Mean-field limits and emergent dynamics of the classical and quantum many-body systems
Lecture 2

François Golse

École polytechnique, CMLS

Summer school "Kinetic and fluid equations for collective dynamics"
France-Korea IRL in Mathematics, August 23rd-26th 2021

Mean Field and Semiclassical Limits of Quantum Systems

Schrödinger

$\downarrow$

$\hbar \to 0$ $\qquad$ $\searrow$

$\downarrow$

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

Lower horizontal arrow: Lecture 1 (Dobrushin's Theorem A)

FROM N-BODY SCHRÖDINGER TO VLASOV

F. G., T. Paul: Archive Rational Mech. Anal. **223** (2017) 57–94

See also
F. G., C. Mouhot, T. Paul: Commun. Math. Phys. **343** (2016), 165–205
P.-L. Lions, T. Paul: Revista Mat. Iberoam. **9** (1993), 553–618

Wave function $\psi \equiv \psi(t,x) \in L^2(\mathbf{R}^d;\mathbf{C}) =: \mathfrak{H}$ s.t. $\|\psi(t,\cdot)\|_{\mathfrak{H}} = 1$

Correspondence principle

Classical	Quantum
Position variable q	Operator on $\mathfrak{H}$: $\psi \mapsto x\psi(x)$
Potential $V(q)$	Operator on $\mathfrak{H}$: $\psi \mapsto V(x)\psi(x)$
Momentum variable p_j	Operator on $\mathfrak{H}$: $-i\hbar\partial_{x_j}$
Kinetic energy $\frac{1}{2m}\|p\|^2$	Operator on $\mathfrak{H}$: $-\frac{\hbar^2}{2m}\Delta_x$

Dirac's bra-ket notation $|\psi\rangle$ is the vector $\psi \in \mathfrak{H}$ while

$$\langle\psi| : \mathfrak{H} \ni \phi \mapsto \langle\psi|\phi\rangle := \int_{\mathbf{R}^d} \overline{\psi(x)}\phi(x)dx$$

With $\|\psi\|_{\mathfrak{H}} = 1$, the orthogonal projection on $\mathbf{C}\psi$ is denoted $|\psi\rangle\langle\psi|$

N-**particle setting** $\Psi \equiv \Psi(x_1,\ldots,x_N) \in \mathfrak{H}_N := L^2(\mathbf{R}^{dN}) \simeq \mathfrak{H}^{\otimes N}$

Let $0 \leq T = T^* \in \mathcal{L}(\mathfrak{H})$ and $(e_n)_{n\geq 1}$ complete orthonormal system

$$\mathrm{trace}_{\mathfrak{H}}(T) := \underbrace{\sum_{n\geq 1} \langle e_n|T|e_n\rangle}_{\text{independent of } (e_n)} \in [0, +\infty]$$

Density operators

$$\mathcal{D}(\mathfrak{H}) := \{R \in \mathcal{L}(\mathfrak{H}) \text{ s.t. } R = R^* \geq 0 \text{ and } \mathrm{trace}_{\mathfrak{H}}(R) = 1\}$$

Finite energy density operators

$$\mathcal{D}_2(\mathfrak{H}) := \{R \in \mathcal{D}(\mathfrak{H}) \text{ s.t. } \mathrm{trace}_{\mathfrak{H}}(R^{1/2}(|x|^2 - \Delta_x)R^{1/2}) < \infty\}$$

Example with (ψ_n) orthonormal system of wave functions

$$R = \sum_{n\geq 1} \lambda_n |\psi_n\rangle\langle\psi_n| \in \mathcal{D}(\mathfrak{H}) \iff \lambda_n \geq 0 \text{ and } \sum_{n\geq 1} \lambda_n = 1$$

Marginals of N-Particle Density Operators

Symmetric N-particle density operators

$$\mathcal{D}^s(\mathfrak{H}_N) := \{R_N \in \mathcal{D}(\mathfrak{H}_N) \text{ s.t. } U_\sigma R_N U_\sigma^* = R_N \text{ for all } \sigma \in \mathfrak{S}_N\}$$

with

$$U_\sigma \Psi_N(X_N) := \Psi_N(x_{\sigma^{-1}(1)}, \ldots, x_{\sigma^{-1}(N)})$$

