

Commuting the mean-field and classical limits in quantum mechanics

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The question and its motivation

We focus on two important limits used to derive evolution laws from microscopic dynamics:

- ▶ The **classical limit** (sometimes called semiclassical limit) when Planck's constant \hbar (which measures the strength of quantum effects) is small with respect to the scale of observation as discussed later. It is closely related to the high-frequency limit of PDEs.
- ▶ The **mean-field limit** (one form of many-body limits, also called sometimes thermodynamical limits) when the number of bodies-particles N is sent to infinity, under some appropriate assumption of low correlations.

In many situations the two regimes are involved: we want to study how they interact. More precisely **we want to quantify the convergence of the mean-field limit uniformly along the classical limit.**

The two limits

Starting point: N -body Schrödinger equation for bosons

$$i\hbar\partial_t\Psi^N = -\frac{\hbar^2}{2m}\sum_{k=1}^N\Delta_{x_k}\Psi^N + \sum_{k,l=1}^N V(x_k - x_l)\Psi^N$$

on **symmetric** N -body wave function $\Psi^N(t, x_1, \dots, x_N)$, $x_k \in \mathbb{R}^d$.

Binary interaction potential V : measurable and even on \mathbb{R}^d .

Rescaling: $\hat{x} = x/L$, $\hat{t} = t/T$, $\hat{V}(\hat{z}) = (NT^2)/(mL^2)V(z)$

$$i\partial_t\tilde{\Psi}_\epsilon^N = -\frac{\epsilon}{2}\sum_{k=1}^N\Delta_{x_k}\tilde{\Psi}_\epsilon^N + \frac{1}{N\epsilon}\sum_{k,l=1}^N\tilde{V}(\tilde{x}_k - \tilde{x}_l)\tilde{\Psi}_\epsilon^N, \quad \epsilon := \frac{\hbar T}{mL^2}$$

Classical limit $\epsilon \rightarrow 0$

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Mean-field limit $N \rightarrow \infty$

The quantum mean-field limit (Hartree equation)

△ N goes to infinity while ϵ is kept fixed △

Assuming initial decorrelation $\Psi_{\epsilon, in}^N \sim \prod_{k=1}^N \psi_{\epsilon, in}(x_k)$ and under various assumptions on V :

$$\int_{x_2, \dots, x_N} \overline{\Psi^N(t, x, x_2, \dots, x_N)} \Psi^N(t, y, x_2, \dots, x_N) dx_2 \cdots dx_N \\ \xrightarrow{N \rightarrow \infty} \overline{\psi(t, x)} \psi(t, y)$$

where ψ solves the **Hartree equation**

$$i\partial_t \psi_\epsilon = -\frac{\epsilon}{2} \Delta_x \psi_\epsilon + \frac{1}{\epsilon} (V * |\psi_\epsilon|^2) \psi_\epsilon, \quad (\psi_\epsilon)|_{t=0} = \psi_{\epsilon, in}$$

Coulomb potential V or even more singular (cf. cubic NLS) covered by existing results, but most of the time non-quantitative apart from restricted cases **and degenerates as $\epsilon \rightarrow 0$**

The classical limit (N -body Liouville equation)

△ ϵ goes to zero while N is kept fixed △

High-frequency limit \Rightarrow one needs to localise oscillations

Wigner transform at scale ϵ :

$$W_\epsilon[\Phi](X, \Xi) := \frac{1}{(2\pi)^n} \int_Y \overline{\Phi\left(X - \frac{Y}{2\epsilon}\right)} \Phi\left(X + \frac{Y}{2\epsilon}\right) e^{-i\Xi \cdot Y} dY$$

If the initial conditions satisfy $W_\epsilon[\Psi_{\epsilon, in}^N] \sim F_{in}^N$ as $\epsilon \rightarrow 0$, and under appropriate conditions on V :

$$W_\epsilon[\Psi_\epsilon^N(t, \cdot)] \sim F^N(t, \cdot) \quad \text{at later times } t \geq 0$$

where F^N satisfies the **N -body Liouville equation**

$$\partial_t F^N + \sum_{k=1}^N \xi_k \cdot \nabla_{x_k} F^N - \frac{1}{N} \sum_{k,l=1}^N \nabla V(x_k - x_l) \cdot \nabla_{\xi_k} F^N = 0.$$

