# IV Dilute mean field.

## Back to dynamics:

* given particles $\{I_{\varepsilon N}^n\}_n = \{X_{\varepsilon N}^n, R_{\varepsilon N}^n\}_n$, compute fluid velocity $u_{\varepsilon N}$:

$$
\begin{cases}
-\Delta u_{\varepsilon N} + \nabla p_{\varepsilon N} = h & \text{in } \mathbb{R}^d \setminus \underbrace{\bigcup_n I_{\varepsilon N}^n}_{\mathcal{I}_{\varepsilon N}} \\
\operatorname{div} u_{\varepsilon, N} = 0 & \\
D u_{\varepsilon N}|_{\mathcal{I}_{\varepsilon N}} = 0, \ \text{ie} \ \ u_{\varepsilon N}|_{I_{\varepsilon N}^n} = V_{\varepsilon N}^n + W_{\varepsilon N}^n \times (x - X_{\varepsilon N}^n), \ \forall n & \\
\int_{\partial I_{\varepsilon N}^n} \sigma_{\varepsilon N} \nu + |I_{\varepsilon N}^n| e = 0 & \forall n \\
\int_{\partial I_{\varepsilon N}^n} (x - X_{\varepsilon N}^n) \times \sigma_{\varepsilon N} \nu = 0 & \forall n
\end{cases}
$$

* update positions / orientations: $\begin{cases} \partial_t X_{\varepsilon N}^n = V_{\varepsilon N}^n \\ \partial_t R_{\varepsilon N}^n = W_{\varepsilon N}^n \times R_{\varepsilon N}^n. \end{cases}$

Rem: global well-posedness -in-time (Hillairet-Sabbagh '23) (in fact: long unsettled in physics community!)

idea: at collision time $t = T_*$

consider right-most collisioning particle

difficulty: no explicit force kernel... but can prove (say for part 1 colliding with 2)

$$\partial_t |X_1 - X_2| = \frac{X_1 - X_2}{|X_1 - X_2|} \cdot (V_1 - V_2) = O(|X_1 - X_2|)$$

$$\Rightarrow \partial_t \log |X_1 - X_2| = O(1)!$$

$\Rightarrow$ no collision ✓

## Recap of previous lectures:

I) $u_{\varepsilon N} \sim \bar{u}$ macro fluid flow (homogenization)

where $\begin{cases} -\nabla \cdot \bar{B} \nabla \bar{u} + \nabla \bar{p} = (1 - \lambda \mu_f) h & \text{in } \mathbb{R}^d \\ \operatorname{div} \bar{u} = 0 \end{cases}$ $\quad (\lambda \equiv N \varepsilon^d)$

where $\bar{B}$ "effective viscosity" depends on microstructure.

II) dilute expansion – to simplify dependence on microstructure

$$\bar{B} = \mathrm{Id} + \underbrace{\bar{B}^{(1)}(f)}_{O(\lambda)} + \bar{B}^{(2)}(f, h_2) + \dots$$

where $\begin{cases} f = \text{1-part distribution of orientations / positions} \in \mathcal{P}(\mathbb{R}^d \times \mathbb{S}^{d-1}) \\ h_2 = \text{micro 2-part correlation fct.} \\ \text{etc.} \end{cases}$ $\quad \Big| \ \mu_f(x) = \int_{\mathbb{S}^{d-1}} f(x, r)\, dS(r)$

**Remaining question**: dynamics of $f, h_2, \ldots$

① $f$ : mean-field problem

consider empirical measure $f_{\varepsilon N} = \frac{1}{N}\sum_n \delta_{(X_{\varepsilon N}^n, R_{\varepsilon N}^n)} \in \mathcal{P}(\mathbb{R}^d \times \mathbb{S}^{d-1})$

& expect $\begin{cases} f_{\varepsilon N} \overset{*}{\rightharpoonup} f \\ \partial_t f + \bar u \cdot \nabla_x f + \nabla_r \cdot (\Omega(\mathrm{D}\bar u, r) f) = 0 \end{cases}$ (macro tsport eqn)

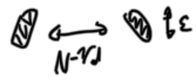
② $h_2, h_3, \ldots$ : micro correlations ($\neq$ macro correlations!)

