From the many-body quantum dynamics to the Vlasov equation

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The Analysis of Complex Quantum Systems:
Large Coulomb Systems and Related Matters

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Fermionic mean-field regime

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General goal

remove the trap 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 regimes in which the evolution can be well approx. by an **effective dynamics**.

Fermionic mean-field regime

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

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

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

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

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Let

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

and multiply by ε^2:

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

Effective equations

M-B Schrödinger Eq.

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$N \to \infty$

1981: Narnhofer & Sewell
Spohn

Vlasov Eq.

$$\partial_t\widetilde{W}_t + v\cdot\nabla_x\widetilde{W}_t + (\nabla V * \widetilde{\rho}_t)\cdot\nabla_v\widetilde{W}_t = 0$$
$$\widetilde{\rho}_t(x) = \int \widetilde{W}_t(x,v)\,dv$$

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$N >> 1$

Hartree-Fock Eq.

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

- MBQ dynamics $\rightarrow$ Hartree-Fock:
  - 2003: Elgart, Erdős, Schlein, Yau;
  - other scalings:
    - 2002: Bardos, Golse, Gottlieb, Mauser;
    - 2010: Fröhlich, Knowles;
    - 2016: Petrat, Pickl; Bach, Breteaux, Petrat, Pickl, Tzaneteas;
  - 2013: Benedikter, Porta, Schlein;
  - 2015: Benedikter, Jaksic, Porta, C.S., Schlein;
  - 2017: Porta, Rademacher, C.S., Schlein;
  - 2018: C.S.

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Goal: singular interactions $V(x) = \frac{1}{|x|^\alpha}$, $\alpha \in (0,1]$

- strong convergence (trace norm)
- explicit rate of convergence

Motivation

Study large atoms and molecules

$$i\,\varepsilon\,\partial_t\,\psi_{N,t} = \left[\sum_{j=1}^{N} -\varepsilon^2\Delta_{x_j} - \frac{1}{|x_j|} + \frac{1}{N}\sum_{i<j}^{N}\frac{1}{|x_i - x_j|}\right]\,\psi_{N,t}$$

Motivation

Pure and mixed states, smooth interaction potential:

Many-body → **Hartree** → **Vlasov-Poisson**

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Semiclassical limit

Compare Hartree-Fock Eq.

$$\begin{cases} i\,\varepsilon\,\partial_t \omega_{N,t}(x;y) = \left[-\varepsilon^2\Delta + \frac{1}{|\cdot|^\alpha} * \rho_t, \omega_{N,t}\right](x;y) \\ \rho_t(x) = \frac{1}{N}\omega_{N,t}(x;x) \end{cases}$$

and Vlasov Eq.

$$\begin{cases} \partial_t \widetilde{W}_t(x,v) + v\cdot\nabla_x \widetilde{W}_t(x,v) + \left(\nabla \frac{1}{|\cdot|^\alpha} * \widetilde{\rho}_t\right)(x)\cdot\nabla_v \widetilde{W}_t(x,v) = 0 \\ \widetilde{\rho}_t(x) = \int \widetilde{W}_t(x,v)\,dv \end{cases}$$

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$\omega_{N,t}$ densities on $L^2(\mathbb{R}^3)$, $0 \leq \omega_{N,t} \leq 1$

vs

$\widetilde{W}_t : \mathbb{R}^3_x \times \mathbb{R}^3_v \to \mathbb{R}_+$ prob. density on the phase space

Weyl and Wigner transforms

Wigner transform

$$W_N(x, v) = \left(\frac{\varepsilon}{2\pi}\right)^3 \int \omega_N\left(x + \varepsilon\frac{y}{2}; x - \varepsilon\frac{y}{2}\right) e^{-iv\cdot y} dy$$

Weyl and Wigner transforms

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Weyl transform

$$\omega_N(x;y) = N \int W_N\left(\frac{x+y}{2}, v\right)\, e^{iv\cdot(x-y)/\varepsilon} dv$$

Remark: when $|x-y| > \varepsilon$, $[x, \omega_N]$ is small

$$\operatorname{tr} |[x,\omega_N]| \lesssim N\varepsilon$$

Weyl and Wigner transforms

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and Weyl-trasformed Vlasov Eq.

$$\begin{cases} i\,\varepsilon\,\partial_t \widetilde{\omega}_{N,t} = \left[-\varepsilon^2\Delta\ ,\ \widetilde{\omega}_{N,t}\right] + A_t \\ A_t(x;y) = \left(\nabla \frac{1}{|\cdot|^\alpha} * \widetilde{\rho}_t\right)\left(\frac{x+y}{2}\right) \cdot (x-y)\,\widetilde{\omega}_{N,t}(x;y) \end{cases}$$

Results

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  - strong convergence
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- For $\alpha \in [1/2, 1]$:
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  - smooth initial **steady** states for the Vlasov equation

Sketch of the proof: step 1

Compare $\omega_{N,t}$ and $\widetilde{\omega}_{N,t}$:

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

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Problem 1. How to get rid of the kinetic term?

