From the Hartree–Fock dynamics to the Vlasov equation

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Consider a system of N interacting fermions with wave function $\psi_N \in L^2_a(\mathbb{R}^{3N})$.

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General goal

switch off the external potential and study the dynamics of the low energy states

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Solution $\psi_{N,t} = e^{-iH_N t}\psi_N$, but N is huge $\Longrightarrow$ look for scaling regimes in which the evolution can be well approx. by an **effective dynamics**.

Fermionic mean-field scaling

Fix λ such that interaction and kinetic energy are of the same order:

$$E_{\mathrm{int}} = \langle \psi_N, \lambda \sum_{i<j}^{N} V(x_i - x_j)\psi_N \rangle \sim \lambda N^2$$

$$E_{\mathrm{kin}} = \langle \psi_N, \sum_{j=1}^{N} -\Delta_{x_j} \psi_N \rangle \sim N^{5/3}$$

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Relevant time scale: $N^{-1/3}$ (typical velocity per particle $\sim N^{1/3}$).
Rescaling time

$$iN^{1/3}\partial_t \psi_{N,t} = (\sum_{j=1}^{N} -\Delta_{x_j} + N^{-1/3}\sum_{i<j}^{N} V(x_i - x_j))\psi_{N,t}\,.$$

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Let

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

and multiplying by ε^2:

$$i\varepsilon\partial_t\psi_{N,t} = \Big(\sum_{j=1}^{N} -\varepsilon^2\Delta_{x_j} + \frac{1}{N}\sum_{i<j}^{N} V(x_i - x_j)\Big)\psi_{N,t}$$

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The mean-field scaling is naturally linked with a **semiclassical limit**

Effective equations

Let $\gamma^{(1)}_{N,t} = N \operatorname{tr} |\psi_{N,t}\rangle\langle\psi_{N,t}|$ be the one-particle density matrix of $\psi_{N,t}$.

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$$\gamma^{(1)}_{N,0} \simeq \omega_N \text{ (minimiser of the Hartree-Fock energy functional)}$$

$$\Downarrow \;\; N \gg 1$$

$\gamma^{(1)}_{N,t} \simeq \omega_{N,t}$, solution of the **Hartree-Fock equation**

$$i\varepsilon\partial_t\omega_{N,t} = \left[-\varepsilon^2\Delta + V * \rho_t - X_t, \omega_{N,t}\right],$$

where $\rho_t(x) := \frac{1}{N}\omega_{N,t}(x;x)$ and $X_t(x;y) = \frac{1}{N}V(x-y)\,\omega_{N,t}(x;y)$.

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As $N \to \infty$?

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The Wigner transform of $\omega_{N,t}$

$$W_{N,t}(x,v) = \frac{\varepsilon^3}{(2\pi)^3}\int dy\, \omega_{N,t}(x+\varepsilon\frac{y}{2}; x-\varepsilon\frac{y}{2})\, e^{-iv\cdot y}$$

for $N \to \infty$ solves the Vlasov equation

$$\partial_t W_t(x,v) + v\cdot\nabla_x W_t(x,v) = \nabla(V*\rho_t)(x)\cdot\nabla_v W_t(x,v)$$

Known results

- ⋆ MBQ dynamics $\to$ Vlasov:
  Narnhofer and Sewell (1981), Spohn (1981).
- ⋆ MBQ dynamics $\to$ Hartree or Hartree–Fock:
  - Elgart, Erdös, Schlein, Yau (2004): mean–field + semiclassical scaling; analytic V, short times.
  - Benedikter, Porta and Schlein (2013): weaker assumption on V, effective estimate on the rate of convergence $\forall\ t$, zero temperature.
  - Petrat, Pickl (2014): similar result with a different method.
  - Benedikter, Porta, Jakšić, S. and Schlein (2015): positive temperature.
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- Golse, Paul (2015) ∇V Lipschitz continuous, explicit estimates on the rate of convergence.

Notations

ω_N sequence of reduced densities on $L^2(\mathbb{R}^3)$

$$\operatorname{tr}\omega_N = N\,, \quad 0 \le \omega_N \le 1$$

Wigner trans.

