Dynamics of extended Fermi gases at high densities.

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Herrsching, June 7, 2022

Joint work with L. Fresta and M. Porta

Mean field limit: N fermions in torus $\Lambda = [0;1]^3$.

Kinetic energy: $\sum_{j=1}^N -\Delta_{x_j} \simeq N^{5/3}$

Potential energy: $\sum_{i<j}^N V(x_i - x_j) \simeq N^2$

Hamilton operator: on $L^2_a(\Lambda^N)$, we consider

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

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

Hartree-Fock theory: restrict to Slater determinants

$$\psi_{\text{slater}}(x_1,\ldots,x_N) \sim \det \Big(f_i(x_j)\Big)_{1\le i,j\le N}$$

with $\{f_j\}_{j=1}^N$ orthonormal system in $L^2(\Lambda)$.

Reduced density matrix: is rank N projection $\omega_N = \sum_{j=1}^N |f_j\rangle\langle f_j|$.

Hartree-Fock functional: energy given by

$$\mathcal{E}_{\text{HF}}(\omega_N) = \text{Tr}\,-\varepsilon^2\Delta\omega_N+\frac{1}{2N}\int V(x-y)\Big[\omega_N(x;x)\omega_N(y;y)-|\omega_N(x;y)|^2\Big]$$

Hartree-Fock energy: $E_{\text{HF}} = \inf_{\omega_N} \mathcal{E}_{\text{HF}}(\omega_N)$.

Correlation energy: defined by

$$E_{\text{corr}} = E_N - E_{\text{HF}}$$

See Niels talk in afternoon.

Dynamics: study evolution after traps are switched off.

Time scale: observe

$$e^{-i\tau\varepsilon^2\Delta}\, x\, e^{i\tau\varepsilon^2\Delta} = x + 2(\varepsilon\tau)(i\varepsilon\nabla)$$

Interested in $t = \varepsilon\tau$ of order one.

Schrödinger equation: on $L^2_a(\mathbb{R}^{3N})$, consider

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

for initial data $\psi_{N,0}$ close to a Slater determinant.

Semiclassical structure: consider Fermi sea

$$\omega_N(x;y) = \sum_{p \in 2\pi\mathbb{Z}^3 : |p| < cN^{1/3}} e^{ip\cdot(x-y)} \simeq N f((x-y)/\varepsilon)$$

Separation of scales: expect interesting states to have form

$$\omega_N(x;y) \simeq N f((x-y)/\varepsilon) \varrho((x+y)/2)$$

Commutators: capture semiclassical structure through bounds

$$\begin{cases} \operatorname{Tr} |[x, \omega_N]| & \lesssim N\varepsilon \\ \\ \operatorname{Tr} |[\varepsilon\nabla, \omega_N]| & \lesssim N\varepsilon \end{cases}$$

Remark: commutator bounds verified for ground states of non-interacting fermions in [Fournais-Mikkelsen 2019]

Theorem [Benedikter, Porta, S. 2013]: let $V : \mathbb{R}^3 \to \mathbb{R}$ with

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

Let ω_N be rank N projection on $L^2(\mathbb{R}^3)$, satisfying **semiclassical** commutator bounds.

Let $\psi_N \in L^2_a(\mathbb{R}^{3N})$ be Slater det. with reduced density ω_N, and

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

Then

$$\left\|\gamma_{N,t} - \omega_{N,t}\right\|_{\text{HS}} \lesssim 1$$

where

$$i\varepsilon\partial_t\omega_{N,t} = \Big[-\varepsilon^2\Delta + (V * \varrho_t), \omega_{N,t}\Big]$$

is **time dependent Hartree-Fock** equation, with $\omega_{N,0} = \omega_N$.

Remarks:

Rate of convergence: compare with $\|\gamma_{N,t}\|_{\text{HS}}, \|\omega_{N,t}\|_{\text{HS}} \simeq N^{1/2}$.

Exchange term: lower order, can be neglected

Vlasov equation: Hartree-Fock equation still depends on N. As $N \to \infty$, it can be approximated by Vlasov equation.

Other works: [Spohn '80], [Narnhofer-Sewell '81], [Bardos-Golse-Gottlieb-Mauser '03], [Elgart-Erdős-S.-Yau '04], [Fröhlich-Knowles '11], [Petrat-Pickl '15], [Porta-Rademacher-Saffirio-S. '16], [Chong-Lafleche-Saffirio, '21]

Norm approximation: obtained for dynamics of almost bosonic excitations of Fermi sea [Benedikter-Nam-Porta-S.-Seiringer, '21].

