A New Approach to Mean-Field Limits for Large Particle Systems

François Golse

CMLS, Ecole polytechnique & CNRS
Université Paris-Saclay

"Kinetic Theory and Fluid Dynamics:
From Micro- to Macroscopic Modeling"
Rakuyu-Kaikan, Kyoto University, May 26th-28th, 2016

In honor of Profs Y. Sone and K. Aoki

Work with C. Mouhot & T. Paul

Motivation

•The Vlasov equation with $C^{1,1}$ interaction potential has been derived from the N-body problem of classical mechanics with $O(1/N)$ coupling constant in the limit $N \to \infty$ (Neunzert-Wick 1973, Braun-Hepp 1977, Dobrushin 1979)

Problem 1: What is the convergence rate?

•The N-body Liouville equation is known to describe the semiclassical limit (as $\hbar \to 0$) of the N-body Schrödinger equation

Problem 2: Can one pass to both limits and derive the Vlasov equation directly from the N-body Schrödinger equation? What is the convergence rate?

•On Pbm 1: see Dobrushin, Func. Anal. 1979, Mischler-Mouhot-Wennberg PTRF 2015

•On Pbm 2: see Pezzotti-Pulvirenti Ann. H. Poincaré 2009, and Graffi-Martinez-Pulvirenti M3AS2003,

The diagram

Schrödinger

$\downarrow$

$\hbar \to 0$ $\searrow$

$\downarrow$

Liouville $\xrightarrow{N\to\infty}$ **Vlasov**

Neunzert-Wick's+Braun-Hepp's approach of the MF limit

•Classical N-body problem with $V \in C^{1,1}(\mathbf{R}^d)$ even ($\Rightarrow \nabla V(0) = 0$)

$$\dot{x}_j = \xi_j \,, \quad \dot{\xi}_j = -\frac{1}{N}\sum_{k=1}^{N} \nabla V(x_j - x_k)$$

•Prove that the time-dependent empirical measure

$$\frac{1}{N}\sum_{k=1}^{N} \delta_{x_k(t),\xi_k(t)} \rightharpoonup f \text{ as } N \to \infty$$

where $f \equiv f(t,x,\xi)$ is a solution of the Vlasov equation

$$\partial_t f(t,x,\xi) + \{\tfrac{1}{2}|\xi|^2 + V_f(t,x), f(t,x,\xi)\} = 0$$

$$V_f(t,x) := \iint V(x-y) f(t,y,\xi) dy d\xi$$

Dobrushin's propagation estimate

Set

$$d_N(t) := \mathrm{dist}_{\mathrm{MK},1}\left(\frac{1}{N}\sum_{k=1}^{N}\delta_{x_k(t),\xi_k(t)}, f(t)\right)$$

Denoting $L := \mathrm{Lip}(\nabla V)$, Dobrushin proves that

$$d_N(t) \le d_N(0)e^{2Lt}$$

Choose $(x_k(0), \xi_k(0))$ for $k \ge 1$ independent with distribution $f\big|_{t=0}$

Law of large numbers $\Rightarrow d_N(0) \to 0$

Convergence rate in LLN in terms of MK distances: Fournier-Guillin PTRF2015

Monge-Kantorovich(-Rubinshtein) or Vasershtein distances

Let $p \geq 1$ and $\mu, \nu \in \mathcal{P}_p(\mathbf{R}^d)$ with bounded moment of order p

Coupling of μ, ν: any $\pi \in \mathcal{P}(\mathbf{R}^d \times \mathbf{R}^d)$ s.t.

$$\iint (\phi(x) + \psi(y))\pi(dxdy) = \int \phi(x)\mu(dx) + \int \psi(y)\nu(dy)$$

Set of couplings of μ, ν denoted $\Pi(\mu, \nu)$; define

$$\text{dist}_{MK,p}(\mu, \nu) = \inf_{\pi \in \Pi(\mu,\nu)} \left(\iint |x - y|^p \pi(dxdy) \right)^{1/p}$$

This distance metrizes the topology of weak convergence on $\mathcal{P}_p(\mathbf{R}^d)$

Difficulties/Shortcomings

•For the MF limit in classical mechanics: the approach with the empirical measure systematically involves the quantization error — e.g. the discrepancy of the sequence of phase-space points

•For the semiclassical+mean-field limit: at present there does not seem to be any convenient analogue of the notion of empirical measure in quantum mechanics. Likewise, is there an analogue of Monge-Kantorovich distance in quantum mechanics?