W_N

Vlasov eq.n

Hatree eq.n

$\tilde{W}_{N,t}$

Weyl quantization

$\omega_{N,t}$

$$i\,\varepsilon\,\partial_t\,\omega_{N,t} = [\,h(t)\,,\,\omega_{N,t}\,]$$

$$h(t) = -\varepsilon^2\,\Delta + V * \rho_t$$

$\tilde{\omega}_{N,t}$

$$i\,\varepsilon\,\partial_t\,\tilde{\omega}_{N,t} = [\,-\varepsilon^2\,\Delta\,,\,\tilde{\omega}_{N,t}\,] + A_t$$

$$A_t(x;y) = \nabla(V * \tilde{\rho}_t)\left(\frac{x+y}{2}\right)\cdot(x-y)\,\tilde{\omega}_{N,t}(x;y)$$

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$$\|W_N\|_{H^s_a} = \sum_{\beta\leq s}\int(1+x^2+v^2)^a|\nabla^\beta W_N(x,v)|^2 dx\,dv$$

Statement of the results: mixed states

Theorem 1 (Benedikter, Porta, S., Schlein)

Let $V \in \mathcal{W}^{2,\infty}(\mathbb{R}^3)$ *and* $\|W_N\|_{H^5_4} < C$.
Then there exists $C = C(\|V\|_{\mathcal{W}^{2,\infty}}, \sup_N \|W_N\|_{H^2_4}) > 0$ *such that*

$$\mathrm{tr}\,|\omega_{N,t} - \tilde{\omega}_{N,t}| \leq CN\varepsilon \exp(C \exp(C|t|))[1 + \sum_{k=1}^{3} \varepsilon^k \sup_N \|W_N\|_{H^{k+2}_4}] .$$

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Relax regularity assumptions on the initial data

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Relax regularity assumptions on the initial data

Theorem 2 (Benedikter, Porta, S., Schlein)

Let $V \in L^1(\mathbb{R}^3)$*such that* $A = \int |\hat{V}(p)|\,(1 + |p|^2)\,dp < \infty$ *and* $\|W_N\|_{H^2_4} < C$.
Then there exists $C = C(\|W_N\|_{H^2_4}, A) > 0$ *such that*

$$\|\omega_{N,t} - \tilde{\omega}_{N,t}\|_{\mathrm{HS}} \leq C\sqrt{N}\varepsilon \exp(C \exp(C|t|)) \,.$$

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$$\|\omega_{N,t} - \tilde{\omega}_{N,t}\|_{\mathrm{HS}} \leq C\sqrt{N}\varepsilon \exp(C \exp(C|t|)).$$

Equivalently,

$$\|W_{N,t} - \tilde{W}_{N,t}\|_{L^2} \leq C\varepsilon \exp(C \exp(C|t|)).$$

Statement of the results: pure states

At zero temperature we prove convergence for the expectation of a class of semiclassical observables, functions of x and $-i\varepsilon\nabla$.

Theorem 3 (Benedikter, Porta, S., Schlein)

Let $V \in L^1(\mathbb{R}^3)$ be such that $\int |\hat{V}(p)|(1+|p|^3)\, dp < \infty$.
Let ω_N satisfy

$$\mathrm{tr}\, |[x\,,\, \omega_N]| \leq CN\varepsilon\,, \quad \mathrm{tr}\, |[\varepsilon\nabla\,,\, \omega_N]| \leq CN\varepsilon\,.$$

Let $W_N \in L^1(\mathbb{R}^3 \times \mathbb{R}^3)$ be such that $\|W_N\|_{\mathcal{W}^{1,1}} \leq C$.
Then there exists $C > 0$ such that

$$|\mathrm{tr}\; e^{ip\cdot x + \varepsilon q \cdot \nabla}(\omega_{N,t} - \tilde{\omega}_{N,t})| \leq CN\varepsilon\, (1 + |p| + |q|)^2 \exp(C|t|)\,,$$

$\forall\ p, q \in \mathbb{R}^3\,,\ \forall\ t \in \mathbb{R}\,.$

Strategy: trace norm convergence

Compare $\omega_{N,t}$ and $\tilde{\omega}_{N,t}$ via Gronwall inequality

Step 1.

$$i\varepsilon\partial_t(\omega_{N,t} - \tilde{\omega}_{N,t}) = [-\varepsilon^2\Delta\,,\,(\omega_{N,t} - \tilde{\omega}_{N,t})] + \dots$$

how to get rid of the kinetic term?

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how to get rid of the kinetic term?