High density limit: consider N fermions in region $\Lambda \subset \mathbb{R}^3$ at density $\rho = N/|\Lambda|$, large but independent of N.

Kinetic energy: $\sum_{j=1}^N -\Delta_{x_j} \simeq \rho^{2/3} N$

Potential energy: $\sum_{i<j}^N V(x_i - x_j) \simeq \rho N$

Schrödinger equation: on $L^2_a(\mathbb{R}^{3N})$, consider

$$i\varepsilon\partial_t \psi_{N,t} = \left[\sum_{j=1}^N -\varepsilon^2 \Delta_{x_j} + \varepsilon^3 \sum_{i<j}^N V(x_i - x_j) \right] \psi_{N,t}$$

where now $\varepsilon = \rho^{-1/3}$ is small, but independent of N.

Initial data: we are interested in evolution of Slater determinant localized in region $\Lambda \subset \mathbb{R}^3$, with volume $|\Lambda| \simeq \varepsilon^3 N$.

Local semiclassical structure: let

$$W_z = \frac{1}{1 + |x - z|^4}$$

and its **free evolution**

$$W_z(t) = \frac{1}{1 + |x(t) - z|^4}, \qquad \text{with } x(t) = x - 2ti\varepsilon\nabla$$

Moreover, let $X_\Lambda(z) = 1 + \text{dist}(z, \Lambda)^4$.

We assume initial data satisfies **local bounds**

$$\sup_{t\in[0;T]} \sup_{z\in\mathbb{R}^3} X_\Lambda(z) \left\| W_z(t)\, \omega_N \right\|_{\text{tr}} \lesssim \varepsilon^{-3}$$

$$\sup_{t\in[0;T]} \sup_{z\in\mathbb{R}^3} X_\Lambda(z) \left\| W_z(t) \left[x, \omega_N\right] \right\|_{\text{tr}} \lesssim \varepsilon^{-2}$$

$$\sup_{t\in[0;T]} \sup_{z\in\mathbb{R}^3} X_\Lambda(z) \left\| W_z(t) \left[\varepsilon\nabla, \omega_N\right] \right\|_{\text{tr}} \lesssim \varepsilon^{-2}$$

Theorem: Assume V smooth and decaying sufficiently fast.

Let ω_N be a rank-N projection on $L^2(\mathbb{R}^3)$, exhibiting the **local semiclassical structure**.

Let $\omega_{N,t}$ be solution of Hartree-Fock equation

$$i\varepsilon\partial_t\omega_{N,t} = \Big[-\varepsilon^2\Delta + (V * \varrho_t), \omega_{N,t}\Big],$$

with $\omega_{N,t=0} = \omega_N$ and $\varrho_t(x) = \varepsilon^3\omega_{N,t}(x;x)$.

Moreover, assume the **no-concentration bound**

$$\sup_{t\in[0;T]} \sup_{z\in\mathbb{R}^3} \operatorname{Tr} W_z\,\omega_{N,t} \lesssim \varepsilon^{-3}$$

Let $\psi_N \in L^2_a(\mathbb{R}^{3N})$ be Slater determinant with reduced density ω_N and $\psi_{N,t}$ the solution of the many-body Schrödinger equation.

Then, for all $t \in [0;T]$,

$$\|\gamma_{N,t} - \omega_{N,t}\|_{\text{HS}} \lesssim \varepsilon^{1/2}N^{1/2}$$

Remarks:

Rates: $\|\gamma_{N,t}\|_{\mathsf{HS}}, \|\omega_{N,t}\|_{\mathsf{HS}} \simeq N^{1/2}$.

No-concentration: for $T > 0$ small enough, the no-concentration condition follows from the assumptions on data ω_N.

Assumptions: can be stated in terms of free evolution $\omega^0_{N,t}$ as

$$\sup_{t\in[0;T]} \sup_{z\in\mathbb{R}^3} X_\Lambda(z) \Big\| W_z \Big[x, \omega^0_{N,t} \Big] \Big\|_{\mathsf{tr}} \lesssim \varepsilon^{-2}$$

Coherent states: approximation for ground states of trapped systems constructed with coherent states satisfies assumptions.

Related work: [Lewin-Sabin,13], [Deckert-Fröhlich-Pickl-Pizzo,18].

