Mean field limit for interacting particles

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Interacting particles

Consider N particles, identical and interacting two by two through the kernel K. Denote $X_i(t) \in \Pi^d$ and $V_i(t) \in \mathbb{R}^d$ the position and velocity of the i-th particle. Then

$$\frac{d}{dt} X_i = V_i, \quad \frac{d}{dt} V_i = \frac{1}{N} \sum_{j \neq i} K(X_i - X_j). \tag{1}$$

The $\frac{1}{N}$ is a renormalization to get the correct time scale.

The most important case is Coulomb interaction

$$K(x) = -\nabla \Phi, \quad \Phi(x) = \frac{\alpha}{|x|^{d-2}} + \textit{regular}.$$

The case $\alpha > 0$ corresponds to the repulsive/electrostatic case (plasmas...) and $\alpha < 0$ to the attractive/gravitational case (cosmology...).

Other kernels of interest exist however...

Well posedness for the dynamics

If K is regular (Lipschitz), then Eq. (1) has a unique solution for all initial data thanks to Cauchy-Lipschitz.

If K is singular, but the potential is repulsive then the same result trivially holds. For example, Coulomb case the energy

$$E(t) = \frac{1}{N}\sum_i |V_i|^2 + \frac{\alpha}{N^2}\sum_i \sum_{j\neq i} \frac{1}{|X_i - X_j|} = E(0),$$

gives

$$|X_i - X_j| \geq \frac{C}{N^2}, \quad \forall i \neq j.$$

This shows that the force is in fact Lipschitz. But notice that this estimate is useless as $N \to +\infty$.

In other cases, one may obtain existence/uniqueness for *a.e.* initial conditions, see DiPerna-Lions, Ambrosio or Hauray.

Formal limit

As $N \to +\infty$, Eq. (1) is even more cumbersome to use and some limit to a PDE is expected.

Definition of the problem :

Take a sequence of initial data
$Z^{N,0} = (X_1^{N,0}, \dots, X_N^{N,0},\ V_1^{N,0}, \dots, V_N^{N,0})$.
Consider the sequence of solutions
$Z^N(t, Z^{N,0}) = (X_1^N, \dots, X_N^N,\ V_1^N, \dots, V_N^N)$ to (1) with corresponding initial data

$$X_i^N(0) = X_i^{N,0}, \quad V_i^N(0) = V_i^{N,0}, \quad i = 1 \dots N.$$

Define the empirical measure (cf P.L. Lions' course)

$$f_N(t,x,v) = \frac{1}{N} \sum_{i=1}^{N} \delta(x - X_i^N(t)) \otimes \delta(v - V_i^N(t)).$$

Can we get an equation for some limit f of f_N ?

Then if $K \in C(\Pi^d)$ or $X_i^N(t) \neq X_j^N(t)$ for every t, $i \neq j$, we get the Vlasov equation (with the convention $K(0) = 0$)

$$\begin{aligned} &\partial_t f_N + v \cdot \nabla_x f_N + (K \star_x \rho_N) \cdot \nabla_v f_N = 0, \\ &\rho_N(t,x) = \int_{\mathbb{R}^3} f_N(t,x,v)\, dv. \end{aligned} \tag{2}$$

As $N \to \infty$, one expects $f_N \longrightarrow f$ in $w - *$ topology, with f a solution to (2) with

$$f(t=0) = \lim_N f_N(t=0).$$

Even for Coulomb potential, Eq. (2) is well posed (existence+uniqueness, at least in 3d) if for example $f(t=0) \in L^1 \cap L^\infty$ with compact support in velocity (see Horst, Lions-Perthame, Pfaffelmoser, Schaeffer,...).
But if $K \notin C(\Pi^d)$ then the limit $f_N \to f$ is extremely difficult because of the product

$$(K \star_x \rho_N)\, f_N.$$

The same question may be asked for the dynamics of particles in the purely physical space, namely

$$\frac{d}{dt}X_i = \frac{1}{N}\sum_{j\neq i}\mu_i\,\mu_j\,K(X_i - X_j), \tag{3}$$

with the μ_i of order 1. Then defining

$$\rho_N(t,x) = \sum_{i=1}^{N}\mu_i\,\delta(x - X_i(t)),$$

one expects as the limit for ρ_N

$$\partial_t\rho + \nabla_x(K\star\rho\,\rho) = 0. \tag{4}$$

The main example is in 2d with $K = x^\perp/|x|^2$, $|\mu_i| = 1$ and then (4) is just the incompressible Euler equation.

