

Quantum Optimal Transport and Sobolev Spaces

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Kinetic and quantum theories

- Classical setting: Phase space $z = (x, v) \in \mathbb{R}^{2d}$
 - ▶ Probability distribution $f = f(t, z)$
 - ▶ Position density $\varrho_f(x) = \int_{\mathbb{R}^d} f(x, v) dv$
 - ▶ pair interaction $K(x - y)$, mean-field potential

$$V_f(x) = (K * \varrho_f)(x) = \int_{\mathbb{R}^d} K(x - y) \varrho_f(y) dy$$

- ▶ Vlasov equation

$$\partial_t f + v \cdot \nabla_x f - \nabla V_f \cdot \nabla_v f = 0$$

- Quantum setting: phase space $(x, \mathbf{p}) = (x, -i\hbar\nabla)$, with $\hbar = h/(2\pi)$
 - ▶ density operator $\rho \in \mathcal{L}^\infty(L^2(\mathbb{R}^d))$

$$\rho \geq 0, \quad h^d \text{Tr}(\rho) = 1$$

- ▶ Position density $\varrho_\rho(x) = h^d \rho(x, x)$
- ▶ Hartree(-Fock) equation

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

with mean-field potential $V_\rho = K * \varrho_\rho$

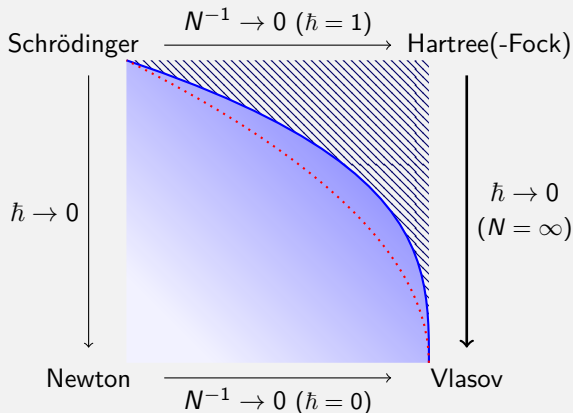
Mean-field and semiclassical limit

Lower densities of bosons and fermions

Higher densities of bosons

$\hbar = N^{-1/3}$

$\hbar = N^{-1/2}$



Weyl quantization and Wigner transform

- Symmetric quantization of operators

$$\rho_f := \int_{\mathbb{R}^{2d}} \widehat{f}(y, v) e^{2i\pi(y \cdot x + w \cdot p)} dy dv$$
$$f_\rho(x, v) := \int_{\mathbb{R}^d} e^{-iy \cdot v / \hbar} \rho(x + \frac{y}{2}, x - \frac{y}{2}) dy$$

- Analogue of the classical kinetic density (see e.g. [Lions–Paul '93])

$$\partial_t f_\rho + v \cdot \nabla_x f_\rho = B_h * f_\rho \xrightarrow{h \rightarrow 0} \nabla V_f \cdot \nabla_v f$$

$$h^d \operatorname{Tr}((A(x) + B(p)) \rho) = \iint_{\mathbb{R}^{2d}} (A(x) + B(v)) f_\rho(x, v) dx dv$$

- But

- ▶ not necessarily positive, Lebesgue norms $L_{x,v}^p$ not preserved ($p \neq 2$)
- ▶ Husimi transform $\widetilde{f}_\rho = \frac{1}{(\pi\hbar)^d} e^{-|z|^2/\hbar} * f_\rho$ positive but worse equation

Classical to quantum dictionary

Classical

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

$$\int_{\mathbb{R}^{2d}} f |v|^n dx dv$$

$$\|f\|_{L^p(\mathbb{R}^{2d})}$$

$$f(z - z_0)$$

$$(f * g)(z') = \int_{\mathbb{R}^{2d}} f(z) g(z' - z) dz$$

$$\nabla_x f = \{-v, f\}, \nabla_v f = \{x, f\}$$

Quantum

$$i\hbar \partial_t \rho = [H_\rho, \rho]$$

$$h^d \text{Tr}(|\rho|^n \rho)$$

$$\|\rho\|_{\mathcal{L}^p} = h^{\frac{d}{p}} \text{Tr}(|\rho|^p)^{\frac{1}{p}}$$

$$T_{z_0} \rho = e^{i(\xi_0 \cdot x - x_0 \cdot p)/\hbar} \rho e^{i(x_0 \cdot p - \xi_0 \cdot x)/\hbar}$$

$$f \star \rho = \int_{\mathbb{R}^{2d}} f(z) T_z \rho dz$$

$$\nabla_x \rho = [\nabla, \rho], \nabla_\xi \rho = \left[\frac{x}{i\hbar}, \rho \right]$$