Propagation of local structure: assuming data exhibits semi-classical structure and no-concentration, we have

$$\sup_{t\in[0;T]} \sup_{z\in\mathbb{R}^3} X_\Lambda(z)\|W_z\,\omega_{N,t}\|_{\mathrm{tr}} \lesssim \varepsilon^{-3}$$

$$\sup_{t\in[0;T]} \sup_{z\in\mathbb{R}^3} X_\Lambda(z)\|W_z\big[x,\omega_{N,t}\big]\|_{\mathrm{tr}} \lesssim \varepsilon^{-2}$$

$$\sup_{t\in[0;T]} \sup_{z\in\mathbb{R}^3} X_\Lambda(z)\|W_z\big[\varepsilon\nabla,\omega_{N,t}\big]\|_{\mathrm{tr}} \lesssim \varepsilon^{-2}$$

Corollary: $F:\mathbb{R}^3\to\mathbb{R}$ smooth and with fast decay. Then

$$\sup_{t\in[0;T]} \sup_{z\in\mathbb{R}^3} X_\Lambda(z)\left\|\Big[F_z(x),\omega_{N,t}\Big]\right\|_{\mathrm{tr}} \lesssim \varepsilon^{-2}$$

where $F_z(x)=F(x-z)$.

Proof: write $F(x)=H(x)G(x)$ and expand

$$\begin{aligned} H_z(x)\Big[G_z(x),\omega_{N,t}\Big] &= \int dp\,\widehat{G}_z(p)H_z(x)\Big[e^{ip\cdot x},\omega_{N,t}\Big] \\ &= i\int dp\,\widehat{G}_z(p)p\cdot\int_0^1 ds\,e^{isp\cdot x}H_z(x)\Big[x,\omega_{N,t}\Big]e^{i(1-s)p\cdot x} \end{aligned}$$

Evolution of localizers: define $U(t;s)$ by

$$i\varepsilon\partial_t U(t;s) = h(t)U(t;s), \qquad h(t) = -\varepsilon^2\Delta + (V * \varrho_t)$$

Then

$$U(t;s)^* W_z^2(t_0) U(t;s) \lesssim W_z^2(t_0 + t - s)$$

Proof: define propagator in interaction picture

$$U_I(t;s) = U_0(t)^* U(t;s) U_0(s)$$

so that

$$i\varepsilon\partial_t U_I(t;s) = U_0^*(t)(V * \varrho_t)U_0(t)U_I(t;s)$$

Claim follows if we can prove that

$$U_I(t;s)^* W_z^2(t_0) U_I(t;s) \lesssim W_z^2(t_0)$$

We find

$$
\begin{aligned}
& i\varepsilon\partial_t U_I(t;s)^* W_z^2(t_0) U_I(t;s) \\
&\qquad = U_I(t;s)^* \left[U_0(t)^*(V * \varrho_t)U_0(t), W_z^2(t_0)\right] U_I(t;s) \\
&\qquad = U_I(t;s)^* U_0(t)^* \left[V * \varrho_t, W_z^2(t_0+t)\right] U_0(t) U_I(t;s)
\end{aligned}
$$

Next observe

$$
\begin{aligned}
& \left[V * \varrho_t, W_z^2(t_0+t)\right] \\
& = W_z(t_0+t)\,[(V * \varrho_t), W_z(t_0+t)] - \text{h.c.} \\
& = W_z(t_0+t)\Big[(V * \varrho_t) - W_z(t_0+t)(V * \varrho_t)W_z^{-1}(t_0+t)\Big]W_z(t_0+t) - \text{h.c.}
\end{aligned}
$$

From **no-concentration** and smoothness of V, we find

$$
\left\|(V * \varrho_t) - W_z(t_0+t)(V * \varrho_t)W_z^{-1}(t_0+t)\right\|_{\mathrm{op}} \lesssim \varepsilon
$$

With **Gronwall**, we conclude

$$
U_I(t;s)^* W_z^2(t_0) U_I(t;s) \lesssim W_z^2(t_0) \qquad \square
$$

Proof of propagation: we compute

$$
\begin{aligned}
i\varepsilon\partial_t U(t;0)^*\big[x,\omega_{N,t}\big]U(t;0) &= U(t;0)^*\Big[\big[x,h(t)\big],\omega_{N,t}\Big]U(t;0) \\
&= 2\varepsilon\, U(t;0)^*\big[\varepsilon\nabla,\omega_{N,t}\big]U(t;0)
\end{aligned}
$$

Thus

$$
U(t;0)^*\big[x,\omega_{N,t}\big]U(t;0) = \big[x,\omega_N\big] + \int_0^t ds\, U(s;0)^*\big[\varepsilon\nabla,\omega_{N,s}\big]U(s;0)
$$

and

$$
\begin{aligned}
\Big\|W_z\big[x,\omega_{N,t}\big]\Big\|_{\mathrm{tr}} \leq{} & \Big\|W_z U(t;0)\big[x,\omega_N\big]U(t;0)^*\Big\|_{\mathrm{tr}} \\
& + \int_0^t ds\, \Big\|W_z U(t;s)\big[\varepsilon\nabla,\omega_{N,s}\big]U(t;s)^*\Big\|_{\mathrm{tr}}
\end{aligned}
$$