The derivation of (4) is usually easier than the one of (2). Indeed the force is typically regular provided that

$$d_{min}(t) = \min_{i \neq j} |X_i(t) - X_j(t)|,$$

is large enough (for example order $N^{1/d}$). And if, for some locally bounded F and fr x close to x_i, an estimate like

$$\|\frac{1}{N}\sum_{j\neq i} \mu_i\, K(x - X_j)\|_{W^{1,\infty}} \leq F(d_{\min}/N^{1/d}),$$

is available, then as for any t, there exists i, k such that $d_{min} = |X_i - X_k|$. Assuming $\mu_i = \mu_k$

$$\begin{aligned}
\frac{d}{dt} d_{\min} &= \frac{d}{dt}|X_i - X_k| \\
&\geq -\frac{1}{N}\Big|\sum_{j\neq i,k} \mu_j (K(X_i - X_j) - K(X_k - X_j))\Big| + \text{small} \\
&\geq -\|\frac{1}{N}\sum_{j\neq i} \mu_j\, K(x - X_j)\|_{W^{1,\infty}}\, d_{min}.
\end{aligned}$$

One deduces then that

$$\frac{d}{dt} d_{\min} \geq -d_{\min}\, F(d_{\min}/N^{1/d}).$$

Gronwall lemma then controls d_{min}, at least for a short time. However for the case in phase space, the force is still controlled by d_{min} the minimal distance in the physical space but it itself only bounds the minimal distance in phase space

$$d^v_{min} = \inf_{i \neq j}(|X_i - X_j| + |V_i - V_j|).$$

Hence it is not possible to close the estimate...

For Euler, see Goodman, Hou and Lowengrub, or Schochet.

Regular case

The easiest way of obtaining the limit is to take enough regularity on K to be able to pass to the limit in $(K \star \rho_N) f_N$.

Theorem

Assume that K is continuous and that $\exists R$ s.t. $|V_i(0)| \leq R, \quad \forall i$.
Then there exists a subsequence σ s.t.
1) $f_{\sigma(N)} \longrightarrow f$ in $w - *L^\infty(\mathbb{R}_+,\ M^1(\Pi^d \times \mathbb{R}^d))$
2) $\rho_{\sigma(N)} \longrightarrow \rho = \int_{\mathbb{R}^d} f\, dv$ in $w - *L^\infty(\mathbb{R}_+,\ M^1(\Pi^d))$
3) f is a solution to (2) in the sense of distribution.

Comments :

1) This provides the existence of measure valued solutions to (2).
2) There is no uniqueness theory for (2) under such a weak assumption for K : no convergence of the full f_N.
3) The particles could be very poorly distributed (all concentrated at 0 for ex.).

Quick proof

- For any t

$$\int_{\Pi^d\times\mathbb{R}^d} f_N(t,x,v)\,dx\,dv = 1.$$

By weak-* compactness of $L^\infty(\mathbb{R}_+,\ M^1(\Pi^d\times\mathbb{R}^d))$ (dual space of $L^1(\mathbb{R}_+,\ C_0(\Pi^d\times\mathbb{R}^d))$), one has σ s.t. $f_{\sigma(N)} \longrightarrow f$.

- One has

$$|V_i(t)| \le |V_i(0)| + \frac{1}{N}\sum_{j\neq i}\int_0^t |K(X_i-X_j)|\,ds \le R + t\,\|K\|_\infty, \qquad \forall i.$$

Therefore $\rho_{\sigma(N)} = \int f_{\sigma(N)}\,dv$ converges weak-* in $L^\infty(\mathbb{R}_+,\ M^1(\Pi^d))$ to $\rho = \int f\,dv$.

