Empirical Measures and Quantum Dynamics

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N-body Schrödinger eqn. Unknown $\Psi_N \equiv \Psi_N(t, x_1, \ldots, x_N) \in \mathbf{C}$

$$i\hbar\partial_t \Psi_N = \mathcal{H}_N \Psi_N \,, \qquad \mathcal{H}_N := \sum_{j=1}^{N} -\tfrac{\hbar^2}{2m}\Delta_{x_N} + \tfrac{1}{N} \sum_{1\le j<k\le N} V(x_j - x_k)$$

Hartree Unknown $\psi \equiv \psi(t,x) \in \mathbf{C}$

$$i\hbar\partial_t \psi = \mathbf{H}_\rho \psi \,, \qquad \mathbf{H}_\rho := -\tfrac{\hbar^2}{2m}\Delta_x + V \star_x \rho(t,\cdot)\,, \quad \rho = |\psi|^2$$

Mean-field limit

$$\int_{(\mathbf{R}^d)^{N-1}} \Psi_N(t, x, z_2, \ldots, z_N)\overline{\Psi_N(t, y, z_2, \ldots, z_N)} dz_2 \ldots dz_N$$

$$\to \psi(t,x)\overline{\psi(t,y)} \quad \text{as } N \to \infty$$

Pbm Convergence rate? Uniform in $\hbar$? recall that $\hbar = 1.1 \cdot 10^{-34} Js$

EMPIRICAL MEASURES IN CLASSICAL MECHANICS

KLIMONTOVICH SOLUTIONS

W. Braun, K. Hepp: Commun. Math. Phys. **56** (1977) 101–113

R.L. Dobrushin: Func. Anal. Appl. **13** (1979), 115–123

The diagram

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

The Mean-Field Limit in Classical Mechanics

Unknown positions+momenta $q_1(t), p_1(t), \ldots, q_N(t), p_N(t)$
Newton's 2nd law

$$\dot{q}_j(t) = \tfrac{1}{m} p_j(t)\,, \quad \dot{p}_j(t) = -\frac{1}{N}\sum_{\substack{k=1\\k\neq j}}^{N} \nabla V(q_j(t) - q_k(t))$$

Vlasov equation distribution function $f \equiv f(t,x,\xi) \geq 0$

$$\partial_t f(t,x,\xi) + \underbrace{\tfrac{1}{m}\xi\cdot\nabla_x f(t,x,\xi) - \nabla_x V_f(t,x)\cdot\nabla_\xi f(t,x,\xi)}_{\{H_f,f\}(t,x,\xi)\ \text{ where } H_f(t,x,\xi):=\frac{1}{2m}|\xi|^2+V_f(t,x)} = 0$$

$$\text{where } V_f(t,x) = \iint_{\mathbf{R}^d\times\mathbf{R}^d} V(x-y)f(t,y,\eta)\,dy\,d\eta$$

From Newton to Vlasov in the limit as $N \to \infty$

$$\frac{1}{N}\sum_{j=1}^{N}\delta_{q_j(0),p_j(0)} \rightharpoonup f(0,\cdot,\cdot) \Rightarrow \frac{1}{N}\sum_{j=1}^{N}\delta_{q_j(t),p_j(t)} \rightharpoonup f(t,\cdot,\cdot)$$

Assume that $V \in C^{1,1}(\mathbf{R}^d)$ is even. Then

$t \mapsto (q_1(t), p_1(t), \ldots, q_N(t), p_N(t))$ satisfies Newton's 2nd law

$$\iff \underbrace{\frac{1}{N}\sum_{j=1}^{N} \delta((x,\xi) - (q_j(t), p_j(t)))}_{=:\mu_N(t,dxd\xi)} \text{ weak solution of Vlasov}$$

