Limiting dynamics of large quantum systems and Egorov-type theorems

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Overview

Part I:

- Some History: Egorov's theorem (1)
- The mean-field limit of classical many-body dynamics revisited (2)
- Quantum spin systems: large-spin limit (3) & continuum limit (4)
- Bose (5) and Fermi (6) gases with Coulomb interaction: the mean-field limit

Part II:

- Bose gases: Sketch of proof of convergence to the mean-field limit

(1) Some history: Egorov's theorem

Classical mechanics:

- Phase space $\Gamma = \mathbb{R}^{2f}$
- Observables $\mathfrak{A}$ = Smooth functions on Γ
- Hamilton function $H \in \mathfrak{A} \quad \Rightarrow \quad$ 1-parameter group on $\mathfrak{A}$: $\quad A \mapsto A \circ \phi_H^t$

Quantum mechanics:

- Observables $\widehat{\mathfrak{A}} = \mathcal{B}(L^2(\mathbb{R}^f))$
- Weyl quantisation $\widehat{(\,\cdot\,)}_\hbar : \mathfrak{A} \to \widehat{\mathfrak{A}}$
- Hamiltonian $\widehat{H}_\hbar \quad \Rightarrow \quad$ 1-parameter group on $\widehat{\mathfrak{A}}$: $\quad \mathbf{A} \;\mapsto\; \mathrm{e}^{\mathrm{i}t\widehat{H}_\hbar/\hbar}\,\mathbf{A}\,\mathrm{e}^{-\mathrm{i}t\widehat{H}_\hbar/\hbar}$

Theorem (Egorov, 1969). For all $A \in \mathfrak{A}$ and $t \in \mathbb{R}$,

$$(\widehat{A \circ \phi_H^t})_\hbar \;=\; \mathrm{e}^{\mathrm{i}t\widehat{H}_\hbar/\hbar}\,\widehat{A}_\hbar\,\mathrm{e}^{-\mathrm{i}t\widehat{H}_\hbar/\hbar} + R_\hbar(t)\,,$$

where $\|R_\hbar(t)\| \to 0$ as $\hbar \to 0$.

(2) Vlasov equation as the mean-field limit of N-body dynamics

- Density on one-particle phase space $f = f_t(x, v)$, $\quad x, v \in \mathbb{R}^3$
- Vlasov equation:

$$\partial_t f + v \cdot \nabla_x f - \frac{1}{m} \nabla U[f] \cdot \nabla_v f \;=\; 0$$

$$U[f](x) \;=\; V(x) + \int \mathrm{d}y \, W(x-y) \int \mathrm{d}v \; f(x, v)$$

- Dynamics of N classical particles $x_1(t), \ldots, x_N(t)$

$$m \ddot{x}_i \;=\; -\nabla V(x_i) - \frac{1}{N} \sum_{j \neq i} \nabla W(x_i - x_j)$$

- Classical result (Braun & Hepp, Neunzert):

$$f_t(x, v) \;=\; \operatorname*{w-lim}_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} \delta(x - x_i(t)) \delta(v - \dot{x}_i(t))$$

The Hamiltonian structure of the Vlasov equation

- Consider $f \in L^1(\mathbb{R}^6)$ and write $f(x,v) = |\alpha(x,v)|^2$
- Phase space $\Gamma = L^2(\mathbb{R}^6)$ with canonical coordinates $\alpha(x,v), \overline{\alpha}(x,v)$
- Poisson bracket $$\{\alpha(x,v), \alpha(y,w)\} = \{\overline{\alpha}(x,v), \overline{\alpha}(y,w)\} = 0$$ $$\{\alpha(x,y), \overline{\alpha}(y,w)\} = \mathrm{i}\delta(x-y)\delta(v-w)$$
- Hamilton function H on Γ: $$H(\alpha) := \mathrm{i}\int \mathrm{d}x\,\mathrm{d}v\;\bar{\alpha}(x,v)\left[-v\cdot\nabla_x + \frac{1}{m}\nabla V(x)\cdot\nabla_v\right]\alpha(x,v)$$ $$+\frac{\mathrm{i}}{m}\int \mathrm{d}x\,\mathrm{d}v\;\bar{\alpha}(x,v)\left[\int \mathrm{d}y\,\mathrm{d}w\;\nabla W(x-y)\,|\alpha(y,w)|^2\right]\cdot\nabla_v\alpha(x,v)\,.$$
- Hamiltonian equations of motion $\dot{\alpha}(x,v) = \{H, \alpha(x,v)\} \quad \Longleftrightarrow \quad$ Vlasov