$\hookrightarrow$ complete open problem!

**Simplification**: neglect 2-particle effects / cluster effects

ie • focus on "dilute mean-field" up to $o(\lambda)$

• assume well-separation of particles $d_{\varepsilon N} := \min_{n\neq m} |X_{\varepsilon N}^n - X_{\varepsilon N}^m| \gtrsim N^{-1/d}$ $(\gg \varepsilon)$




$\hookrightarrow$ expect "Doi model" (Jeffery '22, Hinch-Leal '72, Brenner '74)

$$\begin{cases} u_{\varepsilon N} \sim \bar u + o(\lambda) \\ f_{\varepsilon N} \sim \bar f + o(\lambda) \end{cases} \qquad \begin{cases} -\nabla \cdot \left(\mathrm{Id} + \lambda \bar{\mathrm{B}}^{(1)}(\bar f)\right)\mathrm{D}\bar u + \nabla \bar p = (1-\lambda \mu_f)\, h \\ \operatorname{div} \bar u = 0 \\ \partial_t \bar f + \bar u \cdot \nabla_x \bar f + \nabla_r \cdot \left(\Omega(\mathrm{D}\bar u(x), r)\bar f\right) = 0 \end{cases}$$

where Einstein formula $\begin{cases} \bar{\mathrm{B}}^{(1)}(\bar f) = \int_{\mathbb{S}^{d-1}} \Sigma^\circ(r)\, \bar f(\cdot, r)\, dS(r) \\ E : \Sigma^\circ(r) E = \frac{1}{|I|}\int_{\mathbb{R}^d} |\mathrm{D}\psi^\circ_{r,E}|^2 \text{ with } \psi^\circ_{r,E} \text{ 1-part corrector associated to } I(0,r). \end{cases}$

$\approx \alpha\, (E : r\otimes r)^2$ for elongated particles.

& $\Omega(H, r) = \left(H + \fint_{I(0,R)} \nabla \psi^\circ_{r, H^{sym}}\right) r$

$\Omega(\mathrm{D}\bar u, r) \approx (\mathrm{Id} - r\otimes r)\left(\beta \mathrm{D}\bar u + \frac{1}{2}\nabla\times \bar u\right) r$ for elongated particles.

Difficulties:

① non-explicit, multibody interactions

↳ use cluster expansion + multipole expansion (if well-separated particles)

$$\begin{cases} V^n_{\varepsilon N} = u(X^n_{\varepsilon N}) = \left.\begin{array}{l} G * h(X^n_{\varepsilon N}) \\ - \frac{\lambda}{N} \sum_m G(X^n - X^m)\, h(X^m) \end{array}\right\} G * \left(h(1-\lambda f_{\varepsilon N})\right)(X^n_{\varepsilon N}) \\ \qquad\qquad + \frac{\lambda}{N} \sum_m \nabla G(X^n - X^m)\, \underbrace{\Sigma^\circ(R^m)\, DG * h(X^m)}_{\text{stress difference on } \partial I_m \text{ due to } h} \quad ! \\ \qquad\qquad + O((\lambda+\varepsilon)^2) \\ W^n_{\varepsilon N} = \nabla u(X^n_{\varepsilon N}) = \dots \end{cases}$$

Creates dipole force

② interactions are singular at short distances: $\begin{cases} \text{positions: } \lambda \nabla G \to \text{Coulomb-like singularity} \\ \text{orientation: } \lambda \nabla^2 G \to \text{worse} \dots \end{cases}$

## Intro to mean-field theory

Consider a general particle system (pairwise interaction)

$$\begin{cases} \partial_t X_n = \frac{1}{N} \sum_m^N K(X_n - X_m), \quad 1 \le n \le N \\ X_n|_{t=0} = X_n^\circ \end{cases} \qquad \left(\text{say } \begin{array}{l} K(0) = 0 \\ K(x) = -K(-x) \end{array}\right)$$