The mean-field limit in classical mechanics

$$\triangle \quad \underline{N \rightarrow \infty \text{ while } \epsilon = 0} \quad \triangle$$

Assuming initial decorrelation $F_{in}^N(X, \Xi) \sim \prod_{k=1}^N f_{in}(x_k, \xi_k)$ and under various assumptions on V :

$$F^N(t, X, \Xi) \sim \prod_{k=1}^N f(t, x_k, \xi_k) \quad \text{at later times } t \geq 0 \text{ and}$$
$$\int_{x_2, \xi_2, \dots, x_N, \xi_N} F^N(t, x, \xi, x_2, \xi_2, \dots, x_N, \xi_N) dx_2 d\xi_2 \cdots dx_N d\xi_N$$
$$\xrightarrow{N \rightarrow \infty} f(t, x, \xi)$$

where f solves the **Vlasov equation**

$$\partial_t f + \xi \cdot \nabla_x f - (\nabla V *_x f) \nabla_\xi f = 0, \quad f|_{t=0} = f_{in}.$$

Quantitative results for $V \in C^2$, partial results for some singular V , open for Coulomb-Newton potentials

The classical limit in mean-field mechanics

$$\triangle \quad \underline{\epsilon \rightarrow 0 \text{ while } N = \infty} \quad \triangle$$

High frequency limit again \Rightarrow localise oscillations

Wigner transform at scale ϵ :

$$W_\epsilon[\Phi](X, \Xi) := \frac{1}{(2\pi)^n} \int_Y \overline{\Phi\left(X - \frac{Y}{2\epsilon}\right)} \Phi\left(X + \frac{Y}{2\epsilon}\right) e^{-i\Xi \cdot Y} dY$$

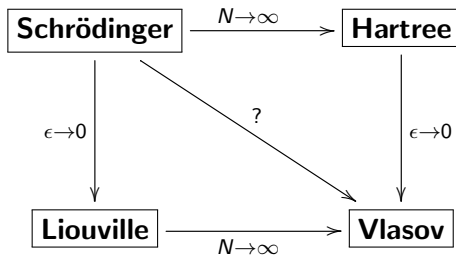
If the initial conditions satisfy $W_\epsilon[\psi_{\epsilon, in}](x, \xi) \sim f_{in}(x, \xi)$ as $\epsilon \rightarrow 0$, and under appropriate conditions on V :

$$W_\epsilon[\psi_\epsilon(t, \cdot)] \sim f(t, x, \xi) \quad \text{at later times } t \geq 0$$

with ψ_ϵ satisfies the Hartree equation, where f satisfies the Vlasov equation

$$\partial_t f + \xi \cdot \nabla_x f - (\nabla V *_x f) \cdot \nabla_\xi f = 0, \quad f|_{t=0} = f_{in}.$$

The diagram of limits



Quantum mean-field limit:

Spohn'80, Bardos-Golse-Mauser'90s, Erdős-Schlein-Yau'00s, Fröhlich-Knowles-Schwarz, Rodnianski-Schlein, Pickl...

Classical limit by Wigner transform (finite or infinite N):

Lions-Paul'90s, Gérard-Markowich-Poupaud-Mauser'90s

Classical mean-field limit:

Neunzert-Wick'74, Braun-Hepp'77, Dobrushin'79, Hauray-Jabin'07, Golse-Mouhot-Ricci'13, Mischler-Mouhot-Ricci

The conceptual difficulties

(1) Classical mean-field limit traditionally reframed as the convergence of **empirical measures**

$$\mu_{(X, \Xi)}^N := \sum_{k=1}^N \delta_{(x_k, \xi_k)} \rightharpoonup f$$

It is based on the use of *weak topologies* and either compactness arguments or stability estimates in associated metrics (e.g. **Monge-Kantorovich-Wasserstein distances**)

(2) Quantum mean-field limit based most often on the **BBGKY hierarchy** written on the wave function, on compactness arguments and in the topology of the **trace-norm** which corresponds as $\epsilon \rightarrow 0$ to **total variation norm**

↪ quantitative results rare and restricted at quantum level

↪ conflict of topologies (weak vs strong topology)

↪ no equivalent of empirical measure at quantum level

↪ Schrödinger equation \sim Newton equations not Liouville!

