From N-Body Schrödinger to Vlasov

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Motivation

The Vlasov equation with Lipschitz continuous interaction force has been derived from the N-body problem of classical mechanics in the large N, small coupling constant limit (Neunzert-Wick 1973, Braun-Hepp 1977, Dobrushin 1979)

Problem: Is it possible to derive the Vlasov equation from the quantum N-body problem by a joint semiclassical ($\hbar \to 0$) and mean field ($N \to \infty$) limit?

[Graffi-Martinez-Pulvirenti M3AS 2003]

[Pezzotti-Pulvirenti Ann IHP 2009]

[Benedikter-Porta-Saffirio-Schlein arXiv:1502.04230]

The diagram

Schrödinger	$\overset{N\to\infty}{\longrightarrow}$	**Hartree**
$\downarrow$		$\downarrow$
$\hbar \to 0$	$\searrow$	$\hbar \to 0$
$\downarrow$		$\downarrow$
Liouville	$\overset{N\to\infty}{\longrightarrow}$	**Vlasov**

Uniformity as $\hbar \to 0$ of the upper horizontal (mean-field) limit:
[FG-Mouhot-Paul CMP **343** (2016), 165–205]

QUANTUM VS CLASSICAL DYNAMICS

Heisenberg/Von Neumann equation

$$i\hbar\partial_t\rho = [\mathcal{H}, \rho]$$

where $\mathcal{H} = \mathcal{H}^* =$Hamiltonian, while $[A, B] := AB - BA$ and

$$\rho = \rho^* \geq 0\,, \quad \operatorname{Tr}_{\mathfrak{H}} \rho = 1 \Leftrightarrow \rho \in \mathcal{D}(\mathfrak{H}) \text{ with } \mathfrak{H} := L^2(\mathbf{R}^d)$$

Liouville equation

$$\partial_t f + \{H, f\} = 0 \qquad H \equiv H(x, \xi) \in \mathbf{R}$$

$$f \equiv f(t, x, \xi) \geq 0\,, \quad \iint_{\mathbf{R}^d\times\mathbf{R}^d} f(t, x, \xi)dxd\xi = 1$$

with

$$\{\mathcal{H}, f\} := \nabla_\xi H \cdot \nabla_x f - \nabla_x H \cdot \nabla_\xi f$$

Comparing quantum and classical densities

WKB ansatz, superpositions of coherent states driven by the classical dynamics produce (local in the case of WKB) **approximate** solutions of the Schrödinger equation, i.e. with source terms

Wigner transform of $\rho \in \mathcal{D}(\mathfrak{H})$

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

satisfies a transport-like equation but is in general not nonnegative

Husimi transform

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

satisfies a transport-like equation involving the complex extension of the potential

Coupling quantum and classical densities

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

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

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

$$\operatorname{Tr}(Q(x,\xi)) = p(x,\xi)\,, \quad \iint_{\mathbf{R}^d \times \mathbf{R}^d} Q(x,\xi) dx d\xi = \rho$$

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

Pseudo-distance between quantum and classical densities

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

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

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 $\mathcal{P}_p(\mathbf{R}^d)$

Töplitz quantization

•**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 $z = q + ip \in \mathbf{C}^d$

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

•Fundamental properties:

$$\mu \geq 0 \Rightarrow \mathrm{OP}^T(\mu) \geq 0 , \quad \mathrm{Tr}(\mathrm{OP}^T(\mu)) = \frac{1}{(2\pi\hbar)^d} \int_{\mathbf{C}^d} \mu(dz)$$

•Important formulas:

$$W_\hbar[\mathrm{OP}^T(\mu)] = \frac{1}{(2\pi\hbar)^d} e^{\hbar\Delta_{q,p}/4} \mu , \quad \tilde{W}_\hbar[\mathrm{OP}^T(\mu)] = \frac{1}{(2\pi\hbar)^d} e^{\hbar\Delta_{q,p}/2} \mu$$