Mean-field: as $N \gg 1$, look for simplified description for averaged "macro" particle density

"law of large numbers" for particle dynamics

Let $\mu_N^t = \frac{1}{N} \sum_n^N \delta_{X_n^t}$ empirical measure
$\in \mathcal{P}(\mathbb{R}^d)$

& assume $\mu_N^\circ \xrightarrow{*} \mu^\circ \in L^1(\mathbb{R}^d)$ in $\mathcal{P}(\mathbb{R}^d)$

(e.g. $X_n^\circ$ iid $\sim \mu^\circ$ by LLN)

Question: what can be said of $\mu_N^t \to \mu^t$ ?? macro eqn?

<u>Theorem</u> (smooth setting – Neunzert '77, Braun-Hepp '77, Dobrushin '79, Maslov '79).

- If $K \in C_b^0(\mathbb{R}^d)$,

  then any weak-$*$ limit point of $\{\mu_N\}$ satisfies (Vlasov) $\begin{cases} \partial_t \mu + \mathrm{div}(\mu\, K*\mu) = 0 \\ \mu|_0 = \mu^0 \end{cases}$

- If $K$ is Lipschitz,

  then $\mu_N \overset{*}{\rightharpoonup} \mu$ in $L^\infty(\mathbb{R}^+, \mathcal{P})$ where $\mu$ is the unique solution of (Vlasov).

<u>Proof</u>: 1) Note that $\mu_N$ satisfies $\partial_t \mu_N = -\mathrm{div}(\mu_N\, K*\mu_N)$ (Klimontovich '60s)

as $$\partial_t \int \varphi \mu_N = \partial_t \frac{1}{N} \sum_n \varphi(X_n)$$
$$= \frac{1}{N} \sum_n \nabla\varphi(X_n) \cdot \frac{1}{N} \sum_m K(X_n - X_m)$$
$$= \iint \nabla\varphi(x) \cdot K(x-y)\, d\mu_N(x)\, d\mu_N(y) \;!$$

$\hookrightarrow$ remains to use stability for Vlasov!

2) If $\mu_N \overset{*}{\rightharpoonup} \mu$, can pass to limit in weak formulation if $K \in C_b^0$.

3) $W_1$-stability (Dobrushin)

– exercise: if $\mu, \nu$ satisfy $\begin{cases} \partial_t \mu + \mathrm{div}(\mu\, K*\mu) = 0 \\ \partial_t \nu + \mathrm{div}(\nu\, K*\nu) = 0 \end{cases}$

then $W_1(\mu^t, \nu^t) \leq e^{2t\|K\|_{Lip}} W_1(\mu^0, \nu^0)$ !

indeed $$\partial_t^+ W_1(\mu^t, \nu^t) \leq \int |K*\mu^t(x) - K*\mu_N^t(T^t(x))|\, d\mu^t(x)$$

where $T^t$ optimal tsp plan, $T^t_*\mu^t = \nu^t$.

$$= \int \left| \int \left( K(x-y) - K(T^t(x) - T^t(y)) \right) d\mu^t(y) \right| d\mu^t(x)$$
$$\leq \|K\|_{Lip} \int \left( |x - T^t(x)| + |y - T^t(y)| \right) d\mu^t(x)\, d\mu^t(y)$$
$$= 2\|K\|_{Lip}\, W_1(\mu^t, \nu^t) \;!$$

$\square$

Of course, this doesn't work for $K$ singular ... even repulsive!
(e.g. Coulomb force, ...)

& the topic is still full of open problems!