Define a unitary operator $\mathcal{U}$,

$$\begin{cases} i\,\varepsilon\,\partial_t\mathcal{U}(t) = h(t)\mathcal{U}(t)\,, \\ \mathcal{U}(0) = 1\,. \end{cases}$$

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Then

$$\begin{aligned} i\,\varepsilon\,\partial_t\mathcal{U}^*(t)\,&(\omega_{N,t} - \tilde{\omega}_{N,t})\mathcal{U}(t) \\ &= -\mathcal{U}^*(t)\,[h(t), \omega_{N,t} - \tilde{\omega}_{N,t}]\mathcal{U}(t) \\ &\quad + \mathcal{U}^*(t)\,([h(t), \omega_{N,t} - \tilde{\omega}_{N,t}] + [V * \rho_t, \tilde{\omega}_{N,t}] - A_t)\,\mathcal{U}(t) \\ &= \mathcal{U}^*(t)\,([V * (\rho_t - \tilde{\rho}_t), \tilde{\omega}_{N,t}] + [V * \tilde{\rho}_t, \tilde{\omega}_{N,t}] - A_t)\,\mathcal{U}(t)\,. \end{aligned}$$

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where

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B_t(x;y)=[V*\tilde{\rho}_t(x)-V*\tilde{\rho}_t(y)-\nabla(V*\tilde{\rho}_t)\left(\frac{x+y}{2}\right)\cdot(x-y)]\tilde{\omega}_{N,t}(x;y)
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Step 2.
Integrate in time and take the trace norm:

$$
\begin{aligned}
\|\omega_{N,t} - \tilde{\omega}_{N,t}\|_{\mathrm{Tr}} \leq \|\omega_{N,0} - \tilde{\omega}_{N,0}\|_{\mathrm{Tr}} \\
&+ \frac{1}{\varepsilon}\int_0^t \|[V * (\rho_s - \tilde{\rho}_s)\,,\,\tilde{\omega}_{N,s}]\|_{\mathrm{Tr}}\,ds \\
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$$\|[V*(\rho_s-\tilde\rho_s)\,,\,\tilde\omega_{N,s}]\|_{\mathrm{Tr}} \leq \|\rho_s-\tilde\rho_s\|_{L^1}\sup_z \|[V(z-\cdot),\tilde\omega_{N,s}]\|_{\mathrm{Tr}}$$

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heuristically

$$\begin{aligned}\|[V(z-\cdot),\tilde\omega_{N,s}]\|_{\mathrm{Tr}} \text{ ``}\le\text{''} \|[x\,,\,\tilde\omega_{N,s}]\|_{\mathrm{Tr}} \text{ ``}=\text{''} N\varepsilon\,\|\nabla\tilde W_{N,s}\|_{L^1_{x,v}} \\ \le C N\varepsilon\,\|\nabla W_{N,0}\|_{L^1}\,e^{C|s|}\end{aligned}$$

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$$\le C N\varepsilon\,\|\nabla W_{N,0}\|_{L^1}\, e^{C|s|}$$

$$\|\rho_s-\tilde\rho_s\|_{L^1} \le \frac{1}{N}\|\omega_{N,t}-\tilde\omega_{N,t}\|_{\mathrm{Tr}}$$

Strategy

$$\frac{1}{\varepsilon}\int_0^t \|[V*(\rho_s-\tilde{\rho}_s)\,,\,\tilde{\omega}_{N,s}]\|_{\mathrm{Tr}}\,ds$$

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$$\begin{aligned}\|[V(z-\cdot),\tilde{\omega}_{N,s}]\|_{\mathrm{Tr}} \;``\le" \;\|[x\,,\,\tilde{\omega}_{N,s}]\|_{\mathrm{Tr}} \;``=" \; N\varepsilon\,\|\nabla\tilde{W}_{N,s}\|_{L^1_{x,v}} \\ \le C\,N\varepsilon\,\|\nabla W_{N,0}\|_{L^1}\,e^{C|s|}\end{aligned}$$

$$\|\rho_s-\tilde{\rho}_s\|_{L^1} \le \frac{1}{N}\|\omega_{N,t}-\tilde{\omega}_{N,t}\|_{\mathrm{Tr}}$$