Basic properties of the pseudo-distance $E_\hbar$

Thm A Let $p =$ probability density on $\mathbf{R}^d \times \mathbf{R}^d$ s.t.

$$\iint_{\mathbf{R}^d \times \mathbf{R}^d} (|x|^2 + |\xi|^2) p(x,\xi) dx d\xi < \infty$$

(1) For each $\rho \in \mathcal{D}(\mathfrak{H})$ one has $E_\hbar(p,\rho) \geq \frac{1}{2} d\hbar$
(2) For each $\mu \in \mathcal{P}(\mathbf{R}^d \times \mathbf{R}^d)$ one has

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

(3) For each $\rho \in \mathcal{D}(\mathfrak{H})$, one has

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

(4) If $\rho_\hbar \in \mathcal{D}(\mathfrak{H})$ and $W_\hbar[\rho_\hbar] \to \mu$ in $\mathcal{S}'$, then $\mu \in \mathcal{P}(\mathbf{R}^d \times \mathbf{R}^d)$ and

$$\varliminf_{\hbar \to 0} E_\hbar(p,\rho) \geq \mathrm{dist}_{\mathrm{MK},2}(p,\mu)$$

QUANTITATIVE CONVERGENCE RATE

Hartree vs Vlasov equations

Hartree equation for density matrices

$$\partial_t \rho_\hbar(t) = -\frac{i}{\hbar}[\mathcal{H}[\rho_\hbar(t)], \rho_\hbar(t)] = 0$$

with

$$\mathcal{H}[\rho] = -\tfrac{1}{2}\hbar^2\Delta + \int_{\mathbf{R}^d} V(x-z)\rho(z,z)dz$$

Vlasov equation for $f \equiv f(t,x,\xi)$ probability density

$$\partial_t f = -\{H_f, f\} = -\xi \cdot \nabla_x f + \nabla_x V_f \cdot \nabla_\xi f$$

with

$$V_f(t,x) = \iint_{\mathbf{R}^d} V(x-z)\rho[f](t,z)dz\,, \qquad \text{where } \rho[f] := \int_{\mathbf{R}^d} f d\xi$$

Thm B Let V be an even, real-valued function of class $C^{1,1}$ on $\mathbf{R}^d$
Let $f^{in} \equiv f^{in}(x,\xi) \in L^1((|x|^2+|\xi|^2)dxd\xi)$ be a probability density on $\mathbf{R}^d \times \mathbf{R}^d$, and let f be the solution of the Vlasov equation with initial data f^{in}. Let $\rho_\hbar$ be a solution of the Hartree equation with initial data $\rho_\hbar^{in} \in \mathcal{D}(\mathfrak{H})$. Then

$$E_\hbar(f(t),\rho_\hbar(t))^2 \le e^{\Lambda t} E_\hbar(f^{in},\rho_\hbar^{in})^2$$

with $\Lambda := 1 + 4\max(1, \mathrm{Lip}(\nabla V))$. If $\rho_\hbar^{in} = \mathrm{OP}_\hbar^T((2\pi\hbar)^d \mu^{in})$, then

$$\mathrm{dist}_{\mathrm{MK},2}(f(t), \tilde{W}_\hbar[\rho_\hbar(t)])^2 \le e^{\Lambda t}(\mathrm{dist}_{\mathrm{MK},2}(f^{in},\mu^{in})^2 + \tfrac{1}{2}d\hbar) + \tfrac{1}{2}d\hbar$$

N-body von Neumann equation

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

where $\rho_{N,\hbar} \in \mathcal{D}(\mathfrak{H}_N)$, with $\mathfrak{H}_N = \mathfrak{H}^{\otimes N} = L^2((\mathbf{R}^d)^N)$ and

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

N-body Liouville equation

$$\partial_t f_N = -\{H_N, f_N\} = -\sum_{j=1}^{N} \xi_j \cdot \nabla_{x_j} f_N + \frac{1}{N} \sum_{j,k=1}^{N} \nabla V(x_j - x_k) \cdot \nabla_{\xi_j} f_N$$