Wick quantisation of the Vlasov equation

- Quantum theory on bosonic Fock space $\mathcal{F}$ over $L^2(\mathbb{R}^6)$
- Quantisation $\widehat{(\,\cdot\,)}_N$: replace $\begin{array}{c} \alpha(x,v) \mapsto \widehat{\alpha}_N(x,v) \\ \overline{\alpha}(x,v) \mapsto \widehat{\alpha}^*_N(x,v) \end{array}$ & Wick order
- CCR:

$$\begin{aligned} \big[\widehat{\alpha}_N(x,v), \widehat{\alpha}_N(y,w)\big] &= \big[\widehat{\alpha}^*_N(x,v), \widehat{\alpha}^*_N(y,w)\big] = 0 \\ \big[\widehat{\alpha}_N(x,y), \widehat{\alpha}^*_N(y,w)\big] &= \frac{1}{N}\delta(x-y)\delta(v-w) \end{aligned}$$

- N^{-1}: deformation parameter of quantisation $\widehat{(\,\cdot\,)}_N$

$$\big[\widehat{A}_N, \widehat{B}_N\big] = \frac{N^{-1}}{\mathrm{i}}\widehat{\{A,B\}}_N + O(N^{-2})$$

Dynamics of the quantised Vlasov equation

- State in Fock space: $\Phi = (\Phi^{(n)})_{n\in\mathbb{N}} \in \mathcal{F}$ with wave functions

  $\Phi^{(n)} \;=\; \Phi^{(n)}(x_1, v_1, \ldots, x_n, v_n)$

- Dynamics given by Schrödinger equation $\quad \mathrm{i}N^{-1}\partial_t\Phi \;=\; \widehat{H}_N\Phi$

- Dynamics of probability density $\rho^{(n)} \;:=\; |\Phi^{(n)}|^2$

$$\partial_t\rho^{(n)} \;=\; \sum_{i=1}^{n}\Big[-v_i\cdot\nabla_{x_i} + \frac{1}{m}\nabla V(x_i)\cdot\nabla_{v_i}\Big]\rho^{(n)} + \frac{1}{N}\sum_{1\leqslant i\neq j\leqslant n}\frac{1}{m}\nabla W(x_i - x_j)\cdot\nabla_{v_i}\rho^{(n)}$$

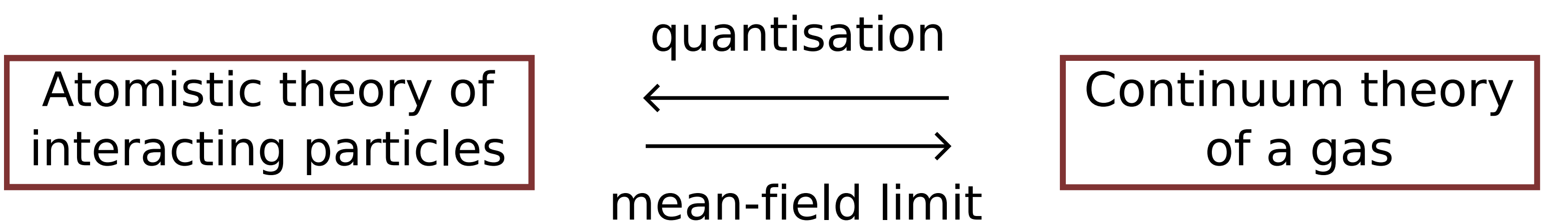
$=$ Liouville equation corresponding to classical n-body dynamics

$$\partial_t x_i \;=\; v_i\,, \qquad m\,\partial_t v_i \;=\; -\nabla V(x_i) - \frac{1}{N}\sum_{j\neq i}\nabla W(x_i - x_j)$$

Moral of the story

- Quantisation of the Vlasov equation $\Longleftrightarrow$ classical n-body dynamics

- Atomism arises as a quantisation of a continuum theory



- Egorov-type theorem for the mean-field limit:

$$(\widehat{A\circ\phi_H^t})_N\Big|_{\mathcal{F}^{(N)}} = \mathrm{e}^{\mathrm{i}tN\widehat{H}_N}\,\widehat{A}_N\,\mathrm{e}^{-\mathrm{i}tN\widehat{H}_N}\Big|_{\mathcal{F}^{(N)}} + R_N(t)\,,$$

where $\|R_N(t)\| \to 0$ as $N \to \infty$.

