From many-body quantum dynamics with singular potentials to Vlasov equation

Regularity and weak-strong uniqueness

(Joint works with C. Saffirio and J. Chong)

Laurent Lafleche

The University of Texas at Austin

Ypatia — Mathematics between France and Italy

8–10 June 2022, LYSM, Rome

Setting

- N-body Schrödinger, Hartree–Fock equation, Vlasov equation [1]

$$i\hbar\,\partial_t \boldsymbol{\rho}_N = [H_N, \boldsymbol{\rho}_N] \quad \text{with} \quad H_N = \sum_{j=1}^{N} -\frac{\hbar^2 \Delta_{x_j}}{2} + \sum_{1\leq j<k\leq N} K(x_j - x_k)$$

$$i\hbar\,\partial_t \boldsymbol{\rho} = [H, \boldsymbol{\rho}] \quad \text{with} \quad H = \frac{-\hbar^2 \Delta}{2} + V_{\boldsymbol{\rho}} - \mathrm{X}_{\boldsymbol{\rho}}$$

$$\partial_t f = \{H_f, f\} \quad \text{with} \quad H_f = \frac{|v|^2}{2} + V_f$$

Potential

$$K(x) = \frac{\pm 1}{|x|^a}\, \mathbb{1}_{x\neq 0} \qquad\qquad a \in (0,1]$$

Mean-field potential $V = K * \varrho$ where

$$\varrho_{\boldsymbol{\rho}}(x) = h^3 \boldsymbol{\rho}(x,x) \qquad\qquad \varrho_f(x) = \int_{\mathbb{R}^3} f(x,v)\,\mathrm{d}v$$

1. Can also be written $\partial_t f + v \cdot \nabla_x f - \nabla V_f \cdot \nabla_v f = 0$

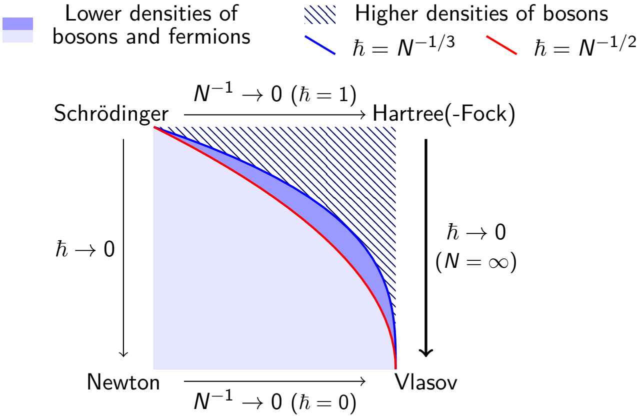
Combined mean-field and semiclassical limit

Smooth interactions

- bosons (Narnhofer–Sewel, Spohn '91, Graffi et al. '03, Golse–Paul '17–19)
- fermions, $\hbar = N^{-1/3}$ (Elgart et al. '04, Benedikter et al. '14–16, Petrat–Pickl '16)

Singular interactions (fermions, $\hbar = N^{-1/3}$)

- conditional (Porta et al '17, Saffirio '18), cutoff (Chen–Lee–Liew '21)



From classical to quantum

Classical	Quantum
$\varrho_f = \int_{\mathbb{R}^3} f \,\mathrm{d}v, \ \int_{\mathbb{R}^3} \varrho_f = 1$	$\varrho_{\boldsymbol{\rho}} = h^3 \boldsymbol{\rho}(x,x), \ h^3 \operatorname{Tr}(\boldsymbol{\rho}) = 1$
$M_n = \int_{\mathbb{R}^6} f \,\lvert v\rvert^n \,\mathrm{d}x \,\mathrm{d}v$	$h^3 \operatorname{Tr}(\lvert \boldsymbol{p}\rvert^n \boldsymbol{\rho})$
$\lVert f\rVert_{L^p(\mathbb{R}^6)}$	$\lVert \boldsymbol{\rho}\rVert_{\mathcal{L}^p} = h^{\frac{3}{p}} \operatorname{Tr}(\lvert\boldsymbol{\rho}\rvert^p)^{\frac{1}{p}}$
$\nabla_x f = \{-v, f\}, \ \nabla_v f = \{x, f\}$	$\boldsymbol{\nabla}_x \boldsymbol{\rho} = [\nabla, \boldsymbol{\rho}], \ \boldsymbol{\nabla}_\xi \boldsymbol{\rho} = \left[\frac{x}{i\hbar}, \boldsymbol{\rho}\right]$

$\Longrightarrow$ Analogous semiclassical inequalities. Example :

$$\int_{\mathbb{R}^6} \frac{\lvert\nabla_v f\rvert}{\lvert x - x_0\rvert^2} \,\mathrm{d}x \,\mathrm{d}v \lesssim \lVert \nabla_v f\rVert_{L^{3,1}_x L^1_v} \quad h^2 \operatorname{Tr}\left\lvert\left[\frac{1}{\lvert x - x_0\rvert}, \boldsymbol{\rho}\right]\right\rvert \lesssim \lVert \varrho_{\lvert\boldsymbol{\nabla}_\xi \boldsymbol{\rho}\rvert}\rVert_{L^{3\pm\varepsilon}}$$

