Effective Equations for Fermions in the Mean-field Limit

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Overview

(Note: subjective overview of results most relevant to this grant/conference)

We consider N fermions without spin in a mean-field limit.

Topics of this talk:

(1) Hartree–Fock equations (for pair interaction).

(2) Vlasov and Thomas–Fermi equations.

(3) Fermions coupled to a bosonic field.

Introduction

We consider:

- N fermions in d dimensions (mostly $d = 3$).
- Configuration space: Ω^N, with either $\Omega = \mathbb{R}^d$ or $\Omega = [0, L]^d$.
- Wave function $\psi \in L^2_{\mathrm{as}}(\Omega^N)$
  $= \left\{ \psi \in L^2(\Omega^N) : \psi(\ldots, x_j, \ldots, x_k, \ldots) = -\psi(\ldots, x_k, \ldots, x_j, \ldots) \right\}$.
- Hamiltonian $H =$ self-adjoint operator on $L^2_{\mathrm{as}}(\Omega^N)$
- Time-independent Schrödinger equation (spectral problem):

  $$H\psi = E\psi.$$

  Especially relevant/accessible: ground state energy $E_0 = \inf \sigma(H)$.
- Time-dependent Schrödinger equation (dynamical problem):

  $$i\partial_t \psi(t) = H\psi(t),$$

  with initial data $\psi(0) \in L^2_{\mathrm{as}}(\Omega^N) \Rightarrow \psi(t) = e^{-iHt}\psi(0)$.

(1) The Hamiltonian

We study Hamiltonians

$$H = \sum_{j=1}^{N}(-\Delta_j) + \lambda_N \sum_{i<j} v(x_i - x_j),$$

with

- Δ the Laplace operator,
- $v : \mathbb{R}^d \to \mathbb{R}$ the pair-interaction potential,
- $\lambda_N > 0$ the coupling constant.

Case (A):

- Choose $v(x) = |x|^{-1}$ (Coulomb potential), $d = 3$.
- Consider initial data localized in volume of $O(N)$.
- Then

$$H\psi = \underbrace{\sum_{j=1}^{N}(-\Delta_j)\psi}_{=O(N)} + \underbrace{\lambda_N \sum_{i<j} \frac{1}{x_i - x_j}\psi}_{=O(N^{5/3})}$$

$\Rightarrow$ choose $\lambda_N = N^{-2/3}$ (mean-field limit)

(1.A) Mean-field Description

Approximation for $\psi(t)$: most simple antisymmetric wave function

$\hookrightarrow$ Choose orthonormal $\varphi_1(t), \ldots, \varphi_N(t) \in L^2(\mathbb{R}^3)$.

$\hookrightarrow$ Effective N-particle state: $\bigwedge_{j=1}^N \varphi_j(t) = \phi_{\mathrm{HF}}(t)$, with

$$\phi_{\mathrm{HF}}(t, x_1, \ldots, x_N) = (N!)^{-1/2} \sum_{\sigma \in S_N} (-1)^\sigma \prod_{j=1}^N \varphi_{\sigma(j)}(t, x_j).$$

Here: the states $\varphi_1(t), \ldots, \varphi_N(t)$ solve the **Hartree-Fock eq.s**

$$i\partial_t \varphi_j(t) = -\Delta \varphi_j(t) + \underbrace{N^{-2/3} \left(|\cdot|^{-1} * \rho(t) \right) \varphi_j(t)}_{\text{direct term}}$$

$$\underbrace{- N^{-2/3} \sum_{k=1}^N \left(|\cdot|^{-1} * \overline{\varphi_k(t)} \varphi_j(t) \right) \varphi_k(t)}_{\text{exchange term}}$$

with density $\rho(t) = \sum_{k=1}^N |\varphi_k(t)|^2$.