With control of **evolution of localizers**, we conclude

$$
\Big\|W_z\big[x,\omega_{N,t}\big]\Big\|_{\mathrm{tr}} \lesssim \Big\|W_z(t)\big[x,\omega_N\big]\Big\|_{\mathrm{tr}} + \int_0^t ds\, \Big\|W_z(t-s)\big[\varepsilon\nabla,\omega_{N,s}\big]\Big\|_{\mathrm{tr}}
$$

Proceed similarly to control commutator with $\varepsilon\nabla$. We find

$$\begin{aligned} i\varepsilon\partial_t U(t;0)^*\Big[\varepsilon\nabla,\omega_{N,t}\Big]U(t;0) &= U(t;0)^*\Big[\Big[\varepsilon\nabla,h(t)\Big],\omega_{N,t}\Big]U(t;0) \\ &= \varepsilon U(t;0)^*\Big[\nabla V * \varrho_t,\omega_{N,t}\Big]U(t;0) \end{aligned}$$

Using **no-concentration**, smoothness and decay of V, we find

$$\Big\|W_z\Big[\varepsilon\nabla,\omega_{N,t}\Big]\|_{\mathrm{tr}} \lesssim \Big\|W_z(t)\Big[\varepsilon\nabla,\omega_N\Big]\Big\|_{\mathrm{tr}} + \int_0^t ds\,\Big\|W_z(t-s)\Big[x,\omega_{N,s}\Big]\Big\|_{\mathrm{tr}}$$

Combined with

$$\Big\|W_z\Big[x,\omega_{N,t}\Big]\Big\|_{\mathrm{tr}} \lesssim \Big\|W_z(t)\Big[x,\omega_N\Big]\Big\|_{\mathrm{tr}} + \int_0^t ds\,\Big\|W_z(t-s)\Big[\varepsilon\nabla,\omega_{N,s}\Big]\Big\|_{\mathrm{tr}}$$

and with **assumptions**, Gronwall implies

$$\Big\|W_z\Big[x,\omega_{N,t}\Big]\Big\|_{\mathrm{tr}},\ \Big\|W_z\Big[\varepsilon\nabla,\omega_{N,t}\Big]\Big\|_{\mathrm{tr}} \lesssim \varepsilon^{-2} \qquad \square$$

Many-body analysis: switch to second quantization.

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: On $\mathcal{F}$, we define

$$\mathcal{H}_N = \varepsilon^2 \int dx \nabla_x a^*_x \nabla_x a_x + \frac{\varepsilon^3}{2} \int dx dy V(x-y)\, a^*_x a^*_y a_y a_x$$

Bogoliubov transformation: find basis $\{f_j\}_{j\in\mathbb{N}}$ of $L^2(\mathbb{R}^3)$ with

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

Unitary implementor: we 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 $u_N = 1 - \omega_N$)

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

For arbitrary $t \in \mathbb{R}$, we also find $R_{\omega_{N,t}}$ with

$$R^*_{\omega_{N,t}} a^*(g) R_{\omega_{N,t}} = a^*(u_{N,t} g) + a(\omega_{N,t} g)$$

Dynamics of excitations: we define $\xi_{N,t}$ s.t.

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

We observe that

$$\|\gamma_{N,t} - \omega_{N,t}\|_{\mathrm{HS}}^2 \leq 2N - 2\mathrm{Tr}\, \gamma_{N,t}\omega_{N,t} = 2\mathrm{Tr}\, \gamma_{N,t}(1 - \omega_{N,t})$$

and that

$$\begin{aligned} \mathrm{Tr}\, \gamma_{N,t}(1 - \omega_{N,t}) &= \langle \psi_{N,t}, d\Gamma(1 - \omega_{N,t})\psi_{N,t}\rangle \\ &= \langle R_{\omega_{N,t}}\xi_{N,t}, d\Gamma(u_{N,t}) R_{\omega_{N,t}}\xi_{N,t}\rangle \\ &= \langle \xi_{N,t}, d\Gamma(u_{N,t})\xi_{N,t}\rangle \\ &\leq \langle \xi_{N,t}, \mathcal{N}\xi_{N,t}\rangle \end{aligned}$$

