Mean field evolution of fermionic systems

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Outline

- Introduction.
- Results:
  1. Derivation of the time-dependent Hartree-Fock equation, for pure and mixed states, with bounded interaction potentials.
  2. Extension to Coulomb interactions.
- Conclusions.

Introduction

Fermionic mean field regime

- N interacting fermionic particles in $\mathbb{R}^3$, $\psi_N \in L^2_{\rm a}(\mathbb{R}^{3N})$.

  $V(x_i - x_j)$ = pair interaction potential, $V_{\rm ext}(x_i)$ = confining potential.

  System confined in $\Lambda \subset \mathbb{R}^3$, $|\Lambda| = O(1)$. Density $= O(N)$.

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- Mean field regime. V varies on scale $O(1)$, and $V \to N^{-1/3}V$. In fact:

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

  $E_{\rm kin} = \langle \psi_N, \sum_{i=1}^{N} -\Delta_{x_i}\psi_N\rangle \gtrsim N^{5/3}$ (by Lieb-Thirring inequality)

Fermionic mean field regime

- N interacting fermionic particles in $\mathbb{R}^3$, $\psi_N \in L^2_{\mathrm{a}}(\mathbb{R}^{3N})$.

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- Mean field Hamiltonian:

$$H_N^{\mathrm{trap}} := \sum_{j=1}^N \big[-\Delta_j + V_{\mathrm{ext}}(x_j) \big] + N^{-1/3} \sum_{i<j}^N V(x_i - x_j)$$

Hartree-Fock theory

- Hartree-Fock ground state energy:

$$E_{\mathrm{HF}}^{N} := \inf_{\psi_{\mathrm{Slater}}} \langle \psi_{\mathrm{Slater}}, H_N^{\mathrm{trap}} \psi_{\mathrm{Slater}} \rangle$$

$$\psi_{\mathrm{Slater}}(x_1, \ldots, x_N) = \frac{1}{\sqrt{N!}} \det f_i(x_j) \;, \qquad \langle f_i, f_j \rangle = \delta_{ij} \;.$$

- Setting $\omega_N := N \operatorname{tr}_{2,\ldots,N} |\psi_{\mathrm{Slater}}\rangle\langle\psi_{\mathrm{Slater}}| = \sum_{i=1}^{N} |f_i\rangle\langle f_i|$,

$$\langle \psi_{\mathrm{Slater}}, H_N^{\mathrm{trap}} \psi_{\mathrm{Slater}} \rangle = \operatorname{tr}(-\Delta + V_{\mathrm{ext}})\omega_N + \frac{1}{2N^{1/3}} \int V(x-y)(\omega_N(x;x)\omega_N(y;y) - |\omega_N(x;y)|^2)$$

One expects that, as $N \to \infty$:

$$E_{\mathrm{GS}}^{N} := \inf_{\psi \in L_{\mathrm{a}}^2(\mathbb{R}^{3N})} \frac{\langle \psi, H_N^{\mathrm{trap}} \psi \rangle}{\langle \psi, \psi \rangle} = E_{\mathrm{HF}}^{N} + \text{smaller order terms} \;,$$

Proven for large atoms: Bach '92, Graf-Solovej '94.

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  Proven for large atoms: Bach '92, Graf-Solovej '94.

- Next: Thomas-Fermi theory (Lieb-Simon '73, Fournais-Lewin-Solovej '15).

Fermionic mean-field dynamics

- Suppose that $V_{\text{ext}} = 0$ at $t = 0$. Dynamics:

$$i\partial_t \psi_{N,\tau} = \Big[\sum_{j=1}^{N} -\Delta_{x_j} + N^{-1/3} \sum_{i<j}^{N} V(x_i - x_j) \Big] \psi_{N,\tau}$$

- $E_{\text{kin}} \sim N^{5/3} \Rightarrow$ velocity $\sim N^{1/3}$. Time scale: $\tau \sim N^{-1/3}$.

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- Introducing the rescaled time $t = N^{1/3}\tau$:

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- Let $\varepsilon = N^{-1/3}$. Multiplying LHS and RHS by ε^2:

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

Mean-field limit coupled with a semiclassical scaling.