- Note: exchange term subleading, we omit it (fermionic Hartree eq.s).
- Mathematical properties of HF eq.s in general: Sabin's talks

(1.A) Convergence

Convergence in terms of reduced one-particle density matrix $\gamma_\psi : L^2 \to L^2$,

$$\gamma_\psi(x,y) = \int dx_2 \dots dx_N \, \psi(x, x_2, \dots, x_N)\overline{\psi(y, x_2, \dots, x_N)}.$$

Note:

- $\gamma_{\wedge\varphi_j} = N^{-1} \sum_{j=1}^{N} |\varphi_j\rangle\langle\varphi_j|$
- $\mathrm{tr}\gamma_\psi = ||\psi|| = 1$

Want to show: $\gamma_{\psi(t)} \to \gamma_{\wedge\varphi_j(t)}$ as $N \to \infty$ in trace norm $||\cdot||_{\mathrm{tr}}$
(assuming $\gamma_{\psi(0)} \to \gamma_{\wedge\varphi_j(0)}$)

Then we can control bounded one-body operators A at time t:

$$\left|\mathrm{tr}(A\gamma_{\psi(t)}) - \mathrm{tr}(A\gamma_{\wedge\varphi_j(t)})\right| \leq ||A|| \left|\left|\gamma_{\psi(t)} - \gamma_{\wedge\varphi_j(t)}\right|\right|_{\mathrm{tr}} \to 0.$$

(1.A) Results

Theorem (Bach, Breteaux, SP, Pickl, Tzaneteas [J. Math. Pures Appl., 2016])
If $\sum_{j=1}^{N} \left|\left|\nabla\varphi_j(0)\right|\right|^2 \leq CN$, *then*

$$\left|\left|\gamma_{\psi(t)} - \gamma_{\phi_{\mathrm{HF}}(t)}\right|\right|_{\mathrm{tr}} \leq e^{Ct}\left(N^{1/3}\left|\left|\gamma_{\psi(0)} - \gamma_{\phi_{\mathrm{HF}}(0)}\right|\right|_{\mathrm{tr}}^{1/2} + N^{-1/6}\right).$$

Theorem (SP [J. Phys. A: Math. Theor., 2017])
If $\sum_{j=1}^{N} \left|\left|\nabla^4\varphi_j(0)\right|\right|^2 \leq CN$, *then*

$$\left|\left|\gamma_{\psi(t)} - \gamma_{\phi_{\mathrm{HF}}(t)}\right|\right|_{\mathrm{tr}} \leq Ce^{e^{Ct}}\left(\left|\left|\gamma_{\psi(0)} - \gamma_{\phi_{\mathrm{HF}}(0)}\right|\right|_{\mathrm{tr}}^{1/2} + N^{-1/2}\right).$$

Remarks:

- Theorems also hold with exchange term.
- Results for N^{-1} scaling: Bardos, Golse, Gottlieb, Mauser (2003, bounded v); Fröhlich, Knowles (2011, Coulomb)

(1.A) Discussion of Mean-field Approximation

$$i\partial_t \varphi_j(t) = -\Delta\varphi_j(t) + N^{-2/3}\left(|\cdot|^{-1} * \rho(t)\right)\varphi_j(t)$$

Note that "force" is small here: think of bounded ρ with support on ball with radius $N^{1/3}$, then

$$N^{-2/3}|\nabla(|\cdot|^{-1} * \rho)| \leq N^{-2/3}|\cdot|^{-2} * \rho \leq CN^{-2/3}\int_0^{N^{1/3}} r^{-2}r^2 dr \propto N^{-1/3},$$

i.e., average force per particle is small, $O(N^{-1/3})$
$\Rightarrow$ closeness to free dynamics with t, x dependent phase

$$\widetilde{\varphi}_j(t) := e^{-i\Phi^t(x)}\varphi_j^{\mathrm{free}}(t), \text{ with } \Phi^t(x) = N^{-2/3}\int_0^t ds \left(|\cdot|^{-1} * \rho^{\mathrm{free}}(s)\right)(x),$$

where

$$i\partial_t \varphi_j^{\mathrm{free}}(t) = -\Delta\varphi_j^{\mathrm{free}}(t).$$