- With t fixed, $K \star_x \rho_{\sigma(N)}$ is equicontinuous in x (same modulous of continuity as K).
- In the sense of distribution, integrating (2) in velocity

$$\partial_t \rho_{\sigma(N)} + \mathrm{div}_x\left(\int_{\mathbb{R}^d} v\, f_{\sigma(N)}\,dv\right) = 0.$$

Therefore $K \star_x \rho_{\sigma(N)}$ is equicontinuous in x and t.

• By Ascoli's theorem, $K \star_x \rho_{\sigma(N)}$ converges uniformly (in $L^\infty([0,\ T] \times \Pi^d)$ for any T) to $K \star_x \rho$.
Consequently in the sense of distributions

$$(K \star_x \rho_{\sigma(N)})\, f_{\sigma(N)} \longrightarrow (K \star_x \rho)\, f$$

Passing to the limit in the other terms of (2) is straightforward.

If K is more regular, the following stability holds (Dobrushin, Braun and Hepp, Spohn...)

Theorem

Assume $K \in W^{1,\infty}$ and $f^1,\ f^2 \in L^\infty(\mathbb{R}_+,\ M^1(\Pi^d \times \mathbb{R}^d))$ are two solutions to (2) with compact support then

$$\|f^1(t) - f^2(t)\|_{W^{-1,1}(\Pi^d\times\mathbb{R}^d)} \leq C\,\|f^1(0) - f^2(0)\|_{W^{-1,1}(\Pi^d\times\mathbb{R}^d)} \times \exp(C\,\|\nabla K\|_{L^\infty}\ t).$$

Comments :

1) Well posedness of measures solutions to (2) and not only convergence.

2) The exponential growth rate is probably not optimal.

3) Controls the concentration of particles.

4) The constant C only depends on the total mass of both solutions.

Idea of the proof

Define the characteristics for each solution

$$\frac{d}{dt}X^\gamma(t,x,v) = V^\gamma(t,x,v), \quad \frac{d}{dt}V^\gamma(t,x,v) = K \star_x \rho^\gamma(t, X^\gamma),$$

$$X(0,x,v) = x, \quad V(0,x,v) = v, \qquad \gamma = 1,\, 2.$$

This is well defined as $K \star \rho^\gamma$ is Lipschitz (K is C^1) and it mimics the dynamics of the particles (1). Moreoever

$$|\nabla X^\gamma| + |\nabla V^\gamma| \le e^{C\,t\,\|\nabla K\|_\infty}.$$

Then denoting

$$\mathcal{L} = \{\phi \in C^1(\Pi^d \times \mathbb{R}^d),\ \|\phi\|_\infty \le 1 \text{ and } \|\nabla\phi\|_\infty \le 1\},$$

one has

$$\|f^1(t) - f^2(t)\|_{W^{-1,1}} = \sup_{\phi\in\mathcal{L}} \int_{\Pi^d\times\mathbb{R}^d} \phi(x,v)\,(f^1(t,x,v) - f^2(t,x,v))$$

$$= \sup_{\phi\in\mathcal{L}} \int (\phi(X^1,\, V^1)\, f^1(0,x,v) - \phi(X^2,\, V^2)\, f^2(0,x,v))\, dx\, dv$$

Therefore

$$\|f^1(t) - f^2(t)\|_{W^{-1,1}} \le \sup_{\phi\in\mathcal{L}} \int_{\Pi^d\times\mathbb{R}^d} \phi(X^1,\, V^1)(f^1(0) - f^2(0))$$
$$+ \sup_{\phi\in\mathcal{L}} \int_{\Pi^d\times\mathbb{R}^d} |\phi(X^1,\, V^1) - \phi(X^2,\, V^2)|\, f^2(0,x,v),$$

so

$$\|f^1(t) - f^2(t)\|_{W^{-1,1}} \le \|\nabla(X^1,\, V^1)\|_\infty\, \|f^1(0) - f^2(0)\|_{W^{-1,1}}$$
$$+ \|(X^1,\, V^1) - (X^2,\, V^2)\|_\infty \int f^2(0,x,v)\, dx\, dv.$$