(3) Spin systems: classical spins on a lattice

- Classical spin system on lattice $\Lambda \subset \mathbb{Z}^d$ with phase space $\Gamma_\Lambda = \prod_{x\in\Lambda} \mathbb{S}^2$
- Γ_Λ is symplectic with Poisson bracket $\{M_i(x), M_i(y)\} = -\varepsilon_{ijk}\,\delta(x,y)\,M_k(x)$
- Observables: $A \in \mathfrak{A}_\Lambda = C(\Gamma_\Lambda)$
- Potential: $V \,:\, \alpha \in \mathbb{N}^{\mathbb{Z}^d \times \{1,2,3\}} \longmapsto V(\alpha) \in \mathbb{R}$
- Hamilton function: $H_\Lambda(M) = \sum_{\alpha\in\mathbb{N}^{\Lambda\times\{1,2,3\}}} V(\alpha)\, M^\alpha$
- Require $\|V\|_r := \sum_{n\in\mathbb{N}} \sup_{x\in\mathbb{Z}^d} \sum_{\alpha\,:\,|\alpha|=n,\,|\alpha(x)|>0} |V(\alpha)|\,\mathrm{e}^{rn} < \infty$

Dynamics of classical spins

- **Lemma.** For finite Λ, H_Λ is well-defined, and the Hamiltonian equation of motion is globally well-posed for all (possible infinite) Λ.

- The spins precess: $|M(t,x)| = |M(0,x)|$

- This generalises to time-dependent potentials $V(t,\alpha)$

- Example: $H_\Lambda(M) = -\sum_{x\in\Lambda} h(t,x)\cdot M(x) - \frac{1}{2}\sum_{x,y\in\Lambda} J(x,y)\, M(x)\cdot M(y)$

  Equation of motion:

$$\partial_t M(t,x) = M(t,x) \wedge \left[h(t,x) + \sum_y J(x,y) M(t,y)\right]$$

(Landau-Lifschitz)

Quantum spins & quantisation

- Quantum spins of magnitude s on Λ: Hilbert space $\mathcal{H}_\Lambda \;=\; \bigotimes_{x\in\Lambda} \mathbb{C}^{2s+1}$
- Observables: $\widehat{\mathfrak{A}}_\Lambda \;=\; \mathcal{B}(\mathcal{H}_\Lambda)$
- Spins (rescaled generators of $\mathrm{su}(2)$ in s-representation): $\widehat{S}_i(x) \in \mathcal{B}(\mathcal{H}_\Lambda)$
- Commutation relations: $\big[\widehat{S}_i(x), \widehat{S}_j(y)\big] \;=\; \frac{\mathrm{i}}{s}\varepsilon_{ijk}\,\delta(x,y)\widehat{S}_k(x)$
- Quantisation $\widehat{(\,\cdot\,)}$ of a polynomial classical observable $A \in \mathfrak{P}_\Lambda \mapsto \widehat{A} \in \widehat{\mathfrak{A}}_\Lambda$ defined by replacement $M_i(x) \mapsto \widehat{S}_i(x)$ & Wick ordering: $M_+ \cdots M_z \cdots M_-$
- s^{-1}: deformation parameter of $\widehat{(\,\cdot\,)}$: $\big[\widehat{A}, \widehat{B}\big] \;=\; \frac{s^{-1}}{\mathrm{i}}\widehat{\{A,B\}} + O(s^{-2})$
- Quantum dynamics given by propagator $U_\Lambda(t) \;=\; \mathrm{e}^{-\mathrm{i}ts\widehat{H}_\Lambda}$

The large-spin limit: a Egorov-type result

Denote by α_Λ^t ($\widehat{\alpha}_\Lambda^t$) the classical (quantum) evolution on observables.

Theorem. Let $A \in \mathfrak{P}_\Lambda$ and $\varepsilon > 0$. Then there exists $A(t) \in \mathfrak{P}_\Lambda$ such that

$$\sup_{t\in\mathbb{R}} \left\|\alpha_\Lambda^t A - A(t)\right\|_\infty \leqslant \varepsilon\,, \qquad \left\|\widehat{\alpha}_\Lambda^t \widehat{A} - \widehat{A(t)}\right\| \leqslant \varepsilon + \frac{C(\varepsilon, A, t)}{s}\,.$$

Comments:

- Thermodynamic limit $\Lambda \nearrow \mathbb{Z}^d$: $\quad \overset{\#}{\alpha}{}_\Lambda^t \to \overset{\#}{\alpha}{}^t \quad$ and the same statement holds.