Proof since V is C^1+even, $\nabla V(0) = 0$, so that

$$\frac{1}{N}\sum_{\substack{k=1\\k\neq j}}^{N} V(q_j(t) - q_k(t)) = \iint_{\mathbf{R}^d\times\mathbf{R}^d} V(q_j(t) - y)\mu_N(t, dyd\eta)$$

Newton's second law for each particle=differential system for the characteristic curves of Vlasov's equation, localized at $(q_j(t), p_j(t))$

A QUANTUM NOTION OF EMPIRICAL MEASURE

Quantum Analog of the Klimontovich Solution

•Set $\mathfrak{H} := L^2(\mathbf{R}^d; \mathbf{C})$, and $\mathfrak{H}_N := L^2(\mathbf{R}^{dN}; \mathbf{C})$ (N-particle H-space)
•For $k = 1, \ldots, N$, set

$$J_k : \mathcal{L}(\mathfrak{H}) \ni A \mapsto \underbrace{I \otimes \ldots \otimes A \otimes \ldots \otimes I}_{= A \text{ acting on the kth variable}} \in \mathcal{L}(\mathfrak{H}_N)$$

Definition For $N > 1$ and $t \in \mathbf{R}$, define $\mathcal{M}_N(t) : \mathcal{L}(\mathfrak{H}) \to \mathcal{L}(\mathfrak{H}_N)$

$$\mathcal{M}_N^{in} := \underbrace{\frac{1}{N}\sum_{k=1}^{N} J_k}_{\text{analog of } \frac{1}{N}\sum_{k=1}^{N}\delta_{z_k}} \quad , \quad \mathcal{M}_N(t)A := e^{it\mathcal{H}_N/\hbar}(\mathcal{M}_N^{in}A)e^{-it\mathcal{H}_N/\hbar}$$

where $\mathcal{H}_N$ is the N-body quantum Hamiltonian

$$\mathcal{H}_N := \sum_{j=1}^{N} -\frac{\hbar^2}{2m}\Delta_{x_N} + \frac{1}{N}\sum_{1\le j<k\le N} V(x_j - x_k) = \mathcal{H}_N^*$$

A Characteristic Property of $\mathcal{M}_N(t)$

•For $\sigma \in \mathfrak{S}_N$, and $\Psi_N \in \mathfrak{H}_N$, define

$$U_\sigma \Psi_N(x_1, \ldots, x_N) = \Psi_N(x_{\sigma^{-1}(1)}, \ldots, x_{\sigma^{-1}(N)})$$

•Symmetric N-particle trace-class operators

$$\mathcal{L}^1_s(\mathfrak{H}_N) := \{T \in \mathcal{L}^1(\mathfrak{H}_N) \,:\, U_\sigma T U_\sigma^* = T \text{ for all } \sigma \in \mathfrak{S}_N\}$$

Lemma Set $T_N(t) := e^{-it\mathcal{H}_N/\hbar} T_N^{in} e^{it\mathcal{H}_N/\hbar}$, for all $T_N^{in} \in \mathcal{L}^1_s(\mathfrak{H}_N)$

$$\mathrm{Tr}_{\mathfrak{H}_N}((\mathcal{M}_N(t)A) T_N^{in}) = \mathrm{Tr}_{\mathfrak{H}}(A T_{N:1}(t)) \qquad \text{for all } A \in \mathcal{L}(\mathfrak{H})$$

where $T_{N:1}(t) = \mathrm{Tr}(T_N(t)|\mathfrak{H}_{N-1}) \in \mathcal{L}^1(\mathfrak{H})$ has integral kernel

$$\int \underbrace{r(t, x, z_2, \ldots, z_N; y, z_2, \ldots, z_N)}_{\text{integral kernel of } T_N(t)} dz_2 \ldots dz_N$$

Thm A Let $V \in \mathcal{F}L^1(\mathbf{R}^d)$ be even+real-valued. Then

$$i\hbar\partial_t \mathcal{M}_N(t) = \mathbf{ad}^*(-\tfrac{1}{2m}\hbar^2\Delta)\mathcal{M}_N(t) - \mathcal{C}[V, \mathcal{M}_N(t), \mathcal{M}_N(t)]$$

