Hartree-Fock dynamics for weakly interacting fermions

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Bosonic systems: described by

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \lambda \sum_{i<j}^{N} V(x_i - x_j)$$

acting on Hilbert space $L^2_s(\mathbb{R}^{3N})$ of symmetric wave functions.

Mean field regime: large number of weak collisions.

Realized when $N \gg 1$, $|\lambda| \ll 1$, $N\lambda \simeq 1$. Study Schrödinger evolution

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

Trapped bosons: ground state approximated by $\varphi^{\otimes N}$, with φ determined by Hartree theory.

For this reason, it makes sense to study evolution of approximately factorized initial data

Dynamics: factorization approximately preserved

$$\psi_{N,t} \simeq \varphi_t^{\otimes N}$$

where φ_t solves Hartree equation

$$i\partial_t \varphi_t = -\Delta \varphi_t + (V * |\varphi_t|^2)\varphi_t, \quad \text{with } \varphi_{t=0} = \varphi$$

One-particle reduced density: defined by kernel

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

Theorem: under appropriate assumptions on potential

$$\text{Tr} \left| \gamma_{N,t}^{(1)} - N|\varphi_t\rangle\langle\varphi_t| \right| \leq Ce^{K|t|}$$

Rigorous works: Hepp, Ginibre-Velo, Spohn, Erdős-Yau, Rodnianski-S., Fröhlich-Knowles-Schwarz, Knowles-Pickl, Grillakis-Machedon-Margetis, Lewin-Nam-S. , . . .

Fermionic systems: described by Hamiltonian

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \lambda \sum_{i<j} V(x_i - x_j)$$

Scaling: kinetic energy is of order $N^{5/3} \Rightarrow$ take $\lambda = N^{-1/3}$

Velocities are order $N^{1/3} \Rightarrow$ consider times of order $N^{-1/3}$;

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

Set $\varepsilon = N^{-1/3}$. We find

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

Hartree-Fock theory: consider trapped fermions, with

$$H_N = \sum_{j=1}^N (-\varepsilon^2 \Delta_{x_j} + V_{\text{ext}}(x_j)) + \frac{1}{N} \sum_{i<j}^N V(x_i - x_j)$$

Ground state $\simeq$ Slater determinant, with reduced density ω_N minimizing the Hartree-Fock energy

$$\begin{aligned} \mathcal{E}_{\text{HF}}(\omega_N) = \; & \text{Tr}(-\varepsilon^2 \Delta + V_{\text{ext}}) \omega_N \\ & + \frac{1}{2N} \int dx dy V(x-y) \left(\omega_N(x,x) \omega_N(y,y) - |\omega_N(x,y)|^2 \right) \end{aligned}$$

Goal: show that evolution of Slater determinant is approximately a Slater determinant, with reduced density $\omega_{N,t}$ s.t.

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

However: cannot be true for arbitrary initial Slater determinants.

Semiclassical structure: consider system of free fermions in box Λ, with volume one.

Ground state: is a Slater determinant

$$\omega_N(x,y) = \sum_{k \in \mathbb{Z}^3 : |k| \leq c N^{1/3}} e^{ik\cdot(x-y)} \simeq \varepsilon^{-3} \int_{|k|\leq c} dk \, e^{ik\cdot(x-y)/\varepsilon}$$

Consequence: $\omega_N(x,y) \simeq \varepsilon^{-3} \varphi((x-y)/\varepsilon)$ concentrates close to diagonal.

General trapping potential: we expect (linear combination of)

$$\omega_N(x,y) \simeq \varepsilon^{-3} \varphi\left(\frac{x-y}{\varepsilon}\right) g\left(\frac{x+y}{2}\right)$$

Conclusion: Slater determinants like ω_N satisfy

$$\begin{cases} \text{Tr}\,|[x,\omega_N]| & \leq CN\varepsilon \\ \text{Tr}\,|[\varepsilon\nabla,\omega_N]| & \leq CN\varepsilon \end{cases}$$

Thomas-Fermi theory: reduced density of ground state of

$$H_N = \sum_{j=1}^{N} (-\varepsilon^2 \Delta_{x_j} + V_{\text{ext}}(x_j)) + \frac{1}{N} \sum_{i<j}^{N} V(x_i - x_j)$$

approximated by

$$\omega_N(x,y) = \text{Op}_M(x,y) = \frac{1}{(2\pi\varepsilon)^3} \int dp\, M(p,(x+y)/2) e^{ip\cdot(x-y)/\varepsilon}$$

with phase-space density $M(p,q) = \chi(|p| \leq c\,\rho_{\text{TF}}^{1/3}(x))$.