The mean-field limit in quantum mechanics is obtained by methods different from Dobrushin's — based on the BBGKY hierarchy, or on 2nd quantization, or on convergence estimates in operator norm (Pickl LMP2009), all of which are not uniform as $\hbar \to 0$

AN EULERIAN CONVERGENCE ESTIMATE

FOR THE MEAN-FIELD LIMIT IN CLASSICAL MECHANICS

F.G.-C. Mouhot-T. Paul: Commun. Math. Phys. **343** (2016), 165–205

An alternative strategy

•Seek to estimate

$$\mathrm{dist}_{\mathrm{MK},2}(f(t), F_N^{\mathbf{1}}(t))$$

where F_N is the solution of the N-body Liouville equation and

$$F_N^{\mathbf{n}}(t) := \int F_N(t) dy_{n+1} d\eta_{n+1} \dots dy_N d\eta_N$$

instead of

$$\mathrm{dist}_{\mathrm{MK},1}\left(f(t), \frac{1}{N}\sum_{k=1}^{N} \delta_{(x_k,\xi_k)(t)}\right)$$

•Look for an Eulerian analogue of the Dobrushin argument, avoiding the use of classical trajectories

•All the steps in the estimate should have clear quantum analogues

•Initial data for Vlasov's equation: $f^{in} \in \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$

•Initial data for N-body Liouville $F_N^{in} \in \mathcal{P}_2^s((\mathbf{R}^d \times \mathbf{R}^d)^N)$ symmetric in the phase-space variables

Notation:

$$X_N := (x_1, \ldots, x_N)\,, \quad \Xi_N := (\xi_1, \ldots, \xi_N)$$
$$Y_N := (y_1, \ldots, y_N)\,, \quad H_N := (\eta_1, \ldots, \eta_N)$$

For each $\sigma \in \mathfrak{S}_N$, set

$$\sigma \cdot X_N := (x_{\sigma(1)}, \ldots, x_{\sigma(N)})$$

Initial coupling: $P^{in} \in \Pi^s((f^{in})^{\otimes N}, F_N^{in})$ — s means invariant by

$$(X_N, \Xi_N, Y_N, H_N) \mapsto (\sigma \cdot X_N, \sigma \cdot \Xi_N, \sigma \cdot Y_N, \sigma \cdot H_N)\,, \quad \sigma \in \mathfrak{S}_N$$

Vlasov vs Liouville dynamics

Vlasov equation:

$$(\partial_t + \xi \cdot \nabla_x) f - \nabla V \star_x \rho_f \cdot \nabla_\xi f = 0 \,, \quad f\big|_{t=0} = f^{in}$$

Hence

$$(\partial_t + \Xi_N \cdot \nabla_{X_N}) f^{\otimes N} = \sum_{j=1}^{N} \nabla V \star_x \rho_f(t, x_j) \cdot \nabla_{\xi_j} f^{\otimes N}$$

Liouville equation

$$(\partial_t + H_N \cdot \nabla_{Y_N}) F_N = \frac{1}{N} \sum_{j,k=1}^{N} \nabla V(y_j - y_k) \cdot \nabla_{\eta_j} F_N \,, \quad F_N\big|_{t=0} = F_N^{in}$$

Theorem A
Assume that the potential V is even with $\nabla V \in W^{1,\infty}(\mathbf{R}^d)$. Let $f(t)$ be the solution of the Vlasov equation with initial data f^{in} and F_N be the solution of the Liouville equation with initial data F_N^{in}. Then

$$\mathrm{dist}_{\mathrm{MK},2}(f(t), F_N^{\mathbf{1}}(t))^2 \leq \frac{1}{N}\,\mathrm{dist}_{\mathrm{MK},2}((f^{in})^{\otimes N}, F_N^{in})^2 e^{\Lambda t} + \frac{(2\|\nabla V\|_{L^\infty})^2}{N}\,\frac{e^{\Lambda t}-1}{\Lambda}$$

for all $t \geq 0$, with

$$\Lambda = 2 + \max(1, 2\,\mathrm{Lip}(\nabla V)^2)$$

•Case of Lipschitz continuous interaction force
Mischler-Mouhot-Wennberg PTRF2015
FG-Mouhot-Ricci KRM2013

$$\mathrm{dist}_{\mathrm{MK},1}(f(t), F_N^{\mathbf{1}}(t)) = O(e^{\Lambda t}/N^{1/(d+4)})$$

•Case of singular interaction force
Hauray-Jabin (Ann. Scient. ENS2015): $O(r^{-\alpha})$ with $\alpha < 1$ if $d \geq 3$

•Singular interaction force with vanishing truncation
Pickl-Lazarovici (arXiv:1502.04608), Lazarovici (arXiv:1502:07047)
Coulomb or Newton with truncation of order $N^{-1/3+\epsilon}$