And consequently it only remains to bound

$$\|(X^1,\, V^1) - (X^2,\, V^2)\|_\infty.$$

First of all

$$\frac{d}{dt}|X^1 - X^2| \le |V^1 - V^2|.$$

And now

$$\frac{d}{dt}|V^1 - V^2| \leq |K \star \rho^1(t, X^1) - K \star \rho^2(t, X^2)|$$

$$\leq |K \star \rho^1(t, X^1) - K \star \rho^1(t, X^2)|$$

$$+|K \star (\rho^1 - \rho^2)(t, X^2)|$$

$$\leq |X^1 - X^2| \, \|\nabla K\|_\infty \int \rho^1 \, dx$$

$$+ \|\nabla K\|_\infty \, \|\rho^1 - \rho^2\|_{W^{-1,1}}.$$

Putting all estimates together

$$\frac{d}{dt}\|f^1(t) - f^2(t)\|_{W^{-1,1}} \leq C \, \|\nabla K\|_\infty \, \|f^1(t) - f^2(t)\|_{W^{-1,1}},$$

and we conclude by Gronwall lemma.

Conclusion

The case $K \in C^1$ is completely solved. However it is very far from the kernels that are used in practice.

The case $K \in C$ is superficially easy but in fact not satisfactory. The well posedness is most probably out of reach (uniqueness of $\dot{X} = b(x)$ with b only continuous ?).

The interesting cases are $K \sim |x|^{-\alpha}$. We don't even have $K \in C$ but in fact $K \in C^1(\Pi^d \setminus \{0\})$.

The problem

Consider the dynamics for $K \sim |x|^{-\alpha}$

$$\frac{d}{dt}X_i = V_i, \quad \frac{d}{dt}V_i = \frac{1}{N}\sum_{j\neq i} K(X_i - X_j). \tag{1}$$

Define

$$f_N = \frac{1}{N}\sum_{i=1}^{N} \delta(x - X_i(t))\,\delta(v - V_i(t)).$$

Can we prove that $f_N \longrightarrow f$ with f solution to

$$\begin{aligned} &\partial_t f + v \cdot \nabla_x f + (K \star_x \rho) \cdot \nabla_v f = 0, \\ &\rho(t,x) = \int_{\mathbb{R}^d} f(t,x,v)\,dv. \end{aligned} \tag{2}$$

Weakly singular case

Still using Gronwall type estimates, we have (Hauray-Jabin)

Theorem

Assume $K \sim \frac{1}{|x|^\alpha}$ with $\alpha < 1$. For any sequence of initial data $Z^{N,0}$ with uniform compact support and such that

$$d_{min}(0) = \min_{i \neq j}(|X_i^{N,0} - X_j^{N,0}| + |V_i^{N,0} - V_j^{N,0}|) \geq cN^{-1/(2d)}.$$

Then for any t we have c' such that $d_{min}(t) \geq c' N^{-1/(2d)}$ and the sequence full f_N converges toward the unique solution f to (2) with $f(t=0) = \lim_N f_N(t=0)$ in $L^1 \cap L^\infty$ and compactly supported.

Comments :

1) The condition $\alpha < 1$ is probably close to optimal even though it is quite far from the Coulombian case. It is used to control the integral of the force along trajectories, even when 2 particles are close :

$$\int_t \frac{dt}{|X + Vt|^\alpha} < \infty$$

2) If the initial positions and velocities are chosen randomly then the probability to satisfy the condition on d_{min} vanishes. Therefore this is not satisfying from a statistical physics point of view but quite all right for numerical purposes.

In fact this assumption even tells a lot on the limit f. For example if

$$d_{min}(0) \geq cN^{1/(2d)},$$

and $f_N(0) \longrightarrow f$, then automatically $f \in L^\infty$.

3) The compact support assumption corresponds to the usual hypothesis for uniqueness on (2) and is rather natural.

The macroscopic equivalent

For macroscopic models, the result is better (see Hauray)

Theorem

Assume $K \sim \frac{1}{|x|^\alpha}$ with $\alpha < d-1$. Take any sequence of initial data $X^{N,0}$ such that

$$d_{min}(0) = \min_{i \neq j}(|X_i^{N,0} - X_j^{N,0}|) \ \geq cN^{-1/d},$$

consider the dynamics (1) with $\mu_i = 1$, $\frac{d}{dt}X_i = \frac{1}{N}\sum_{j\neq i} K(X_i - X_j)$. Then for any $t \leq T$ we have c' such that $d_{min}(t) \geq c' N^{-1/(d)}$ and the sequence full ρ_N converges toward the unique solution ρ to (4). If $\operatorname{div} K = 0$, then $T = \infty$.