(1.A) Results

Theorem (SP [J. Phys. A: Math. Theor., 2017])
If $\sum_{j=1}^{N} \left|\left|\nabla^4 \widetilde{\varphi}_j(0)\right|\right|^2 \leq CN$*, then*

$$\left|\left|\gamma_{\psi(t)} - \gamma_{\wedge\widetilde{\varphi}_j(t)}\right|\right|_{\mathrm{tr}} \leq Ce^{Ct}\left(\left|\left|\gamma_{\psi(0)} - \gamma_{\wedge\widetilde{\varphi}_j(0)}\right|\right|_{\mathrm{tr}}^{1/2} + N^{-1/3}\right).$$

Remarks:

- convergence rate $N^{-1/3}$ expected to be optimal
- simple examples for initial states:
  $\hookrightarrow$ plane waves in a box $[0, N^{1/3}]^3$
  $\hookrightarrow$ $\widetilde{\varphi}_j(0)$ with non-overlapping compact support and $\left|\left|\nabla^4 \widetilde{\varphi}_j(0)\right|\right| \leq C$

(1.B) Scaling Limit

Force $O(N^{-1/3})$ felt only on time scales $O(N^{1/3})$.

$\Rightarrow$ Case (B):

- Consider Schrödinger equation

$$iN^{-1/3}\partial_t\psi(t) = \sum_{j=1}^{N}(-\Delta_{x_j})\psi(t) + N^{-2/3}\sum_{i<j}|x_i - x_j|^{-1}\,\psi(t).$$

- More convenient: rescale $x \to N^{-1/3}x$, i.e, initial data localized in volume of $O(1)$.

$$iN^{-1/3}\partial_t\psi(t) = \sum_{j=1}^{N} N^{-2/3}(-\Delta_{x_j})\psi(t) + N^{-1}\sum_{i<j}|x_i - x_j|^{-1}\,\psi(t).$$

- Since initial data localized in volume $O(1)$, we can in fact consider a more general v:

$$iN^{-1/3}\partial_t\psi(t) = \sum_{j=1}^{N} N^{-2/3}(-\Delta_{x_j})\psi(t) + N^{-1}\sum_{i<j}v(x_i - x_j)\,\psi(t).$$

$\Rightarrow$ Coupled mean-field and semi-classical limit

(1.B) Results

$$iN^{-1/3}\partial_t\psi(t) = \sum_{j=1}^{N} N^{-2/3}(-\Delta_{x_j})\psi(t) + N^{-1}\sum_{i<j} v(x_i - x_j)\,\psi(t).$$

Overview of results:

- Elgart, Erdös, Schlein, Yau (2004) $\Rightarrow$ small times, analytic v
- Benedikter, Porta, Schlein (2013) $\Rightarrow$ all times, v in particular bounded, explicit error estimates
- SP, Pickl (2014) $\Rightarrow$ similar result; can be stated without reference to Fock-space construction

Theorem (Benedikter, Porta, Schlein [Commun. Math. Phys., 2014])
Assume $v \in L^1(\mathbb{R}^3)$, $\int d^3k\,(1+|k|^2)|\hat{v}(k)| < \infty$, *and*

$$\sup_{k\in\mathbb{R}^3}(1+|k|)^{-1}\left|\left|\left[\gamma_{\phi_{\mathrm{HF}}(0)}, e^{ikx}\right]\right|\right|_{\mathrm{tr}} \le CN^{-1/3},$$

$$\left|\left|\left[\gamma_{\phi_{\mathrm{HF}}(0)}, \nabla\right]\right|\right|_{\mathrm{tr}} \le C.$$

$$\textit{Then}\ \left|\left|\gamma_{\psi(t)} - \gamma_{\phi_{\mathrm{HF}}(t)}\right|\right|_{\mathrm{tr}} \le e^{e^{Ct}}\left(\left|\left|\gamma_{\psi(0)} - \gamma_{\phi_{\mathrm{HF}}(0)}\right|\right|_{\mathrm{tr}}^{1/2} + N^{-1/2}\right).$$

(1.B) Results

What about Coulomb interaction?

