Part III: Upscaling of dislocation evolutions

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Starting point: (semi)-discrete interaction energy

$$I_n(x) = \frac{1}{2n^2} \sum_{i,j=1}^{n} b_i b_j V(x_i - x_j), \quad b_i \in \{\pm 1\}, \; \underbrace{x_i \in \mathbb{T}^2}_{\text{periodic}}$$

$\underline{b}_i \cdot \underline{b}_j$

V ? e.g. $V(x) = -\log|x|$ or $V(x) = -\log|x| + \frac{x_1^2}{|x|^2}$

screw, vortices   edge, $\underline{b} = \underline{e}_1$

Associated evolutions   GF (Orowan's; $\underline{v} = BF$)

$$\dot{x} = -n \nabla I(x)$$

$$\begin{cases} \dot{x}_i = -\frac{1}{n} \sum_{j=1}^{n} b_i b_j \nabla V(x_i - x_j) \quad (*) & \text{isotropic} \sim \text{screw} \\ \dot{x}_i = -\frac{1}{n} \sum_{j=1}^{n} b_i b_j (\partial_1 V)(x_i - x_j) & \sim \text{edge} \end{cases}$$

GF: Alicandro - De Luca - Garroni - Ponsiglione
Blass - Fonseca - Leoni - Morandotti;
Dipierro, Figalli, Palatucci, Patrizi, Valdinoci

R.I: Mora - Peletier - Scardia

Set $\mu_n^{\pm} = \frac{1}{n} \sum_{\substack{i=1 \\ b_i = \pm 1}}^{n} \delta_{x_i}$ densities of $\pm$ d.d.

solutions of ⊛

Q: If $\mu_n^{\pm} \longrightarrow \rho^{\pm}$, then $\rho^{\pm}$ solutions of

$$\partial_t \rho^{\pm} = \pm \operatorname{div}\left(\rho^{\pm}\left(\nabla V * (\rho^{+} - \rho^{-})\right)\right) \; ? \quad (**)$$

- Groma-Balogh
- agreement with DDD

Note: Formally $\mu_n^{\pm}$ are solution of (**)

$$\frac{d}{dt} \int_{\mathbb{T}^2} \varphi(x)\, d\mu_n^{+}(x) = \frac{d}{dt} \frac{1}{n} \sum_{i=1}^{n} \varphi(x_i)$$

$$= \frac{1}{n} \sum \nabla \varphi(x_i) \boxed{\dot{x}_i} \quad \text{use ⊛}$$

$$= \frac{1}{n} \sum_i \nabla \varphi(x_i) \left[-\frac{1}{n} \sum_j b_i b_j \nabla V(x_i - x_j) \right]$$

$$= -\int_{\mathbb{T}^2} \nabla \varphi(x)\, d\mu_n^{+}(x) \left[\int_{\mathbb{T}^2} \nabla V(x-y)\, d(\mu_n^{+} - \mu_n^{-})(y) \right]$$

✓

- If V smooth Yes

- If V singular (log) and $b_i = 1 \ \forall i$ Yes

  If $b_i = \pm 1$ $\Rightarrow$ tricky

  $\exists$ in (*) up to first collision.

  $\Rightarrow$ regularisation needed!

  $\hookrightarrow$ $\delta_n > 0$.

AIM: Prove convergence

$$\dot{x}_i = -\frac{1}{n} \sum_j b_i b_j \nabla V_{\delta_n}(x_i - x_j)$$

rigorously solutions of $(GB)_{\delta_n}$

$$\downarrow \ n \to \infty$$

$$\partial_t \rho^{\pm} = \pm \operatorname{div}\Big(\underbrace{\rho^{\pm}(\nabla V * (\rho^+ - \rho^-))}_{\text{well defined?}}\Big)$$