Dynamics of couplings

Lemma 1 Let $t \mapsto P(t) \in \mathcal{P}((\mathbf{R}^d \times \mathbf{R}^d)^2)$ satisfy $P\big|_{t=0} = P^{in}$ and

$$(\partial_t + \Xi_N \cdot \nabla_{X_N} + H_N \cdot \nabla_{Y_N})P$$
$$= \sum_{j=1}^{N} \left(\nabla V \star_x \rho_f(t, x_j) \cdot \nabla_{\xi_j} + \frac{1}{N} \sum_{k=1}^{N} \nabla V(y_j - y_k) \cdot \nabla_{\eta_j} \right) P$$

Then $P(t) \in \Pi^s(f(t)^{\otimes N}, F_N(t))$ for each $t \geq 0$, i.e.

$$\int P(t) dY_N dH_N = f(t)^{\otimes N}, \qquad \int P(t) dX_N d\Xi_N = F_N(t)$$

Proof: Integrate both sides of the equation for P in (Y_N, H_N) and in (X_N, Ξ_N), and use the uniqueness property for the Vlasov and the Liouville equations

The quantity $D_N(t)$

Definition For each $P^{in} \in \Pi^s((f^{in})^{\otimes N}, F_N^{in})$, set

$$D_N(t) := \int \frac{1}{N} \sum_{j=1}^{N} (|x_j - y_j|^2 + |\xi_j - \eta_j|^2) P(t)$$

Lemma 2

$$D_N(t) \geq \mathrm{dist}_{\mathrm{MK},2}(f(t), F_N^{\mathbf{1}}(t))^2$$

Proof: By symmetry of $P(t)$, one has

$$D_N(t) := \int (|x_j - y_j|^2 + |\xi_j - \eta_j|^2) P(t) \quad \text{for all } j = 1, \ldots, N$$

Bound on $\mathrm{dist}_{\mathrm{MK},2}(f, F_N^{\mathbf{1}})$ = moment bound for a 1st order PDE

Notation for $Y_N=(y_1,\ldots,y_N)$, we set

$$\mu_{Y_N}:=\frac{1}{N}\sum_{j=1}^N\delta_{y_j}$$

•Multiplying by $\frac{1}{N}(|X_N-Y_N|^2+|\Xi_N-H_N|^2)$ each side of the equation for P and integrating in all variables

$$\begin{aligned}\dot{D}_N(t)&\le D_N(t)\\&+\int\frac{2}{N}\sum_{j=1}^N(\nabla V\star_x\rho_f(x_j)-\nabla V\star\mu_{X_N}(x_j))\cdot(\xi_j-\eta_j)P(t)\\&+\int\frac{2}{N}\sum_{j=1}^N(\nabla V\star\mu_{X_N}(x_j)-\nabla V\star\mu_{Y_N}(y_j))\cdot(\xi_j-\eta_j)P(t)\\&=:D_N(t)+I_N(t)+J_N(t)\end{aligned}$$

Since ∇V is Lipschitz continuous

$$J_N(t) \leq \max(1, 2\,\mathrm{Lip}(\nabla V)^2) D_N(t)$$

On the other hand

$$I_N(t) \leq \int \frac{1}{N} \sum_{j=1}^{N} |\nabla V \star (\rho_f - \mu_{X_N})(x_j))|^2 \rho_f(t)^{\otimes N} + D_N(t)$$

Lemma 3 [Quantitative LLN] Elementary computations show that

$$\int |\nabla V \star (\rho_f - \mu_{X_N})(x_1)|^2 \rho_f(t)^{\otimes N} \leq \frac{(2\|\nabla V\|_{L^\infty})^2}{N}$$

Conclude with Gronwall's lemma.

FROM N-BODY SCHRÖDINGER TO VLASOV

F.G.-T. Paul: arXiv:1510.06681

The method

Task 1: define a "pseudo-distance" between a quantum density (operator), and a classical probability density

Task 2: bound the amplification of this pseudo-distance under the joint quantum and classical dynamics

Task 2 will be formally similar to the classical computation above — replacing Poisson brackets with commutators, integrals with traces. . .

