Mean-Field Dynamics of Fermionic Systems

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joint work with Vojkan Jakšić, Marcello Porta, Chiara Saffirio and Benjamin Schlein

Motivation

- Many physical systems can be modelled as fermionic many-body theories.
  Many non-rigorous approximation schemes exist.
- Rigorous understanding of approximations is difficult, in particular in non-equilibrium.

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- Many physical systems can be modelled as fermionic many-body theories.
  Many non-rigorous approximation schemes exist.
- Rigorous understanding of approximations is difficult, in particular in non-equilibrium.
- We establish one of the most fundamental approximations: time-dependent Hartree-Fock theory.
- Central requirement: quantitative understanding of 'semi-classicality'.
- Ideas turn out to apply very generally (extension to mixed states, derivation of Vlasov equation, . . .).

Outline

1. Fermionic Many-Body Systems
2. Main Result: Hartree-Fock Theory is a Valid Approximation.
3. . . . assuming certain Semi-Classical Estimates
4. Proof of Hartree-Fock Theory
5. Mixed States, Vlasov Equation

Outline

Fermionic Many-Body System

- N fermions in $\mathbb{R}^3$ are described by wavefunction

$$\psi \in L^2_a(\mathbb{R}^{3N}), \qquad \|\psi\|_2 = 1,$$

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- One-particle density matrix

$$\gamma_\psi := \mathrm{tr}_{2,\ldots,N} |\psi\rangle\langle\psi|.$$

Sufficient for calculating one-particle observables.

Time Evolution

- Schrödinger equation

$$i\partial_t \psi_t = H\psi_t, \qquad \psi_0 \in L^2_{\mathrm{a}}(\mathbb{R}^{3N}),$$

with Hamilton operator

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

Goal

Approximate one-particle density matrix γ_{ψ_t} by time-dependent Hartree-Fock equation and estimate error as $N \to \infty$.

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- Weak, but nontrivial, interaction:

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

Physical Regime

- Rescale time to scale of order $N^{-1/3}$

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- Introduce semi-classical parameter $\hbar := N^{-1/3}$, multiply by $\hbar^2$:

Mean-field scaling is coupled to semi-classical scaling

$$i\hbar\partial_t\psi_t = \left[\sum_{j=1}^{N} -\hbar^2\Delta_{x_j} + \frac{1}{N} \sum_{1\le i<j\le N} V(x_i - x_j)\right]\psi_t$$

$$\hbar = N^{-1/3}, \quad N \to \infty.$$

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Hartree-Fock Approximation

Restrict to Slater determinants

$$\psi(x_1, x_2, \ldots) = \frac{1}{\sqrt{N!}} \det\left(\varphi_i(x_j)\right)_{1\leq i,j\leq N},$$

and optimize the choice of the $\varphi_i \in L^2(\mathbb{R}^3)$.

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- Approximate time evolution

$$\frac{1}{\sqrt{N!}} \det\left(\varphi_{i,t}(x_j)\right) :\simeq e^{-iHt/\hbar} \frac{1}{\sqrt{N!}} \det\left(\varphi_{i,0}(x_j)\right)$$

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- Hartree-Fock equation

$$i\hbar\partial_t\varphi_{i,t} = -\hbar^2\Delta\varphi_{i,t} + \frac{1}{N}\sum_{j=1}^{N}\left(V * |\varphi_{j,t}|^2\right)\varphi_{i,t} - \frac{1}{N}\sum_{j=1}^{N}\left(V * (\varphi_{i,t}\overline{\varphi_{j,t}})\right)\varphi_{j,t}$$

$$i\hbar\partial_t\gamma_t^{\mathrm{HF}} = \left[-\hbar^2\Delta + V * \rho_t - X_t, \gamma_t^{\mathrm{HF}}\right]$$

Validity of HF Approximation

Is γ_t^{HF} close to γ_{ψ_t}, in mean-field scaling as $N \to \infty$?

- *Narnhofer-Sewell* '81: Convergence to Vlasov equation ($=$ semi-classical limit of HF). Analytic V.
- *Spohn* '81: more general V.

- *Erdős-Elgart-Schlein-Yau* '04: Convergence to HF for short times, $t < t_0$. Analytic V.
- *B-Porta-Schlein* '13: more general V. Arbitrary times t.

other physical regimes:
Bardos-Golse-Gottlieb-Mauser '03, *Fröhlich-Knowles* '11, *Pickl-Petrat* '14, *Bach-Breteaux-Petrat-Pickl-Tzaneteas* '15.

Validity of HF Approximation

Theorem (B-Porta-Schlein '13)

Let $V \in L^1(\mathbb{R}^3)$ *with* $\int |\hat{V}(p)|(1+|p|)^2 dp < \infty$.