AIM: Prove convergence

$$\partial_t \mu_n^\pm = \pm \operatorname{div}\Big(\overbrace{\mu_n^\pm\big(\overbrace{\nabla V_{\delta_n} * (\mu_n^+ - \mu_n^-)}^{\text{unif. cont}}\big)}^{\text{measure}}\Big) \qquad (GB)_{\delta_n}$$

$$\Big\downarrow \; n \to \infty \qquad ?$$

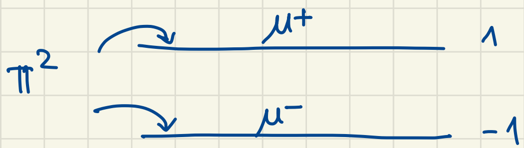
$$\partial_t \rho^\pm = \pm \operatorname{div}\Big(\underbrace{\rho^\pm\big(\nabla V * (\rho^+ - \rho^-)\big)}_{\text{well defined ?}}\Big) \qquad (GB)$$

Assumptions:

- $V_\delta \in W^{2,\infty}(\mathbb{T}^2) \longrightarrow \nabla V_\delta$ Lip
- $\sup_{k \in \mathbb{Z}^2} (1+|k|^2)\, \hat{V}_k < \infty$ $\hat{V}_{\delta,k}$ $\sim$ V log. singularity, $\hat{V}_k \sim \frac{1}{|k|^2}$
- $\hat{V}_k, \; \hat{V}_{\delta,k} \geq 0 \quad k \neq 0$

Notation:

- $\mathcal{P}(\mathbb{T}^2 \times \{\pm 1\}) = \{ \underline{\mu} = (\mu^+, \mu^-) : \mu^+(\mathbb{T}^d) + \mu^-(\mathbb{T}^d) = 1 \}$



"separate $\mu^\pm$"

no sources / sinks
no annihilation
$\mu^+(\mathbb{T}^2)$, $\mu^-(\mathbb{T}^2)$ conserved

- $\mathbb{W}^2(\underline{\mu}, \underline{\nu})$ Wasserstein distance

$$\mathbb{W}^2(\underline{\mu}, \underline{\nu}) \, / \! / \quad \text{if } \mu^{\pm}(\mathbb{T}^2) = \nu^{\pm}(\mathbb{T}^2)$$

$$W^2(\mu^+, \nu^+) + W^2(\mu^-, \nu^-)$$

- $\mathrm{Ent}(\underline{\mu}) = \int_{\mathbb{T}^2} \mu^+ \log \mu^+ + \int_{\mathbb{T}^2} \mu^- \log \mu^-$

$$\mu^{\pm} \ll dx$$

Definition

- $$\mathbb{W}^2(\underline{\mu}, \underline{\nu}) = \inf_{\gamma \in \Gamma(\underline{\mu}, \underline{\nu})} \int_{(\mathbb{T}^2 \times \{\pm 1\})^2} d^2(x', y') \, d\gamma(x', y')$$

$$x' = (x, a) \in \mathbb{T}^2 \times \{\pm 1\}$$

$$y' = (y, b) \in \mathbb{T}^2 \times \{\pm 1\}$$

$$d^2(x', y') = \| x - y \|_{\mathbb{T}^2}^2 + |a - b|^2$$

AIM : Prove convergence

$$\partial_t \mu_n^\pm = \pm \operatorname{div}\Big(\overbrace{\mu_n^\pm \big(\underbrace{\nabla V_{\delta_n} * (\mu_n^+ - \mu_n^-)}_{\text{unif. cont}}\big)}^{\text{measure}}\Big) \quad (GB)_{\delta_n}$$

$$\Big\downarrow \; n \to \infty \; ?$$

$$\partial_t \rho^\pm = \pm \operatorname{div}\big(\underbrace{\rho^\pm(\nabla V * (\rho^+ - \rho^-))}_{\text{well defined ?}}\big) \quad (GB)$$

Difficulty : • discrete-to-continuum

• regularised → unregularised

Strategy : separate them!!!

Introduce $\boxed{\rho_n}$: a.c. solution of $(GB)_{\delta_n}$

$$\partial_t \rho_n^\pm = \pm \operatorname{div}\big(\rho_n^\pm (\nabla V_{\delta_n} * (\rho_n^+ - \rho_n^-))\big)$$

1) Estimate $W(\mu_n, \rho_n)$ ← same equation!

using GF structure of $(GB)_{\delta_n}$

2) Estimate $W(\rho_n, \rho)$ ← both a.c.

using entropy estimates

1) Regularised problem $(GB)_\delta$, $\delta > 0$ fixed

$$\boxed{\partial_t \rho^\pm = \pm \operatorname{div}\left(\rho^\pm \left(\nabla V_\delta * (\rho^+ - \rho^-)\right)\right)}$$

$\exists!$ Gronwall: $\forall \mu_0 \in \mathcal{P}$, $\exists!$ $f_\delta \in C([0,T]; \mathcal{P})$ of $(GB)_\delta$ with i.c. μ_0.

