Dynamics of interacting fermions at high density

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Summary

- Introduction: many-body Fermi gases. Extended systems with long-range interactions (Kac scaling). Equivalent to high density regime.
- Nonlinear effective theory at high-density: Hartree-Fock theory.
- Main result: Derivation of the time-dependent Hartree equation for extended systems at high density.
- Sketch of the proof. Control of fluctuations around limiting equation, local semiclassical structure.
- Conclusions.

Introduction

Many-body Fermi gases

- Consider a system of N fermionic particles, in a domain $\Lambda \subset \mathbb{R}^3$. State of the system: $\psi_N \in L^2_{\mathrm{a}}(\mathbb{R}^{3N})$,

$$\psi_N(x_1, \ldots, x_N) = \mathrm{sgn}(\pi)\psi_N(x_{\pi(1)}, \ldots, x_{\pi(N)}) \ .$$

- Many-body Hamiltonian:

$$H_N^{\mathrm{trap}} = \sum_{j=1}^{N}(-\Delta_j + V_{\mathrm{ext}}(x_j)) + \sum_{i<j}^{N} V(x_i - x_j) \ ,$$

where V_{ext} confines the particles in Λ, and V is a bounded two-body interaction.

- The average particle density of the system is:

$$\varrho = \frac{N}{|\Lambda|} \ .$$

For the moment, we shall suppose that the density is order 1.

Equilibrium and dynamical properties

- The spectral properties of H_N^{trap} play an important role in understanding the behavior of the system at low temperature. Ground state energy:

$$E_N := \inf_{\psi_N \in L^2_{\mathrm{a}}(\mathbb{R}^{3N})} \frac{\langle \psi_N, H_N \psi_N \rangle}{\|\psi_N\|_2^2} \; .$$

- Quantum dynamics. Suppose that ψ_N equal, or close, to the ground state of H_N^{trap}. Remove the trap at $t = 0$. Evolution:

$$i\partial_t \psi_{N,t} = H_N \psi_{N,t} \; , \qquad \psi_{N,0} = \psi_N \; .$$

The existence and uniqueness of the solution is provided by the spectral theorem, $\psi_{N,t} = e^{-iH_N t}\psi_N$.

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- For realistic values of N, it is extremely hard to gain quantitative information about the system. Typical questions, for large N:
  - Computation of E_N?
  - Evolution of local observables?
  - How to describe correlations among particles?

Long range interactions

- Such problems are way too hard from the analytic viewpoint. The analysis becomes more accessible in suitable scaling regimes.

- Kac scaling. Replace $V(x-y)$ by

$$V_\varepsilon(x-y) = \varepsilon^3 V(\varepsilon(x-y)) \qquad \text{for } \varepsilon \ll 1.$$

  Each particle interacts with $O(\varepsilon^{-3})$ particles. By the rescaling of the coupling, $\|V\|_1 = \|V_\gamma\|_1$.

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- The simplification introduced by the scaling is that one expects a local averaging mechanism to take place (later).
- **Rmk.** ε is independent of N! Not mean-field (where $\varepsilon = N^{-1/3}$). Still, one expects that some of the predictions of mean-field are recovered.

  In classical stat-mech: Lebowitz-Penrose '66. Derivation of van der Waals theory for the liquid/vapor transition. Lieb '66: extension to quantum.

Quantum dynamics

- The Fermi velocity in a gas with density ϱ grows as $\varrho^{1/3}$ (Lieb-Thirring). Macroscopic time scale: $\tau = \varepsilon^{-1} t$ with $t = O(1)$. Schrödinger equation:

$$i\varepsilon\partial_t \psi_{N,t} = \Big(\sum_{j=1}^{N} -\Delta_j + \varepsilon^3 \sum_{i<j}^{N} V(\varepsilon(x_i - x_j)) \Big) \psi_{N,t} \; .$$