⇒ Quantum Sobolev norms

$$\|\rho\|_{\dot{W}^{1,p}} = \|\nabla \rho\|_{\mathcal{L}^p} \simeq \|\nabla_x \rho\|_{\mathcal{L}^{1,p}} + \|\nabla_\xi \rho\|_{\mathcal{L}^{1,p}}$$

Quantum Sobolev inequalities

Gagliardo and Bessel semi-norms

$$\|\rho\|_{\dot{\mathcal{W}}^{s,p}}^p := \gamma_{s,p} \int_{\mathbb{R}^{2d}} \frac{h^d \operatorname{Tr}(|T_z \rho - \rho|^p)}{|z|^{2d+sp}} dz \quad s \in (0, 1)$$

$$\|\rho\|_{\dot{\mathcal{H}}^{s,p}} := \left\| (-\Delta)^{s/2} \rho \right\|_{\mathcal{L}^p} \quad s \in [0, 2]$$

with $(-\Delta)^s \rho := \rho_{(-\Delta_z)^s f_\rho}$, that is $\Delta = \Delta_x + \Delta_\xi = \nabla \cdot \nabla$ and

$$(-\Delta)^s \rho = c_s \int_{\mathbb{R}^d} \frac{\rho - T_z \rho}{|z|^{2d+2s}} dz \quad s \in (0, 1)$$

Theorem (LL '22)

Let $s \in [0, 1]$, $1 \leq p \leq q < \infty$ such that $\frac{1}{p} - \frac{1}{q} = \frac{s}{2d}$, then there exists $C_{s,p}$ and $C'_{s,p}$ independent of \hbar such that for any compact operator ρ ,

$$\begin{aligned} \|\rho\|_{\mathcal{L}^q} &\leq C_{s,p} \|\rho\|_{\dot{\mathcal{W}}^{s,p}} \\ \|\rho\|_{\mathcal{L}^q} &\leq C'_{s,p} \|\rho\|_{\dot{\mathcal{H}}^{s,p}} \quad \text{if } p > 1 \end{aligned}$$

Uncertainty for the skew information

In the case $s = 1$,

$$\|\rho\|_{\mathcal{L}^q} \leq C_{d,p} \|\nabla_x \rho\|_{\mathcal{L}^p}^{1/2} \|\nabla_\xi \rho\|_{\mathcal{L}^p}^{1/2} \quad \text{if } \frac{1}{q} = \frac{1}{p} - \frac{1}{2d}$$

Wigner–Yanase skew information: for an operator $A \geq 0$,

$$I_A(\rho) = \frac{1}{2} \text{Tr} \left(|[A, \sqrt{\rho}]|^2 \right)$$

Smaller than the variance $I_A(\rho) \leq \sigma_A(\rho)^2 := \text{Tr} \left(\rho |A - \text{Tr}(\rho A)|^2 \right)$, but Sobolev inequality with $p = 2$ still implies

$$\sqrt{I_x(\rho) I_p(\rho)} \geq \frac{1}{8\pi C_{1,2}^2} \hbar \|\rho\|_{\frac{d}{d-1}}$$

In the case of projection operators $\rho = \rho^2$ in dimension $d = 3$ with $\text{Tr}(\rho) = N$

$$\|[x, \rho]\|_2 \|\nabla, \rho\|_2 \geq \frac{N^{2/3}}{4\pi (\tilde{C}_{1,2}^S)^2}$$

Semiclassical convolution

$$f \star \rho = \int_{\mathbb{R}^{2d}} f(z) T_z \rho \, dz$$

- Convolution inequalities.