Conclusion: need to control growth of number of excitations

$$\langle \xi_{N,t}, \mathcal{N}\xi_{N,t}\rangle$$

Growth of excitations: a computation shows that

$$\begin{aligned} i\varepsilon\, \partial_t \langle\, \xi_{N,t}, \mathcal{N}\, \xi_{N,t}\rangle &= \text{Re } \varepsilon^3 \int dx dy V(x-y) \\ &\quad \times \Big\langle\, \xi_{N,t}, \Big\{ a^*(u_{N,t,y}) a^*(\omega_{N,t,y}) a^*(\omega_{N,t,x}) a(\omega_{N,t,x}) \\ &\qquad\qquad + a^*(u_{N,t,x}) a(u_{N,t,x}) a(\omega_{N,t,y}) a(u_{N,t,y}) \\ &\qquad\qquad + a(u_{N,t,x}) a(\omega_{N,t,x}) a(\omega_{N,t,y}) a(u_{N,t,y}) \Big\}\, \xi_{N,t} \Big\rangle \end{aligned}$$

Bound for last term: we write

$$V(x-y) = \int dz\, V^{(1)}(x-z) V^{(2)}(z-y)$$

and

$$\begin{aligned} \mathrm{III} = \varepsilon^3 \int dz \Big\langle \Big[\int dx V^{(1)}(x-z) a^*(u_{N,t,x}) a^*(\omega_{N,t,x}) \Big] \xi_{N,t}, \\ \times \Big[\int dy V^{(2)}(y-z) a(u_{N,t,y}) a(\omega_{N,t,y}) \Big] \xi_{N,t} \Big\rangle \end{aligned}$$

Hence

$$\mathrm{III} \leq \varepsilon^3 \int dz \left\| A_z^{(1)*} \xi_{N,t} \right\| \left\| A_z^{(2)} \xi_{N,t} \right\|$$

with

$$\begin{aligned} A_z^{(j)} &= \int dx V^{(j)}(x-z) a(u_{N,t,x}) a(\omega_{N,t,x}) \\ &= \int dr ds \Big\{ u_{N,t} V_z^{(j)}(x) \omega_{N,t} \Big\}(r,s) a_r a_s \end{aligned}$$

where $V_z^{(j)}(x) = V^{(j)}(x-z)$ $(j = 1,2)$.

We estimate

$$\left\| A_z^{(j)} \right\|_{\text{op}} \lesssim \left\| u_{N,t} V_z^{(j)} \omega_{N,t} \right\|_{\text{tr}} \lesssim \left\| [V_z^{(j)}, \omega_{N,t}] \right\|_{\text{tr}}$$

We conclude that

$$\mathrm{III} \lesssim \varepsilon^3 \int dz X_\Lambda(z)^{-2} \prod_{j=1,2} \sup_{z \in \mathbb{R}^3} X_\Lambda(z) \left\| \left[\omega_{N,t}, V_z^{(j)} \right] \right\|_{\text{tr}} \lesssim \varepsilon^{-1} |\Lambda| \lesssim \varepsilon^2 N$$

Bound for second term: let

$$\mathrm{I} = \varepsilon^3 \int dxdy\, V(x-y) \langle \xi_{N,t}, a^*(u_{N,t,x}) a(\omega_{N,t,y}) a(u_{N,t,y}) a(u_{N,t,x}) \xi_{N,t} \rangle$$
$$= \varepsilon^3 \int dx \, \Big\langle \xi_{N,t}, a^*(u_{N,t,x}) \Big[\int dy V_x(y) a(\omega_{N,t,y}) a(u_{N,t,y}) \Big] a(u_{N,t,x}) \xi_{N,t} \Big\rangle$$

Estimating

$$\Big\| \int dy V_x(y) a(\omega_{N,t,y}) a(u_{N,t,y}) \Big\|_{\mathrm{op}} \lesssim \Big\| \big[V_x, \omega_{N,t} \big] \Big\|_{\mathrm{tr}} \lesssim \varepsilon^{-2}$$

we conclude that

$$\mathrm{II} \lesssim \varepsilon \int dx \, \| a(u_{N,t,x}) \xi_{N,t} \|^2 \lesssim \varepsilon \langle \xi_{N,t}, \mathcal{N} \xi_{N,t} \rangle$$

Conclusion: we find

$$\partial_t \langle \xi_{N,t}, \mathcal{N} \xi_{N,t} \rangle \lesssim N\varepsilon + \langle \xi_{N,t}, \mathcal{N} \xi_{N,t} \rangle$$

Thus

$$\langle \xi_{N,t}, \mathcal{N} \xi_{N,t} \rangle \lesssim N\varepsilon$$

$\square$