U(x) = C_R e^{-\frac{|x|}{\ell_R}} - C_A e^{-\frac{|x|}{\ell_A}}$ with either $\ell_A < \ell_R$ and $\frac{C_A}{C_R} < \left(\frac{\ell_R}{\ell_A}\right)^d$,

with the convention $\frac{|x|^0}{0} = \log|x|$.

Discrete To Continuum: Power-law Case

(C., Chipot, Huang; preprint 2014)

Discrete Setting: Find

$$I_N = \inf_{x\in(\mathbb{R}^d)^N} \mathcal{F}_N(x)\,,$$

with

$$\mathcal{F}_N(x_1,\cdots,x_N) = \sum_{i\neq j}^{N}\left(\frac{|x_i-x_j|^a}{a} - \frac{|x_i-x_j|^b}{b}\right)\,.$$

Uniform Control of the support

Suppose that $1\leq b<a$. Then the diameter of any global minimizer of $\mathcal{F}_N$ achieving the infimum I_N is bounded independently of N.

Key Idea: use Euler-Lagrange and a convexity argument for the repulsive potential to estimate the distance between the two particles the furthest away.

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Regularity of Local Minimizers

(H3) The function $U_a(x) := U(x) - V(x)$ with V being the Newtonian potential in dimension d satisfies:

$$\Delta U_a \in L^p_{loc}(\mathbb{R}^d) \quad \text{for some } p \in (d, \infty]$$

with ΔU_a bounded below.

Main Theorem

Assume that the potential U satisfies Hypotheses (H1) and (H3). Then any μ compactly supported W_∞ local minimizer of the energy $\mathcal{F}$ is bounded uniformly, i.e., $\mu = \rho(x) d\mathcal{L}^d$ with $\rho \in L^\infty(\mathbb{R}^d)$.

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Main ideas: Obstacle problems to obtain information out of the Euler-Lagrange conditions (Nash equilibria conditions).

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Obstacle Problem

Continuity of the potential

Assume that the potential U satisfies Hypotheses (H1) and (H3). Let μ be a W_∞ local minimizer of E. Then the potential $\psi(x) := U * \mu(x)$ associated to μ is a continuous function in $\mathbb{R}^N$.

Implicit Obstacle Problem

For all $x_0 \in \text{supp}(\mu)$, the potential function ψ is equal, in $B_\varepsilon(x_0)$, to the unique solution of the obstacle problem

$$\begin{cases} \varphi \geq C_0, & \text{in } B_\varepsilon(x_0) \\ -\Delta\varphi \geq -F(x), & \text{in } B_\varepsilon(x_0) \\ -\Delta\varphi = -F(x), & \text{in } B_\varepsilon(x_0) \cap \{\varphi > C_0\} \\ \varphi = \psi, & \text{on } \partial B_\varepsilon(x_0), \end{cases}$$

where $C_0 = \psi(x_0)$ and $F(x) = \Delta U_a * \mu \in L^p_{loc}(\mathbb{R}^d)$. Furthermore, the density μ is given by

$$\mu = -\Delta\psi + F.$$

Particular Case: Newtonian repulsion and quadratic confinement, the global minimizer is the characteristic of a ball with unit mass upto translations.

Obstacle Problem

Continuity of the potential

Assume that the potential U satisfies Hypotheses (H1) and (H3). Let μ be a W_∞ local minimizer of E. Then the potential $\psi(x) := U * \mu(x)$ associated to μ is a continuous function in $\mathbb{R}^N$.

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Conclusions

- The dimensionality of the support of local minimizers of the interaction energy can be classified in terms of the repulsion strength of the potential near zero.
- If the strength of the repulsion is stronger than or equal to Newtonian, they are bounded uniformly.
- Compactly supported global minimizers exist under the reasonable condition that it costs less energy to be near the origin than to be at infinity.
- References:

1. C.-Huang-Patacchini-Wolansky (work in preparation).
2. Balagué-C.-Laurent-Raoul (Physica D & ARMA 2013).
3. Cañizo-C.-Patacchini (preprint 2014).
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