Back to microscopic Hamiltonian dynamics

- ▶ Binary interactions through a potential V depending only on the distance between two interacting bodies
- ▶ External forces with some potential ϕ (time, position)
- ▶ Hamilton equations (Newton laws)

$$\frac{dx_k}{dt} = \frac{\partial H^N}{\partial \xi_k} \quad \frac{d\xi_k}{dt} = -\frac{\partial H^N}{\partial x_k} \quad \text{in } \mathbb{R}^d, \quad 1 \leq k \leq N$$

$$H^N(X, \Xi) = \underbrace{\sum_{k=1}^N \frac{\xi_k^2}{2}}_{\text{kinetic energy}} + \underbrace{\sum_{k < l} V(x_k - x_l)}_{\text{interaction energy}} + \underbrace{\sum_{k=1}^N \phi(t, x_k)}_{\text{potential energy}}$$

- ▶ This corresponds to the set of N second-order ODEs in \mathbb{R}^d

$$\dot{x}_k = \xi_k, \quad \dot{\xi}_k = -\sum_{k \neq l} \nabla_x V(x_k - x_l) - \nabla_x \phi(x_k), \quad 1 \leq k \leq N$$

The N -body Liouville equation (I)

Statistical solution to the previous ODEs, i.e. evolution of a *distribution* of trajectories:

$$\frac{\partial F^N}{\partial t} + \sum_{k=1}^N \left(\frac{\partial H^N}{\partial \xi_k} \cdot \frac{\partial F^N}{\partial x_k} - \frac{\partial H^N}{\partial x_k} \cdot \frac{\partial F^N}{\partial \xi_k} \right) = 0$$

on joint microscopic probability distribution function $F^N(t, X, \Xi)$

Liouville's theorem

For any $t \in \mathbb{R}$ one has $F^N(t, S_t(X, \Xi)) = F^N(0, X, \Xi)$, where S_t is the flow of the Hamilton equations, and S_t preserves volume

Consequence: statistical Casimir invariants (for $\Theta : \mathbb{R} \mapsto \mathbb{R}$)

$$\int_{\mathbb{R}^{2dN}} \Theta \left(F^N(t, X, \Xi) \right) dX dV = \int_{\mathbb{R}^{2dN}} \Theta \left(F^N(0, X, \Xi) \right) dX dV$$

including Boltzmann's entropy for $\Theta(r) = r \log r$

The N -body Liouville equation (II)

Proof: Differentiate in time $F^N(t, S_t(X, \Xi)) = F^N(t, X_t, \Xi_t)$:

$$\begin{aligned} \left(\frac{\partial}{\partial t} F^N \right) (t, X_t, \Xi_t) + \left(\frac{\partial}{\partial t} X_t \right) \cdot \left(\frac{\partial}{\partial X} F^N \right) (t, X_t, \Xi_t) \\ + \left(\frac{\partial}{\partial t} \Xi_t \right) \cdot \left(\frac{\partial}{\partial \Xi} F^N \right) (t, X_t, \Xi_t) = 0 \end{aligned}$$

which means, using the equations on X_t and Ξ_t :

$$\begin{aligned} \left(\frac{\partial}{\partial t} F^N \right) (t, X_t, \Xi_t) + \left(\frac{\partial}{\partial \Xi} H \right) \cdot \left(\frac{\partial}{\partial X} F^N \right) (t, X_t, \Xi_t) \\ - \left(\frac{\partial}{\partial X} H \right) \cdot \left(\frac{\partial}{\partial \Xi} F^N \right) (t, X_t, \Xi_t) = 0 \end{aligned}$$

which is the desired equation at the point (t, X_t, Ξ_t) .