- Take expectation in coherent spin states: a more "down-to-earth" statement.

(4) A continuum theory of spins

- $\Lambda \subset \mathbb{R}^d$ bounded and open
- Configuration of classical spins: (measurable) function $M : \Lambda \to \mathbb{S}^2$
- $\Gamma_\Lambda = \{M\}$ is symplectic: $\{M_i(x), M_j(y)\} = -\mathrm{i}\,\varepsilon_{ijk}\,\delta(x-y)\,M_k(x)$
- Good class of observables given by symmetric functions $f = f_{i_1 \dots i_p}(x_1, \dots, x_p)$:

$$M_\Lambda(f) := \sum_{i_1,\dots,i_p} \int \mathrm{d}x_1 \cdots \mathrm{d}x_p \, f_{i_1 \dots i_p}(x_1, \dots, x_p)\, M_{i_1}(x_1) \cdots M_{i_p}(x_p)$$

- Generate a polynomial Abelian algebra $\mathfrak{P}_\Lambda$

Dynamics of the continuum spin system

- Family of real potentials $V = (V^{(n)})_{n\in\mathbb{N}}$ with $V^{(n)} = V^{(n)}_{i_1\dots i_n}(x_1,\dots,x_n)$
- Hamilton function $H_\Lambda = \sum_{n\in\mathbb{N}} M_\Lambda(V^{(n)})$
- Natural assumptions on $V \implies$ Hamiltonian equation of motion is globally well-posed & $|M(t,x)| = |M(0,x)|$
- Example: $H_\Lambda = -\int_\Lambda \mathrm{d}x\, h(t,x)\cdot M(x) - \frac{1}{2}\int_{\Lambda\times\Lambda} \mathrm{d}x\,\mathrm{d}y\; J(x,y)\, M(x)\cdot M(y)$

$$\implies \partial_t M(t,x) = M(t,x)\wedge\left[h(t,x) + \int_\Lambda \mathrm{d}y\; J(x,y) M(t,y)\right]$$

(Landau-Lifschitz)

A system of quantum spins on a fine lattice

- Lattice constant $h > 0$ $\rightsquigarrow$ lattice $\Lambda^{(h)} := h\mathbb{Z}^d \cap \Lambda$
- Spins of fixed magnitude s on $\mathcal{H}_\Lambda^{(h)} = \bigotimes_{x \in \Lambda^{(h)}} \mathbb{C}^{2s+1}$
- Observables: $\widehat{\mathfrak{A}}_\Lambda = \mathcal{B}(\mathcal{H}_\Lambda)$
- Rescaled spin generators: $\left[\widehat{S}_i(x), \widehat{S}_j(y)\right] = \mathrm{i}\,\frac{h^d}{s}\,\varepsilon_{ijk}\,\delta(x,y)\,\widehat{S}_k(x)$
- Good observables given by:

$$\widehat{S}_\Lambda(f) := \sum_{i_1,\ldots,i_p} \sum_{x_1,\ldots,x_p \in \Lambda^{(h)}} f_{i_1 \ldots i_p}(x_1,\ldots,x_p)\widehat{S}_{i_1}(x_1)\cdots\widehat{S}_{i_p}(x_p)$$

Quantisation & continuum limit

- Quantisation $A \in \mathfrak{P}_\Lambda \to \widehat{A} \in \widehat{\mathfrak{A}}_\Lambda$ defined by $M_\Lambda(f) \mapsto \widehat{S}_\Lambda(f)$ & Wick ordering
- $h^d s^{-1}$: deformation parameter of $\widehat{(\,\cdot\,)}$: $\quad [\widehat{A}, \widehat{B}] \;=\; \dfrac{h^d s^{-1}}{\mathrm{i}} \widehat{\{A, B\}} + O\big((h^d s^{-1})^2\big)$
- Quantum dynamics given by propagator $\quad U_\Lambda(t) \;=\; \mathrm{e}^{-\mathrm{i} s h^{-d} t \widehat{H}_\Lambda}$

Theorem. Let $A \in \mathfrak{P}_\Lambda$ and $\varepsilon > 0$. Then there exists $A(t) \in \mathfrak{P}_\Lambda$ such that

$$\sup_{t \in \mathbb{R}} \big\|\alpha_\Lambda^t A - A(t)\big\|_\infty \;\leqslant\; \varepsilon\,, \qquad \big\|\widehat{\alpha}_\Lambda^t \widehat{A} - \widehat{A(t)}\big\| \;\leqslant\; \varepsilon + C(\varepsilon, A, t)\, h^d s^{-1}\,.$$

Same comments as before.