Notation for each $\Lambda : \mathcal{L}(\mathfrak{H}) \to \mathcal{L}(\mathfrak{H}_N)$, each unbounded operator H on $\mathfrak{H}$ and each $A \in \mathcal{L}(\mathfrak{H})$

$$(\mathbf{ad}^*(H)\Lambda)A := -\Lambda([H, A]), \qquad \text{if } [H, A] := HA - AH \in \mathcal{L}(\mathfrak{H})$$

$$\mathcal{C}[V, \Lambda_1, \Lambda_2]A := \int_{\mathbf{R}^d} ((\Lambda_1 E_\omega^*)\Lambda_2(E_\omega A) - \Lambda_2(AE_\omega)(\Lambda_1 E_\omega^*))\hat{V}(\omega)\frac{d\omega}{(2\pi)^d}$$

where

$$E_\omega\psi(x) := e^{i\omega\cdot x}\psi(x) \quad \text{for each } \psi \in \mathfrak{H}, \qquad E_\omega^* = E_{-\omega}$$

Hartree equation $\subset$ equation for $\mathcal{M}_N^*(t)$

Thm B For $t \mapsto R(t)$ time-dependent density operator on $\mathfrak{H}$, define

$$\mathcal{R}(t)A := \mathrm{Tr}_{\mathfrak{H}}(R(t)A)I_{\mathfrak{H}_N}\,, \quad A \in \mathcal{L}(\mathfrak{H})\,, \qquad \text{(chaotic K soln)}$$

Then R is a solution of the Hartree equation (for density operators)

$$i\hbar\partial_t R(t) := [-\tfrac{1}{2m}\hbar^2\Delta + V_{R(t)}, R(t)]$$

$$\text{with } V_{R(t)}(x) = \int_{\mathbf{R}^d} V(x-z) \underbrace{r(t,z,z)}_{\text{integral kernel of } R(t)} dz$$

$$\iff i\hbar\partial_t\mathcal{R}(t) = \mathbf{ad}^*(-\tfrac{1}{2m}\hbar^2\Delta)\mathcal{R}(t) - \mathcal{C}[V, \mathcal{R}(t), \mathcal{R}(t)]$$

i.e. iff $\mathcal{R}$ is a solution of the equation obtained in Thm A

Ideas for the proofs

•Thm A $\Longrightarrow$ Thm B: if $\mathcal{R}(t)A = \mathrm{Tr}_{\mathfrak{H}}(R(t)A)I_{\mathfrak{H}_N}$ then

$$
\begin{aligned}
((\mathcal{R}(t)E_\omega^*)\mathcal{R}(t)(E_\omega A) - \mathcal{R}(t)(AE_\omega)(\mathcal{R}(t)E_\omega^*))\hat{V}(\omega) \\
= -\widehat{V \star_x \rho}(t,\omega)\,\mathrm{Tr}_{\mathfrak{H}}([R(t),E_\omega]A) \\
= -\mathrm{Tr}_{\mathfrak{H}}([R(t),\widehat{V_R(t)}(\omega)E_\omega])
\end{aligned}
$$

•to prove Thm A, write the 1st equation in the BBGKY hierarchy, think of $\mathcal{M}_N(t)$ as the adjoint of the map

$$
\mathcal{L}^1_s(\mathfrak{H}_N) \ni R_N\big|_{t=0} \mapsto R_{N:1}(t) \in \mathcal{L}^1(\mathfrak{H})
$$

and use the identity

$$
[\mathcal{M}_N(t)A, \mathcal{M}_N(t)B] = \frac{1}{N}\mathcal{M}_N(t)[A,B] \quad \text{for all } A,B \in \mathcal{L}(\mathfrak{H})
$$

THE QUANTUM MEAN-FIELD LIMIT

UNIFORMITY IN $\hbar$ OF THE CONVERGENCE RATE

From Schrödinger to Hartree

Let $V \in C_b(\mathbf{R}^d)$ be even and real-valued. Assume that $\|\psi_\hbar^{in}\|_{L^2} = 1$.