Indistinguishable particles and symmetries

Notation

$$X_N := (x_1, \dots, x_N), \quad \Xi_N := (\xi_1, \dots, \xi_N)$$
$$\sigma \cdot X_N := (x_{\sigma(1)}, \dots, x_{\sigma(N)}) \quad \text{for } \sigma \in \mathfrak{S}_N$$

Classical N-body symmetric probability density: for all $t \geq 0$

$$f_N(t, \sigma \cdot X_N, \sigma \cdot \Xi_N) = f_N(t, X_N, \xi_N) \quad \text{for all } \sigma \in \mathfrak{S}_N$$

Quantum symmetric N-body density: for all $t \geq 0$

$$U_\sigma \rho_{N,\hbar}(t) U_\sigma^* = \rho_{N,\hbar}(t)$$

where U_σ is the operator on $\mathfrak{H}_N$ defined by

$$U_\sigma \psi(X_N) = \psi(\sigma \cdot X_N)$$

Symmetric densities and $k-$particle marginals

For $\rho_N \in \mathcal{D}^s(\mathfrak{H}_N)$, its k-particle marginal is $\rho_N^{\mathbf{k}} \in \mathcal{D}^s(\mathfrak{H}_k)$ such that

$$\mathrm{Tr}_{\mathfrak{H}_k}(A\rho_N^{\mathbf{k}}) = \mathrm{Tr}_{\mathfrak{H}_N}((A \otimes I_{\mathfrak{H}_{N-k}})\rho_N)$$

for each $A \in \mathcal{L}(\mathfrak{H}_k)$

Symmetric classical density $f_N \equiv f_N(X_N, \Xi_N)$; its k-particle marginal:

$$f_N^{\mathbf{k}}(X_k, \Xi_k) = \int f_N(X_N, \Xi_N) dx_{k+1} d\xi_{k+1} \dots dx_N d\xi_N$$

Thm C Let V be an even, real-valued function of class $C^{1,1}$ on $\mathbf{R}^d$. Let $\rho^{in}_{N,\hbar} \in \mathcal{D}^s(\mathfrak{H}_N)$ and F^{in}_N be a symmetric probability density on $(\mathbf{R}^d \times \mathbf{R}^d)^N$ in $L^1((|X_N|^2 + |\Xi_N|^2)dX_N d\Xi_N)$. Let $\rho_{N,\hbar}$ and F_N be the solutions of the von Neumann and the Liouville equations resp. with initial data $\rho^{in}_{N,\hbar}$ and F^{in}_N.

Setting $\Lambda = 1 + 4\max(1, \mathrm{Lip}(\nabla(V))^2$, one has

$$E_\hbar(F^{\mathbf{1}}(t), \rho^{\mathbf{1}}_{N,\hbar}(t))^2 \leq \frac{1}{N} E_\hbar(F^{in}_N, \rho^{in}_{N,\hbar})^2 e^{\Lambda t}$$

If $\rho^{in}_{N,\hbar} = \mathrm{OP}^T_\hbar[(2\pi\hbar)^{Nd}\mu^{in}]$, then

$$\begin{aligned} &\mathrm{dist}_{\mathrm{MK},2}(F^{\mathbf{1}}(t), \tilde{W}_\hbar[\rho^{\mathbf{1}}_{N,\hbar}(t)])^2 \\ &\leq \left(\frac{1}{N}\mathrm{dist}_{\mathrm{MK},2}((F^{in}_N, \tilde{W}_\hbar[\rho^{in}_{N,\hbar}]) + \tfrac{1}{2}d\hbar\right) e^{\Lambda t} + \tfrac{1}{2}d\hbar \end{aligned}$$

Thm D Let $f^{in} \equiv f^{in}(x,\xi) \in L^1((|x|^2+|\xi|^2)dxd\xi)$ be a probability density on $\mathbf{R}^d \times \mathbf{R}^d$, an $\rho^{in}_{N,\hbar} \in \mathcal{D}^s(\mathfrak{H}_N)$. 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 $\rho^{in}_{N,\hbar}$.