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- Next, we rescale lengths, so that the range of the potential is 1. Let:

$$(U_\varepsilon\psi_N)(x_1,\ldots,x_N) := \varepsilon^{-3N/2}\psi_N(\varepsilon^{-1}x_1,\ldots,\varepsilon^{-1}x_N)$$

we write:

$$\begin{aligned} i\varepsilon U_\varepsilon\partial_t\psi_{N,t} &= U_\varepsilon\Big(\sum_{j=1}^{N} -\Delta_j + \varepsilon^3 \sum_{i<j}^{N} V(\varepsilon(x_i - x_j))\Big)U_\varepsilon^* U_\varepsilon\psi_{N,t} \\ &= \Big(\sum_{j=1}^{N} -\varepsilon^2\Delta_j + \varepsilon^3 \sum_{i<j}^{N} V(x_i - x_j)\Big)U_\varepsilon\psi_{N,t} \equiv H_N U_\varepsilon\psi_{N,t}\ . \end{aligned}$$

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- **Rmk.** The effective density is: $\varrho = \frac{N}{\varepsilon^3 |\Lambda|} = O(\varepsilon^{-3}) \gg 1.$

One-particle density matrix

- Consider one-particle observables $\mathcal{O}_N = \sum_{j=1}^{N} 1^{\otimes(N-j)} \otimes O \otimes 1^{\otimes(j-1)}$. We have:

$$\langle \psi_{N,t}, \mathcal{O}_N \psi_{N,t} \rangle = \mathrm{tr}_{L^2(\mathbb{R}^3)}\, O \gamma^{(1)}_{N,t}$$

where $\gamma^{(1)}_{N,t}$ is the reduced one-particle density matrix. It has the kernel:

$$\gamma^{(1)}_{N,t}(x;y) = N \int dx_2 \dots dx_N \psi_{N,t}(x, x_2, \dots, x_N) \overline{\psi_{N,t}(y, x_2, \dots, x_N)}\,.$$

Properties: $\quad 0 \leq \gamma^{(1)}_{N,t} \leq 1, \qquad \mathrm{tr}\, \gamma^{(1)}_{N,t} = N.$

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- Unfortunately, $\gamma^{(1)}_{N,t}$ does not solve a closed equation: it involves $\gamma^{(2)}_{N,t}$, whose evolution involves $\gamma^{(3)}_{N,t}$ etc. (BBGKY hierarchy).
- However, in some scaling regimes one expects $\gamma^{(1)}_{N,t}$ to be well approximated by the solution of a suitable non-linear evolution equation.

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- However, in some scaling regimes one expects $\gamma^{(1)}_{N,t}$ to be well approximated by the solution of a suitable non-linear evolution equation.
- Advantage wrt to Schrödinger: the solution is an operator on $L^2(\mathbb{R}^3)$ with trace N instead of a function on $L^2(\mathbb{R}^{3N})$.

Slater determinants

- Recall the Schrödinger equation:

$$i\varepsilon\partial_t\psi_{N,t} = \Big(\sum_{j=1}^{N} -\varepsilon^2\Delta_j + \varepsilon^3\sum_{i<j}^{N} V(x_i - x_j)\Big)\psi_{N,t}$$

The initial datum lives in $\Lambda \subset \mathbb{R}^3$, density $\varrho = O(\varepsilon^{-3})$. On uncorrelated states, one expects a local averaging mechanism to take place:

$$\Big\langle \psi_{N,t}, \sum_{i<j}^{N} V(x_i - x_j)\psi_{N,t}\Big\rangle \simeq \frac{1}{2}\int dxdy\, V(x-y)\rho_t(x)\rho_t(y)\ ,$$

with $\rho_t(x) = \gamma_{N,t}(x;x) =$ density of particles at x.

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- The most uncorrelated fermionic states are Slater determinants:

$$\psi_{\mathrm{Slater}}(x_1,\ldots,x_N) = \frac{1}{\sqrt{N!}}\sum_{\pi}\mathrm{sgn}(\pi) f_1(x_{\pi(1)})\cdots f_N(x_{\pi(N)})\ ,$$

with orthonormal $f_i \in L^2(\mathbb{R}^3)$.