Thomas-Fermi density: ρ_{TF} minimizes

$$\mathcal{E}_{\text{TF}}(\rho) = \frac{3}{5}\gamma \int dx \rho^{5/3}(x) + \int dx V_{\text{ext}}(x)\rho(x) + \frac{1}{2} \int dxdy\, V(x-y)\rho(x)\rho(y).$$

Semiclassics: since $[x, \omega_N] = i\varepsilon \text{Op}_{\nabla_p M}$, $[\varepsilon\nabla, \omega_N] = \varepsilon \text{Op}_{\nabla_q M}$,

$$\text{Tr}|[x, \omega_N]| \simeq \frac{\varepsilon}{(2\pi\varepsilon)^3} \int dpdq |\nabla_p M(p,q)| = CN\varepsilon \int \rho_{\text{TF}}^{2/3}(x)dx \leq CN\varepsilon$$

$$\text{Tr}|\varepsilon\nabla, \omega_N]| \simeq \frac{\varepsilon}{(2\pi\varepsilon)^3} \int dpdq |\nabla_q M(p,q)| = CN\varepsilon \int |\nabla \rho_{\text{TF}}(x)|dx \leq CN\varepsilon$$

Fock space: we introduce

$$\mathcal{F} = \bigoplus_{n \geq 0} L^2_a(\mathbb{R}^{3n}, dx_1 \dots dx_n)$$

Creation and annihilation operators: for $f \in L^2(\mathbb{R}^3)$ we define $a^*(f)$ und $a(f)$, satisfying the CAR

$$\{a(f), a^*(g)\} = \langle f, g \rangle, \quad \{a(f), a(g)\} = \{a^*(f), a^*(g)\} = 0$$

We also introduce operator valued distributions a^*_x, a_x so that

$$a^*(f) = \int dx\, f(x)\, a^*_x \quad \text{and} \quad a(f) = \int dx\, \overline{f(x)}\, a_x$$

Hamilton operator: Using these distributions, we define

$$\mathcal{H}_N = \varepsilon^2 \int dx \nabla_x a^*_x \nabla_x a_x + \frac{1}{2N} \int dx dy V(x-y)\, a^*_x a^*_y a_y a_x$$

Bogoliubov transformations: let

$$\omega_N = \sum_{j=1}^{N} |f_j\rangle\langle f_j|$$

be orthogonal projection onto $L^2(\mathbb{R}^3)$ with $\text{Tr}\,\omega_N = N$.

Let $\{f_j\}_{j\in\mathbb{N}}$ be an orthonormal basis of $L^2(\mathbb{R}^3)$.

Unitary implementor: find unitary map R_{ω_N} on $\mathcal{F}$ such that

$$R_{\omega_N}\Omega = a^*(f_1)\dots a^*(f_N)\Omega$$

and

$$R^*_{\omega_N} a^*(f_j) R_{\omega_N} = \begin{cases} a(f_j) & \text{if } j \leq N \\ a^*(f_j) & \text{if } j > N \end{cases}$$

For general $g \in L^2(\mathbb{R}^3)$, we have (with $u_N = 1 - \omega_N$)

$$R_{\omega_N} a^*(g) R_{\omega_N^*} = a^*(u_N g) + a(\omega_N g)$$

Theorem: let $V : \mathbb{R}^3 \to \mathbb{R}$ s.t.

$$\int |\widehat{V}(p)|(1+p^2)dp < \infty$$

Initial data: let ω_N be family of projections with $\text{Tr}\,\omega_N = N$ and

$$\text{Tr}\,|[x, \omega_N]| \leq CN\varepsilon \qquad \text{and} \qquad \text{Tr}\,|[\varepsilon\nabla, \omega_N]| \leq CN\varepsilon$$

Let ξ_N be a sequence in $\mathcal{F}$, with $\langle \xi_N, \mathcal{N}\xi_N \rangle \leq C$.