Coupling quantum and classical densities

Density operators on $\mathfrak{H} := L^2(\mathbf{R}^d)$

$$\rho = \rho^* \geq 0\,, \quad \mathrm{tr}(\rho) = 1 \quad \Leftrightarrow \rho \in \mathcal{D}(\mathfrak{H})$$

Couplings of $\rho \in \mathcal{D}(\mathfrak{H})$ and p probability density on $\mathbf{R}^d \times \mathbf{R}^d$

$$(x,\xi) \mapsto Q(x,\xi) = Q(x,\xi)^* \in \mathcal{L}(\mathfrak{H}) \text{ s.t.} Q(x,\xi) \geq 0$$
$$\mathrm{tr}(Q(x,\xi)) = p(x,\xi)\,, \quad \iint_{\mathbf{R}^d\times\mathbf{R}^d} Q(x,\xi)dxd\xi = \rho$$

The set of all couplings of the densities ρ and p is denoted $\mathcal{C}(\rho, p)$

Task 1: defining the pseudo-distance

Cost function comparing classical and quantum "coordinates" (i.e. position and momentum)

$$c_\hbar(x,\xi) := |x-y|^2 + |\xi + i\hbar\nabla_y|^2$$

Define a pseudo-distance "à la" Monge-Kantorovich

$$E_\hbar(p,\rho) := \left(\inf_{Q\in\mathcal{C}(p,\rho)} \iint_{\mathbf{R}^d\times\mathbf{R}^d} \operatorname{tr}(c_\hbar(x,\xi)Q(x,\xi))dxd\xi\right)^{1/2}$$

Analogous to the quadratic Monge-Kantorovich distance $\operatorname{dist}_{MK,2}$

Quantum Hamiltonian

$$\mathcal{H}_N := \sum_{j=1}^{N} -\tfrac{1}{2}\hbar^2\Delta_{y_j} + \frac{1}{N}\sum_{1\le j<k\le N} V(y_j - y_k)$$

N-body von Neumann equation

$$\partial_t \rho_{N,\hbar} = -\frac{i}{\hbar}[\mathcal{H}_N, \rho_{N,\hbar}]$$

Vlasov equation

$$\partial_t f(t,x,\xi) + \{\tfrac{1}{2}|\xi|^2 + V_f(t,x), f(t,x,\xi)\} = 0$$
$$V_f(t,x) := \iint V(x-y) f(t,y,\xi)\, dy d\xi$$

Symmetric densities and marginals in the quantum formalism

The density operator $\rho_{\hbar,N}$ is an integral operator with integral kernel

$$R_{\hbar,N}(t,x_1,\dots,x_N,y_1,\dots,y_N)$$

Since particles are indistinguishable, $\rho_{\hbar,N}(t)$ is a symmetric density operator for all t:

$$\begin{aligned}R_{\hbar,N}&(t,x_{\sigma(1)},\dots,x_{\sigma(N)},y_{\sigma(1)},\dots,y_{\sigma(N)})\\&=R_{\hbar,N}(t,x_1,\dots,x_N,y_1,\dots,y_N)\,,\text{ for all }\sigma\in\mathfrak{S}_N\end{aligned}$$

The 1st marginal density operator $\rho^{\mathbf{k}}_{\hbar,N}$ has integral kernel

$$R^{\mathbf{1}}_{\hbar,N}(t,x_1,y_1):=\int R_{\hbar,N}(t,x_1,z_2,\dots,z_N,y_1,z_2,\dots,z_N)dz_2\dots dz_N$$

Thm B Let $f^{in} \equiv f^{in}(x,\xi) \in L^1((|x|^2 + |\xi|^2)dxd\xi)$ be a probability density, and $\rho^{in}_{N,\hbar} \in \mathcal{D}^s(\mathfrak{H}_N)$. Let f and $\rho_{N,\hbar}$ be the solutions of the Vlasov equation and the von Neumann equation resp. with initial data f^{in} and $\rho^{in}_{N,\hbar}$. Then

$$E_\hbar(f(t), \rho^{\mathbf{1}}_{\hbar,N}(t)) \leq \frac{1}{N} E_\hbar((f^{in})^{\otimes N}, \rho^{in}_{\hbar,N}) e^{\Gamma t} + \frac{(2\|\nabla V\|_{L^\infty})^2}{N-1} \frac{e^{\Gamma t} - 1}{\Gamma}$$

Here $\Gamma = 2 + 4\max(1, \mathrm{Lip}(\nabla(V))^2$.