Marginals If $r_N(X_N, Y_N)$ is an integral kernel of $R_N \in \mathcal{D}^s(\mathfrak{H}_N)$, its k-th marginal is $R_{N:k} \in \mathcal{D}^s(\mathfrak{H}_k)$ with integral kernel

$$r_k(X_k, Y_k) = \int_{\mathbf{R}^{d(N-k)}} r_k(X_k, Z_{k,N}, Y_k, Z_{k,N}) dZ_{k,N}$$

In particular

$$\operatorname{trace}_{\mathfrak{H}_N}(R_N) = \int_{\mathbf{R}^{dN}} r_N(Z_N, Z_N) dZ_N = \operatorname{trace}_{\mathfrak{H}_k}(R_{N:k}) = 1$$

Dynamics of N-Body Density Operators

Quantum Hamiltonian on $\mathfrak{H}_N = L^2(\mathbf{R}^{dN})$ with V satisfying (H1-2) of lecture 1 — i.e. $V(z) = V(-z) \in \mathbf{R}$ and $\nabla V \in W^{1,\infty}(\mathbf{R}^d)$

$$\mathcal{H}_N = \sum_{k=1}^{N} -\tfrac{1}{2}\hbar^2\Delta_{x_k} + \tfrac{1}{N}\sum_{1\le k<l\le N} V(x_k - x_l) = \mathcal{H}_N^*$$

Starting from $R_N^{in} \in \mathcal{D}(\mathfrak{H}_N)$, we define

$$R_N(t) = e^{-\frac{it\mathcal{H}_N}{\hbar}} R_N^{in} e^{+\frac{it\mathcal{H}_N}{\hbar}} \in \mathcal{D}(\mathfrak{H}_N)$$

Example

$$e^{-\frac{it\mathcal{H}_N}{\hbar}}(|\Psi_N^{in}\rangle\langle\Psi_N^{in}|)e^{+\frac{it\mathcal{H}_N}{\hbar}} = \left|e^{-\frac{it\mathcal{H}_N}{\hbar}}\Psi_N^{in}\right\rangle\left\langle e^{-\frac{it\mathcal{H}_N}{\hbar}}\Psi_N^{in}\right|$$

Coupling Quantum and Classical Densities

Following Dobrushin's 1979 derivation of Vlasov's equation, we seek to measure the difference between the quantum and the classical dynamics by a Monge-Kantorovich type distance.

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

$$(x,\xi) \mapsto Q(x,\xi) = Q(x,\xi)^* \in \mathcal{L}(\mathfrak{H}) \text{ s.t.} Q(x,\xi) \geq 0$$

$$\text{trace}(Q(x,\xi)) = f(x,\xi)\,, \quad \int_{\mathbf{R}^{2d}} Q(x,\xi)dxd\xi = R$$

The set of all couplings of the densities f and R is denoted $\mathcal{C}(f,R)$

Example: the map

$$f \otimes F : (x,\xi) \mapsto f(x,\xi)R \qquad \text{belongs to } \mathcal{C}(f,R)$$

Cost function compares classical and quantum "coordinates" — in other words, position and momentum

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

Definition for $f \in \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$ and $R \in \mathcal{D}_2(\mathfrak{H})$

$$E_\hbar(f,R) := \inf_{Q\in\mathcal{C}(f,R)} \sqrt{\int_{\mathbf{R}^{2d}} \operatorname{trace}(Q(x,\xi)^{\frac{1}{2}} c_\hbar(x,\xi) Q(x,\xi)^{\frac{1}{2}}) dx d\xi}$$

Triangle inequality [F.G.-T. Paul, JMPA **151** (2021), 257–311]
For all $f, g \in L^1 \cap \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$ and $R \in \mathcal{D}_2(\mathfrak{H})$

$$E_\hbar(f,R) \le \mathbf{W}_2(f,g) + E_\hbar(g,R)$$

Wigner and Husimi transforms of $R \in \mathcal{D}(\mathfrak{H})$

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

$$\widetilde{W_\hbar}[R] := e^{\hbar \Delta_{x,\xi}/4} W_\hbar[R] \geq 0$$

Thm A For $f \in L^1 \cap \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$ and $R \in \mathcal{D}_2(\mathfrak{H})$

$$E_\hbar(f,R)^2 \geq \max\left(d\hbar\,,\ \mathbf{W}_2(f, \widetilde{W_\hbar}[R])^2 - d\hbar\right)$$