Time evolution: consider $\psi_{N,t} = e^{-i\mathcal{H}_N t/\varepsilon} R_{\nu_N} \xi_N$

Convergence in Hilbert-Schmidt norm: we have

$$\|\gamma^{(1)}_{N,t} - \omega_{N,t}\|_{\text{HS}} \leq C \exp(c_1 \exp(c_2|t|))$$

Convergence in trace norm: if additionally $\langle \xi_N, \mathcal{N}^2 \xi_N \rangle \leq C$ and $d\Gamma(\omega_{N,t})\xi_N = 0$, we have

$$\text{Tr}\left|\gamma^{(1)}_{N,t} - \omega_{N,t}\right| \leq CN^{1/6} \exp\left(c_1 \exp\left(c_2|t|\right)\right)$$

Extension: weaker bounds also hold if

$$\langle \xi_N, \mathcal{N} \xi_N \rangle \leq C N^\alpha, \qquad \text{for } 0 \leq \alpha < 1.$$

Corollary: let $\psi_N \in L^2_a(\mathbb{R}^{3N})$ be s.t.

$$\text{Tr} \left| \gamma^{(1)}_N - \omega_N \right| \leq C N^\alpha$$

for $0 \leq \alpha < 1$ and for orthogonal projection ω_N with $\text{Tr}\, \omega_N = N$, satisfying semiclassical bounds.

Then $\psi_{N,t} = e^{-iH_N t/\varepsilon} \psi_N$ is such that

$$\| \gamma^{(1)}_{N,t} - \omega_{N,t} \|_{\text{HS}} \leq C N^\alpha \exp(c_1 \exp(c_2 |t|))$$

Proof: set $\xi_N = R^*_{\omega_N} \psi_N$ and observe that

$$\langle \xi_N, \mathcal{N} \xi_N \rangle \leq \text{Tr} \left| \gamma^{(1)}_N - \omega_N \right| \leq C N^\alpha$$

Remarks:

Higher order densities: similar bounds can be proven for $\gamma^{(k)}_{N,t}$, for any fixed $k \in \mathbb{N}$.

Hartree-Fock versus Hartree: Exchange term in Hartree-Fock equation is of smaller order. Bounds continue to hold for

$$i\varepsilon\partial_t \widetilde{\omega}_{N,t} = \left[-\varepsilon^2\Delta + (V * \widetilde{\rho}_t), \widetilde{\omega}_{N,t}\right]$$

Vlasov dynamics: Hartree-Fock equation still depend on N. Let

$$W_{N,t}(x,v) = \frac{1}{(2\pi\varepsilon)^3}\int dy\, \omega_{N,t}\left(x + \frac{\varepsilon y}{2}, x - \frac{\varepsilon y}{2}\right)\, e^{iv\cdot y}$$

Then $W_{N,t} \to W_{\infty,t}$ as $N \to \infty$, where

$$\partial_t W_{\infty,t} + v\cdot\nabla_x W_{\infty,t} + \nabla\left(V * \rho_t\right)\cdot\nabla_v W_{\infty,t} = 0$$

is classical Vlasov equation.

Previous works:

Narnhofer-Sewell (1980) proved convergence towards Vlasov dynamics for smooth potentials.

Spohn (1982) extended convergence to bounded potentials.

Elgart-Erdős-S.-Yau (2003) proved convergence to Hartree but only for short times and analytic potentials.

Bardos-Golse-Gottlieb-Mauser (2002) and **Fröhlich-Knowles** (2010) showed convergence to Hartree-Fock dynamics, but with different scaling (no semiclassical limit).

Bach (1992) and **Graf-Solovej** (1994) proved that Hartree-Fock theory approximates ground state energy of systems of matter, up to relative error $o(\varepsilon^2)$.