Husimi transform and lower bound for $E_\hbar$

Wigner transform: if $\rho \in \mathcal{D}(L^2(\mathbf{R}^d))$ with integral kernel R

$$W_\hbar[\rho](x,\xi) := \frac{1}{(2\pi\hbar)^d} \int_{\mathbf{R}^d} e^{-i\xi\cdot y} R(x + \tfrac{1}{2}\hbar y, x - \tfrac{1}{2}\hbar y) dy$$

Husimi transform:

$$\tilde{W}_\hbar[\rho](x,\xi) := e^{\hbar\Delta_{x,\xi}/4} W_\hbar[\rho](x,\xi) \geq 0$$

Lemma 1: Let p be a probability density on $\mathbf{R}^d \times \mathbf{R}^d$ with finite 2nd order moment, and $\rho \in \mathcal{D}(\mathfrak{H})$. Then

$$E_\hbar(p,\rho)^2 \geq \mathrm{dist}_{\mathrm{MK},2}(p, \tilde{W}_\hbar[\rho])^2 - \tfrac{1}{2} d\hbar$$

Töplitz operators and upper bound for $E_\hbar$

•**Coherent state** with $q, p \in \mathbf{R}^d$:

$$|q + ip, \hbar\rangle = (\pi\hbar)^{-d/4} e^{-|x-q|^2/2\hbar} e^{ip\cdot x/\hbar}$$

•With the identification $z = q + ip \in \mathbf{C}^d$

$$\mathrm{OP}^T(\mu) := \frac{1}{(2\pi\hbar)^d} \int_{\mathbf{C}^d} |z, \hbar\rangle\langle z, \hbar|\mu(dz), \quad \mathrm{OP}^T(1) = I$$

Lemma 2: Let p be a probability density on $\mathbf{R}^d \times \mathbf{R}^d$ with finite 2nd order moment and μ a Borel probability measure on $\mathbf{R}^d \times \mathbf{R}^d$. Then

$$E_\hbar(p, \mathrm{OP}^T_\hbar((2\pi\hbar)^d \mu))^2 \leq \mathrm{dist}_{\mathrm{MK},2}(p, \mu)^2 + \tfrac{1}{2} d\hbar$$

Corollary Let $f^{in} \equiv f^{in}(x,\xi) \in L^1((|x|^2+|\xi|^2)dxd\xi)$ be a probability density. Let $\rho^{in}_{N,\hbar} = \mathrm{OP}^T_\hbar[(f^{in})^{\otimes N}]$. Let f and $\rho_{N,\hbar}$ be the solutions of the Vlasov equation and the von Neumann equation resp. with initial data f^{in} and $\rho^{in}_{N,\hbar}$. Then

$$\mathrm{dist}_{\mathrm{MK},2}(f(t), \tilde{W}_\hbar[\rho^{\mathbf{1}}_{N,\hbar}(t)])^2 \leq \tfrac{1}{2} d\hbar(e^{\Gamma t}+1) + \frac{(2\|\nabla V\|_{L^\infty})^2}{N-1}\frac{e^{\Gamma t}-1}{\Gamma}$$

with $\Gamma = 2 + 4\max(1, \mathrm{Lip}(\nabla(V))^2$.

Conclusion (in the form of an advertisement...)

We have presented a new method for deriving mean-field limits of large particle systems

•no hierarchies, no CK syndrome $\Rightarrow$ global in time

•Eulerian formulation $\Rightarrow$ also works for the quantum pbm

•measures convergence rate with MK-type distances $\Rightarrow$ uniform in $\hbar$

The most important message in this talk...

BEST WISHES TO PROFS. SONE AND AOKI

Figure: Profs. Y. Sone and M. Cannone (Kyoto 2013)

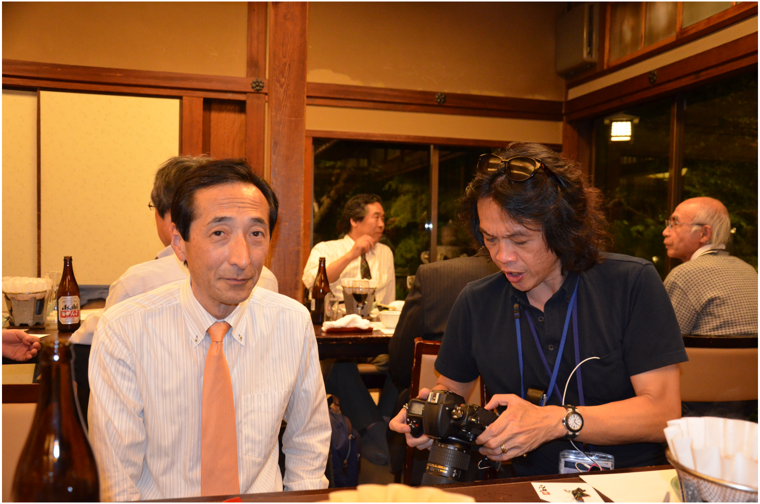

Figure: Profs K. Aoki and S.-H. Yu (Kyoto 2013)