Semiclassical Kinetic Theory

From Many body Quantum Dynamics to the Vlasov Equation with Singular Potentials

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Quantum versus Kinetic Hamiltonian systems

Both the N-body Schrödinger and Liouville equations, and the mean-field Hartree-Fock and Vlasov equations can be written under the form

$$\partial_t \boldsymbol{f} = \{H, \boldsymbol{f}\}$$

- Classical setting, $\boldsymbol{f} = f(t, x, \xi)$ is a measure on the phase space. Bracket: the Poisson Bracket $\{H, f\} = \nabla_x H \cdot \nabla_\xi f - \nabla_\xi H \cdot \nabla_x f$. Momentum: $\boldsymbol{p} = \xi$.
- Quantum setting $\boldsymbol{f} = \boldsymbol{\rho}(t)$ is a compact operator acting on $L^2(\mathbb{R}^d)$. Bracket: the scaled commutator $\{H, \boldsymbol{\rho}\} = \frac{1}{i\hbar}(H\boldsymbol{\rho} - \boldsymbol{\rho}H)$. Momentum: $\boldsymbol{p} = -i\hbar\nabla$.

Hamiltonian

Mean-field case: $$H_{\boldsymbol{f}} = \frac{|\boldsymbol{p}|^2}{2} + V_{\boldsymbol{f}} - h^d \mathsf{X}_{\boldsymbol{f}}$$

N-Body case: $$H_N = \sum_{j=1}^N \frac{|\boldsymbol{p}_{x_j}|^2}{2} + \sum_{1\leq j<k\leq N} K(x_j - x_k)$$

Potential

- Pair interaction potential K. Example: singular potential
$$K(x) = \frac{\pm 1}{|x|^a}\, \mathbb{1}_{x\neq 0} \quad \text{with} \quad a \in (0, 1]$$
- Mean-field potential $V_{\boldsymbol{f}} = K * \varrho_{\boldsymbol{f}}$ where $\varrho_{\boldsymbol{f}}$ is the spatial density.
- Exchange term $\mathsf{X}_{\boldsymbol{f}}$ (additional corrector in the case of fermions)

The Kinetic–Quantum dictionnary

- Spatial density
$$\varrho_f(x) = \int_{\mathbb{R}^d} f(x,\xi)\,\mathrm{d}\xi \qquad\qquad \varrho_{\boldsymbol{\rho}}(x) = h^d \boldsymbol{\rho}(x,x)$$
- Moments
$$M_n = \int_{\mathbb{R}^{2d}} f\,|\xi|^n\,\mathrm{d}x\,\mathrm{d}\xi \qquad\qquad M_n = h^d\,\mathrm{Tr}(|\boldsymbol{p}|^n\,\boldsymbol{\rho})$$
- Lebesgue norms
$$\|f\|_{L^p(\mathbb{R}^6)} \qquad\qquad \|\boldsymbol{\rho}\|_{\mathcal{L}^p} = h^{\frac{d}{p}}\,\mathrm{Tr}(|\boldsymbol{\rho}|^p)^{\frac{1}{p}}$$
- Gradients
$$\nabla_x f = \{-\xi, f\},\ \nabla_\xi f = \{x, f\} \qquad\qquad \boldsymbol{\nabla}_x\boldsymbol{\rho} = \{-\boldsymbol{p}, \boldsymbol{\rho}\},\ \boldsymbol{\nabla}_\xi\boldsymbol{\rho} = \{x, \boldsymbol{\rho}\}$$

Weak-strong stability and classical limit

Proposition (LL, Saffirio [LS21])

Let f_1 and f_2 be solutions of Vlasov equation with f_2 initially sufficiently smooth. Then
$$\|f_1 - f_2\|_{L^1(\mathbb{R}^6)} \leq \left\|f_1^{\mathrm{in}} - f_2^{\mathrm{in}}\right\|_{L^1(\mathbb{R}^6)} \exp\left(C\int_0^T \|\nabla_\xi f_2\|_{L^{3,1}_x L^1_\xi}\,\mathrm{d}t\right),$$

Proof: Compute the equation for the difference of two solutions
$$\left(\partial_t + \xi\cdot\nabla_x - \nabla V_1\cdot\nabla_\xi\right)(f_1 - f_2) = (\nabla V_1 - \nabla V_2)\cdot\nabla_\xi f_2,$$
so that, since $V = K * \varrho$, it holds
$$\partial_t \int_{\mathbb{R}^{2d}} |f_1 - f_2|\,\mathrm{d}x\,\mathrm{d}\xi = -\int_{\mathbb{R}^{2d}} (\varrho_1 - \varrho_2)\,\nabla K * \int_{\mathbb{R}^d} \mathrm{sgn}(f_1 - f_2)\,\nabla_\xi f_2\,\mathrm{d}\xi\,\mathrm{d}x$$
$$\leq \|f_1 - f_2\|_{L^1}\left\|\nabla K * \int_{\mathbb{R}^d}|\nabla_\xi f_2|\,\mathrm{d}\xi\right\|_{L^\infty}$$