Hartree-Fock and Vlasov dynamics

- Let $\gamma_N^{(1)} = N \operatorname{tr}_{2,\dots,N} |\psi_N\rangle\langle\psi_N| \simeq \omega_N$, with $\omega_N = \omega_N^2$ (Slater det.).
- Expect: for $N \gg 1$, $\gamma_{N,t}^{(1)} \simeq \omega_{N,t} =$ solution of time dep. HF equation:

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

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

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- Wigner transform of $\omega_{N,t}$:

$$W_{N,t}(x,p) := \frac{\varepsilon^3}{(2\pi)^3}\int dy\,\omega_{N,t}\Big(x+\varepsilon\frac{y}{2}, x-\varepsilon\frac{y}{2}\Big)e^{-ip\cdot y}$$

As $N\to\infty$, Vlasov equation:

$$\boxed{\partial_t W_{\infty,t}(x,p) + p\cdot\nabla_x W_{\infty,t}(x,p) = \big(\nabla_x V * \rho_t\big)(x)\cdot\nabla_p W_{\infty,t}(x,p)}$$

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- Narnhofer-Sewell '81, Spohn '81; Elgart-Erdős-Schlein-Yau '04; Bardos-Golse-Gottlieb-Mauser '03, Fröhlich-Knowles '11

Results

Hartree-Fock dynamics of pure states

1. (interaction) $V \in L^1(\mathbb{R}^3)$, such that $\int dp\, |\widehat{V}(p)|(1+|p|)^2 < \infty$.
2. (initial data) $\psi_N \in L^2_{\mathrm{a}}(\mathbb{R}^{3N})$ s.t. $\mathrm{tr}\,|\gamma_N^{(1)} - \omega_N| \leq C$, with $\omega_N = \omega_N^2$ and

$$\mathrm{tr}\,|[e^{iq\cdot x}, \omega_N]| \leq CN\varepsilon\,(1+|q|)\,, \qquad \mathrm{tr}\,|[\varepsilon\nabla, \omega_N]| \leq CN\varepsilon$$

Theorem (Benedikter-P-Schlein, Comm. Math. Phys. '14)

Let $\gamma_{N,t}^{(1)}$ be the reduced 1PDM of $\psi_{N,t} = e^{-iH_N t/\varepsilon}\psi_N$. Let $\omega_{N,t}$ be the sol. of

$$i\varepsilon\partial_t \omega_{N,t} = [-\varepsilon^2\Delta + V * \rho_t - X_t, \omega_{N,t}]\,, \qquad \omega_{N,0} \equiv \omega_N$$

Then, for some constant $c > 0$ and for all $t \in \mathbb{R}$:

$$\|\gamma_{N,t}^{(1)} - \omega_{N,t}\|_{HS} \leq \exp(c\exp(c|t|))\,, \quad \mathrm{tr}\,|\gamma_{N,t}^{(1)} - \omega_{N,t}| \leq N^{1/2}\exp(c\exp(c|t|))$$

Remarks

1. Result still holds replacing Hartree-Fock with Hartree:

$$i\varepsilon\partial_t\widetilde{\omega}_{N,t} = [-\varepsilon^2\Delta + V * \rho_t, \widetilde{\omega}_{N,t}]$$

2. Pseudorelativistic case [Benedikter-P-Schlein, J. Math. Phys. '14]:

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

with $m = O(1)$. Under similar assumptions, we proved the emergence of the pseudorelativistic time-dependent HF equation:

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

3. Commutator estimates $\equiv$ semiclassical structure. Implied by

$$\omega_N(x;y) \simeq N\varphi\Big(\frac{x-y}{\varepsilon}\Big)\xi\Big(\frac{x+y}{2}\Big) \qquad \text{for suitable } \varphi,\ \xi.$$

true for the semiclassical approximation of the HF ground state.

4. Similar result: Petrat-Pickl '14.

Hartree-Fock dynamics of mixed states

1. (interaction) $V \in L^1(\mathbb{R}^3)$, $\int dp\, |\widehat{V}(p)|(1+|p|^2) < +\infty$.
2. (initial data) Quasi-free mixed state with 1PDM ω_N, s.t. $0 \leq \omega_N \leq 1$ and

$$\mathrm{tr}\,|[x, \sqrt{\omega_N}]|^2 \leq CN\varepsilon^2 \qquad \mathrm{tr}\,|[\varepsilon\nabla, \sqrt{\omega_N}]|^2 \leq CN\varepsilon^2$$
$$\mathrm{tr}\,|[x, \sqrt{1-\omega_N}]|^2 \leq CN\varepsilon^2 \qquad \mathrm{tr}\,|[\varepsilon\nabla, \sqrt{1-\omega_N}]|^2 \leq CN\varepsilon^2$$

Theorem (Benedikter-Jaksic-P-Saffirio-Schlein, CPAM '15)

Let $\gamma^{(1)}_{N,t}$ be the 1PDM of the many-body evolution of the initial state. Let $\omega_{N,t}$ be the solution of

$$i\varepsilon\partial_t \omega_{N,t} = \left[-\varepsilon^2\Delta + V * \rho_t - X_t, \omega_{N,t}\right], \qquad \omega_{N,0} \equiv \omega_N$$