(5) Quantum Bose gas with mean-field scaling

N bosons with mean-field scaling:

- Hamiltonian $H_N = -\sum_{i=1}^{N} \Delta_i + \frac{1}{N} \sum_{i<j} w(x_i - x_j)$ on $L^2(\mathbb{R}^3)^{\otimes_+ N}$
- Dynamics: $\mathrm{i}\partial_t \Psi_{N,t} = H_N \Psi_{N,t}$
- Start in a product state: $\Psi_{N,t=0} = \psi^{\otimes N}$, $\quad \psi \in H^1(\mathbb{R}^3)$
- ψ_t satisfies the Hartree equation

$$\mathrm{i}\partial_t \psi_t \;=\; -\Delta \psi_t + (w * |\psi_t|^2)\psi_t\,, \qquad \psi_{t=0} = \psi$$

- One expects $\Psi_{N,t} \approx \psi_t^{\otimes N}$ for large N

The mean-field limit with Coulomb interaction: previous results

p-particle marginals: $\gamma_{N,t}^{(p)} := \mathrm{Tr}_{p+1,\dots,N} |\Psi_{N,t}\rangle\langle\Psi_{N,t}|$

Error between microscopic and mean-field marginals:

$$R_{N,t}^{(p)} := \mathrm{Tr}\left|\gamma_{N,t}^{(p)} - |\psi_t\rangle\langle\psi_t|^{\otimes p}\right|$$

Set $w(x) = |x|^{-1}$ (Coulomb)

Theorem (Erdős & Yau, 2001). $\lim_{N\to\infty} R_{N,t}^{(p)} = 0$

Theorem (Rodnianski & Schlein, 2007). $R_{N,t}^{(p)} \leqslant C\frac{\mathrm{e}^{Kt}}{\sqrt{N}}$

Formulation in terms of Heisenberg-picture observables

Fock space $\mathcal{F} = \bigoplus_{n \in \mathbb{N}} \mathcal{F}^{(n)} = \bigoplus_{n \in \mathbb{N}} L^2(\mathbb{R}^3)^{\otimes_+ n}$

Creation and annihilation operators $\widehat{\psi}^*$, $\widehat{\psi}$. Rescale by $1/\sqrt{N} \;\Rightarrow\; \widehat{\psi}^*_N$, $\widehat{\psi}_N$

CCR: $[\widehat{\psi}^*_N(x), \widehat{\psi}^*_N(y)] = [\widehat{\psi}_N(x), \widehat{\psi}_N(y)] = 0\,, \quad [\widehat{\psi}_N(x), \widehat{\psi}^*_N(y)] = \frac{1}{N}\,\delta(x-y)$

Second quantisation: $a^{(p)}$ on $\mathcal{F}^{(p)} \quad \Longrightarrow \quad \widehat{\mathrm{A}}_N(a^{(p)})$ on $\mathcal{F}$

$$\widehat{\mathrm{A}}_N(a^{(p)}) := \int \prod_{j=1}^{p} \mathrm{d}x_j\, \widehat{\psi}^*_N(x_j)\, a^{(p)}(x_1, \dots, x_p; y_1, \dots, y_p) \prod_{j=1}^{p} \mathrm{d}y_j\, \widehat{\psi}_N(y_j)$$

Hamiltonian $\widehat{H}_N := \widehat{\mathrm{A}}_N(-\Delta) + \frac{1}{2}\widehat{\mathrm{A}}_N(W)$, where $W = |x_1 - x_2|^{-1}$

$$N\widehat{H}_N\Big|_{\mathcal{F}^{(N)}} = H_N$$

Heisenberg evolution of p-particle observable: $\mathrm{e}^{\mathrm{i}tN\widehat{H}_N}\,\widehat{\mathrm{A}}_N(a^{(p)})\,\mathrm{e}^{-\mathrm{i}tN\widehat{H}_N}$

Hartree as a classical Hamiltonian equation & quantisation

Classical phase space: $\Gamma = H^1(\mathbb{R}^3)$ with Poisson bracket

$$\{\psi(x), \psi(y)\} \;=\; \{\bar\psi(x), \bar\psi(y)\} \;=\; 0\,, \qquad \{\psi(x), \bar\psi(y)\} \;=\; \mathrm{i}\delta(x-y)$$