The N -body Liouville equation (III)

Then compute time derivative of $J(t, X, \Xi) := \det \nabla_{X, \Xi} S_t(X, \Xi)$:

$$\frac{d}{dt} J(t, X, \Xi) = \left[\sum_i \left(\frac{\partial^2 H^N}{\partial x_k \partial \xi_k} - \frac{\partial^2 H^N}{\partial \xi_k \partial x_k} \right) \right] J(t, X, \Xi) = 0$$

Together with $J(0, X, \Xi) = \det \text{Id} = 1$, it yields $J(t, X, \Xi) \equiv 1$

One deduces by change of variable

$$\int_{\mathbb{R}^{2dN}} \Theta \left(F^N(t, X, \Xi) \right) dX dV = \int_{\mathbb{R}^{2dN}} \Theta \left(F^N(0, X, \Xi) \right) dX dV$$

→ conservation of Lebesgue norms, Boltzmann entropy...

This reflects the time-reversibility of the Liouville equation:

invariance under the change of variable $(t, X, \Xi) \mapsto (-t, X, -V)$

Cf. reversibility of Newton laws at microscopic level

The BBGKY hierarchy (I)

- ▶ N -particle Liouville equation allows for considering superpositions of all trajectories at once, still contains same amount of information as the Newton equations
- ▶ Desirable to simplify description of the system by throwing away information: (Hopefully) the system is described by a one-particle distribution (first marginal):

$$f_1^N(t, x, v) := \int_{\mathbb{R}^{2d(N-1)}} F^N(t, X, \Xi) dx_2 dx_3 \dots dx_N dv_2 \dots dv_N$$

(Observe that it still depends on N)

- ▶ Why the marginal according to the first variable? No loss of generality since F^N symmetric (invariant under permutations) by indistinguishability of the particles

The BBGKY hierarchy (II)

- ▶ How can we interpret this equation?
- ▶ Binary collisions \Rightarrow evolution of first marginal (f_1^N) depends on second marginal f_2^N : interactions \Rightarrow correlations
- ▶ Similarly f_2^N 's evolution depends on f_3^N and so on:

$$\begin{aligned}\frac{\partial f_1^N}{\partial t} &= \mathcal{L}_1(f_1^N) + \mathcal{B}_1(f_2^N) \\ \dots \\ \frac{\partial f_k^N}{\partial t} &= \mathcal{L}_k(f_k^N) + \mathcal{B}_k(f_{k+1}^N) \\ \dots \\ \frac{\partial f_N^N}{\partial t} &= \frac{\partial F^N}{\partial t} = \{H^N, F^N\}\end{aligned}$$

- ▶ This is the **BBGKY hierarchy** (Bogoliubov, Born, Green, Kirkwood, Yvon) for

$$f_1^N, f_3^N, \dots, f_k^N, \dots, f_N^N = F_N.$$

The Many-particle or “Thermodynamic” Limit

- ▶ **Goal of thermodynamical limit:** perform $N \rightarrow \infty$ and recover closed equations on reduced distribution $f_1^N \sim f_1$ as $N \sim \infty$
- ▶ Natural to ask whether (low correlations)

$$f_2^N = f_1^N \otimes f_1^N := f_1^N(t, x, v) f_1^N(t, y, w)?$$

- ▶ However the probability independence assumption **not preserved** along time for interacting particle systems
- ▶ Boltzmann discovered (and Kac formulated mathematically. . .) that this could hold **in the limit** $N \rightarrow \infty$

$$f_2^N \sim f_1^N \otimes f_1^N \quad \text{as } N \rightarrow +\infty \quad (\text{“near-product structure”})$$

→ this is the idea of **molecular chaos**

- ▶ **Formally chaos** \Rightarrow closed equation on f_1 as $N \rightarrow \infty$
(Vlasov in mean-field scaling, Boltzmann with $Nr(N)^2 = 1$)

Empirical distribution solutions to the Vlasov equation (I)

Crucial property uncovered by Dobrushin: the empirical distribution following the microscopic trajectories is a weak solution to the nonlinear Vlasov equation

Let $Z_t^N = (X_t, \Xi_t)$ be the solutions to the microscopic equations with initial data Z_0^N , then the corresponding empirical distribution μ_t^N satisfies

$$\frac{\partial \mu_t^N}{\partial t} + v \cdot \nabla_x \mu_t^N - [\nabla_x V *_{x,\xi} \mu_t^N](t, x) \cdot \nabla_v \mu_t^N = 0$$

in the weak sense with

$$[V *_{x,\xi} \mu_t^N](t, x) := \int_{y,\xi} V(x-y) d\mu_t^N(y, \xi)$$

Empirical distribution solutions to the Vlasov equation (II)