If μ_0, ν_0 i.c. & μ_δ, ν_δ are solutions, then

$$\mathbb{W}(\mu_\delta(t), \nu_\delta(t)) \leq e^{3\lambda_\delta t} \, \mathbb{W}(\mu_0, \nu_0)$$

large

$$\lambda_\delta = \| D^2 V_\delta \|_\infty \sim \frac{1}{\delta^2}$$

Idea: Use GF structure!

$$\frac{d}{dt} \mathbb{W}(\mu_\delta(t), \nu_\delta(t)) \leq \square$$

Gronwall (derivative of W along solutions)

$\exists!$ by spatial discretisation.

2) $(GB)_\delta \to (GB)$ for a.c. evolutions

Main ingredient: entropy estimates:

If $\underline{\rho_{0,\delta} \in} \underline{(L\log L(\mathbb{T}^2))^2} \cap \mathcal{P}$

$\Rightarrow$ unique solution $\rho_\delta \in C([0,T];\mathcal{P})$ of $(GB)_\delta$

$$\mathrm{Ent}(\rho_\delta(t)) + \int_0^t \|\nabla V_\delta * (\rho_\delta^+ - \rho_\delta^-)(\tau)\|_{H^1}^2 \leq \mathrm{Ent}(\rho_{0,\delta})$$

Orlicz space ~ space where entropy finite

<u>Idea of proof</u> (formal!)

$$\frac{d}{dt}\mathrm{Ent}(\rho_\delta^+) = \frac{d}{dt}\int_{\mathbb{T}^2} \rho_\delta^+ \log \rho_\delta^+$$

$$= \int_{\mathbb{T}^2} \partial_t \rho_\delta^+ \log \rho_\delta^+ + \cancel{\rho_\delta^+} \frac{\partial_t \rho_\delta^+}{\cancel{\rho_\delta^+}}$$

$$= \int (\log \rho_\delta^+ + 1) \boxed{\partial_t \rho_\delta^+} = \mathrm{div}\left(\rho_\delta^+ (\nabla V_\delta * (\rho_\delta^+ - \rho_\delta^-))\right)$$

$$= -\int \underbrace{\nabla(\log \rho_\delta^+ + 1)}_{\frac{\nabla \rho_\delta^+}{\cancel{\rho_\delta^+}}} \cdot \left(\cancel{\rho_\delta^+}(\nabla V_\delta * (\rho_\delta^+ - \rho_\delta^-))\right)$$

$$= \int \rho_\delta^+ \, \Delta V_\delta * (\rho_\delta^+ - \rho_\delta^-)$$

$$\Rightarrow \frac{d}{dt} \mathrm{Ent}(\rho_\delta) = \int (\rho_\delta^+ - \rho_\delta^-) \, \Delta V_\delta * (\rho_\delta^+ - \rho_\delta^-)$$

$$\leq - c \, \| \nabla V_\delta * (\rho_\delta^+ - \rho_\delta^-) \|_{H^1}^2$$

In "Fourier" terms

$$\int_{\mathbb{T}^2} f \, \Delta V_\delta * f = \sum_{k \in \mathbb{Z}^d} \widehat{\Delta V_\delta * f}_k \, \overline{\hat{f}_k}$$

use assumpt's on V_δ

$$\leq - c \, \| \nabla V_\delta * f \|_{H^1}^2$$

$$\boxed{\mathrm{Ent}(\rho_\delta(t)) + \int_0^t \|\nabla V_\delta * (\rho_\delta^+ - \rho_\delta^-)(\tau)\|_{H^1}^2 \leq \mathrm{Ent}(\rho_{0,\delta})}$$

What can we deduce ?