**Theorem** (Sub-Coulomb setting – Hauray & Jabin '07, Choi-Carrillo-Hauray '14, etc.)

If $\begin{cases} |K(x)| \lesssim |x|^{-\alpha} \\ |\nabla K(x)| \lesssim |x|^{-\alpha-1} \end{cases}$ for some $\alpha < d-1$ (Coulomb force is $\alpha = d-1$)

& if initial data are "well-prepared" in sense of $\dfrac{W_\infty(\mu_N^\circ, \mu^\circ)^d}{\left(\min_{n\neq m} |X_n^\circ - X_m^\circ|\right)^{\alpha+1}} \xrightarrow{N\uparrow\infty} 0$

then $\mu_N \overset{*}{\rightharpoonup} \mu$ unique Vlasov solution as long as $\mu \in L^\infty(\mathbb{R}^d)$

where $W_\infty(\mu_N, \mu) \equiv \inf_{\substack{T:\mathbb{R}^d\to\mathbb{R}^d \\ T_\# \mu = \mu_N}} \left( \operatorname{ess\,sup}_{(\mu)} |x - T(x)| \right)$


**Rem**: many improvements of this statement are possible
e.g. Hauray-Jabin '11 for reduced well-preparedness
Höfer-Schubert '23 for $W_p$-version, $p<\infty$, etc.

**Rem**. for $\mu = 1$ on $\Omega$ & $\mu_N = \frac{1}{N} \sum_{z \in N^{-1/d}\mathbb{Z}^d \cap \Omega} \delta_z$

get $\begin{cases} W_\infty(\mu_N, \mu) \sim N^{-1/d} \\ d_N := \min_{n\neq m} |X_n - X_m| \sim N^{-1/d} \end{cases}$ $\Rightarrow$ well-preparedness cannot hold for $\alpha = d-1$. (Coulomb)

**Rem**. well-posedness of Vlasov follows from Loeper '06:

$\begin{cases} \text{If } \mu, \nu \text{ satisfy (Vlasov)}, \ \alpha < d-1, \\ \text{Then } \partial_t W_1(\mu,\nu) \lesssim (\|\mu\|_{L^\infty} + \|\nu\|_{L^\infty}) W_1(\mu,\nu). \end{cases}$

**Rem**: Results for more singular kernels?

- $K = -\nabla V$ or $\nabla^\perp V$, $V =$ Coulomb $|x|^{2-d}$, $|x|^{-\beta}$, $0<\beta<d$ $\Big\}$ $\Rightarrow$ mean field is known – modulated energy (need good structure)

Cf. see Serfaty-Rosenzweig, Bresch-Jabin-Wang.

- inertial particles – Newton $\begin{cases} \partial_t X_i = V_i \\ \partial_t V_i = \frac{1}{N}\sum_j K(X_i - X_j) \end{cases}$ $\Rightarrow$ mean field is wide open! for Coulomb $K = -\nabla V$ (even for $|\nabla V(x)| \sim |x|^{-1}$, $d \geq 3$)

**Rem**: What about more singular kernels?

$\partial_t \mu + \operatorname{div}(\mu K * \mu) = 0$ makes no sense for $K = -\nabla V$, $V(x) \sim |x|^{-d}$.

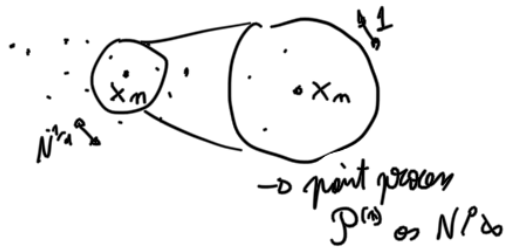
In fact: mean-field breaks down!
– macro dynamics dependence on micro geometry! (no universality)

Indeed compute:

$$\partial_t \int \varphi \, \mu_N = \frac{1}{N}\sum_n \nabla\varphi(X_n)\cdot \frac{1}{N}\sum_m K(X_n - X_m)$$

$$= \frac{1}{2N^2}\sum_{n,m}\big(\nabla\varphi(X_n) - \nabla\varphi(X_m)\big)\cdot K(X_n - X_m)$$