Proof: in the sense of distribution for a test function $\varphi \in C_c^\infty(E)$

$$\begin{aligned}\partial_t \langle \mu_t^N, \varphi \rangle &= \partial_t \left(\frac{1}{N} \sum_{k=1}^N \varphi(x_k, \xi_k) \right) \\ &= \frac{1}{N} \sum_{k=1}^N \left(\frac{\partial x_k}{\partial t} \cdot \nabla_x \varphi(x_k, \xi_k) + \frac{\partial \xi_k}{\partial t} \cdot \nabla_\xi \varphi(x_k, \xi_k) \right) \\ &= \frac{1}{N} \sum_{k=1}^N \left(\xi_k \cdot \nabla_x \varphi(x_k, \xi_k) - \frac{1}{N} \sum_{l=1}^N \nabla_x V(x_k - x_l) \cdot \nabla_\xi \varphi(x_k, \xi_k) \right) \\ &= \langle \mu_t^N, \xi \cdot \nabla_x \varphi \rangle - \langle \mu_t^N, [\nabla_x V * \mu_t^N] \nabla_\xi \varphi \rangle \\ &= - \langle \xi \cdot \nabla_x \mu_t^N, \varphi \rangle + \langle [\nabla_x V * \mu_t^N] \cdot \nabla_\xi \mu_t^N, \varphi \rangle\end{aligned}$$

Proof of classical mean-field limit (I)

Convergence of μ_t^N by compactness and weak-strong uniqueness stability of Vlasov equation

⇒ Frontier between classical and statistical mechanics is in the topology M^1 / L^1 (strong distance is too crude for handling Dirac masses $\|\delta_x - \delta_y\| = 2 \mathbf{1}_{x \neq y} \dots$)

$$W_p(\mu, \nu) = \left(\inf_{\pi \in \Pi(\mu, \nu)} \int_{E \times E} |Z - Z'|^p d\pi(Z, Z') \right)^{1/p}$$

$\Pi(\mu, \nu)$ set of probability with marginals μ and ν (“coupling”)

$$W_p(\mu, \nu) = \left(\inf_{(Z, Z') \sim \pi \in \Pi(\mu, \nu)} \mathbb{E} (|Z - Z'|^p) \right)^{1/p}$$

Observe that $W_p(\delta_x, \delta_y) = |x - y|_p$ (sensitive to the distance)

Proof of classical mean-field limit (II)

To avoid using empirical measure: new Eulerian proof of Dobrushin's estimate in W_p on the BBGKY hierarchy

Start from an optimal coupling π_{in}^N between f^N and g^N at time zero, and derive at later time π_t^N by the evolution

$$\partial_t \pi^N + \left\{ (H^{MF})_1^{\otimes N} + H_2^N, \pi^N \right\}_{2N} = 0$$

Study $D^N(t) := \frac{1}{N} \int \left(\sum_{k=1}^N |x_k - y_k|^p + |\xi_k - \eta_k|^p \right) d\pi_t^N$

$$\frac{d}{dt} D^N(t) = -\frac{p}{N} \sum_{j=1}^N \int (\xi_j - \eta_j) \cdot (x_j - y_j) |x_j - y_j|^{p-2} d\pi_t^N$$

$$-\frac{p}{N} \sum_{j=1}^N \int (\xi_j - \eta_j) \cdot \left([\nabla V * f](x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(y_j - y_k) \right) |\xi_j - \eta_j|^{p-2} d\pi_t^N$$

Proof of classical mean-field limit (III)

Use Young inequality to reduce RHS to $D^N(t)$ and

$$\frac{1}{N} \sum_{j=1}^N \int \left| [\nabla V * f](x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(y_j - y_k) \right| d\pi_t^N$$

Use Lipschitz constant on V to reduce it to $D^N(t)$ and

$$\frac{1}{N} \sum_{j=1}^N \int \left| [\nabla V * f](x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right| d\pi_t^N$$