- ρ_δ bdd $L^\infty((L\log L)^2)$

$$\rho_\delta \xrightarrow{*} \rho \in L^\infty((L\log L)^2)$$

- $\nabla V_\delta * (\rho_\delta^+ - \rho_\delta^-)$ bdd $L^2(H^1)$

$$\nabla V_\delta * (\rho_\delta^+ - \rho_\delta^-) \xrightarrow{w} \nabla V * (\rho^+ - \rho^-)$$

not enough to pass to limit

$(GB)_\delta \to (GB)$ in nonlinear term!

improve it !! $\to$ $\partial_t(\quad)$

Aubin-Lions-Simon $\to$ strong $L^2(\underbrace{EXP}_{\text{pre-dual of } L\log L})$ ✓

$\Rightarrow$ ρ solves (GB) !

Put the steps together!

- Given $f_0 \in (L\log L)^2$, approximate in $\mathbb{W}$ with $\underbrace{\mu_{0,n}}_{\text{empirical}}$ and $\underbrace{f_{0,n}}_{\text{bdd entropy}}$

* μ_n, f_n unique solutions of $(GB)_{f_n}$ with i.c $\mu_{0,n}, f_{0,n}$

$\lambda_n = \| D^2 V_{f_n} \|_\infty$

$$\mathbb{W}(\mu_n(t), f_n(t)) \leq c e^{3\lambda_n t} \mathbb{W}(\mu_{0,n}, f_{0,n})$$

* $\mathbb{W}(f_n(t), f(t)) \to 0$ (entropy estimates)

* limit of f_n, f solves (GB)

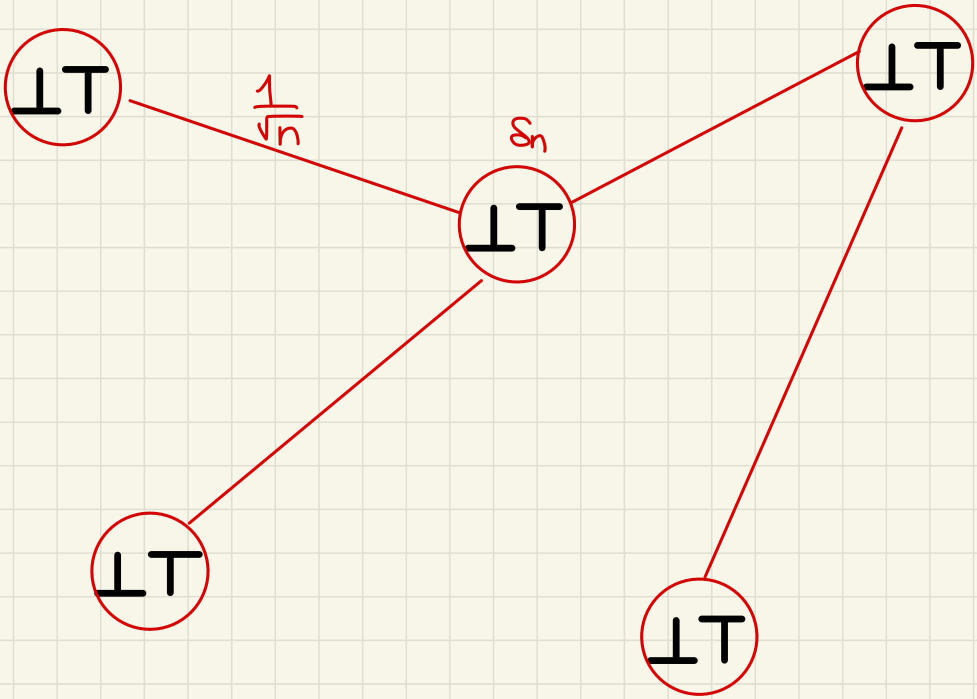
$\Rightarrow \mu_n \longrightarrow f$, f solves (GB) ✓

⊛ Slowness condition on f_n!

So that $\mathbb{W}(\mu_n(t), f_n(t)) \to 0$

Counterexample: If $\delta_n \to 0$ too fast

$\Rightarrow$ no convergence
(due to dipoles!)



- $\delta_n \ll \frac{1}{\sqrt{n}}$