Hartree-Fock theory

- The HF approx. consists in replacing $L^2_{\mathrm{a}}(\mathbb{R}^{3N})$ by the set of Slater dets.
- At equilibrium, the HF ground state energy of a confined system is:

$$E_N^{\mathrm{HF}} = \inf_{\psi_{\mathrm{Slater}}} \langle \psi_{\mathrm{Slater}}, H_N \psi_{\mathrm{Slater}} \rangle = \inf_{\omega_N} \mathcal{E}_N^{\mathrm{HF}}(\omega_N)\;,$$

with $\omega_N = \sum_{i=1}^N |f_i\rangle\langle f_i|$ the reduced 1PDM of a Slater, and:

$$\mathcal{E}_N^{\mathrm{HF}}(\omega_N) = \mathrm{tr}(-\varepsilon^2\Delta + V_{\mathrm{ext}})\omega_N + \frac{\varepsilon^3}{2}\int dxdy\, V(x-y)\big[\rho(x)\rho(y) - |\omega_N(x;y)|^2\big]$$

(Hartree-Fock energy functional.)

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(Hartree-Fock energy functional.)

- Proof of validity of the HF approximation (for the ground state energy)
  - Bach '92: large atoms/molecules (analogous to mean-field)
  - Graf-Solovej '94: extens. to Jellium (extended Coulomb system).

Time-dependent Hartree-Fock equation

- Let ψ_N be given by the HF minimizer, and let $V_{\text{ext}} = 0$ at $t = 0$.
- If one assumes that $\psi_{N,t}$ is a Slater determinant for all times, it is not difficult to derive a self-consistent evolution equation for the 1PDM:

$$i\varepsilon\partial_t\omega_{N,t} = \big[-\varepsilon^2\Delta + \varepsilon^3\rho_t * V - X_t \, , \, \omega_{N,t}\big]$$

with $\rho_t(x) = \omega_{N,t}(x;x)$ and $X_t(x;y) = \varepsilon^3 V(x-y)\omega_{N,t}(x;y)$.
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- The assumption that $\psi_{N,t}$ is a Slater determinant is of course nontrivial. In the mean-field regime, $|\Lambda| = O(1)$ and $\varepsilon = N^{-1/3}$, for a suitable class of initial data, the validity of the HF equation has been proved:

$$\|\gamma^{(1)}_{N,t} - \omega_{N,t}\|_{\text{HS}} \leq C(t) \qquad \text{for all times } t = O(1)$$

which has to be compared with the trivial bounds:

$$\|\gamma^{(1)}_{N,t}\|_{\text{HS}} \leq N^{1/2} \, , \qquad \|\omega_{N,t}\|_{\text{HS}} = N^{1/2} \, .$$

Rigorous results about the validity of tHF equation

We shall only discuss the mean-field/semiclassical scaling:

$$i\varepsilon\partial_t\psi_{N,t} = \Big(\sum_{j=1}^{N} -\varepsilon^2\Delta_j + \varepsilon^3 \sum_{i<j}^{N} V(x_i - x_j)\Big)\psi_{N,t}$$

with $\varepsilon = N^{-1/3}$ and initial datum confined in $|\Lambda| = O(1)$.

- Elgart, Erdős, Schlein, Yau '07: analytic V, short times. BBGKY.
- Benedikter, P., Schlein '14: $V \in C^2$, all times. Fock space methods.
- Petrat, Pickl '16: similar result, first quantization.
- Benedikter, Jaksic, P., Saffirio, Schlein '16: ext. of [BPS] to mixed states.
- P., Rademacher, Saffirio, Schlein '17: Coulomb, conditional result.
- Chong, Laflèche, Saffirio '21: singular potentials, mixed states.
- Benedikter, Nam, P., Schlein, Seiringer '22: bounded potentials, norm approximation for a special class of pure states (bosonization).

Remarks

- As $N \to \infty$, the solution of the time-dependent HF equation converges to the solution of the Vlasov equation (after Wigner transf.)

$$\partial_t W_t(x,p) + 2v \cdot \nabla_x W_t(x,p) = \nabla_x (V * \rho_t^{\mathrm{Vl}}) \cdot \nabla_p W_t(x,p)$$

with $\rho^{\mathrm{Vl}}(x) = \int dp\, W_t(x,p)$. (Under suitable regularity assumptions)

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- All the previous results hold for the mean-field regime, $\varepsilon = N^{-1/3}$. In particular, the coupling constant scales as N^{-1}.

- High density regime: $N/|\Lambda| = \varrho$ and $\varepsilon = O(\varrho^{-1/3})$. In contrast to the mean-field regime, here one has three length scales:
  - The size of the support of the initial datum, $L \sim |\Lambda|^{1/3}$
  - The range of the interaction potential, $\ell = O(1)$
  - The interparticle distance, $\delta = O(\varrho^{-1/3})$.