- ▶ Young's inequality (Werner '84)
- ▶ Hardy–Littlewood–Sobolev's inequality. Let $(p, q, r) \in (1, \infty)^3$. There exists C independent of \hbar such that for any $f \in L^{q, \infty}$ and $\rho \in \mathcal{L}^r$,

$$\|f \star \rho\|_{\mathcal{L}^p} \leq C \|f\|_{L^{q, \infty}} \|\rho\|_{\mathcal{L}^r} \quad \text{if } 1 + \frac{1}{p} = \frac{1}{q} + \frac{1}{r}$$

- Toeplitz operators (Wick quantization)

$$\tilde{\rho}_f = \frac{1}{h^d} \int_{\mathbb{R}^{2d}} f(z) |\psi_z\rangle \langle \psi_z| \, dz = g_h \star \rho_f, \quad g_h(z) = \frac{1}{(\pi \hbar)^d} e^{-|z|^2/\hbar}$$

$$\|\tilde{\rho}_f\|_{\mathcal{L}^p} \leq \|f\|_{L^p(\mathbb{R}^{2d})}$$

- Sobolev inequalities - idea of the proof: Since $\tilde{\rho} = \tilde{\rho}_{\tilde{f}_\rho}$,

$$\|\rho\|_{\mathcal{L}^q} \leq \|\tilde{f}_\rho\|_{L^q(\mathbb{R}^{2d})} + \|\rho - \tilde{\rho}\|_{\mathcal{L}^q}$$

Quantum optimal transport

- Quantum pseudo-distance [Golse–Mouhot–Paul '16]
 - ▶ Quantum–quantum coupling $\gamma \in \mathcal{C}(\rho, \rho_2) \subset \mathcal{L}^1(L^2(\mathbb{R}^d) \otimes L^2(\mathbb{R}^d))$

$$h^d \operatorname{Tr}_1(\gamma) = \rho_2, \quad h^d \operatorname{Tr}_2(\gamma) = \rho$$

- ▶ Analogue to Monge–Kantorovich–Wasserstein distance

$$W_{2,h}(\rho, \rho_2) = \min_{\gamma \in \mathcal{C}(\rho, \rho_2)} h^{2d} \operatorname{Tr}(\mathbf{c}_h \gamma) \geq 2 d \hbar$$

$$\text{with cost } \mathbf{c}_h \varphi(y_1, y_2) = (|y_1 - y_2|^2 + |\mathbf{p}_1 - \mathbf{p}_2|^2) \varphi(y_1, y_2)$$

- Semiclassical pseudo-distance [Golse–Paul '17]
 - ▶ Semiclassical coupling $\gamma \in \mathcal{C}(f, \rho)$

$$h^d \operatorname{Tr}(\gamma(z)) = f(z), \quad \int_{\mathbb{R}^{2d}} \gamma(z) dz = \rho$$

- ▶ Classical to quantum pseudo-distance

$$W_{2,h}(f, \rho)^2 = \min_{\gamma \in \mathcal{C}(f, \rho)} h^d \int_{\mathbb{R}^{2d}} \operatorname{Tr}(\mathbf{c}_h(z) \gamma(z)) dz \geq d \hbar$$

$$\text{with } \mathbf{c}_h(z) \varphi(y) = (|x - y|^2 + |v - \mathbf{p}|^2) \varphi(y)$$

Application to mean-field and semiclassical limits

- Regular potentials: ∇K Lipschitz

- ▶ If $f \in L^1(|x|^2 + |v|^2)$ is solution of Vlasov and ρ of Hartree [Golse–Paul '17]

$$W_{2,\hbar}(f, \rho) \leq W_{2,\hbar}(f^{\text{in}}, \rho^{\text{in}}) e^{\lambda t} + C(t) \sqrt{\hbar}$$

- ▶ Mean-field limit: similar statements [Golse–Mouhot–Paul '16, Golse–Paul '17]

- Singular potentials: $K(x) = \frac{\pm 1}{|x|^a}$, with $a \in (-1, 1]$ [LL '19 '21]

- ▶ If f solution of Vlasov with $(1 + |v|^n)f^{\text{in}} \in L^1 \cap L^\infty$ and ρ solution of Hartree with $(1 + |\rho|^n)\rho^{\text{in}} \in \mathcal{L}^1 \cap \mathcal{L}^\infty$, there exists $T > 0$ such that

$$W_{2,\hbar}(f, \rho) \leq W_{2,\hbar}(f^{\text{in}}, \rho^{\text{in}})^{c(t)} e^{\lambda(t)} \quad \text{for all } t \in [0, T]$$