Use quantitative law of large number at each time on π_t^N

$$\mathbf{E}_{\pi_t^N} \left[\left| [\nabla V * f](x_k) - \frac{1}{N} \sum_{l=1}^N \nabla V(x_k - x_l) \right| \right] = O \left(N^{-\min(1/2, p/d)} \right)$$

[Fournier-Guillin PTRF to appear]

Proof of classical mean-field limit (IV)

Finally differential inequality of the form:

$$\frac{d}{dt} D^N(t) \lesssim D^N(t) + O\left(N^{-\min(1/2, p/d)}\right)$$

\Rightarrow control over time by Gronwall lemma

Then use that

$$W_p\left(\mu_t^N, f_t^{\otimes N}\right)^p \leq D^N(t)$$

(particular coupling) to conclude

The quantum N -body Von Neumann-Liouville equation

Functional setting: $\mathfrak{H} = L^2(\mathbb{R}^d)$, $\mathfrak{H}^N = L^2(\mathbb{R}^{dN})$

$\mathcal{L}(\mathfrak{H})$ bounded linear operators

$\mathcal{D}(\mathfrak{H})$ subset where $A^* = A$ and $\text{trace}(A) = 1$

Von-Neumann-Liouville equation

$$i\partial_t \rho_\epsilon^N = \left[-\frac{\epsilon}{2} \sum_{k=1}^N \Delta_k + \frac{1}{N\epsilon} \sum_{k,l=1}^N V(x_k - x_l), \rho_\epsilon^N \right]$$

(commutator bracket) with $\rho_\epsilon^N \in \mathcal{D}(\mathfrak{H})$

In the mean-field limit

$$i\partial_t \rho_\epsilon = \left[-\frac{\epsilon}{2} \Delta + \frac{1}{\epsilon} \mathcal{V}(\rho_\epsilon), \rho_\epsilon \right], \quad \mathcal{V}(\rho_\epsilon) := \int_z V(x-z) \rho_\epsilon(t, z, z)$$

Concept of marginal replaced by **partial traces** $\rho_\epsilon^{N,n} \in \mathcal{D}(\mathfrak{H}^n)$:

$$\text{trace}_{\mathfrak{H}^n} \left(A \rho_\epsilon^{N,n} \right) = \text{trace} \left((A \otimes I_{N-n}) \rho^N \right) \quad \text{where } A \in \mathcal{L}(\mathfrak{H}^n)$$

A semi-classical Monge-Kantorovich quasi-distance

Concept of quantum coupling between ρ_1 and ρ_2 :

$R \in \mathcal{D}(\mathfrak{H}^2)$ with partial traces respectively ρ_1 and ρ_2

Monge-Kantorovich quantum quasi-distance:

$$MK_2(\rho_1, \rho_2) = \inf_R \text{trace}_{\mathfrak{H}^2} ((Q^*Q + P^*P)R)^{1/2}$$

with $Q\psi = (x_1 - x_2)\psi(x_1, x_2)$ and $P\psi = -i\epsilon(\nabla_{x_1} - \nabla_{x_2})\psi$

Properties:

(i) $MK_2(\rho_1, \rho_2) \geq 2d\epsilon$

(ii) If $\rho_{1/2}$ Töplitz operators at scale ϵ with symbols $(2\pi\epsilon)^d \mu_{1/2}$ then

$$MK_2(\rho_1, \rho_2) \leq W_2(\mu_1, \mu_2) + 2d\epsilon$$

(iii) Husimi transforms at scale ϵ : $\tilde{W}_\epsilon[\rho_{1/2}]$ then

$$MK_2(\rho_1, \rho_2) \geq W_2(\tilde{W}_\epsilon[\rho_1], \tilde{W}_\epsilon[\rho_2]) - 2d\epsilon$$

The main result

Similar Gronwall estimate on quantum total cost

$$D^N(t) := \text{trace}_{\mathfrak{H}^2} ((Q^*Q + P^*P)R_t)$$

where the coupling R_t evolves according to

$$\partial_t R_t + \left[(H^{MF})_1^{\otimes N} + H_2^N, R_t \right]_{2N} = 0$$

and use the same other ingredients. . .