One has to capture the mean-field behavior at the $O(1)$ scale.

Main result

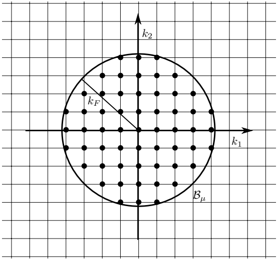
Interlude: the free Fermi gas

- We consider initial data that are expected to describe ground states of confined systems. Example: the free Fermi gas (homogeneous system). Non-interacting ground state on $\mathbb{T}^3_L$ (3-torus of side L):

$$\psi = f_{k_1} \wedge \ldots \wedge f_{k_N} \,,$$

where $f_k(x) = e^{ik\cdot x}/L^{\frac{3}{2}}$ and $k \in (2\pi/L)\mathbb{Z}^3$ (plane waves).

- The points k fill the Fermi ball:



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- The points k fill the Fermi ball.
    - $|\mathcal{B}(k_F)| = N = L^3 \varrho$. The spacing between the lattice points is L^{-1}, hence the Fermi momentum k_F grows as $k_F \sim \varrho^{1/3}$.
    - Up to subleading corrections in L, we can assume that the Fermi ball is completely filled.
    - For interacting, homogeneous models, the free Fermi gas agrees in energy with the HF ground state, up to corrections that are exp. small in the density. [Gontier, Hainzl, Lewin '18.]

The free Fermi gas - density matrix

- Reduced one-particle density matrix:

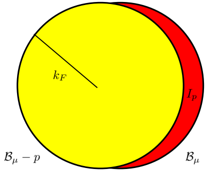
$$\omega_N(x;y) = \frac{1}{L^3} \sum_{k \in \mathcal{B}(k_F)} e^{ik\cdot(x-y)} \; .$$

- Consider the operator $[e^{ip\cdot x}, \omega_N]$. A simple computation shows that:

$$|[e^{ip\cdot x}, \omega_N]| = |[e^{ip\cdot x}, \omega_N]|^2 = \sum_{k \in I_p} |f_k\rangle\langle f_k|$$

with $I_p = \{k \in \mathcal{B}(k_F) \mid k + p \notin \mathcal{B}(k_F)\}$ (see figure). Also,

$$|[e^{ip\cdot x}, \omega_N]|(x;x) = \frac{1}{L^3} \, \mathrm{tr} \, |[e^{ip\cdot x}, \omega_N]| = \frac{1}{L^3} |I_p| = O(|p|\varrho^{2/3})$$



Semiclassical structure

- Given $\Lambda \subset \mathbb{R}^3$ and $\varepsilon > 0$ let $N = [\varepsilon^{-3}|\Lambda|]$. Hence, $\varrho \simeq \varepsilon^{-3}$.
  We would like to capture the fact that ω_N is concentrated in Λ and:
$$\omega_N(x;y) \simeq \varepsilon^{-3}\varphi\Big(\frac{x-y}{\varepsilon}\Big)\xi\Big(\frac{x+y}{2}\Big)\,.$$

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$$\omega_N(x;y) \simeq \varepsilon^{-3}\varphi\Big(\frac{x-y}{\varepsilon}\Big)\xi\Big(\frac{x+y}{2}\Big)\,.$$
- Let us define the localizer $\mathcal{W}_z$ and the weight $X_\Lambda(z)$ as:
$$\mathcal{W}_z(\hat{x}) := \frac{1}{1+|z-\hat{x}|^4}\,, \qquad X_\Lambda(z) := 1 + \mathrm{dist}(\Lambda, z)^4\,.$$

(i) We suppose that, for $t \in [0,T]$:
$$X_\Lambda(z)\big\|\mathcal{W}_z(t)\omega_N\big\|_{\mathrm{tr}} \leq C\varepsilon^{-3}\,.$$
with $\mathcal{W}_z(t) = e^{-i\varepsilon\Delta t}\mathcal{W}_z e^{i\varepsilon\Delta t}$ (free evolution).