Comments :

1) The condition $\alpha < d-1$ is now very reasonable as 2d Euler is just the limit case. Moreover no symmetry is needed on K contrary to the previous derivations.

2) All other remarks concerning d_{min} unfortunately still hold.

A partial proof

Let us only show the estimate on the minimal distance. Of course

$$\frac{d}{dt}|X_i - X_k| \geq -\frac{1}{N}\sum_{j\neq i,k} |K(X_i - X_j) - K(X_k - X_j)| \\ + \frac{1}{N}(|K(X_i - X_k)| + |K(X_k - X_i)|).$$

If $K \sim |x|^\alpha$ then

$$|K(X_i - X_k)| \leq \frac{C}{|X_i - X_k|^\alpha} \leq \frac{C}{d_{min}^\alpha},$$

and on the other hand

$$|K(X_i - X_j) - K(X_k - X_j)| \leq |X_i - X_k| \\ \times \left(\frac{C}{|X_i - X_j|^{\alpha+1}} + \frac{C}{|X_k - X_j|^{\alpha+1}}\right).$$

The main point is to control

$$\frac{1}{N}\sum_{j\neq i} \frac{C}{|X_i - X_j|^{\alpha+1}}.$$

We simply mimic the usual convolution estimates. Denote

$$N_k = |\{j,\ j \neq i \text{ and } 2^k\, d_{min} \leq |X_i - X_j| \leq 2^{k+1}\, d_{min}\}.$$

By the definition of d_{min} we of course have $N_k = 0$ for any $k < 0$ and as we are in Π^d, $N_k = 0$ for $k > k_0 = -\ln d_{min}/\ln 2$. Decomposing we get

$$\frac{1}{N}\sum_{j\neq i}\frac{1}{|X_i - X_j|^{\alpha+1}} \leq \frac{C_d}{N}\sum_{k=0}^{k_0} 2^{-k(\alpha+1)}\, d_{min}^{-\alpha-1}\, N_k.$$

Again by the definition of d_{min}

$$N_k \leq C_d\, 2^{kd},$$

so as $\alpha + 1 < d$

$$\frac{1}{N}\sum_{j\neq i}\frac{1}{|X_i - X_j|^{\alpha+1}} \leq \frac{C_d}{N}\sum_{k=0}^{k_0} 2^{k(d-\alpha-1)}\, d_{min}^{-\alpha-1}$$

$$\leq \frac{C_d}{N}\, 2^{k_0(d-\alpha-1)}\, d_{min}^{-\alpha-1} \leq C_d\, \frac{N^{-1}}{d_{min}^{d}}.$$

Putting all the estimates together, one gets

$$\frac{d}{dt}|X_i - X_k| \geq -|X_i - X_k| \; C_d \; \frac{N^{-1}}{d_{min}^d} - C \, \frac{d_{min}^{-\alpha}}{N}.$$

Therefore taking the i and k such that $|X_i - X_k| = d_{min}$

$$\begin{aligned}\frac{d}{dt} d_{min} &\geq -d_{min} \; C_d \; \left(\frac{N^{-1}}{d_{min}^d} \right) - C \, \frac{d_{min}^{-\alpha}}{N} \\ &\geq -d_{min} \; \frac{N^{-1}}{d_{min}^d} \; \left(C_d + C \, d_{min}^{d-\alpha} \right),\end{aligned}$$

and we conclude by Gronwall lemma.