- ▶ Also works for Hartree–Fock by [Chong–Lafleche–Saffirio '22]

- *Semiclassical limit - idea of the proof*

- ▶ Propagation of moments and weighted norms
- ▶ Interpolation inequality $\|\varrho_\rho\|_{L^p} \leq \|\rho\|_{\mathcal{L}^r}^\theta \left(h^d \text{Tr}(|\rho|^n \rho) \right)^{1-\theta}$
- ▶ Adapt [Loeper '06] uniqueness estimate

Quantum optimal pseudometrics properties

Theorem (Golse–Mouhot–Paul '16, Golse–Paul '17 '22)

- *Bound by below*

$$W_2(f, \tilde{f}_\rho)^2 \leq W_{2, \hbar}(f, \rho)^2 + d \hbar$$
$$W_2(\tilde{f}_{\rho_1}, \tilde{f}_{\rho_2})^2 \leq W_{2, \hbar}(\rho_1, \rho_2)^2 + 2 d \hbar$$

- *Special case: Toeplitz operators $\rho = \tilde{\rho}_f$*

$$W_{2, \hbar}(f, \tilde{\rho}_g)^2 \leq W_2(f, g)^2 + d \hbar$$
$$W_{2, \hbar}(\tilde{\rho}_f, \tilde{\rho}_g)^2 \leq W_2(f, g)^2 + 2 d \hbar$$

- *Triangle inequalities*

$$W_{2, \hbar}(f, \rho) \leq W_2(f, g) + W_{2, \hbar}(g, \rho)$$
$$W_{2, \hbar}(\rho, \rho_2) \leq W_{2, \hbar}(\rho, g) + W_{2, \hbar}(g, \rho_2)$$

In particular,

$$W_{2, \hbar}(f, \tilde{\rho}_f)^2 = d \hbar \quad \text{and} \quad W_{2, \hbar}(\tilde{\rho}_f, \tilde{\rho}_f)^2 = 2 d \hbar$$

Quantum optimal transport versus Sobolev norms

Theorem (LL '23)

- "Self-distance bound"

$$W_{2,\hbar}(\tilde{f}_\rho, \rho)^2 \leq d \hbar + \hbar^2 \|\nabla \sqrt{\rho}\|_{\mathcal{L}^2}^2$$

$$W_{2,\hbar}(\rho, \rho)^2 \leq 4 d \hbar + 4 \hbar^2 \|\nabla \sqrt{\rho}\|_{\mathcal{L}^2}^2$$

- If $0 \leq \rho, \rho_2 \leq 1$ then

$$\|\rho - \rho_2\|_{\dot{W}^{-1}} < W_{2,\hbar}(\rho, \rho_2) + 2 \sqrt{d \hbar}$$

- If $h^d \operatorname{Tr}((|x|^n + |\mathbf{p}|^n)(\rho + \rho_2))$ is bounded uniformly in \hbar

$$W_{2,\hbar}(\rho, \rho_2) \leq C \|\rho - \rho_2\|_{\dot{W}^{-1,1}}^\theta + \sqrt{2 d \hbar} + \hbar \|\nabla \sqrt{\rho}\|_{\mathcal{L}^2} + \hbar \|\nabla \sqrt{\rho_2}\|_{\mathcal{L}^2}$$

⇒ Small self-distances for thermal states, powers of Toeplitz operators, Slater determinants ...

- Self-distance bound - Idea of proof: Use the coupling

$$\gamma(z) := \rho^{1/2} T_z \rho_{g_h} \rho^{1/2}$$

The case of projection operators

- Slater determinants

- $\rho_N = |\Psi_N\rangle \langle \Psi_N|$ with $Nh^d = 1$ and $\Psi_N(x_1, \dots, x_N) := \frac{1}{\sqrt{N!}} \det(\psi_j(x_k))_{1 \leq j, k \leq N}$
- First marginal is not "semiclassically smooth" [LL '23]