Fluctuation dynamics: we define $\xi_{N,t}$ s.t.

$$e^{-i\mathcal{H}_N t/\varepsilon} R_{\omega_N} \xi_N = R_{\omega_{N,t}} \xi_{N,t}$$

Equivalently $\xi_{N,t} = \mathcal{U}_N(t)\xi_N$ with unitary evolution

$$\mathcal{U}_N(t) = R^*_{\omega_{N,t}} e^{-i\mathcal{H}_N t/\varepsilon} R_{\omega_N}$$

We want to compute

$$\begin{aligned}
\gamma^{(1)}_{N,t}(x,y) &= \langle e^{-i\mathcal{H}_N t/\varepsilon} R_{\omega_N} \psi_N, a^*_x a_y \, e^{-i\mathcal{H}_N t/\varepsilon} R_{\omega_N} \psi_N \rangle \\
&= \langle R_{\omega_{N,t}} \xi_{N,t}, a^*_x a_y R_{\omega_{N,t}} \xi_{N,t} \rangle \\
&= \left\langle \xi_{N,t}, \left(a^*(u_{N,t,x}) + a(\omega_{N,t,x} \right) \left(a(u_{N,t,y}) + a^*(\omega_{N,t,y}) \right) \xi_{N,t} \right\rangle \\
&= \omega_{N,t}(x,y) + \text{normally ordered terms}
\end{aligned}$$

Conclusion: need to control

$$\langle \xi_{N,t}, \mathcal{N} \xi_{N,t} \rangle = \langle \xi_N, \mathcal{U}^*_N(t) \mathcal{N} \mathcal{U}_N(t) \xi_N \rangle$$

uniformly in N.

Growth of fluctuations: we compute

$$
\begin{aligned}
i\varepsilon\,\partial_t \langle \mathcal{U}_N(t)\xi_N, \mathcal{N}\,\mathcal{U}_N(t)\xi_N\rangle
&= i\varepsilon\,\partial_t \left\langle R_{\omega_N}\xi_N, e^{i\mathcal{H}_N t/\varepsilon} \left(\mathcal{N} - 2d\Gamma(\omega_{N,t}) + N\right) e^{-i\mathcal{H}_N t/\varepsilon} R_{\omega_N}\xi_N \right\rangle \\
&= -2 \left\langle e^{-i\mathcal{H}_N t/\varepsilon} R_{\omega_N}\xi_N, \left\{ [\mathcal{H}_N, d\Gamma(\omega_{N,t})] + d\Gamma(i\varepsilon\,\partial_t \omega_{N,t}) \right\} \right. \\
&\qquad\qquad \left. \times\, e^{-i\mathcal{H}_N t/\varepsilon} R_{\omega_N}\xi_N \right\rangle
\end{aligned}
$$

Identity for derivative: We obtain

$$
\begin{aligned}
i\varepsilon\,\partial_t \langle \mathcal{U}_N(t)\xi_N, \mathcal{N}\,\mathcal{U}_N(t)\xi_N\rangle
&= \mathrm{Re}\, \frac{1}{N} \int dx dy V(x-y) \\
&\quad \times \left\langle \mathcal{U}_N(t)\xi_N, \left\{ a^*(u_{N,t,y}) a^*(\omega_{N,t,y}) a^*(\omega_{N,t,x}) a(\omega_{N,t,x}) \right.\right. \\
&\qquad + a^*(u_{N,t,x}) a(u_{N,t,x}) a(\omega_{N,t,y}) a(u_{N,t,y}) \\
&\qquad \left.\left. + a(u_{N,t,x}) a(\omega_{N,t,x}) a(\omega_{N,t,y}) a(u_{N,t,y}) \right\} \mathcal{U}_N(t)\xi_N \right\rangle
\end{aligned}
$$

Consider for example, the last contribution

$$
\frac{1}{N} \int dx dy V(x-y) \left\langle a(u_{N,t,x}) a(\omega_{N,t,x}) a(\omega_{N,t,y}) a(u_{N,t,y}) \right\rangle
$$

Expanding V in Fourier space, we find

$$\frac{1}{N}\int dxdyV(x-y)\left\langle a(u_{N,t,x})a(\omega_{N,t,x})a(\omega_{N,t,y})a(u_{N,t,y})\right\rangle$$
$$= \frac{1}{N}\int dp\,\widehat{V}(p)\Big\langle \int dr_1 ds_1 (\omega_{N,t}e^{ip\cdot x}u_{N,t})(r_1,s_1)a^*_{r_1}a^*_{s_1}\mathcal{U}_N(t)\xi_N,$$
$$\int dr_2 ds_2 (\omega_{N,t}e^{ip\cdot x}u_{N,t})(r_2,s_2)a_{r_2}a_{s_2}\mathcal{U}_N(t)\xi_N\Big\rangle$$