An almost everywhere approach

We would like to still derive a stability estimate, *i.e.* showing that $|X_i^N(t,Z^{N,0})-X_i^N(t,Z^{N,0}+\delta)|$ remains of order δ for shifts δ that may go to 0.
However as we do not want to use Cauchy-Lipschitz/Gronwall like estimates, this can only be true for almost all initial data.
More precisely (following Crippa-De Lellis) one is looking for an estimate like

$$\int_{\Pi^{dN}\times\mathbb{R}^{dN}} P(Z^{N,0})\ \log\Big(1+\frac{1}{N\,|\delta|_\infty}\sum_{i=1}^N (|X_i^N(t,Z^{N,0})-X_i^N(t,Z^{N,0}+\delta)| \\ +|V_i^N(t,Z^{N,0})-V_i^N(t,Z^{N,0}+\delta)|)\Big)\leq C\,(1+t). \tag{5}$$

The function P of the initial configuration determines the notion of almost everywhere and so must be chosen with care...

Idea of the proof

Differentiate in time and for a given t use the change of variables

$$Z^{N,0} \longrightarrow Z^N(t, Z^{N,0}),$$

which has jacobian 1. Then, as the measure e^{-H_N} is invariant under the flow, one has to control quantities like

$$\int_{\Pi^{dN}\times\mathbb{R}^{dN}} \frac{P_t(Z^{N,0})}{|X_1^0 - X_2^0|^{\alpha+1}}\, dZ^{N,0},$$

with P_t the image by the flow of at time t of P. This should be all right if $\alpha + 1 < d$.

If one is not careful, one ends up instead with

$$\int_{\Pi^{dN}\times\mathbb{R}^{dN}} P_t(Z^{N,0})\ \max_i \Big(\frac{1}{N}\sum_{j\neq i} \frac{1}{|X_i^0 - X_j^0|^{\alpha+1}}\Big)\, dZ^{N,0} = +\infty \ldots$$

The choice of P

From the details of the proof one gets the following condition on P

$$\int_{\Pi^{d(N-k)}\times\mathbb{R}^{dN}} P_t(Z^{N,0})\, dX^0_{N-k}\dots dX_N\, dV^0_1\dots dV^0_N \le C^k.$$

The simplest (and more or less only reasonable) way of satisfying this is to choose P invariant for the flow. For instance if $K=-\nabla\Phi$ with $\Phi\ge 0$

$$P(Z^{N,0})=\beta_N\, e^{-H_N(Z^{N,0})},$$

Where the hamiltonian H_N can be one of the two

$$H_N=E_N=\frac{1}{N}\sum_{i=1}^N |V_i^N|^2+\frac{1}{N^2}\sum_{i=1}^N\sum_{j\neq i}\Phi(X_i^N-X_j^N)\qquad \text{(easy)}.$$

or

$$H_N=N\,E_N=\sum_{i=1}^N |V_i^N|^2+\frac{1}{N}\sum_{i=1}^N\sum_{j\neq i}\Phi(X_i^N-X_j^N)\qquad \text{(much harder)}.$$

Interpretation of the estimate

Take $K = -\nabla\Phi$ with $\Phi \geq 0$ and $K \sim |x|^{-\alpha}$ with $\alpha < d - 1$.

• First of all one can replace $Z^N(t, Z^{N,0} + \delta)$ in (5) by $Z^{N,\delta}$ the solution to the dynamics with a regularized kernel K_δ. Hence (5) controls

$$\int_{\Pi^{3N}\times\mathbb{R}^{3N}} P(Z^{N,0}) \log\Big(1 + \frac{1}{|\delta|}\|f_N(t) - f_\delta(t)\|_{W^{-1,1}}\Big),$$

with f_δ the solution to (2) with the regularized kernel K_δ.

$\Longrightarrow$ Convergence to the solutions of (2) with $f^0 = \lim_N f_N(0)$.

• But in general one expects some sort of concentration of the measure P so that the possible limits f^0 are very limited.

• For $H_N = E_N$ one has almost always

$$f_N(0) \longrightarrow 0.$$

For $H_N = N\,E_N$ one has almost always

$$f_N(0) \longrightarrow \rho(x)\, e^{-|v|^2},$$

with ρ the minimizer of

$$\int_{\Pi^6} \frac{1}{2}\, \Phi(x-y)\, \rho(x)\, \rho(y)\, dx\, dy + \int_{\Pi^3} \rho(x)\, \log \rho(x)\, dx.$$

• For the moment this gives only a stability of the two stationary solutions through perturbation by Dirac masses.

$\Longrightarrow$ Interest of having non invariant measures instead of H_N.