(ii) We shall say that ω_N satisfies the local semiclassical structure if:
$$X_\Lambda(z)\big\|\mathcal{W}_z(t)\big[e^{ip\cdot x},\omega_N\big]\big\|_{\mathrm{tr}} \leq C|p|\varepsilon^{-2}$$
$$X_\Lambda(z)\big\|\mathcal{W}_z(t)\big[\varepsilon\nabla,\omega_N\big]\big\|_{\mathrm{tr}} \leq C\varepsilon^{-2}$$

Derivation of the Hartree equation for extended systems

Theorem (Fresta, P., Schlein 2022)

Let $V \in L^1(\mathbb{R}^3)$ *such that:*

$$\max_{\alpha:|\alpha|\leq 8} \int_{\mathbb{R}^3} dp\, (1 + |p|^{15}) |\partial_p^\alpha \hat{V}(p)| < \infty \,.$$

Let $\psi_N \in L^2_a(\mathbb{R}^{3N})$*, and suppose that:*

$$\| \gamma_N^{(1)} - \omega_N \|_{tr} \leq C \varepsilon^\delta N \qquad \text{for some } \delta > 0,$$

where ω_N *is a rank-*N *orthogonal projection, and it satisfies the assumptions (i), (ii). Let* $\omega_{N,t}$ *be the solution of the time-dep. Hartree equation:*

$$i\varepsilon \partial_t \omega_{N,t} = \big[-\varepsilon^2 \Delta + \varepsilon^3 V * \rho_t \,,\, \omega_{N,t} \big] \,.$$

Then, there exists $T_* > 0$ *independent of* ε *such that, for* $|t| \leq T_*$*:*

$$\boxed{\| \gamma_{N,t}^{(1)} - \omega_{N,t} \|_{HS} \leq C \max\{ \varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\delta}{2}} \} N^{\frac{1}{2}} \,.}$$

Remarks

- The result should be compared with the trivial estimates

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- The result actually holds for all times for which there exists $C > 0$ s.t.:

$$\mathrm{tr}\,\mathcal{W}_z\omega_{N,t} \leq \varepsilon^{-3}C\;. \qquad \text{[Non-concentration estimate.]}$$

  We are able to prove this bound for $|t| \leq T_*$, with $T_* \equiv T_*(V)$, which can be made arb. large for V small enough.

  Another challenge: propagation of the local semiclassical structure.

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  Recall that $\varrho \simeq \varepsilon^{-3}$. With respect to previous work [BPS14] we are able to control the rate of convergence uniformly in the system size.

- The result actually holds for all times for which there exists $C > 0$ s.t.:

$$\operatorname{tr} \mathcal{W}_z \omega_{N,t} \leq \varepsilon^{-3} C\,. \qquad \text{[Non-concentration estimate.]}$$

  We are able to prove this bound for $|t| \leq T_*$, with $T_* \equiv T_*(V)$, which can be made arb. large for V small enough.

  Another challenge: propagation of the local semiclassical structure.

- Our estimates are not strong enough to resolve the exchange term.

Sketch of the proof

Fermionic Fock space

- Fermionic Fock space:

$$\mathcal{F} = \mathbb{C} \oplus \bigoplus_{n\geq 1} L^2_{\mathrm{a}}(\mathbb{R}^{3n})$$

$$\mathcal{F} \ni \psi = (\psi^{(0)}, \psi^{(1)}, \ldots, \psi^{(n)}, \ldots)\,, \qquad \text{Vacuum: } \Omega = (1, 0, 0, \ldots)$$

- Fermonic creation/annihilation operators $a(f)$, $a^*(f)$ ($f \in L^2(\mathbb{R}^3)$):

$$(a^*(f)\psi)^{(n)}(x_1, \ldots, x_n) = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} (-1)^j f(x_j) \psi^{(n-1)}(x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_n)$$

$$(a(f)\psi)^{(n)}(x_1, \ldots, x_n) = \sqrt{n+1} \int dx \overline{f}(x) \psi^{(n+1)}(x, x_1, \ldots, x_n).$$

Operator valued distributions: $a_x \equiv a(\delta_x)$, $a^*_x \equiv a^*(\delta_x)$,

$$a(f) = \int dx\, a_x\, \overline{f(x)}\,, \qquad a^*(f) = \int dx\, a^*_x f(x)\,.$$

- Canonical anticommutation relations:

$$\{a(f), a^*(g)\} = \langle f, g\rangle_{L^2(\mathbb{R}^3)} \qquad \{a(f), a(g)\} = \{a^*(f), a^*(g)\} = 0$$