Then, for some constant $c > 0$ and for all $t \in \mathbb{R}$:

$$\|\gamma^{(1)}_{N,t} - \omega_{N,t}\|_{HS} \leq \exp(c\exp(c|t|)), \quad \mathrm{tr}\,|\gamma^{(1)}_{N,t} - \omega_{N,t}| \leq N^{1/2}\exp(c\exp(c|t|))$$

HF dynamics of pure states - sketch of the proof

- Fock space representation:

$$\mathcal{F}(L^2(\mathbb{R}^3)) = \bigoplus_{n\geq 0} L^2_{\mathrm{a}}(\mathbb{R}^{3n}) \,, \qquad \mathcal{F} \ni \varphi = (\varphi^{(0)}, \varphi^{(1)}, \ldots, \varphi^{(n)}, \ldots)$$

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

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- For simplicity: $\psi_N = \psi_{\text{Slater}}$. On $\mathcal{F}$, $\psi_{\text{Slater}} \rightsquigarrow R_{\omega_0}\Omega$, with R_{ω_0} = Bogoliubov transformation and $\Omega = (1, 0, \ldots, 0, \ldots)$.

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- We get:

$$\|\gamma^{(1)}_{N,t} - \omega_{N,t}\|_{HS} \leq C\langle \mathcal{U}_N(t)\Omega, \mathcal{N}\mathcal{U}_N(t)\Omega\rangle$$

with $\mathcal{U}_N(t) = R^*_{\omega_t} e^{-i\mathcal{H}_N t/\varepsilon} R_{\omega_0}$ and $(\mathcal{N}\varphi)^{(n)} = n\varphi^{(n)}$.
- Goal: prove $\langle \mathcal{U}_N(t)\Omega, \mathcal{N}\mathcal{U}_N(t)\Omega\rangle \leq C(t)$, uniformly in N. Implied by:

$$\big|i\varepsilon\partial_t \langle \mathcal{U}_N(t)\Omega, \mathcal{N}\mathcal{U}_N(t)\Omega\rangle\big| \leq C\varepsilon\langle \mathcal{U}_N(t)\Omega, \mathcal{N}\mathcal{U}_N(t)\Omega\rangle$$

HF dynamics of pure states - sketch of the proof

- We have:

$$i\varepsilon\partial_t\langle\mathcal{U}_N(t)\Omega,\mathcal{N}\mathcal{U}_N(t)\Omega\rangle = \langle\mathcal{U}_N(t)\Omega,[\mathcal{N},\mathcal{L}_N(t)]\,\mathcal{U}_N(t)\Omega\rangle$$

with $\mathcal{L}_N(t)$ the generator of $\mathcal{U}_N(t)$. The largest contribution comes from:

$$\frac{1}{2N}\int dxdy\,V(x-y)a(u_x)a(u_y)a(\bar{v}_x)a(\bar{v}_y) + \text{h.c.}$$

with $u = 1-\omega_{N,t}$, $v^*v = \omega_{N,t}$ and $vu = 0$.

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$$\frac{1}{2N}\int dp\,\hat{V}(p)\int d\underline{r}\,(ve^{ipx}u)(r_1,r_3)(ve^{-ipx}u)(r_2,r_4)a_{r_1}a_{r_2}a_{r_3}a_{r_4}$$

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with $u = 1 - \omega_{N,t}$, $v^*v = \omega_{N,t}$ and $vu = 0$. Expectation bounded by:

$$N^{-1}\sup_p \frac{\mathrm{tr}\,|[\omega_{N,t}, e^{ipx}]|^2}{1+|p|}\langle \mathcal{U}_N(t)\Omega, \mathcal{N}\mathcal{U}_N(t)\Omega\rangle \le C(t)\varepsilon\langle \mathcal{U}_N(t)\Omega, \mathcal{N}\mathcal{U}_N(t)\Omega\rangle\ ,$$

thanks to the propagation of the semiclassical structure:

$$\mathrm{tr}\,|[\omega_{N,t},\, e^{ipx}]| \le Ce^{c|t|}N\varepsilon(1+|p|)\ , \qquad \mathrm{tr}\,|[\omega_{N,t},\, \varepsilon\nabla]| \le Ce^{c|t|}N\varepsilon\ .$$

■

Coulomb interactions?