Theorem (Porta, Rademacher, Saffirio, Schlein [J. Stat. Phys., 2017])
Assume $\mathrm{tr}(-\Delta)\gamma_{\phi_{\mathrm{HF}}(t)} \leq CN^{2/3}$*, and assume that* **there exists** $T > 0$ *and* $p > 5$ *such that*

$$\sup_{t\in[0,T]} \sum_{i=1}^{3} \left(\|\rho_{|[x_i,\gamma_{\phi_{\mathrm{HF}}(t)}]|}\|_1 + \|\rho_{|[x_i,\gamma_{\phi_{\mathrm{HF}}(t)}]|}\|_p \right) \leq CN^{-1/3},$$

and $\left|\left|\gamma_{\psi(0)} - \gamma_{\phi_{\mathrm{HF}}(0)}\right|\right|_{\mathrm{tr}} \leq C$*. Then for every* $\delta > 0$ *there exits* $C(\delta, T) > 0$ *such that*

$$\sup_{t\in[0,T]} \left|\left|\gamma_{\psi(t)} - \gamma_{\phi_{\mathrm{HF}}(t)}\right|\right|_{\mathrm{tr}} \leq C(\delta, T)\, N^{-1/12+\delta}.$$

Note: Condition at time t holds for plane wave initial data in a box $\Omega = [0,1]^3$, but otherwise unclear.

Open problem: Proof only under (reasonable) assumption on initial data.

(1.B) Results

More results:

- Relativistic dispersion (Benedikter, Porta, Schlein 2014)
- Mixed states (Benedikter, Jaksic, Porta, Saffirio, Schlein 2014)
- Norm approximation for homogeneous Fermi gas using bosonization of particle-hole excitations (Benedikter, Nam, Porta, Schlein, Seiringer 2022); also ground state energy
- Fermions in magnetic fields: Perice's talk

(2) Setup

What is the semiclassical limit of

$$i\partial_t N^{-1/3}\varphi_j(t) = -N^{-2/3}\Delta\varphi_j(t) + N^{-1}\left(v * \rho(t)\right)\varphi_j(t) \quad ?$$

Consider Wigner transform

$$W_N(t,x,v) = N^{-1}(2\pi)^{-3}\int \gamma_{\phi_{\mathrm{HF}(t)}}(x+N^{-1/3}y/2, x-N^{-1/3}y/2)e^{-ivy}dy.$$

(Its inverse is the Weyl quantization.) In the limit $N \to \infty$, it should satisfy the Vlasov equation

$$\partial_t W(t) + 2v\cdot\nabla_x W(t) = \nabla(v * \rho(t))\cdot\nabla_v W(t).$$

(Note that $W_N(t,x,v)$ is not a probability density, but $W(t,x,v)$ is.)

Theorem (Benedikter, Porta, Saffirio, Schlein [ARMA, 2016])
Assume $v \in L^1(\mathbb{R}^3)$, $\int d^3k\,(1+|k|^2)|\hat{v}(k)| < \infty$, $\|W_N\|_{H^2_4} \le C$, $\|W_0\|_{H^2_4} \le C$, *and* $\|W_N - W_0\|_1 \le CN^{-1/6}$, $\|W_N - W_0\|_2 \le CN^{-1/6}$.
Then

$$\|W_N(t) - W(t)\|_2 \le N^{-1/3}e^{e^{Ct}} + N^{-1/6}e^{Ct}.$$

Note: $v(x) = |x|^{-\alpha}$, for $\alpha \in [0, \frac{1}{2})$ (Chong, Lafleche, Saffirio, 2021–2023)

(2) Ground State Energy

Ground state energy of

$$H_N = \sum_{j=1}^{N} \Big(- N^{-2/3} \Delta_{x_j} + V^{\mathrm{ext}}(x_j) \Big) + N^{-1} \sum_{i<j} v(x_i - x_j).$$