Fock space dynamics

- The Hamiltonian can be lifted to the Fock space in a natural way:

$$\begin{aligned}\mathcal{H}_N &= \bigoplus_{n=0}^{\infty} H_N^{(n)} \\ &\equiv \int dx\, \varepsilon\nabla_x a_x^* \varepsilon\nabla_x a_x + \frac{\varepsilon^3}{2}\int dxdy\, V(x-y) a_x^* a_y^* a_y a_x \;.\end{aligned}$$

That is:

$$e^{-i\mathcal{H}_N t/\varepsilon}\psi = (\psi^{(0)}, e^{-iH_N^{(1)} t/\varepsilon}\psi^{(1)}, \ldots, e^{-iH_N^{(n)} t/\varepsilon}\psi^{(n)}, \ldots) \;.$$

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- For simplicity, suppose that the initial datum is a Slater determinant:

$$\psi = (0, 0, \ldots, 0, \psi_{\text{Slater}}, 0, \ldots)$$

  where the only nontrivial entry is the one associated to $n = N$.

- Slater determinants can be conveniently represented via Bogoliubov transformations.

Bogoliubov transformations

- Let $\mathcal{F} \ni \psi = (0, 0, \ldots, \psi_{\text{Slater}}, 0, \ldots)$. There exists $R : \mathcal{F} \to \mathcal{F}$ s.t.:

  1. $\psi = R\Omega$ with $R^* R = 1$

  2. Let $\{f_i\}_{i=1}^{\infty}$ = basis of $L^2(\mathbb{R}^3)$, with $\{f_i\}_{i=1}^{N}$ orbitals of ψ_{Slater}. Then:

$$Ra(f_i)R^* = \begin{cases} a^*(f_i) & \text{for } i \leq N \\ a(f_i) & \text{for } i > N \end{cases}$$

- Equivalently, $Ra(g)R^* = a(ug) + a^*(\overline{vg})$, with

$$u \equiv u_N = 1 - \omega_N \;, \qquad v \equiv v_N = \sum_{i=1}^{N} |\overline{f_i}\rangle\langle f_i| \;.$$

Important properties: $u_N \overline{v}_N = 0, \qquad \overline{v}_N v_N = \omega_N.$

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  Important properties: $\quad u_N \overline{v}_N = 0, \qquad \overline{v}_N v_N = \omega_N.$

- In general, $R_t :=$ Bogoliubov transf. corresp. to $\omega_{N,t} = \sum_{i=1}^{N} |f_{i,t}\rangle\langle f_{i,t}|$. The state $R_t\Omega$ is the vacuum for the new operators $R_t a(f_i) R_t^*$.

Estimating the distance between density matrices

- The quantity $\mathrm{tr}_{L^2(\mathbb{R}^3)}\, \gamma^{(1)}_{N,t}(1-\omega_{N,t})$ allows to estimate the distance between the states. In fact:

$$\begin{aligned}\|\gamma^{(1)}_{N,t} - \omega_{N,t}\|^2_{\mathrm{HS}} &= \mathrm{tr}(\gamma^{(1)2}_{N,t} + \omega^2_{N,t} - \omega_{N,t}\gamma^{(1)}_{N,t} - \gamma^{(1)}_{N,t}\omega_{N,t}) \\ &\leq 2\,\mathrm{tr}\,\gamma^{(1)}_{N,t}(1-\omega_{N,t})\end{aligned}$$

where we used $\gamma^{(1)}_{N,t} \leq 1$, $\omega_{N,t} \leq 1$, together with $\mathrm{tr}\,\gamma^{(1)}_{N,t} = \mathrm{tr}\,\omega_{N,t} = N$.

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- On the other hand,

$$2\,\mathrm{tr}\,\gamma^{(1)}_{N,t}(1-\omega_{N,t}) = \langle \mathcal{U}(t)\Omega, \mathcal{N}\mathcal{U}(t)\Omega\rangle$$

  where:

$$\mathcal{N} = \bigoplus_{n\geq 0} n\mathbb{1}_{L^2(\mathbb{R}^{3n})} = \sum_{i=1}^{\infty} a^*(f_i)a(f_i) \qquad \text{[Number operator.]}$$

$$\mathcal{U}(t) = R^*_t e^{-i\mathcal{H}_N t/\varepsilon} R_0 \qquad \text{[Fluctuation dynamics.]}$$

- **Rmk.** $\mathcal{U}(t)$ does not preserve the number of particles!

