From N-body Schrödinger to Vlasov equation with singular potentials

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Setting

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

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

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

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

Potential

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

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

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

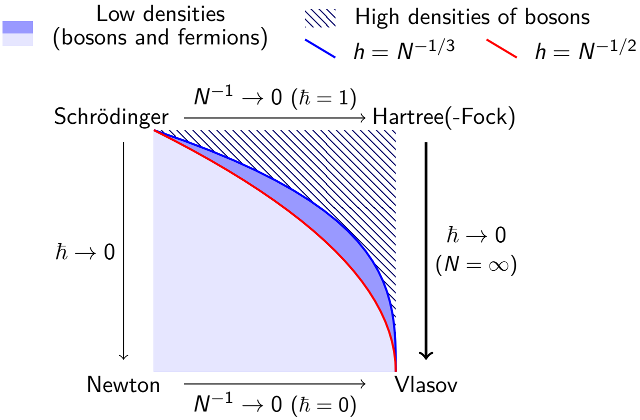
1. Can also be written $\partial_t f + v\cdot\nabla_x f - \nabla V_f \cdot \nabla_v f = 0$

Combined mean-field and semiclassical limit

Smooth interactions

- bosons (Narnhofer-Sewel '81, Spohn '91, Graffi et al. '03, Golse-Paul '17-19)
- fermions $h = N^{-\frac{1}{3}}$ (Elgart et al. '04, Benedikter et al. '14-16, Petrat-Pickl '16)

Singular interactions : conditional results (Porta et al '17, Saffirio '18)



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

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

From classical to quantum

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

$\Longrightarrow$ Analogous semiclassical inequalities. Example :

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

Results

Theorem (LL, Saffirio '20)

Let f solution of Vlasov equation initially sufficiently smooth, $\boldsymbol{\rho}$ a solution of Hartree-(Fock) equation and $\boldsymbol{\rho}_f$ be the Weyl quantization of f. Then

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

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 $T > 0$, $\boldsymbol{\rho}_{N,\boldsymbol{\rho}}^{\mathrm{in}} \in \mathcal{L}^1(\mathcal{F})$ such that for any $\boldsymbol{\rho}_N$ solution of Schrödinger equation with initial condition $\boldsymbol{\rho}_N^{\mathrm{in}} \in \mathcal{L}^1(\mathcal{F})$ commuting with $\mathcal{N}$, for any $t \in [0, T]$

$$\|\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho}\|_{\mathcal{L}^1} \lesssim \frac{C\, e^{\lambda\, t}}{N^{1/2}} \left(1 + \left\|(\mathcal{N} + N)^7 \left(\boldsymbol{\rho}_N^{\mathrm{in}} - \boldsymbol{\rho}_{N,\boldsymbol{\rho}}^{\mathrm{in}}\right)\right\|_{\mathcal{L}^1(\mathcal{F})}\right)$$

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

Ideas of the proofs :

- First theorem
  - Weak-strong uniqueness + regularity of f
- Second theorem
  - Propagate regularity for $\boldsymbol{\rho}$

$$\left(1+|\boldsymbol{p}|^n\right)\boldsymbol{\rho},\ \left(1+|\boldsymbol{p}|^n\right)\boldsymbol{\nabla}_x\boldsymbol{\rho},\ \left(1+|\boldsymbol{p}|^n\right)\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\in\mathcal{L}^p$$

  - Purification of mixed states

$$\boldsymbol{\rho}_N\in\mathcal{L}^1(\mathcal{F}(L^2))\to\Psi_{\boldsymbol{\rho}_N}\in\mathcal{F}\left(L^2\oplus L^2\right)$$

  - Bogoliubov transformation $\mathrm{R}_t=\mathrm{R}_{\boldsymbol{\rho}_t}$

$$\Psi_t=\mathrm{R}_t^*\,e^{i\,t\,\mathrm{L}_N}\,\mathrm{R}_t\Psi^{\mathrm{in}}$$

  - Number of particules outside the Bogoliubov state $\boldsymbol{\rho}_{N,\boldsymbol{\rho}}$ such that

$$\Psi_{\boldsymbol{\rho}_{N,\boldsymbol{\rho}}}=\mathrm{R}_t^*\,e^{it\mathrm{L}_N}\,\mathrm{R}_t\Omega$$

Questions ?