$\forall n$, consider rescaling around $X_n$: let $X_m^{(n)} := N^{1/d}(X_m - X_n)$




$\hookrightarrow$ get $\displaystyle \partial_t \int \varphi\, \mu_N \simeq \frac{1}{2N}\sum_n \frac{1}{N}\sum_m \underbrace{\big(\nabla\varphi(X_n + N^{-1/d}X_m^{(n)}) - \nabla\varphi(X_n)\big)\cdot K(N^{-1/d}X_m^{(n)})}_{\simeq\, \nabla^2\varphi(X_n) : N^{-1/d} X_m^{(n)} \otimes K(N^{-1/d}X_m^{(n)})}$

$$\simeq \frac{1}{2N}\sum_n \nabla^2\varphi(X_n) : \underbrace{\sum_m X_m^{(n)} \otimes K(X_m^{(n)})}$$

$\simeq \displaystyle\sum_{z\in P^{(n)}} z\otimes K(z)$ as $N\uparrow\infty$

depends on micro geometry ...

(in 1D: no geometry $\to$ mean field holds
see Oelschläger '81)

Proof of theorem (mb. Coulomb case).

Consider $\begin{cases} d_N(t) = \min\limits_{n\neq m} |X_n^t - X_m^t| \\ W_\infty(t) = W_\infty(\mu_N^t, \mu^t) = \operatorname{ess\,sup}\limits_{(\mu^t)} |x - T^t(x)|, \quad T^t_\# \mu^t = \mu_N^t \end{cases}$

Idea: - control on $W_\infty$ requires info on $d_N$ (cf singular interaction)

- control on $d_N$ improves if we know $W_\infty \ll 1$.

- At a time around which $d_N = |X_n - X_m|$,

we compute $\displaystyle |\partial_t d_N| = \Big|\underbrace{\frac{1}{N}\sum_k\big(K(X_n - X_k) - K(X_m - X_k)\big)}_{\int (K(X_n - x) - K(X_m - x))\, d\mu_N(x)}\Big|$

$$\leq \int |K(X_n - T(y)) - K(X_m - T(y))|\, d\mu(y)$$

use $|K(a) - K(b)| \leq |a-b|\,\big(|a|^{-\alpha-1} + |b|^{-\alpha-1}\big)$

$$\lesssim \int_{\substack{|X_n-y|\geq 2W_\infty \\ |X_m-y|\geq 2W_\infty}} \underbrace{|X_n - X_m|}_{\leq d_N} \Big( \underbrace{|X_n - T(y)|^{-\alpha-1}}_{\lesssim |X_n-y|^{-\alpha-1}} + \underbrace{|X_m - T(y)|^{-\alpha-1}}_{\lesssim |X_m-y|^{-\alpha-1}} \Big)\, d\mu(y)$$

as $\Big[\, |X_n-y|\geq 2W_\infty \Rightarrow |X_n - Ty| \geq |X_n-y| - \underbrace{|y-Ty|}_{\leq W_\infty} \geq \frac{1}{2}|X_n-y|$

$$+ \int_{\underbrace{|X_n-y|\leq 2W_\infty}_{\lesssim W_\infty^d}} \Big( \underbrace{|X_n - Ty|^{-\alpha} \mathbb{1}_{X_n\neq Ty}}_{\lesssim d_N^{-\alpha}} + \underbrace{|X_m-Ty|^{-\alpha} \mathbb{1}_{X_m\neq Ty}}_{\lesssim d_N^{-\alpha}} \Big)\, d\mu(y) \; + \text{sym}$$

$$\Rightarrow |\partial_t d_N| \lesssim d_N \left(1 + W_\infty^d / d_N^{\alpha+1}\right) \|\mu\|_\infty$$

- Similarly, can prove $\partial_t W_\infty \lesssim W_\infty \left(1 + W_\infty^d / d_N^{\alpha+1}\right) \|\mu\|_\infty$ ] exercise! (see e.g. Choi-Carrillo-Hauray)