Töplitz Quantization and Upper Bound for $E_\hbar$

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

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

Töplitz operator with symbol μ (positive Borel measure on $\mathbf{C}^d$):

$$\mathrm{OP}^T_\hbar(\mu) := \tfrac{1}{(2\pi\hbar)^d} \int_{\mathbf{C}^d} |z,\hbar\rangle\langle z,\hbar|\mu(dz) \geq 0$$

Thm B Let $f, \mu \in \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$ such that $f \in L^1(\mathbf{R}^d \times \mathbf{R}^d)$ is a probability density. Then $\mathrm{OP}^T_\hbar((2\pi\hbar)^d \mu) \in \mathcal{D}_2(\mathfrak{H})$ and

$$E_\hbar(f, \mathrm{OP}^T_\hbar((2\pi\hbar)^d\mu))^2 \leq \mathbf{W}_2(f,\mu)^2 + d\hbar$$

Thm C Let $R_{\hbar,N}(t) = e^{-\frac{it\mathcal{H}_N}{\hbar}} R^{in}_{\hbar,N} e^{+\frac{it\mathcal{H}_N}{\hbar}}$, where $R^{in}_{\hbar,N} \in \mathcal{D}^s_2(\mathfrak{H}_N)$, and let f be the solution of the Vlasov equation with initial data $f^{in} \in L^1 \cap \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$. Let $\Gamma := 2 + 4\max(1, \mathrm{Lip}(\nabla V))^2$.

(1) Then, for each $t \geq 0$ one has

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

(2) If moreover $R^{in}_{\hbar,N} = \mathrm{OP}^T_\hbar[(2\pi\hbar)^{dN}(f^{in})^{\otimes N}]$, then

$$\mathbf{W}_2(f(t), \widetilde{W}_\hbar[R_{\hbar,N:1}(t)])^2 \leq d\hbar(1 + e^{\Gamma t}) + \frac{(2\|\nabla V\|_{L^\infty})^2}{N-1} \frac{e^{\Gamma t} - 1}{\Gamma}$$

FROM N-BODY SCHRÖDINGER TO EULER-POISSON

F. G. - T. Paul: Comm. on Pure and Appl. Math. (2022) to appear

See also S. Serfaty: Duke Math. J. **169** (2020), 2887–2935.

From Quantum Coulomb Gas to Pressureless Euler-Poisson

Quantum Hamiltonian on $L^2(\mathbf{R}^{3N})$ (by Kato's Thm $\mathcal{H}_N = \mathcal{H}_N^*$)

$$\mathcal{H}_N = \sum_{k=1}^{N} -\tfrac{1}{2}\hbar^2 \Delta_{x_k} + \tfrac{1}{N} \sum_{1\le k<l\le N} \tfrac{1}{|x_k - x_l|}$$

***N*-body wave function**

$$\Psi_{\hbar,N}(t,\cdot) = e^{-it\mathcal{H}_N/\hbar}(\psi_\hbar^{in})^{\otimes N} \quad \text{with } (\psi_\hbar^{in})^{\otimes N}(X_N) = \prod_{k=1}^{N} \psi_\hbar^{in}(x_k)$$

Assume that the **Wigner function of the initial 1-particle state**

$$W_\hbar[|\psi_\hbar^{in}\rangle\langle\psi_\hbar^{in}|](x,\xi) \to \rho^{in}(x)\delta(\xi - u^{in}(x))$$

Satisfied by **WKB initial data** with $\|a^{in}\|_{L^2} = 1$ and $S^{in} \in W^{1,\infty}(\mathbf{R}^3)$

$$\psi_\hbar^{in}(x) = a^{in}(x)e^{iS^{in}(x)/\hbar} \text{ with } \rho^{in}(x) = a^{in}(x)^2 \text{ and } u^{in} = \nabla S^{in}$$

Unknown $\rho(t,x)\geq 0$ (density) and $u(t,x)\in\mathbf{R}^d$ (velocity field)

$$\begin{cases}\partial_t\rho+\operatorname{div}_x(\rho u)=0\,, & \rho\big|_{t=0}=\rho^{in}\\ \partial_t u+u\cdot\nabla_x u=-\nabla_x\frac{1}{|x|}\star_x\rho\,, & u\big|_{t=0}=u^{in}\end{cases}$$