Towards quantum. Analogous semiclassical inequalities. Example with $d = 3$
$$\int_{\mathbb{R}^{2d}} \frac{|\nabla_\xi f|}{|x - x_0|^2}\,\mathrm{d}x\,\mathrm{d}\xi \lesssim \|\nabla_\xi f\|_{L^{3,1}_x L^1_\xi} \qquad\qquad h^2\,\mathrm{Tr}\left|\left[\tfrac{1}{|x-x_0|}, \boldsymbol{\rho}\right]\right| \lesssim \left\|\varrho_{|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}|}\right\|_{\mathcal{L}^{3\pm\varepsilon}}$$

Theorem (LL, Saffirio [LS21])

Let f solution of Vlasov equation initially sufficiently smooth, $\boldsymbol{\rho}$ a solution of the Hartree-(Fock) equation and $\boldsymbol{\rho}_f$ be the Weyl quantization of f. Then
$$\left\|\boldsymbol{\rho} - \boldsymbol{\rho}_f\right\|_{\mathcal{L}^1} \leq \left(\left\|\boldsymbol{\rho}^{\mathrm{in}} - \boldsymbol{\rho}_f^{\mathrm{in}}\right\|_{\mathcal{L}^1} + C_f(t)\,\hbar\right) e^{\lambda_f(t)}$$

Towards the mean-field limit. Go to an L^2 setting to use Fock spaces and Bogoliubov transformations. Weak-strong stability? Yes, for square roots! If both solutions are bounded in phase space and f is regular enough, then [CLS22],
$$\left\|\sqrt{\boldsymbol{\rho}} - \boldsymbol{\rho}_{\sqrt{f}}\right\|_{\mathcal{L}^2} \leq \left(\left\|\sqrt{\boldsymbol{\rho}^{\mathrm{in}}} - \boldsymbol{\rho}_{\sqrt{f^{\mathrm{in}}}}\right\|_{\mathcal{L}^2} + C_f(t)\,\hbar\right) e^{\lambda_f(t)}$$

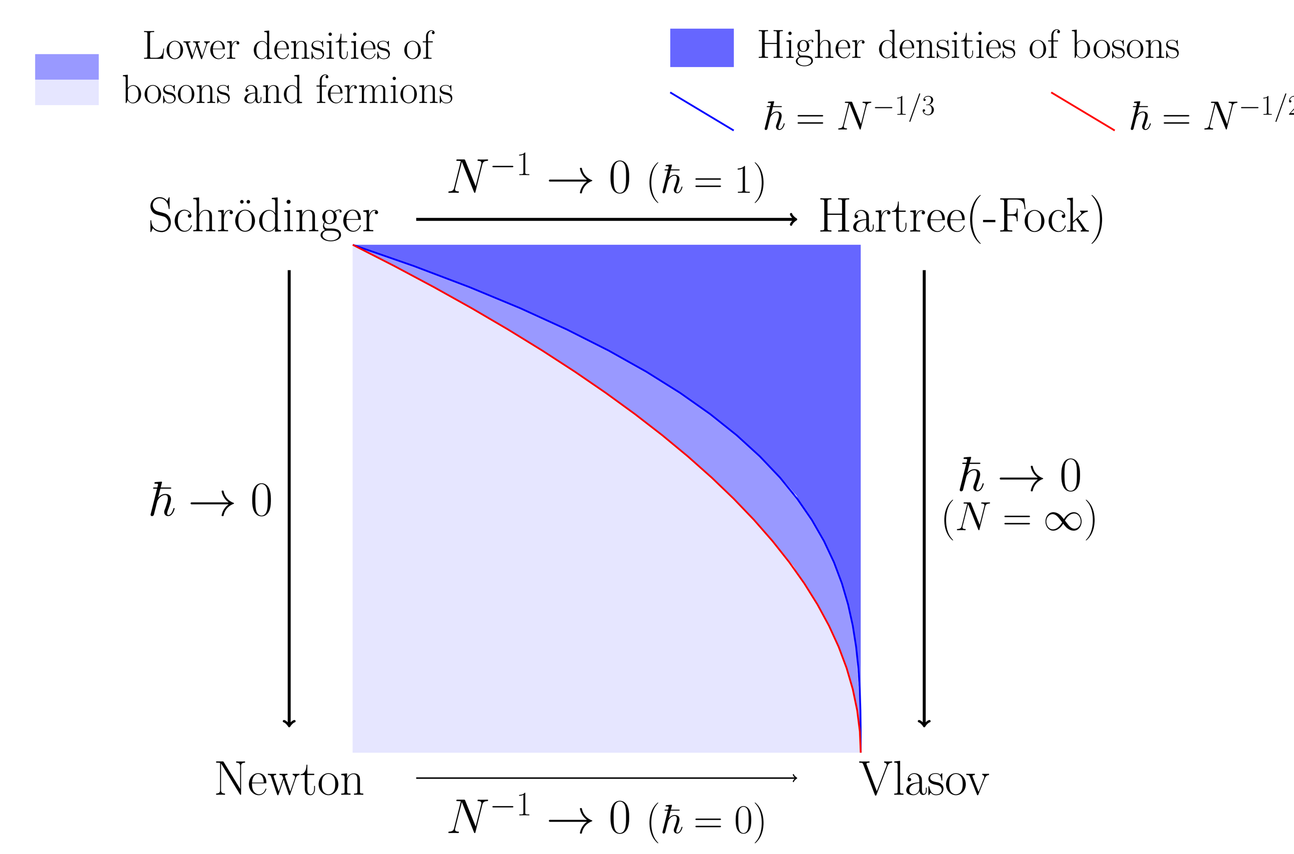
Combined mean-field and semiclassical limit