Polynomial functions on phase space

$$\mathrm{A}(a^{(p)})(\psi) \;:=\; \int \prod_{j=1}^{p} \mathrm{d}x_j\, \bar\psi(x_j)\, a^{(p)}(x_1,\dots,x_p; y_1,\dots,y_p) \prod_{j=1}^{p} \mathrm{d}y_j\, \psi(y_j)$$

Hamiltonian $H \;:=\; \mathrm{A}(-\Delta) + \dfrac{1}{2}\mathrm{A}(W)$ flow $\phi^t : \Gamma \to \Gamma$

Hamiltonian equation of motion $=$ Hartree equation

Wick quantisation $\widehat{(\,\cdot\,)}_N$: replace $\bar\psi, \psi$ with $\widehat\psi_N^*, \widehat\psi_N$ & Wick order

Mean-field limit

Theorem. Let $a^{(p)}$ be a bounded p-particle operator. Then

$$\left\| \left(\mathrm{A}(a^{(p)}) \circ \phi^t \right)\widehat{\ }_N - \mathrm{e}^{\mathrm{i}tN\widehat{H}_N}\, \widehat{\mathrm{A}}_N(a^{(p)})\, \mathrm{e}^{-\mathrm{i}tN\widehat{H}_N} \Big|_{\mathcal{F}^{(N)}} \right\| \to 0$$

as $N \to \infty$.

Corollary. $\lim_{N\to\infty} R_{N,t}^{(p)} = 0$ (Erdős & Yau).

Proof. Take expectation in state $\psi^{\otimes N}$.

(6) Quantum Fermi gase with low density mean-field scaling

N fermions with low density mean-field scaling:

- Hamiltonian $H_N = -\sum_{i=1}^{N} \Delta_i + \frac{1}{N} \sum_{i<j} w(x_i - x_j)$ on $L^2(\mathbb{R}^3)^{\otimes -N}$
- Initial state described by an orthonormal sequence $\Phi_N = (\varphi_1, \ldots, \varphi_N)$:

  Slater determinant $\Psi_{N,0} = \varphi_1 \wedge \cdots \wedge \varphi_N$
- Dynamics: $\mathrm{i}\partial_t \Psi_{N,t} = H_N \Psi_{N,t}$
- One expects that $\Psi_{N,t} \approx \varphi_1(t) \wedge \cdots \wedge \varphi_N(t)$, where

$$\mathrm{i}\partial_t \varphi_i = h\varphi_i + \frac{1}{N} \sum_{j=1}^{N} (w * |\varphi_j|^2)\varphi_i - \frac{1}{N} \sum_{j=1}^{N} (w * (\varphi_i \bar{\varphi}_j))\varphi_j$$

(Hartree-Fock)

Mean-field limit for Fermi gas

Set

$$\Gamma_N^{(p)}(t) \;:=\; \mathrm{Tr}_{p+1\ldots N}\Big(\mathrm{e}^{-\mathrm{i}tH_N}\,|\varphi_1\wedge\cdots\wedge\varphi_N\rangle\langle\varphi_1\wedge\cdots\wedge\varphi_N|\,\mathrm{e}^{\mathrm{i}tH_N}\Big)$$

and

$$\tilde{\Gamma}_N^{(p)}(t) \;:=\; \mathrm{Tr}_{p+1\ldots N}\Big(|\varphi_1(t)\wedge\cdots\wedge\varphi_N(t)\rangle\langle\varphi_1(t)\wedge\cdots\wedge\varphi_N(t)|\Big)$$

Theorem. Let $t\in\mathbb{R}$, $p\in\mathbb{N}$ and $w(x)=|x|^{-1}$. Then

$$\mathrm{Tr}\left|\Gamma_N^{(p)}(t)-\tilde{\Gamma}_N^{(p)}(t)\right| \;\to\; 0\,, \qquad N\to\infty\,.$$

Previously proven by Bardos, Golse, Gottlieb and Mauser for bounded w.

Remark. The limit $N\to\infty$ of $\Gamma_N^{(p)}(t)$ does not exist in $\mathrm{Tr}|\cdot|$:

$\lim_{N\to\infty}\|\Gamma_N^{(p)}(t)\|=0$ but $\mathrm{Tr}\,\Gamma_N^{(p)}(t)=1\,.$