Growth of number of fluctuations

- $\langle \mathcal{U}(t)\Omega, \mathcal{N}\mathcal{U}(t)\Omega\rangle$ can be controlled with a Gronwall-type inequality. The operator $\mathcal{N}$ commutes with most of the terms in the generator of $\mathcal{U}(t)$.

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$$
\begin{aligned}
&i\varepsilon\partial_t \big\langle \mathcal{U}(t)\Omega, \mathcal{N}\mathcal{U}(t)\Omega\big\rangle \\
&\quad = -4i\varepsilon^3 \mathrm{Im} \int dxdy\, V(x-y) \Big\langle \mathcal{U}(t)\Omega, \Big(a(\overline{v}_{t;x}) a(\overline{v}_{t;y}) a(u_{t;y}) a(u_{t;x}) \\
&\qquad + a^*(u_{t;x}) a(\overline{v}_{t;y}) a(u_{t;y}) a(u_{t;x}) + a^*(u_{t;y}) a^*(\overline{v}_{t;y}) a^*(\overline{v}_{t;x}) a(\overline{v}_{t;x}) \Big)\, \mathcal{U}(t)\Omega \Big\rangle \\
&\qquad + 4i\varepsilon^3 \mathrm{Im} \int dxdy\, V(x-y) \Big\langle \mathcal{U}(t)\xi, \Big(\omega_{N,t}(y;x) a^*(u_{t,y}) a^*(\overline{v}_{t,x}) \Big) \mathcal{U}(t)\Omega \Big\rangle
\end{aligned}
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- The largest term appearing in $i\varepsilon\partial_t\langle \mathcal{U}(t)\Omega, \mathcal{N}\mathcal{U}(t)\Omega\rangle$ is:

$$(*) = \varepsilon^3 \int dxdy\, V(x-y) \Big\langle \mathcal{U}(t)\Omega, a(u_{x;t})a(u_{y;t})a(\overline{v}_{y;t})a(\overline{v}_{x;t})\mathcal{U}(t)\Omega \Big\rangle$$

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Growth of number of fluctuations

- $\langle \mathcal{U}(t)\Omega, \mathcal{N}\mathcal{U}(t)\Omega\rangle$ can be controlled with a Gronwall type inequality. The operator $\mathcal{N}$ commutes with most of the terms in the generator of $\mathcal{U}(t)$.
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It would be zero, if V was constant. We want to gain from orthonormality in both x and y integrations. First try:

$$\begin{aligned}(*) &= \varepsilon^3 \int dp\, \hat{V}(p)\Big\langle \mathcal{U}(t)\Omega, \Big(\int dx\, a(u_{x;t})e^{ipx}a(\overline{v}_{x;t})\Big) \\ &\qquad\qquad \cdot \Big(\int dy\, a(u_{y;t})e^{-ipy}a(\overline{v}_{y;t})\Big)\mathcal{U}(t)\Omega\Big\rangle \\ &\leq \varepsilon^3 \int dp\, \hat{V}(p)\big\|u_t e^{ipx}\overline{v}_t\big\|_{\mathrm{tr}}^2\end{aligned}$$

where we used that $\big\|\int dr_1 dr_2 A(r_1,r_2)a_{r_1}a_{r_2}\big\|_{\mathrm{op}} \leq \|A\|_{\mathrm{tr}}$.

Global commutator estimates

- By orthonormality of u and v,

$$\varepsilon^3 \int dp\, \hat{V}(p) \big\| u_t e^{ipx} \overline{v}_t \big\|_{\mathrm{tr}}^2 \leq \varepsilon^3 \int dp\, \hat{V}(p) \big\| [\omega_{N,t}, e^{ipx}] \big\|_{\mathrm{tr}}^2 \leq C \varepsilon^3 (N\varepsilon)^2 \,,$$

provided $\big\| [\omega_{N,t}, e^{ipx}] \big\|_{\mathrm{tr}} \leq C N \varepsilon |p|$ [Global s.c. structure.]