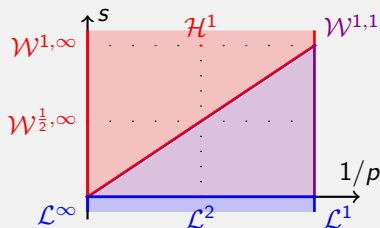
$$\rho_{N:1} = \sum_{j=1}^N |\psi_j\rangle \langle \psi_j| \implies \rho_{N:1}^2 = \rho_{N:1} \text{ and } \rho_{N:1} \notin \mathcal{W}^{s,p}, \quad s > \frac{1}{p}, \quad p > 1$$

- Spectral functions with V nice [Fournais–Mikkelsen '20]

$$\rho_V := \mathbb{1}_{\mathbb{R}_-}(-\hbar^2 \Delta + V) \in \mathcal{W}^{1,1} \implies \|\nabla \rho_V\|_{\mathcal{L}^2} \leq C_V / \sqrt{\hbar}$$

- By the "self-distance bound" for $W_{2,\hbar}$,

$$W_{2,\hbar}(\tilde{f}_\rho, \rho)^2 \leq d \hbar + C_V \hbar$$



Thank you for your attention!

Schatten norm estimates

Theorem (LL, Saffirio '20)

If f is initially sufficiently smooth, ρ a solution of Hartree(-Fock) equation and ρ_f is the Weyl quantization of f , then

$$\|\rho - \rho_f\|_{\mathcal{L}^1} \leq (\|\rho^{\text{in}} - \rho_f^{\text{in}}\|_{\mathcal{L}^1} + C_f(t) \hbar) e^{\lambda_f(t)}$$

Classical case: weak-strong uniqueness

$$\|f_1 - f_2\|_{L^1(\mathbb{R}^6)} \leq \|f_1^{\text{in}} - f_2^{\text{in}}\|_{L^1(\mathbb{R}^6)} \exp\left(C \int_0^T \|\nabla_v f_2\|_{L_x^{3,1} L_v^1} dt\right),$$

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 $V = K * \rho$, we obtain

$$\begin{aligned} \partial_t \int_{\mathbb{R}^{2d}} |f_1 - f_2| dx dv &= - \int_{\mathbb{R}^{2d}} (\rho_1 - \rho_2) \nabla K * \int_{\mathbb{R}^d} \text{sgn}(f_1 - f_2) \nabla_v f_2 dv dx \\ &\leq \|f_1 - f_2\|_{L^1} \left\| \nabla K * \int_{\mathbb{R}^d} |\nabla_v f_2| dv \right\|_{L^\infty}, \end{aligned}$$

Mean-field limit

Theorem (Chong–LL–Saffirio '21)

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

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

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

- Other \mathcal{L}^p estimates possible with $p > 1$ and other rates
- Schrödinger to Vlasov?
 - ▶ For $a < 1/2$ and "regular" mixed states
Example: thermal states [Chong–LL–Saffirio '21]
 - ▶ Pure states cannot be that regular!

Main steps of the proof of the mean-field

- Uniform-in- \hbar regularity for the Hartree–Fock equation
 - ▶ Let $m = 1 + |\rho|^n$ with $n \geq 3$ and ρ such that

$$\rho^{\text{in}}, \sqrt{\rho^{\text{in}}} \in \mathcal{L}^\infty(m) \cap \mathcal{W}^{1,2}(m) \cap \mathcal{W}^{1,4}(m).$$

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

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

- Mean-Field

- ▶ Purification of mixed states: take an appropriate square root

$$\rho_N \in \mathcal{L}^1(\mathcal{F}(L^2)) \rightarrow \nu_N \in \mathcal{L}^2(\mathcal{F}(L^2)) \text{ such that } |\nu_N|^2 = \rho_N$$

- ▶ Identify the kernel of the operator with a function of a double Fock space

$$\nu_N \in \mathcal{L}^2(\mathcal{F}(L^2)) \rightarrow \Psi_{\rho_N} \in \mathcal{F}(L^2 \oplus L^2)$$

- ▶ Bogoliubov transformation $R_t = R_{\rho_t}$

$$\Psi_t = R_t^* e^{itL_N} R_t \Psi^{\text{in}}$$

- ▶ Number of particles outside the Bogoliubov state $\rho_{N,\rho}$ such that

$$\Psi_{\rho_{N,\rho}} = R_t^* e^{itL_N} R_t \Omega$$

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