$$\begin{aligned}\|[V(z-\cdot),\tilde{\omega}_{N,s}]\|_{\mathrm{Tr}} &\le \|(1-\varepsilon^2\Delta)^{-1}(1+x^2)^{-1}\|_{\mathrm{HS}}\|(1+x^2)(1-\varepsilon^2\Delta)[V(z-\cdot),\tilde{\omega}_{N,s}]\|_{\mathrm{HS}} \\ &\le C\sqrt{N}\,\|(1+x^2)(1-\varepsilon^2\Delta)[V(z-\cdot),\tilde{\omega}_{N,s}]\|_{\mathrm{HS}} \\ &\le C\exp\left(C|s|\right)N\varepsilon\,[\|W_N\|_{H^1_4}+\varepsilon\,\|W_N\|_{H^2_4}+\varepsilon^2\,\|W_N\|_{H^3_4}+\varepsilon^3\|W_N\|_{H^4_4}]\end{aligned}$$

Strategy

$$\begin{aligned}\|\omega_{N,t} - \tilde{\omega}_{N,t}\|_{\mathrm{Tr}} \leq \|\omega_{N,0} - \tilde{\omega}_{N,0}\|_{\mathrm{Tr}} \\ + \frac{1}{\varepsilon}\int_0^t \|[V * (\rho_s - \tilde{\rho}_s)\,,\, \tilde{\omega}_{N,s}]\|_{\mathrm{Tr}} ds \\ + \frac{1}{\varepsilon}\int_0^t \|B_s\|_{\mathrm{Tr}} ds\end{aligned}$$

Strategy

$$\frac{1}{\varepsilon}\int_0^t \|B_s\|_{\mathrm{Tr}} ds$$

with

$$B_t(x;y) = \left[V * \tilde{\rho}_t(x) - V * \tilde{\rho}_t(y) - \nabla(V * \tilde{\rho}_t)\left(\frac{x+y}{2}\right)\cdot(x-y)\right]\tilde{\omega}_{N,t}(x;y)$$

Strategy

$$\frac{1}{\varepsilon}\int_0^t \|B_s\|_{\mathrm{Tr}}\, ds$$

with

$$B_t(x;y) = \left[V * \tilde{\rho}_t(x) - V * \tilde{\rho}_t(y) - \nabla(V * \tilde{\rho}_t)\left(\frac{x+y}{2}\right)\cdot(x-y)\right]\tilde{\omega}_{N,t}(x;y)$$

$$\|[x\,,\,[x\,,\,\tilde{\omega}_{N,s}]\,]\|_{\mathrm{Tr}}\text{ “}=\text{” } N\,\varepsilon^2\|\nabla^2\tilde{W}_s\|_{L^1_{x,v}}$$

Strategy

$$\frac{1}{\varepsilon}\int_0^t \|B_s\|_{\mathrm{Tr}}\, ds$$

with

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$$\|[x\,,\,[x\,,\,\tilde{\omega}_{N,s}]\,]\|_{\mathrm{Tr}} \text{ “} = \text{''}\, N\,\varepsilon^2 \|\nabla^2 \tilde{W}_s\|_{L^1_{x,v}}$$

Strategy

$$\frac{1}{\varepsilon}\int_0^t \|B_s\tilde{\omega}_{N,s}\|_{\mathrm{Tr}}\,ds$$

with

$$B_t(x;y) = V*\tilde{\rho}_t(x) - V*\tilde{\rho}_t(y) - \nabla(V*\tilde{\rho}_t)\left(\frac{x+y}{2}\right)$$

$$\|[x\,,\,[x\,,\,\tilde{\omega}_{N,s}]]\|_{\mathrm{Tr}}\,\text{``}=\text{''}\,N\,\varepsilon^2\|\nabla^2\tilde{W}_s\|_{L^1_{x,v}}$$

Hence we conclude by Gronwall Lemma:

$$\begin{aligned}\|\omega_{N,t}-\tilde{\omega}_{N,t}\|_{\mathrm{Tr}} \le C\int_0^t ds\,\|\omega_{N,s}-\tilde{\omega}_{N,s}\|_{\mathrm{Tr}}\exp(C|s|)\\ + C\,N\,\varepsilon\,[\|W_N\|_{H^2_4}+\varepsilon\,\|W_N\|_{H^3_4}+\varepsilon^2\,\|W_N\|_{H^4_4}+\varepsilon^3\|W_N\|_{H^5_4}]\,\exp(C|s|)\end{aligned}$$