If (ρ,u) is a classical solution of the pressureless Euler-Poisson system, the monokinetic distribution function

$$f(t,x,\xi):=\rho(t,x)\delta(\xi-u(t,x))$$

is a solution of the Vlasov-Poisson system

$$\begin{cases}\partial_t f+\xi\cdot\nabla_x f-\nabla_x V_f(t,x)\cdot\nabla_\xi f=0\\ -\Delta_x V_f(t,x)=4\pi\int_{\mathbf{R}^3}f(t,x,\xi)d\xi\end{cases}$$

Let $u^{in} \in L^\infty(\mathbf{R}^3)$ be s.t. $\nabla_x u^{in} \in H^{2m}(\mathbf{R}^3)$, and $\rho^{in} \in H^{2m}(\mathbf{R}^3)$ s.t.

$$\rho^{in}(x) \geq 0 \text{ for a.e. } x \in \mathbf{R}^3, \quad \text{and} \quad \int_{\mathbf{R}^3} \rho^{in}(y)dy = 1$$

(1) There exists $T \equiv T[\|\rho^{in}\|_{H^{2m}(\mathbf{R}^3)} + \|\nabla_x u^{in}\|_{H^{2m}(\mathbf{R}^3)}] > 0$, and a unique solution (ρ, u) of the Euler-Poisson system s.t.

$$u \in L^\infty([0,T] \times \mathbf{R}^3) \quad \text{while } \rho \text{ and } \nabla_x u \in C([0,T], H^{2m}(\mathbf{R}^3))$$

(2) Besides, for all $t \in [0,T]$, one has

$$\rho(t,x) \geq 0 \text{ for a.e. } x \in \mathbf{R}^3, \quad \text{and} \quad \int_{\mathbf{R}^3} \rho(t,y)dy = 1$$

Thm [F.G.-T. Paul 2022]
Let $\rho^{in} \in H^4(\mathbf{R}^3) \cap \mathcal{P}(\mathbf{R}^3)$ and $u^{in} \in L^\infty(\mathbf{R}^3)^3$ s.t. $\nabla u^{in} \in H^4(\mathbf{R}^3)^3$.
Let (ρ, u) be the (classical) solution on $[0, T] \times \mathbf{R}^3$ for some $T > 0$ of the pressureless Euler-Poisson system initial data (ρ^{in}, u^{in}).

Let $\Psi^{in}_{\hbar,N} = (\psi^{in}_\hbar)^{\otimes N}$, with $\|\psi_\hbar\|_{L^2} = 1$ satisfying

$$\sup_{0<\hbar<1} \|\hbar^2 \Delta_x \psi^{in}_\hbar\|_{L^2(\mathbf{R}^3)} < \infty \,, \qquad \lim_{\hbar\to 0^+} \||i\hbar\nabla_x + u^{in}|^2 \psi^{in}_\hbar\|_{L^2(\mathbf{R}^3)} = 0$$

$$\lim_{\hbar\to 0} \iint_{\mathbf{R}^3\times\mathbf{R}^3} \frac{(|\psi^{in}_\hbar(x)|^2 - \rho^{in}(x))(|\psi^{in}_\hbar(y)|^2 - \rho^{in}(y))}{|x-y|} dxdy = 0$$

Remark test these assumptions on WKB initial states of the form

$$\psi^{in}(x) = a^{in}(x) \exp\left(\frac{iS^{in}(x)}{\hbar}\right) \,, \qquad |a^{in}|^2 = \rho^{in} \,, \quad u^{in} = \nabla S^{in}$$

Let $\mathcal{H}_N :=$ N-body Hamiltonian with Coulomb potential and set

$$\Psi_{\hbar,N}(t) := e^{\frac{it\mathcal{H}_N}{\hbar}} \Psi^{in}_{\hbar,N}$$

Then, in the limit as $\hbar + \frac{1}{N} \to 0$, one has

$$\int_{\mathbf{R}^{3(N-1)}} |\Psi_{\hbar,N}(t,\cdot,X_{2,N})|^2 dX_{2,N} \to \rho(t,\cdot)$$

$$\hbar \int_{\mathbf{R}^{3(N-1)}} \Im \left(\overline{\Psi_{\hbar,N}} \nabla_{x_1} \Psi_{\hbar,N} \right) (t,\cdot,X_{2,N}) dX_{2,N} \to \rho u(t,\cdot)$$