Smooth interactions

- bosons (Narnhofer-Sewel [NS81], Spohn [Spo91], Graffi et al. [GMP03], Golse-Mouhot-Paul [GMP16, GP17])
- fermions, $\hbar = N^{-1/3}$ (Elgart et al. [EESY04], Benedikter et al. [BPS14, BJP+16], Petrat-Pickl [PP16])

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

- conditional results (Porta et al [PRSS17], Saffirio [Saf18])



Theorem (Chong, LL, Saffirio [CLS21])

Let $\boldsymbol{\rho}$ be a solution of the Hartree–Fock equation initially smooth in a semiclassical sense. Then there exists $k, T > 0$, $\boldsymbol{\rho}^{\mathrm{in}}_{N,\boldsymbol{\rho}} \in \mathcal{L}^1(\mathcal{F})$ 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 $t \in [0, T]$
$$\|\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho}\|_{\mathcal{L}^1} \lesssim \frac{C\,e^{\lambda t}}{N^{1/2}}\left(1 + \left\|(\mathcal{N} + N)^k\left(\boldsymbol{\rho}^{\mathrm{in}}_N - \boldsymbol{\rho}^{\mathrm{in}}_{N,\boldsymbol{\rho}}\right)\right\|_{\mathcal{L}^1(\mathcal{F})}\right)$$
where λ is independent of $\hbar$ if $a < 1/2$ and $N^{-1/2} \ll h \leq N^{-1/3}$.

Main steps of the proof

- Propagate regularity for $\boldsymbol{\rho}$ uniformly in $\hbar$
$$\boldsymbol{\rho},\ \boldsymbol{\nabla}_x\boldsymbol{\rho},\ \boldsymbol{\nabla}_\xi\boldsymbol{\rho} \in \mathcal{L}^p(1 + |\boldsymbol{p}|^n)$$
- Purification of mixed states
  - » Take an appropriate square root
$$\boldsymbol{\rho}_N \in \mathcal{L}^1(\mathcal{F}(L^2)) \to \boldsymbol{\nu}_N \in \mathcal{L}^2(\mathcal{F}(L^2)) \text{ such that } |\boldsymbol{\nu}_N|^2 = \boldsymbol{\rho}_N$$
  - » Identify the kernel of the operator with a function of a double Fock space
$$\boldsymbol{\nu}_N \in \mathcal{L}^2(\mathcal{F}(L^2)) \to \Psi_{\boldsymbol{\rho}_N} \in \mathcal{F}\big(L^2 \oplus L^2\big)$$
- Bogoliubov transformation $\mathsf{R}_t = \mathsf{R}_{\boldsymbol{\rho}_t}$
$$\Psi_t = \mathsf{R}_t^*\,e^{i\,t\,\mathsf{L}_N}\,\mathsf{R}_t\Psi^{\mathrm{in}}$$
- Number of particles outside the Bogoliubov state $\boldsymbol{\rho}_{N,\boldsymbol{\rho}}$ such that
$$\Psi_{\boldsymbol{\rho}_{N,\boldsymbol{\rho}}} = \mathsf{R}_t^*\,e^{it\mathsf{L}_N}\,\mathsf{R}_t\Omega$$

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