- This strategy works for the mean-field regime, where $\varepsilon^3 = N^{-1}$. It gives:

$$\big| \varepsilon \partial_t \langle \mathcal{U}(t)\Omega, \mathcal{N} \mathcal{U}(t)\Omega \rangle \big| \leq C N \varepsilon^2 \Rightarrow \langle \mathcal{U}(t)\Omega, \mathcal{N} \mathcal{U}(t)\Omega \rangle \leq C N \varepsilon \ll N.$$

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- The strategy however fails for extended systems, since there $\varepsilon^3 = \varrho^{-1}$ and we lose two volume factors! It would lead to the useless bound:

$$\big| \varepsilon \partial_t \langle \mathcal{U}(t)\Omega, \mathcal{N} \mathcal{U}(t)\Omega \rangle \big| \lesssim |\Lambda|^2 \varepsilon^{-1} \,.$$

To improve, we need the exploit orthonormality at a smaller scale.

Local commutator estimate

- Using that, for $n \in \mathbb{N}$ suitably large:

$$V(x-y) = \int dp\, e^{ip\cdot(x-y)} \frac{1}{1+|p|^{2n}} (1+|p|^{2n}) \hat{V}(p) \equiv \int dz\, G(x-z) F(y-z)$$

for two nice functions F, G localized at 0, we have:

$$\varepsilon^3 \int dxdy\, V(x-y) \langle \mathcal{U}(t)\Omega, a(u_{x;t}) a(u_{y;t}) a(\overline{v}_{y;t}) a(\overline{v}_{x;t}) \mathcal{U}(t)\Omega \rangle =$$

$$\varepsilon^3 \int dz\, \langle \mathcal{U}(t)\Omega, \Big(\int dx\, a(u_{x;t}) F_z(x) a(\overline{v}_{x;t}) \Big) \Big(\int dy\, a(u_{y;t}) G_z(y) a(\overline{v}_{y;t}) \Big) \mathcal{U}(t)\Omega \rangle$$

with $F_z(x) \equiv F(x-z)$ and $G_z(y) \equiv G(y-z)$.

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with $F_z(x) \equiv F(x-z)$ and $G_z(y) \equiv G(y-z)$.

- Proceeding as before: (with $X_\Lambda(z) = 1 + \mathrm{dist}(z,\Lambda)^4$)

$$(*) \leq \varepsilon^3 \int dz \frac{1}{X_\Lambda(z)^2}\Big(X_\Lambda(z)\big\|[\omega_{N,t}, F_z]\big\|_{\mathrm{tr}}\Big)\Big(X_\Lambda(z)\big\|[\omega_{N,t}, G_z]\big\|_{\mathrm{tr}}\Big)$$

and we would like to estimate each parenthesis with $C\varepsilon^{-2}$.

Propagation of the local semiclassical structure

- By some algebra with commutators, and by the monotonicity properties of the trace norm, it turns out that it is enough to control:

$$X_\Lambda(z) \big\| \mathcal{W}_z [\omega_{N,t}, e^{ip\cdot x}] \big\|_{\mathrm{tr}} \qquad (**)$$

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We prove that, for $\hat{x}(t) = \hat{x} - ti\varepsilon\nabla$, for times for which excessive concentration does not occurr:

$$U_{\mathrm{H}}(t;0)^*\mathcal{W}_z(\hat{x})U_{\mathrm{H}}(t;0) \leq C\mathcal{W}_z(\hat{x}(t))$$

which is the key ingredient to show that (**) can be controlled by:

$$X_\Lambda(z)\big\|\mathcal{W}_z(\hat{x}(t))[\omega_N, e^{ip\cdot x}]\big\|_{\mathrm{tr}} + X_\Lambda(z)\big\|\mathcal{W}_z(\hat{x}(t))[\omega_N, \varepsilon\nabla]\big\|_{\mathrm{tr}} \lesssim \varepsilon^{-2}. \quad \blacksquare$$

Conclusions

- We discussed the derivation of the time-dependent Hartree equation for extended systems, at high density.
- The analysis builds on previous work [BPS14] for the mean-field regime, with the main crucial addition of exploiting a local semiclassical structure of the initial datum.
- Much more difficult to propagate along the Hartree flow. Need to rule out excessive concentration of particles, which we do for short times (Long times?)
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- **Thank you!**