Bound for operators on $\mathcal{F}$: if $A(x,y)$ is kernel of operator A, we have

$$\left\|\int drdsA(r,s)a_r a_s\psi\right\| \leq \|A\|_{\text{HS}}\,\|(\mathcal{N}+1)^{1/2}\psi\|$$

Hence, we conclude that

$$\left|\frac{1}{N}\int dxdyV(x-y)\left\langle\, a(u_{N,t,x})a(\omega_{N,t,x})a(\omega_{N,t,y})a(u_{N,t,y})\,\right\rangle\right|$$
$$\leq \frac{1}{N}\int dp\,|\widehat{V}(p)|\,\|\omega_{N,t}\,e^{ip\cdot x}u_{N,t}\|^2_{\text{HS}}\,\|(\mathcal{N}+1)^{1/2}\mathcal{U}_N(t)\xi_N\|^2$$

Since $\|\omega_{N,t}\, e^{ip\cdot x} u_{N,t}\|_{\text{HS}}^2 \leq \|\omega_{N,t}\|_{\text{HS}}^2 = N$, we easily conclude that

$$\left| \frac{1}{N} \int dx dy V(x-y) \left\langle \, a(u_{N,t,x}) a(\omega_{N,t,x}) a(\omega_{N,t,y}) a(u_{N,t,y}) \, \right\rangle \right| \\ \leq C \langle \mathcal{U}_N(t)\xi_N, (\mathcal{N}+1)\mathcal{U}_N(t)\xi_N \rangle$$

However: this is still not enough, since we are computing $i\varepsilon\, \partial_t \ldots$

We need to extract an additional ε from $\|\omega_{N,t}\, e^{ip\cdot x} u_{N,t}\|_{\text{HS}}^2$.

Improved estimate: we notice that

$$\begin{aligned} \|\omega_{N,t}\, e^{ip\cdot x} u_{N,t}\|_{\text{HS}}^2 &= \|\omega_{N,t}\, [e^{ip\cdot x}, u_{N,t}]\|_{\text{HS}}^2 = \|\omega_{N,t}\, [e^{ip\cdot x}, \omega_{N,t}]\|_{\text{HS}}^2 \\ &\leq \|[e^{ip\cdot x}, \omega_{N,t}]\|_{\text{HS}}^2 \leq \text{Tr}|[e^{ip\cdot x}, \omega_{N,t}]| \\ &\leq C(1+|p|)\text{Tr}\,|[x, \omega_{N,t}]| \end{aligned}$$

Desired bound for growth of $\mathcal{N}$ follows, if we can show propagation of semiclassical structure

$$\text{Tr}\,|[x, \omega_{N,t}]| \leq C(t) N\varepsilon$$

Propagation of semiclassical structure: we observe

$$\begin{aligned} i\varepsilon\, \partial_t [x, \omega_{N,t}] &= [x, [-\varepsilon^2 \Delta + (V * \rho_t), \omega_{N,t}]] \\ &= [\omega_{N,t}, [x, \varepsilon^2 \Delta]] + [-\varepsilon^2 \Delta + (V * \rho_t), [x, \omega_{N,t}]] \\ &= \varepsilon [\varepsilon \nabla, \omega_{N,t}] + [-\varepsilon^2 \Delta + (V * \rho_t), [x, \omega_{N,t}]] \end{aligned}$$

The second term cannot change the trace norm (it acts as unitary conjugation). Hence

$$\mathrm{Tr}\, |[x, \omega_{N,t}]| \leq \mathrm{Tr}\, |[x, \omega_{N,0}]| + \int_0^t ds\, \mathrm{Tr}\, |[\varepsilon \nabla, \omega_{N,s}]|$$

Analogously, from assumption on the potential, we find

$$\mathrm{Tr}\, |[\varepsilon \nabla, \omega_{N,t}]| \leq \mathrm{Tr}\, |[\varepsilon \nabla, \omega_{N,0}]| + C \int_0^t ds\, \mathrm{Tr}\, |[x, \omega_{N,s}]|$$

Gronwall's Lemma: implies that

$$\begin{cases} \mathrm{Tr}\, |[x, \omega_{N,t}]| & \leq C N \varepsilon \exp(c|t|) \\ \mathrm{Tr}\, |[\varepsilon \nabla, \omega_{N,t}]| & \leq C N \varepsilon \exp(c|t|) \end{cases}$$