Let $\{\varphi_{j,0}\}_{j=1}^{\infty}$ *be orthonormal in* $L^2(\mathbb{R}^3)$. *Let* $\psi_0 = \frac{1}{\sqrt{N!}} \det(\varphi_{i,0}(x_j))$.

Assume 'semi-classical commutators'

$$\|[\hat{x}, \gamma_{\psi_0}]\|_{\mathrm{tr}} \leq \hbar C, \qquad \|[-i\hbar\nabla, \gamma_{\psi_0}]\|_{\mathrm{tr}} \leq \hbar C.$$

Start with the same initial data ψ_0 *for Schrödinger equation and HF. Then*

$$\|\gamma_{\psi_t} - \gamma_t^{HF}\|_{\mathrm{tr}} \leq \frac{C}{N^{5/6}} e^{ce^{c|t|}}.$$

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The Semi-Classical Commutators

- e. g. ground state of trapped systems (with trap to be removed to observe evolution).
- non-interacting fermions in a box

$$\varphi_{j,0}(x) = e^{ik_j x}, \quad k_j \in 2\pi\mathbb{Z}^3.$$

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$$\gamma_{\psi_0}(x;y) = \frac{1}{N}\sum_{j=1}^{N} \varphi_{j,0}(x)\overline{\varphi_{j,0}}(y) = \frac{1}{N}\sum_{|k|\leq cN^{1/3}} e^{ik(x-y)}$$

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- more rigorously by coherent states quantization

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Particle-Hole Transformation

- embed in Fock space using 2nd quantization (for convenience)

Redefine 'particle' as 'excitation w. r. t. Slater determinant', using a unitarily implemented Bogoliubov transformation $\mathbb{U}_t$.

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- v_t = projection on $\operatorname{span}\{\varphi_{1,t}, \ldots, \varphi_{N,t}\}$ $\qquad v_{t,x}(y) = v_t(y; x)$
  $u_t = v_t^{\perp}$

$$\mathbb{U}_t a_x^* \mathbb{U}_t^* = a(v_{t,x}) + a^*(u_{t,x}).$$

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- Number of excitations w. r. t. HF-evolved Slater determinant

$$\mathcal{N}_t^{\mathrm{exc}} = \mathbb{U}_t \mathcal{N} \mathbb{U}_t^*.$$

- Error $\leq$ Number of Excitations

$$\|\gamma_{\psi_t} - \gamma_t^{\mathrm{HF}}\|_{\mathrm{tr}} \leq \frac{C}{N^{1/2}} \underbrace{\langle e^{-i\mathcal{H}t/\hbar}\psi_0, \mathcal{N}_t^{\mathrm{exc}}\, e^{-i\mathcal{H}t/\hbar}\psi_0 \rangle}_{=:\, r(t)} .$$

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- sufficient to prove (Grönwall)

$$r'(t) \leq C_t\, r(t) \quad \text{with } C_t = \mathcal{O}(N^0).$$

- most terms in $r'(t)$ cancel, remaining

$$\frac{1}{\hbar N} \int \mathrm{d}x\mathrm{d}y\; V(x-y) a^*(u_{t,y}) a(u_{t,y}) a(v_{t,x}) a(u_{t,x})$$

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- Semi-classical commutators: $V(x-y) = \int \hat{V}(p)\, e^{ip\cdot x} e^{-ip\cdot y} \mathrm{d}p$

$$\int \mathrm{d}x\, v_{t,x} e^{ip\cdot\hat{x}} u_{t,x} = \int \mathrm{d}x\, v_{t,x} [e^{ip\cdot\hat{x}}, u_t](\cdot, x) = \int \mathrm{d}x\, v_{t,x} \underbrace{[e^{ip\cdot\hat{x}}, N\gamma_t^{\mathrm{HF}}](\cdot, x)}_{\text{gain } \hbar}.$$

Outline

Hartree-Fock for Mixed States

- e. g. positive temperature
- described by density matrices

$$\Gamma : \mathcal{F}\left(L^2(\mathbb{R}^3)\right) \to \mathcal{F}\left(L^2(\mathbb{R}^3)\right).$$

- Purification: density matrix $\simeq$ vector in bigger Fock space

$$\mathcal{F}\left(L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)\right).$$

- Araki-Wyss representation of the dynamics.
- Replace p-h transformation by general Bogoliubov transformation.

Vlasov Equation as Semi-Classical Limit

$$\text{Hartree-Fock equation} \xrightarrow{\hbar \to 0} \text{Vlasov equation}$$

Summary

- Time-dependent Hartree-Fock theory is valid.
- Requires semi-classical structure (e. g. trapped ground states).
- Extension to mixed initial data; Derivation of Vlasov equation.