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Problem 1. How to get rid of the kinetic term?

Idea 1. Define a unitary operator $\mathcal{U}(t)$

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

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$$i\,\varepsilon\,\partial_t\,\mathcal{U}^*(t)\,(\omega_{N,t}-\widetilde{\omega}_{N,t})\,\mathcal{U}(t) = \ldots \text{ compute } \ldots$$

$$= \mathcal{U}^*(t)\left[\frac{1}{|\cdot|^\alpha} * (\rho_t - \widetilde{\rho}_t), \widetilde{\omega}_{N,t}\right]\mathcal{U}(t) + \mathcal{U}^*(t) B_t\,\mathcal{U}(t)\,.$$

where

$$B_t(x;y) = \left[\frac{1}{|\cdot|^\alpha} * \widetilde{\rho}_t(x) - \frac{1}{|\cdot|^\alpha} * \widetilde{\rho}_t(y) - \nabla\left(\frac{1}{|\cdot|^\alpha} * \widetilde{\rho}_t\right)\left(\frac{x+y}{2}\right)\cdot(x-y)\right]\widetilde{\omega}_{N,t}(x;y)$$

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Duhamel + trace norm:

$$\begin{aligned}\mathrm{tr}\,|\omega_{N,t}-\widetilde{\omega}_{N,t}| \leq \frac{1}{\varepsilon}\int_0^t \mathrm{tr}\,\left|\left[\frac{1}{|\cdot|^\alpha} * (\rho_s - \widetilde{\rho}_s), \widetilde{\omega}_{N,s}\right]\right|\,ds \\ + \frac{1}{\varepsilon}\int_0^t \mathrm{tr}\,|B_s|\,ds\end{aligned}$$

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dominant term

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$i\,\varepsilon\,\partial_t\,\mathcal{U}^*(t)\,(\omega_{N,t} - \widetilde{\omega}_{N,t})\,\mathcal{U}(t) = \ldots$ compute $\ldots$

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error term

Sketch of the proof: step 2

Focus on the dominant term

$$\frac{1}{\varepsilon}\int_0^t \mathrm{tr}\ \left|\left[\frac{1}{|\cdot|^\alpha} * (\rho_s - \widetilde{\rho}_s), \widetilde{\omega}_{N,s}\right]\right| ds$$

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Problem 2. Find a handier representation for the dominant term.

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Idea 2. Generalised Fefferman - de la Llave representation formula

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$$\frac{1}{|x-y|^\alpha} = C\int_0^\infty \frac{1}{r^{1+\alpha}}\,\chi_{(r,y)}(x)\,dr$$

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$$\frac{1}{|x-y|^\alpha} = C\int_0^\infty \frac{1}{r^{1+\alpha}}\,\chi_{(r,y)}(x)\,dr$$

$$\chi_{(r,y)}(x) = \exp\left(-|x-y|^2/r^2\right)$$

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Hence

$$\begin{aligned}&\mathrm{tr}\,\left|\left[|\cdot|^{-\alpha} * (\rho_s - \widetilde{\rho}_s), \widetilde{\omega}_{N,s}\right]\right| \\ &\quad\lesssim \int_0^\infty \frac{1}{r^{1+\alpha}} \int |\rho_s(y) - \widetilde{\rho}_s(y)|\,\mathrm{tr}\,|[\chi_{(r,y)}, \widetilde{\omega}_{N,t}]|\,dy\,dr\end{aligned}$$

Sketch of the proof: step 3

$$\operatorname{tr} |\omega_{N,t} - \widetilde{\omega}_{N,t}| \lesssim \frac{1}{\varepsilon} \int_0^t \int_0^\infty \frac{1}{r^{1+\alpha}} \int |\rho_s(y) - \widetilde{\rho}_s(y)| \operatorname{tr} |[\chi_{(r,y)}, \widetilde{\omega}_{N,t}]| \, dy \, dr \, ds + \text{ error term}$$