- For Coulomb interactions, $\hat{V}(p) = p^{-2}$: slow decay in p.
- Instead of Fourier, use (smoothed) Fefferman-de la Llave representation:

$$\frac{1}{|x-y|} = \frac{4}{\pi^2}\int_0^\infty dr\,\frac{1}{r^5}\int dz\,\chi(|x-z|/r)\chi(|y-z|/r), \qquad \chi(\rho) = e^{-\rho^2}\,.$$

  Here, one has to control commutators $[\chi(|x|/r), \omega_{N,t}]$. Need to:

  - use the smallness of the support of $\chi(|x|/r)$ to control the r^{-5},
  - extract a factor ε from the commutator.

- $\Rightarrow$ A more local notion of semiclassical structure is needed to control the commutators.

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- $\Rightarrow$ A more local notion of semiclassical structure is needed to control the commutators.
- Results on short time scales, without semiclassical structure:

  Bach-Breteaux-Petrat-Pickl-Tzaneteas '14, Petrat '16.

Hartree-Fock dynamics for Coulomb interactions

- Let $\psi_N \in L^2_{\rm a}(\mathbb{R}^{3N})$ s.t. $\mathrm{tr}\,|\gamma^{(1)}_N - \omega_N| \leq C$, with $\omega_N = \omega_N^2$.

  Let $\rho_{|[\omega_{N,t},x]|}(x) := |[\omega_{N,t},x]|(x;x)$. Suppose that $\exists\, T>0$ s.t.:

$$\sup_{t\in[0,T]} \|\rho_{|[\omega_{N,t},x]|}\|_1 + \|\rho_{|[\omega_{N,t},x]|}\|_p \leq CN\varepsilon, \qquad \text{for some } p>5\,.$$

Theorem (P-Rademacher-Saffirio-Schlein, `arXiv:1608.05268`)

Let $\gamma^{(1)}_{N,t}$ be the reduced 1PDM of $\psi_{N,t} = e^{-iH_N t/\varepsilon}\psi_N$. Let $\omega_{N,t}$ be the sol. of

$$i\varepsilon\partial_t \omega_{N,t} = \left[-\varepsilon^2\Delta + V*\rho_t - X_t, \omega_{N,t}\right], \qquad \omega_{N,0}\equiv\omega_N$$

with $V(x-y) = |x-y|^{-1}$. Then, for every $\delta>0$ there exists $C>0$ s.t.:

$$\sup_{t\in[0,T]} \|\gamma^{(1)}_{N,t} - \omega_{N,t}\|_{HS} \leq CN^{5/12+\delta}\,, \qquad \sup_{t\in[0,T]} \mathrm{tr}\,|\gamma^{(1)}_{N,t} - \omega_{N,t}| \leq CN^{11/12+\delta}$$

Conclusions

Conclusions

- We proved the convergence of many-body dynamics to the Hartree-Fock dynamics, for pure and mixed states, in the mean field scaling.
- A crucial role is played by the semiclassical structure of the initial data, which can be propagated along the HF flow, for bounded potentials.
- Extension to Coulomb interactions, if the semiclassical structure holds at positive times (trivially true for translation invariant systems).
- Other results. Derivation of the Vlasov equation, staring from the HF equation, for pure and mixed states: Benedikter-P-Saffirio-Schlein, ARMA '16
- Open problems.
  - Propagation of the semiclassical structure for Coulomb potentials?
  - Stability of BCS initial data?
  - Other scaling regimes (quantum Boltzmann)?
  - ....

Thank you!

Mixed states

- So far, we considered initial data close to ψ_{Slater} (pure quasi-free state). OK for $T = 0$. What happens at $T > 0$?

Mixed states

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- However, we can still represent it with a pure state as follows. Let

$$\kappa_N := \rho_N^{1/2} = \sum_{n \geq 0} \lambda_n^{1/2} |\psi_n\rangle\langle\psi_n| \simeq \sum_{n \geq 0} \lambda_n^{1/2} \psi_n \otimes \overline{\psi}_n \in \mathcal{F} \otimes \mathcal{F}$$

  The state of the system is represented by a vector in $\mathcal{F} \otimes \mathcal{F}$:

$$\langle O \rangle_{\rho_N} = \mathrm{tr}_{\mathcal{F}}\, O \rho_N = \langle \kappa_N, O \otimes 1\, \kappa_N \rangle$$

Mixed states

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- It follows that

$$\|\gamma^{(1)}_{N,t} - \omega_{N,t}\|_{HS} \leq C \langle \mathcal{U}_N(t)\Omega, \mathcal{N}\,\mathcal{U}_N(t)\Omega\rangle$$

  with $\mathcal{U}_N(t) := R_t^* e^{-i\mathcal{L}_N t/\varepsilon} R_0$.

- Grönwall-type estimate plus propagation of semiclassical structure implies:

$$\langle \mathcal{U}_N(t)\Omega, \mathcal{N}\,\mathcal{U}_N(t)\Omega\rangle \leq C(t)$$