On the Mean-Field and Semiclassical Limits of the N-Body Schrödinger Equation

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Motivation

$$
\begin{tikzcd}[row sep=huge, column sep=huge]
\boxed{\textbf{Schrödinger}} \arrow[r, "N\to\infty"] \arrow[d, "\hbar \to 0"] \arrow[dr, red] & \boxed{\textbf{Hartree}} \arrow[d, "\hbar \to 0"] \\
\boxed{\textbf{Liouville}} \arrow[r, "N\to\infty"] & \boxed{\textbf{Vlasov}}
\end{tikzcd}
$$

Problem: To derive Vlasov equation from quantum N-body problem by a joint semiclassical ($\hbar \to 0$) + mean field ($N \to \infty$) limit

[Graffi-Martinez-Pulvirenti M3AS 2003]

[Pezzotti-Pulvirenti Ann IHP 2009]

$\boxed{\text{DISTANCE BETWEEN CLASSICAL AND QUANTUM STATES}}$

Quantum density operator

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

Classical density=probability density on $\mathbf{R}^d \times \mathbf{R}^d$

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

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

not nonnegative in general

Husimi transform

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

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 (or Vasershtein) type distance

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

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

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

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

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

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

Pseudo-distance "à la" Monge-Kantorovich (with exponent 2)

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

Töplitz quantization

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

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

•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

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

(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

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

PSEUDO-DISTANCE AND DYNAMICS

Vlasov and N-body von Neumann equations

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

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

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

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

Notation for $\sigma \in \mathfrak{S}_N$

$$X_N := (x_1, \ldots, x_N)\,, \quad \sigma \cdot X_N := (x_{\sigma(1)}, \ldots, x_{\sigma(N)})$$

Quantum symmetric N**-body density** for all $\sigma \in \mathfrak{S}_N$

$$U_\sigma \rho_N U_\sigma^* = \rho_N\,, \qquad \text{where } U_\sigma \psi(X_N) = \psi(\sigma \cdot X_N)$$

Notation $\rho_N \in \mathcal{D}^s(\mathfrak{H}_N)$

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

$$\mathrm{tr}_{\mathfrak{H}_k}(A\rho_N^{\mathbf{k}}) = \mathrm{tr}_{\mathfrak{H}_N}((A \otimes I_{\mathfrak{H}_{N-k}})\rho_N) \text{ for all } A \in \mathcal{L}(\mathfrak{H}_k)$$

Thm B 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 $\rho^{in}_{N,\hbar}$.

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

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

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

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

Amplification In fact, one has a quantitative statement on propagation of chaos for this problem: for each **fixed** $n \geq 1$ and all $N > n$

$$\frac{1}{n}\mathrm{dist}_{\mathrm{MK},2}(f(t)^{\otimes n}, \widetilde{W_\hbar}[\rho^{\mathbf{n}}_{\hbar,N}(t)])^2 \leq \tfrac{1}{n}E_\hbar(f(t)^{\otimes n}, \rho^{\mathbf{n}}_{\hbar,N}(t))$$
$$\leq \frac{1}{N}E_\hbar((f^{in})^{\otimes n}, \rho^{in}_{\hbar,N})e^{\Gamma t} + \frac{(2\|\nabla V\|_{L^\infty})^2}{N-1}\frac{e^{\Gamma t}-1}{\Gamma}$$

This follows from
(1) the symmetry of the classical and quantum densitie is, and
(2) the **structure of the cost** which is the sum of costs in each variable

$\boxed{\text{SOME IDEAS FOR THE PROOF}}$

Dynamics of couplings

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

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

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

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

$$D(t) := \frac{1}{N} \iint_{(\mathbf{R}^d \times \mathbf{R}^d)^N} \sum_{k=1}^{N} \operatorname{tr}_{\mathfrak{H}_N}(c_\hbar(x_j, \xi_j, y_j, \nabla_{y_j}) Q_{N,\hbar}(t)) dX_N d\Xi_N$$
$$\geq \frac{1}{N} E_\hbar(f(t)^{\otimes N}, \rho_{N,\hbar}(t))$$

The evolution of D

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

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

provided that $Q_{N,\hbar}$ is a **symmetric** coupling (propagated by the dynamics of couplings).

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

Other approaches

•Same methods gives (1) a quantitative convergence rate for the semiclassical limit Hartree $\to$ Vlasov, and (2) a uniform in N quantitative convergence rate for the semiclassical limit of the N-body von Neumann equation to the N-body Liouville equation

•Uniform in $\hbar \to 0$ convergence rate for the Hartree (mean-field) limit of the quantum N-body problem
[F.G., C. Mouhot, T. Paul, CMP, to appear]

•Work in preparation with T. Paul and M. Pulvirenti

Final remarks/open questions

Advantage/Shortcoming of the pseudo-distance $E_\hbar$ between classical and quantum densities (or of the pseudo-distance between quantum densities considered in FG-Mouhot-Paul) is not a distance, but is a distance mod. $O(\hbar)$

Can one use instead a real distance between quantum objects (in the style of Connes' distance in NC geometry, or Biane-Voiculescu (free probabilities), or Carlen-Maas) to obtain a uniform in $\hbar$ convergence rate for the quantum mean field limit?

Is there a Benamou-Brenier variational formulation for the pseudo-distance $E_\hbar$?