Sketch of the proof: step 3

$$\operatorname{tr}|\omega_{N,t} - \widetilde{\omega}_{N,t}|$$
$$\lesssim \frac{1}{\varepsilon}\int_0^t \int_0^\infty \frac{1}{r^{1+\alpha}} \int |\rho_s(y) - \widetilde{\rho}_s(y)| \operatorname{tr}|[\chi_{(r,y)}, \widetilde{\omega}_{N,t}]|\, dy\, dr\, ds + \text{ error term}$$

$$\|\rho_s - \widetilde{\rho}_s\|_{L^1} \leq \frac{1}{N}\operatorname{tr}|\omega_{N,s} - \widetilde{\omega}_{N,s}|$$

Sketch of the proof: step 3

$$\operatorname{tr}|\omega_{N,t} - \widetilde{\omega}_{N,t}| \lesssim \frac{1}{\varepsilon}\int_0^t\int_0^\infty \frac{1}{r^{1+\alpha}}\int |\rho_s(y) - \widetilde{\rho}_s(y)| \operatorname{tr}|[\chi_{(r,y)}, \widetilde{\omega}_{N,t}]|\, dy\, dr\, ds + \text{ error term}$$

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$$\operatorname{tr}|[\chi_{(r,y)}, \widetilde{\omega}_{N,s}]| \lesssim \begin{cases} r^{\frac{1}{2}}\, N\varepsilon + \text{error terms} & \Longrightarrow \quad \alpha \in (0, 1/2) \\ r^{\frac{3}{2}-\delta} \sum_{i=1}^3 \|\rho_{|[x_i,\widetilde{\omega}_{N,t}]|}\|_{L^1}^{\frac{1}{6}+\delta} \|\rho_{|[x_i,\widetilde{\omega}_{N,t}]|}\|_{L^\infty}^{\frac{5}{6}-\delta} & \Longrightarrow \quad \alpha \in [1/2, 1] \end{cases}$$

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Propagation of regularity for the Vlasov equation:

- smooth initial data (mixed states);
- smooth steady states for the Vlasov system.

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Therefore, for $k > 0$,

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Trace norm convergence

Theorem 1 (C.S., *CMP 2019*)

Let $\alpha \in (0, \frac{1}{2})$.

Let ω_N *a sequence of fermionic operators on* $L^2(\mathbb{R}^3)$ *with* $\mathrm{tr}\,\omega_N = N$ *and* $\mathrm{tr}\,(-\varepsilon^2\Delta)\omega_N \lesssim N$.

Let W_N*, Wigner transform of* ω_N*, satisfy:*

- $W_N \in L^1 \cap L^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$ *and* $\mathcal{H}_2 = \iint |v|^2\, W_N(x,v)\, dx\, dv < \infty$;
- *Let* $m_0 > \frac{6\alpha}{2-\alpha}$. *For* $m < m_0$, $\mathcal{H}_m < \infty$;
- *For all* $R,\ T > 0$, $0 \le l \le 5$ *and* $k = 0, 2$,

$$\sup\{(1+x^2+v^2)^k |\nabla^l W_N|(y+tv, w)\ :\ |y-x| \le Rt^2, |w-v| \le Rt\} \in L^\infty((0,T)\times\mathbb{R}^3_x; L^1 \cap L^2(\mathbb{R}^3_v));$$

- *For* $k = 0, \ldots, 6$, $W_N \in H^4(\mathbb{R}^3 \times \mathbb{R}^3, (1+x^2+v^2)^4 dxdv)$.

Then there exists $C > 0$ *such that*

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Let ω_N be a sequence of fermionic operators on $L^2(\mathbb{R}^3)$, $0 \leq \omega_N \leq 1$, with $\mathrm{tr}\,\omega_N = N$ and with Wigner transform W_N satisfying:

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iv) $\exists\, T, C > 0$ *s.t.*

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Then, there exits a constant C_T depending on $T > 0$ and $\|W_N\|_{H^2_4}$ such that

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Outlooks

- Beyond steady states (with L. Laflèche):

  propagation of regularity for $\|\varrho_{|[x_i,\widetilde{\omega}_{N,t}]|}\|_{L^p}$

- Pure states - zero temperature (with D. Dimonte);

- From many-body quantum dynamics to Hartree-Fock with Coulomb interaction for more general initial data.