- By Gronwall, conclude $\begin{cases} d_N(t) \geq e^{-Ct} d_N(0) \\ W_\infty(t) \leq e^{Ct} W_\infty(0) \end{cases}$ as long as $W_\infty^d / d_N^{\alpha+1} \lesssim 1$ & $\mu \in L^\infty$ $\square$

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## Back to suspensions

Force in $\begin{cases} \text{position} : \lambda \nabla G \text{ ] Coulomb-like singularity : tolerable perturbatively } (\lambda \ll 1) \text{ by sub-Coulomb theory} \\ \text{orientation} : \lambda \nabla^2 G \text{ ] too singular : no mean-field description!} \end{cases}$

2 limitations:
- need strong separation — Otherwise: cluster effects change the $O(\lambda)$ dynamics (cf Mecherbet '21)
- accuracy of mean-field description: $\begin{cases} O(\lambda^2) \text{ for fluid flow} \\ O(\lambda) \text{ for orientation} \end{cases}$ ] beyond: micro geometry becomes important...

**Theorem.** Höfer, Mecherbet, MD-23

Assume $\begin{cases} \text{diluteness: } \lambda = \varepsilon^d N, \; \lambda \log N \ll 1 \\ \text{strong separation: } \min_{n\neq m} |X^n_{\varepsilon N} - X^m_{\varepsilon N}| \gtrsim N^{-1/d} \gg \varepsilon \text{ at } t=0 \\ \text{well-preparedness} \dots \; (W_\infty(\mu^\circ_N, \mu^\circ) \text{ small enough}) \end{cases}$

Then $\begin{cases} u_{\varepsilon N} \approx \bar{u} + O((\lambda+\varepsilon)^2 \log N) \\ f_{\varepsilon N} \approx f + O(\lambda+\varepsilon) \text{ — only!} \end{cases}$ convergence to Doi model

# Non-Newtonian properties from Doi model

Doi model yields $\bar f^t = \bar f(\{\nabla \bar u^s\}_{s\le t}) \Rightarrow$ effective viscosity $\mathrm{Id} + \lambda \bar B^{(1)}(\bar f^t)$
depends on $\{\nabla \bar u^s\}_{s \le t}$
$\hookrightarrow$ nonlinearity + memory (// ketchup)

<u>Question</u> : can we make this more explicit ?

$\hookrightarrow$ consider the model with diffusion for clearer relaxation

$$\begin{cases} -\operatorname{div}\left(1 + \lambda \bar B^{(1)}(f)\right) D\bar u + \nabla \bar p = h + \dfrac{1}{Wi} \operatorname{div}_x \left( \displaystyle\int_r (r \otimes r) f(\cdot, r)\, dS(r) \right) \\ \operatorname{div} \bar u = 0 \\ \partial_t f + \bar u \cdot \nabla f + \operatorname{div}_r \left( \Omega(\nabla \bar u(x), r) f \right) = \underbrace{\dfrac{1}{Wi} \Delta_r f}_{\text{diffusion in orientation}} \end{cases}$$

" $Wi$ = Weissenberg number "
= relaxation time in orientation

$\hookrightarrow$ hydrodynamic limit : Hilbert expansion in $Wi \ll 1$

$$\bar u = \bar v + O(Wi), \quad \begin{cases} -\operatorname{div} \bar\sigma = h \\ \operatorname{div} \bar v = 0 \\ \bar\sigma = \eta\, D\bar v + \beta (D\bar v)^2 + \alpha \left( (\partial_t + \bar v \cdot \nabla) D\bar v + (\nabla \bar v)(D\bar v) + (D\bar v)(\nabla \bar v)^T \right). \end{cases}$$

$\hookrightarrow$ recover " ordered fluid models "
explicit non-Newtonian effects : $\begin{cases} \text{strain-thickening} \\ \text{shear-thinning} \\ \text{phase shift} \end{cases}$

(see MD - Ertzbischoff - Girodroux-Lavigne - Höfer '23)