for the narrow topology of Radon measures on $\mathbf{R}^3$, with the notation

$$X_{2,N} = (x_2, \ldots, x_N)$$

With the notation $J_1 A = A \otimes \overbrace{I \otimes \ldots \otimes I}^{N-1 \text{ terms}}$, define

$$\mathcal{E}[\Psi_{\hbar,N},\rho,u](t) := \langle \Psi_{\hbar,N}(t) | J_1 |\hbar D_x - u(t,\cdot)|^2 + F[X_N,\rho(t,\cdot)] | \Psi_{\hbar,N}(t) \rangle$$

where $D := -i\nabla$ and

$$F[X_N,\rho] = \iint_{x\neq y} \frac{(\mu_{X_N}-\rho)(dx)(\mu_{X_N}-\rho)(dy)}{|x-y|}$$

Denoting $\Sigma := \nabla_x u + (\nabla_x u)^T$, rather long computations show that

$$\frac{d\mathcal{E}}{dt} = -\langle \Psi_{\hbar,N} | J_1((\hbar D_x - u)^T \Sigma (\hbar D_x - u)) + G[X_N,\rho,u] | \Psi_{\hbar,N} \rangle$$

with

$$G[X_N,\rho,u] := -\iint_{x\neq y} \frac{(u(x)-u(y))\cdot(x-y)}{|x-y|^3} (\mu_{X_N}-\rho)(dx)(\mu_{X_N}-\rho)(dy)$$

Serfaty's Inequality (DMJ2020)

For all $\rho \in L^\infty(\mathbf{R}^3)$, all $u \in W^{1,\infty}(\mathbf{R}^3)^3$ and all $X_N \in \mathbf{R}^{3N}$, set

$$\begin{cases} F[X_N,\rho] := \iint_{x\neq y} \dfrac{(\mu_{X_N}-\rho)(dx)(\mu_{X_N}-\rho)(dy)}{|x-y|} \\ G[X_N,\rho,u] := \iint_{x\neq y} \frac{(u(x)-u(y))\cdot(x-y)}{|x-y|^3}(\mu_{X_N}-\rho)(dx)(\mu_{X_N}-\rho)(dy) \end{cases}$$

There exists $C>2$ such that, for all $\rho \in L^\infty(\mathbf{R}^3)$, all $u \in W^{1,\infty}(\mathbf{R}^3)^3$ and a.e. $X_N \in \mathbf{R}^{3N}$

$$|G[X_N,\rho,u]| \le C\|\nabla u\|_{L^\infty} F_N[X_N,\rho] + \frac{C}{N^{1/3}}(1+\|\rho\|_{L^\infty})(1+\|u\|_{W^{1,\infty}})$$

Besides, there exists $C'>0$ such that

$$F[X_N,\rho] \ge -\frac{C'}{N^{2/3}}(1+\|\rho\|_{L^\infty(\mathbf{R}^3)})$$

By Gronwall's and Serfaty's inequalities, one arrives at the bound

$$
\begin{aligned}
0 \leq \mathcal{E}[\Psi_{\hbar,N},\rho,u](t) + \frac{C'}{N^{2/3}}(1+\|\rho\|_{L^\infty(\mathbf{R}^3)}) \\
\leq e^{CT\|\nabla u\|_{L^\infty}} \left(\underbrace{\mathcal{E}[\Psi_{\hbar,N},\rho,u](0)}_{\to 0} + \frac{C'}{N^{2/3}}(1+\|\rho\|_{L^\infty(\mathbf{R}^3)}) \right) \\
+ Te^{CT\|\nabla u\|_{L^\infty}} \frac{C}{N^{1/3}}(1+\|\rho\|_{L^\infty})(1+\|u\|_{W^{1,\infty}}) \\
+ Te^{CT\|\nabla u\|_{L^\infty}} \tfrac{1}{2}\hbar^2 \|\Delta_x \operatorname{div}_x u\|_{L^\infty}
\end{aligned}
$$

Conclusions/Perspectives

(1) Uniformity of the mean-field limit (for classical and quantum systems) as $t \to \infty$?

(2) Can one extend the techniques presented in this lectures to treat the case of non monokinetic distribution functions AND of a singular repulsive potential (Coulomb, or screened Coulomb)?