Let $\psi_\hbar \equiv \psi_\hbar(t,x)$ be a solution of the Hartree equation

$$i\hbar\partial_t\psi_\hbar = -\tfrac{1}{2m}\hbar^2\Delta_x\psi_\hbar + (V \star_x |\psi_\hbar|^2)\psi_\hbar\,, \quad \psi_\hbar\big|_{t=0} = \psi_\hbar^{in}$$

where $\star_x$ is the convolution in the variable x, and define

$$\Psi_{N,\hbar}(t,X_N) := e^{-it\mathcal{H}_N/\hbar}\prod_{j=1}^N \psi_\hbar^{in}(x_j)$$

where

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

Uniform in $\hbar$ convergence rate for the MF limit

Thm C Let $\Gamma := \max(1, \|\nabla^2 V\|_{L^\infty}) < \infty$ and assume that

$$\mathbf{V} := \frac{1}{(2\pi)^d} \int_{\mathbf{R}^d} |\hat{V}(\xi)|(1+|\xi|)^{[d/2]+3} d\xi < \infty$$

Then

$$\left\| W_\hbar[|\Psi_{N,\hbar}\rangle\langle\Psi_{N,\hbar}|_{:1}] - W_\hbar[|\psi_\hbar\rangle\langle\psi_\hbar|] \right\|'_{[d/2]+2}(t) \leq \frac{c[d]e^{c[d]\mathbf{V}te^{t\Gamma}}}{\sqrt{N}}$$

where

$$\|\cdot\|'_n \text{ dual norm of } \|f\|_n := \max_{|\alpha|,|\beta|\leq n} \|\partial_x^\alpha \partial_\xi^\beta f\|_{L^\infty(\mathbf{R}^d\times\mathbf{R}^d)}$$

Wigner transform of a density R with integral kernel $r \equiv r(X,Y)$

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

Sketch of the proof of Thm C

(1) Let $A \equiv A(t)$ satisfy

$$i\hbar\partial_t A(t) := [-\tfrac{1}{2m}\hbar^2\Delta + V \star_x |\psi_\hbar(t,\cdot)|^2, A(t)]$$

Let $\mathcal{R}(t)B := \langle\psi_\hbar(t)|B|\psi_\hbar(t)\rangle I_{\mathfrak{H}_N}$ where $\psi_\hbar =$Hartree solution

$$(\mathcal{M}_N^*(t) - \mathcal{R}(t))A(t) = (\mathcal{M}_N^*(0) - \mathcal{R}(0))A(0)$$
$$-\frac{i}{\hbar}\int_0^t \mathcal{C}[V, \mathcal{M}_N^*(s) - \mathcal{R}(s), \mathcal{M}_N^*(s)]A(s)ds$$

(2) Introduce the metric

$$d_N^T(t) := \sup_{t\mapsto A(t)} \|(\mathcal{M}_N^*(t) - \mathcal{R}(t))A(t)|\Psi_{N,\hbar}\rangle\langle\Psi_{N,\hbar}|(0)\|_{\mathcal{L}^1(\mathfrak{H}_N)}$$

where $A(\tau) = \mathrm{OP}_\hbar^W[a]$ with $\|a\|_n \leq 1$ for some $\tau \in [0, T]$

(3) Use semiclassical estimates to propagate an estimate for

$$\frac{1}{\hbar}\|[E_\omega, A(t)]\| \le \frac{\sqrt{d}}{\hbar}|\omega| \max_{1\le k\le d}(\|[x_k, A(t)]\| + \|[-i\hbar\partial_{\xi_k}, A(t)]\|)$$

as in Appendix C of Benedikter-Porta-Saffirio-Schlein ARMA2016, starting from τ (since $A(\tau)$ is a Weyl operator, so that the r.h.s. is $O(1)$ by standard commutator estimates)