Classical case : weak-strong uniqueness

Theorem

$$\|f_1 - f_2\|_{L^1(\mathbb{R}^6)} \leq \left\|f_1^{\mathrm{in}} - f_2^{\mathrm{in}}\right\|_{L^1(\mathbb{R}^6)} \exp\left(C \int_0^T \|\nabla_v f_2\|_{L^{3,1}_x L^1_v} \,\mathrm{d}t\right),$$

Proof :

$$(\partial_t + v \cdot \nabla_x - \nabla V_1 \cdot \nabla_v)(f_1 - f_2) = (\nabla V_1 - \nabla V_2) \cdot \nabla_v f_2,$$

so that, since $V = K * \varrho$, we obtain

$$\partial_t \int_{\mathbb{R}^6} |f_1 - f_2| \,\mathrm{d}x \,\mathrm{d}v = - \int_{\mathbb{R}^6} (\varrho_1 - \varrho_2)\, \nabla K * \int_{\mathbb{R}^3} \mathrm{sgn}(f)\, \nabla_v f_2 \,\mathrm{d}v \,\mathrm{d}x$$
$$\leq \|f_1 - f_2\|_{L^1} \left\|\nabla K * \int_{\mathbb{R}^3} |\nabla_v f_2| \,\mathrm{d}v\right\|_{L^\infty},$$

Application : semiclassical limit

Theorem (LL, Saffirio '20)

If f is initially sufficiently smooth and $\boldsymbol{\rho}_f$ is the Weyl quantization of f, then

$$\|\boldsymbol{\rho} - \boldsymbol{\rho}_f\|_{\mathcal{L}^1} \leq \left(\left\|\boldsymbol{\rho}^{\mathrm{in}} - \boldsymbol{\rho}_f^{\mathrm{in}}\right\|_{\mathcal{L}^1} + C_f(t)\,\hbar\right) e^{\lambda_f(t)}$$

- Idea of the proof :
  - Weak-strong uniqueness in $\mathcal{L}^1$
  - Classical Regularity of $f \implies$ semiclassical regularity of $\boldsymbol{\rho}_f$
- Other candidate ? The Hellinger distance $H_2(f,g) = \left\|\sqrt{f} - \sqrt{g}\right\|_{L^2}$

Theorem (Chong, LL, Saffirio '22)

If $\boldsymbol{\rho} \in \mathcal{L}^1 \cap \mathcal{L}^\infty$ and $f_{\boldsymbol{\rho}}$ is the Wigner transform of f, then

$$\|f_{\boldsymbol{\rho}} - f\|_{\mathcal{L}^2} \lesssim \left\|f_{\sqrt{\boldsymbol{\rho}^{\mathrm{in}}}} - \sqrt{f^{\mathrm{in}}}\right\|_{\mathcal{L}^2} + \hbar$$

Mean-field limit

Theorem (Chong, LL, Saffirio '21)

Let $\boldsymbol{\rho}$ be a solution of the Hartree–Fock equation initially smooth in a semiclassical sense. Then there exists $k, T > 0$, $\boldsymbol{\rho}^{\mathrm{in}}_{N,\rho} \in \mathcal{L}^1(\mathcal{F})$ such that for any $\boldsymbol{\rho}_N$ solution of Schrödinger equation with initial condition $\boldsymbol{\rho}^{\mathrm{in}}_N \in \mathcal{L}^1(\mathcal{F})$ commuting with $\mathcal{N}$, for any $t \in [0, T]$

$$\|\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho}\|_{\mathcal{L}^1} \lesssim \frac{C\, e^{\lambda\, t}}{N^{1/2}} \left(1 + \left\|(\mathcal{N} + N)^k \left(\boldsymbol{\rho}^{\mathrm{in}}_N - \boldsymbol{\rho}^{\mathrm{in}}_{N,\rho}\right)\right\|_{\mathcal{L}^1(\mathcal{F})}\right)$$

where λ is independent of $\hbar$ if $a < 1/2$.

Main steps of the proof

- Regularity uniform in $\hbar$: quantum Sobolev spaces

$$\|\boldsymbol{\rho}\|_{\dot{\mathcal{W}}^{1,p}(m)} = \|\boldsymbol{\nabla}_\xi \boldsymbol{\rho}\, m\|_{\mathcal{L}^{1,p}} + \|\boldsymbol{\nabla}_x \boldsymbol{\rho}\, m\|_{\mathcal{L}^{1,p}}$$

Theorem (Propagation of regularity)

Let $a \in (0,1]$, $m = 1 + |\boldsymbol{p}|^n$ with $n \in \mathbb{N}$ verifying $n \geq 3$ and $\boldsymbol{\rho}$ be a solution to the Hartree–Fock equation with initial condition $\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{L}^\infty(m)$ such that

$$\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{W}^{1,2}(m) \cap \mathcal{W}^{1,4}(m).$$

Then there exists $T > 0$ such that uniformly in $\hbar$ it holds

$$\boldsymbol{\rho} \in L^\infty([0,T], \mathcal{W}^{1,2}(m) \cap \mathcal{W}^{1,4}(m)),$$

- Mean-Field : Purification of mixed states and Bogoliubov transformation

Thank you for your attention !