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

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

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

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

SKETCH OF THE PROOFS

Dynamics of couplings

If F_N is a symmetric classical N-particle density and $\rho_N \in \mathcal{D}^s(\mathfrak{H}_N)$, a coupling $Q_N \in \mathcal{C}(F_N, \rho_N)$ is symmetric, denoted $Q_N \in \mathcal{C}^s(F_N, \rho_N)$

$$U_\sigma Q_N(\sigma \cdot X_N, \sigma \cdot \Xi_N) U_\sigma^* = Q_N(X_N, \Xi_N) \quad \text{for all } \sigma \in \mathfrak{S}_N$$

Let $Q_{N,\hbar}^{in} \in \mathcal{C}^s((f^{in})^{\otimes N}, \rho_{N,\hbar}^{in})$; solve

$$\partial_t Q_{N,\hbar} + \left\{ \sum_{j=1}^N H_f(x_j, \xi_j), Q_{N,\hbar} \right\} + \frac{i}{\hbar}[\mathcal{H}_N, Q_{N,\hbar}] = 0$$

with $Q_{N,\hbar}\big|_{t=0} = Q_{N,\hbar}^{in}$ and

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

$$H_f(x,\xi) := \tfrac{1}{2}|\xi|^2 + \iint_{\mathbf{R}^d \times \mathbf{R}^d} V(x-z) f(t,z,\zeta)\, dz d\zeta$$

The functional $D(t)$

Lemma For each $t \geq 0$, one has

$$Q_{N,\hbar}(t) \in \mathcal{C}^s(f(t)^{\otimes N}, \rho_{N,\hbar}(t))$$

where f is the solution of the Vlasov equation and $\rho_{N,\hbar}$ is the solution of the N-body von Neumann equation

Define

$$D(t) := \frac{1}{N} \iint_{(\mathbf{R}^d \times \mathbf{R}^d)^N} \sum_{k=1}^{N} \mathrm{Tr}_{\mathfrak{H}_N}(c_\hbar(x_j, \xi_j, y_j, \nabla_{y_j}) Q_{N,\hbar}(t)) dX_N d\Xi_N$$

$$= \iint_{(\mathbf{R}^d \times \mathbf{R}^d)^N} (c_\hbar(x_1, \xi_1, y_1, \nabla_{y_1}) Q_{N,\hbar}(t)) dX_N d\Xi_N$$

$$= \iint_{(\mathbf{R}^d \times \mathbf{R}^d)} \mathrm{Tr}_{\mathfrak{H}}(c_\hbar(x_1, \xi_1, y_1, \nabla_{y_1}) Q^{\mathbf{1}}_{N,\hbar}(t)) dx_1 d\xi_1$$

$$\geq E_\hbar(f(t), \rho^{\mathbf{1}}_{N,\hbar}(t))$$

The evolution of D

Multiply both sides of the equation for $Q_{N,\hbar}$ and "integrate by parts":

$$\dot{D} = \iint \mathrm{Tr}_{\mathfrak{H}}(\{H_f(x_1,\xi_1), c_\hbar(x_1,\xi_1,y_1,\nabla y_1)\} Q^{\mathbf{1}}_{N,\hbar}) dx_1 d\xi_1$$
$$-\tfrac{1}{2} i\hbar \iint \mathrm{Tr}_{\mathfrak{H}}([\Delta_{y_1}, c_\hbar(x_1,\xi_1,y_1,\nabla y_1)] Q^{\mathbf{1}}_{N,\hbar}) dx_1 d\xi_1$$
$$+\frac{i}{\hbar} \iint \mathrm{Tr}_{\mathfrak{H}_2}([\tfrac{N-1}{N} V(y_1 - y_2), c_\hbar(x_1,\xi_1,y_1,\nabla y_1)]) Q^{\mathbf{2}}_{N,\hbar}) dX_2 d\Xi_2$$