Theorem (Fournais, Lewin, Solovej [Calc. Var. PDE, 2018])
(Confining case.) Assume

$$v, V_-^{\mathrm{ext}} \in L^{1+d/2} + L^\infty_\varepsilon, \quad V_+^{\mathrm{ext}} \in L^1_{\mathrm{loc}}, \quad \lim_{|x|\to\infty} V_+^{\mathrm{ext}}(x) = \infty.$$

Then

$$\lim_{N\to\infty} \frac{E_0(N)}{N} = \inf \Big\{ \mathcal{E}_{\mathrm{TF}}(\rho) : 0 \le \rho \in L^1 \cap L^{1+2/d}, \int \rho = 1 \Big\},$$

where

$$\mathcal{E}_{\mathrm{TF}}(\rho) = \frac{c_{\mathrm{TF}}\, d}{d+2} \int \rho^{1+2/d} + \int V^{\mathrm{ext}} \rho + \frac{1}{2} \int\int v(x-y)\rho(x)\rho(y) dx dy,$$

and c_{TF} the Thomas–Fermi constant.

Note: This is also a minimizer of the Vlasov energy with
$W(x,p) = \mathbb{1}\Big(p^2 \le c_{\mathrm{TF}} \rho(x)^{2/d} \Big)$.

(3) Microscopic Model: Nelson with UV cutoff

Dynamics:

- Hilbert space $\mathscr{H}^{(N)} = L^2_{as}(\mathbb{R}^{3N}) \otimes \mathcal{F} \ni \Psi_{N,t}$, with $\mathcal{F}$ = bosonic Fock space
- Schrödinger equation

$$i\partial_t N^{-1/3}\Psi_{N,t} = H_N \Psi_{N,t},$$

with Hamiltonian

$$H_N = N^{-2/3}\sum_{j=1}^{N}\Big(-\Delta_j + \widehat{\Phi}_\Lambda(x_j)\Big) + N^{-1/3}\int d^3k\, \omega(k) a^*(k) a(k)$$

with

- bosonic creation and annihilation operators $a^*(k)$, $a(k)$ with

$$[a(k), a(l)] = 0 = [a^*(k), a^*(l)], \quad [a(k), a^*(l)] = \delta(k - l)$$

- free dispersion relation $\omega(k) = \sqrt{k^2 + m^2}$, mass $m \geq 0$
- field operator $\widehat{\Phi}_\Lambda(x) = \int d^3k\, \widetilde{\eta}(k)\Big(e^{ikx} a(k) + e^{-ikx} a^*(k)\Big)$,

  with cutoff in momentum space: $\widetilde{\eta}(k) = \frac{(2\pi)^{-3/2}}{\sqrt{2\omega(k)}} \mathbb{1}_{|k|\leq\Lambda}(k)$, $\Lambda > 1$.

(3) Effective Equations

Consider initial state

$$\Psi_N(0) \approx \bigwedge_{j=1}^{N} \varphi_j(0) \otimes W(N^{2/3}\alpha(0))\Omega$$

- $\bigwedge_{j=1}^{N} \varphi_j(0)$ antisymm. product of orthonormal $\varphi_1, \ldots, \varphi_N \in L^2(\mathbb{R}^3)$
- $\alpha(0) \in L^2(\mathbb{R}^3)$
- $\Omega =$ vacuum in $\mathcal{F}$, i.e., $a(k)\Omega = 0$
- Weyl operator $W(f) = \exp\Big(\int d^3k \left(f(k)a^*(k) - \overline{f(k)}a(k) \right) \Big)$. Note:

  $a(k)W(f)\Omega = f(k)W(f)\Omega, \quad a^*(k)W(f)\Omega = \overline{f(k)}W(f)\Omega + W(f)a^*(k)\Omega$