(4) The dual norm

$$\left\| W_\hbar[|\Psi_{N,\hbar}\rangle\langle\Psi_{N,\hbar}|_{:1}](T,\cdot) - W_\hbar[|\psi_\hbar\rangle\langle\psi_\hbar|](T,\cdot)\right\|'_{[d/2]+2} \le d_N^T(T)$$

while Boulkhemair's (JFA1999) variant of the Calderon-Vaillancourt theorem implies that

$$d_N^T(0) \le c[d]/\sqrt{N}$$

Comparison with earlier results

(1) Rodnianski-Schlein (CMP 2009) for $\hbar = 1$

$$\operatorname{Tr}\left||\Psi_N\rangle\langle\Psi_N|_{:1} - |\psi\rangle\langle\psi|\right|(t) \le \frac{Ce^{Kt}}{\sqrt{N}}$$

assuming that $V(x)^2 \le D(1-\Delta_x)$ and $\|\psi^{in}\|_{H^1(\mathbf{R}^3)} = 1$

(2) Pickl (LMP 2009) for $\hbar = 1$

$$\operatorname{Tr}\left(|\Psi_N\rangle\langle\Psi_N|_{:1}(I - |\psi\rangle\langle\psi|)\right)(t) \le \frac{1}{N}\left(\exp\int_0^t 10\|V\|_{L^{2r}}\|\psi(s,\cdot)\|_{L^{2r'}}ds - 1\right)$$

assuming that $V \in L^{2r}(\mathbf{R}^3)$ with $r \ge 1$ and $V \in L^\infty(\mathbf{R}^3 \setminus B(0,R))$

(3) FG-Mouhot-Paul (CMP 2016) Assume $V \in C^{1,1}(\mathbf{R}^d)$

$$\mathrm{dist}_{MK,2}\left(e^{\hbar\Delta_{x,\xi}/4}W_\hbar[R_{N:1,\hbar}], e^{\hbar\Delta_{x,\xi}/4}W_\hbar[R_\hbar]\right)^2(t)$$
$$\leq 2d\hbar(e^{\Lambda t}+1)+\frac{8}{N}\|\nabla V\|^2_{L^\infty}\frac{e^{\Lambda t}-1}{\Lambda}$$

Töplitz initial 1-body density, with $\Lambda := 3 + 4(\mathrm{Lip}\,\nabla V)^2$

(4) Earlier uniform in $\hbar$ convergence results: local in time and for WKB initial data (Graffi-Martinez-Pulvirenti M3AS2003), formal semi-classical expansion (Pezzotti-Pulvirenti Ann. IHP2009)

Conclusion/Open pbms

We have

(a) extended the Klimontovich Theorem to the quantum setting, and

(b) used it to obtain an $O(1/\sqrt{N})$ convergence rate for the quantum mean-field limit **uniformly in** $\hbar \in (0,1]$

•Singular potentials? e.g. Coulomb

•The formula for the interaction term $\mathcal{C}[V, \mathcal{M}_N^*(t), \mathcal{M}_N^*(t)]$ involves

$$V(x_1 - x_2) = \int_{\mathbf{R}^d} \hat{V}(\omega) E_\omega(x_1) E_\omega^*(x_2) \tfrac{d\omega}{(2\pi)^d}$$

Other representations of V involving tensor products — e.g. Pólya (1949), Fefferman-de la Llave (1986), Hainzl-Seiringer (2002)...

$$\frac{1}{|x|} = \tfrac{1}{\pi} \int_0^\infty \int_{\mathbf{R}^3} \mathbf{1}_{B(0,r)} \star \mathbf{1}_{B(0,r)} \tfrac{dr}{r^5}$$