since $Q_{N,\hbar}$ is a **symmetric** coupling

In other words

$$\begin{aligned}\dot{D} \le D - \tfrac{N-1}{2N} \int \mathrm{Tr}_{\mathfrak{H}_2}(Q^2_{N,\hbar}(\xi_1 + i\hbar\nabla_{y_1}) \vee \mathcal{W}(X_2, Y_2)) dX_2 d\Xi_2 \\ -\tfrac{1}{2} \int \mathrm{Tr}_{\mathfrak{H}_2}(Q^2_{N,\hbar}(\xi_1 + i\hbar\nabla_{y_1}) \vee \mathcal{V}(t, x_1, x_2)) dX_2 d\Xi_2 \\ \le D - \tfrac{N-1}{2N} \int \mathrm{Tr}_{\mathfrak{H}_2}(Q^2_{N,\hbar}(\xi_1 + i\hbar\nabla_{y_1}) \vee \mathcal{W}(X_2, Y_2)) dX_2 d\Xi_2 \\ -\tfrac{1}{2} \int \mathrm{Tr}_{\mathfrak{H}_2}(Q_{N,\hbar}(\xi_1 + i\hbar\nabla_{y_1}) \vee \tfrac{1}{N-1} \sum_{k=2}^{N} \mathcal{V}(t, x_1, x_k)) dX_N d\Xi_N\end{aligned}$$

with $a \vee b := ab + ba$ is the anticommutator while

$$\begin{aligned}\mathcal{V}(t, x_1, x_2) &:= \nabla V \star \rho_f(t, x_1) - \tfrac{N-1}{N} \nabla V(x_1, x_2) \\ \mathcal{W}(X_2, Y_2) &:= \nabla V(x_1 - x_2) - \nabla V(y_1 - y_2)\end{aligned}$$

Stability vs consistency

$$
\begin{aligned}
\dot{D} \leq 3D + \tfrac{N-1}{2N} \int \mathrm{Tr}_{\mathfrak{H}_2}(Q^{\mathbf{2}}_{N,\hbar} |\mathcal{W}(X_2, Y_2)|^2) dX_2 d\Xi_2 \\
+ \tfrac{1}{2} \int \left| \tfrac{1}{N-1} \sum_{k=2}^{N} \mathcal{V}(t, x_1, x_k) \right|^2 \rho_f^{\otimes N} dX_N \\
\leq 3D + \tfrac{N-1}{2N} L^2 \int \mathrm{Tr}_{\mathfrak{H}_2}(Q^{\mathbf{2}}_{N,\hbar} |X_2 - Y_2|^2) dX_2 d\Xi_2 \\
+ \tfrac{1}{2} \int \left| \tfrac{1}{N-1} \sum_{k=2}^{N} \mathcal{V}(t, x_1, x_k) \right|^2 \rho_f^{\otimes N} dX_N \\
\leq (3 + 2L^2) D + \tfrac{1}{2} \int \left| \tfrac{1}{N-1} \sum_{k=2}^{N} \mathcal{V}(t, x_1, x_k) \right|^2 \rho_f^{\otimes N} dX_N
\end{aligned}
$$

Summarizing...

•The stability part of the analysis (leading to the exponential amplification by Gronwall's inequality) is seen at the level of the 1st equation in the BBGKY hierarchy

•The consistency part of the analysis requires distributing the interaction term $\mathcal{V}$ on **all** the particles, and because the $\mathcal{V}$ term depends on the X_N variables only, and the X_N marginal of $Q_{N,\hbar}$ is the N-fold tensor power of the Vlasov solution, one concludes by LLN

•Because the cost function in D is a **sum** of quantities depending on x_j, y_j, ξ_j, there is a "**localization in degree**" effect in the BBGKY hierarchy: no Cauchy-Kovalevska effect when estimating D