Schrödinger–Klein-Gordon equations:

$$N^{-1/3} i\partial_t \varphi_j(t) = \Big(-N^{-2/3}\Delta + \phi_\Lambda(x,t) \Big)\varphi_j(t), \quad j = 1, \ldots, N$$

$$\phi_\Lambda(x,t) := \int d^3k \, \widetilde{\eta}(k) \Big(e^{ikx}\alpha(t,k) + e^{-ikx}\overline{\alpha(t,k)} \Big)$$

$$i\partial_t \alpha(t,k) = \omega(k)\alpha(t,k) + (2\pi)^{3/2} N^{-1} \widetilde{\eta}(k) \mathcal{F}[\rho(t)](k),$$

with $\mathcal{F} =$ Fourier trafo, and electron density $\rho(t,x) := \sum_{j=1}^{N} |\varphi_j(t,x)|^2$

(3) Effective Equations

Well-posedness:

- $H^k(\mathbb{R}^3)$ = k-th Sobolev space
- $L^2_k(\mathbb{R}^3) = \{f \in L^2 : \|(1+|\cdot|)^{k/2} f\| < \infty\}$
- Theorem: If $\varphi_1^0, \ldots, \varphi_N^0 \in H^2(\mathbb{R}^3)$ orthonormal, $\alpha^0 \in L^2_1(\mathbb{R}^3)$, then so are $\varphi_1^t, \ldots, \varphi_N^t$ and α^t; solutions also strongly differentiable.

Alternatively:

$$\begin{aligned}&\left(\partial_t^2 - \Delta_x + m^2\right)\phi_\Lambda(x,t)\\ &\qquad = -(2\pi)^{-3/2}\int d^3k\, e^{ikx}\,\mathbb{1}_{|k|\leq\Lambda}(k) N^{-1}\mathcal{F}[\rho^t](k)\end{aligned}$$

Note: $\Lambda = \infty$, $m = 0$, with physical constants:

$$\left(c^{-2}\partial_t^2 - \Delta_x\right)\phi(x,t) = -\frac{e^2}{\varepsilon_0} N^{-1}\rho^t(x)$$

As $c \to \infty$: Poisson eq., i.e., $\phi(x,t) = -N^{-1}\frac{e^2}{4\pi\varepsilon_0}(|\cdot|^{-1} * \rho^t)(x)$ (attractive Hartree-Coulomb)

(3) Main Result

Theorem (Leopold, SP [Ann. H. Poincaré, 2019])
Let $p(0) := \sum_{j=1}^{N} |\varphi_j(0)\rangle\langle\varphi_j(0)|$, $q(0) := 1 - p(0)$. *We assume*

$$\|p(0)e^{ikx}q(0)\|_{\mathrm{Tr}} \leq C(1+|k|)N^{2/3} \; \forall k \in \mathbb{R}^3, \quad \|p(0)\nabla q(0)\|_{\mathrm{Tr}} \leq CN$$

and well-posedness. Let

$$\Psi_N(0) = \bigwedge_{j=1}^{N} \varphi_j(0) \otimes W(N^{2/3}\alpha(0))\Omega.$$

Then

$$\|\gamma_N^{\mathrm{fermion}}(t) - N^{-1}p(t)\|_{\mathrm{Tr}} \leq C_\Lambda(t)N^{-1/2},$$
$$\|\gamma_N^{\mathrm{boson}}(t) - |\alpha(t)\rangle\langle\alpha(t)|\|_{\mathrm{Tr}} \leq C_\Lambda(t)N^{-2/3},$$

where $p(t) = \sum_{j=1}^{N} |\varphi_j(t)\rangle\langle\varphi_j(t)|$.

Open questions:

- No cutoff?
- Relativistic Fermions?
- Convergence to Vlasov–Klein-Gordon?

Related questions:

- UV cutoff (not mean-field): talks by Schach Møller
- Other limits: Farhat' talk (classical limit)
- One particle in radiation field: Bach's and Breteaux's talks

Thank you for your attention!