Mean-Field Evolution of Fermionic Systems

Derivation of the time-dependent Hartree-Fock equation.

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joint work with Marcello Porta and Benjamin Schlein

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Quantum Mechanical Fermions

- We consider N particles in a fixed volume, e. g. electromagnetic trap.
- State of QM system $\sim$ wavefunction

$$\psi \in L^2(\mathbb{R}^{3N}) \simeq L^2(\mathbb{R}^3)^{\otimes N}.$$

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- Let $\mathcal{A} =$ projection on antisymmetric subspace. Restrict to

$$\psi \in \mathcal{A}L^2(\mathbb{R}^{3N}).$$

- $\rightsquigarrow$ Pauli exclusion principle: no two particles in the same orbital!

$$\mathcal{A}(\varphi \otimes \varphi \otimes \varphi_1 \dots \otimes \varphi_{N-2}) = 0.$$

Measurements and the Reduced Density

- In QM: observable $\sim$ self-adjoint operator O on $\mathcal{A}L^2(\mathbb{R}^{3N})$.
- Experiments to be compared to expectation values

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- One-particle observables O on $L^2(\mathbb{R}^3)$:

$$\begin{aligned}\langle \psi, O_1\psi \rangle &= \int \mathrm{d}x_1 \ldots \mathrm{d}x_N \, \overline{\psi}(x_1, x_2, \ldots) \int \mathrm{d}y \, O(x_1; y) \, \psi(y, x_2, \ldots) \\ &= \int \mathrm{d}x_1 \mathrm{d}y \, O(x_1; y) \underbrace{\int \mathrm{d}x_2 \ldots \mathrm{d}x_N \, \psi(y, x_2, \ldots) \overline{\psi}(x_1, x_2, \ldots)}_{= \operatorname{tr}_{2,\ldots,N} |\psi\rangle\langle\psi| \; =: \; \gamma_\psi \quad \text{partial trace}} \\ &= \int \mathrm{d}x_1 \mathrm{d}y \, O(x_1; y) \, \gamma_\psi(y; x_1) = \operatorname{tr} O\gamma_\psi.\end{aligned}$$

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&= \int \mathrm{d}x_1 \mathrm{d}y \, O(x_1; y) \, \gamma_\psi(y; x_1) = \mathrm{tr}\, O\gamma_\psi.
\end{aligned}$$

Expectation values can be calculated from the reduced density

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

Time Evolution

- Exact time evolution: Schrödinger equation

$$i\partial_t \psi_t = H\psi_t, \qquad \psi_{t=0} = \psi_0,$$

where H is the Hamilton operator

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

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- Solution:

$$\psi_t = e^{-iHt}\psi_0.$$

- In physical systems N is huge, $N \sim 10^3 - 10^{58}$.

Goal: Find more accessible equation that gives an approximation to γ_{ψ_t}.
Estimate error for $N \gg 1$.

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$$\sum_{j=1}^{N} -\Delta_{x_j} = \sum_{j=1}^{N} k_j^2 \simeq \mathcal{O}(N^{5/3}) \qquad \text{(c. f. bosons: } \mathcal{O}(N)\text{).}$$

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- For $N \gg 1$: Evolution non-trivial if kinetic and potential energy are same order of N. $\rightsquigarrow \lambda = N^{-1/3}$.

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

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- Introduce semiclassical time τ such that physical time t is $\mathcal{O}(N^{-1/3})$:

$$t = N^{-1/3}\tau \quad \leadsto$$

$$iN^{1/3}\partial_\tau\psi_\tau = \left[\sum_{j=1}^{N} -\Delta_{x_j} + \frac{1}{N^{1/3}} \sum_{1\leq i<j\leq N} V(x_i - x_j)\right]\psi_\tau.$$

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- Introduce semiclassical parameter $\varepsilon = N^{-1/3}$ and multiply with ε^2:

Combined Semiclassical and Mean-Field scaling:

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

Hartree-Fock Approximation

- Model with weak interaction should be close to model without interaction.
- N non-interacting fermions in a trap:
  $H = \sum_{j=1}^{N} h_j$, one-particle Hamiltonian $h = -\Delta + V_{\text{trap}}$ on $L^2(\mathbb{R}^3)$.
  Fill N eigenstates $\varphi_1, \ldots, \varphi_N \in L^2(\mathbb{R}^3)$ of h with lowest energy $\rightsquigarrow$

$$\psi_0 = \mathcal{A}(\varphi_1 \otimes \ldots \otimes \varphi_N) \in L^2(\mathbb{R}^{3N}).$$

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- N weakly interacting fermions in a trap:

$$\psi_0 \simeq \mathcal{A}(\varphi_1 \otimes \ldots \otimes \varphi_N) \in L^2(\mathbb{R}^{3N}).$$

Hartree-Fock approximation

Restrict attention to Slater determinants

$$\psi_0 = \mathcal{A}(\varphi_1 \otimes \ldots \otimes \varphi_N).$$

Hartree-Fock Energy Functional

Reminder:
$H = \sum_j -\varepsilon^2 \Delta_j + \frac{1}{N} \sum_{i,j} V(x_i - x_j)$

- For any Slater determinant ψ_0:

$$\begin{aligned}\langle \psi_0, \Big(H + \sum_{j=1}^N V_{\text{trap}}(x_j)\Big)\psi_0\rangle &= \int \mathrm{d}x \sum_{j=1}^N \Big(\varepsilon^2 |\nabla \varphi_j|^2 + V_{\text{trap}} |\varphi_j|^2\Big) \\ &\quad + \frac{1}{2N} \int \mathrm{d}x\mathrm{d}y \sum_{i,j=1}^N V(x-y) |\varphi_j(x)|^2 |\varphi_i(y)|^2 \\ &\quad - \frac{1}{2N} \int \mathrm{d}x\mathrm{d}y \sum_{i,j=1}^N V(x-y)\, \overline{\varphi_j(x)} \varphi_j(y)\, \varphi_i(x) \overline{\varphi_i(y)} \\ &=: \mathcal{E}_{\text{HF}}(\varphi_1, \ldots, \varphi_N).\end{aligned}$$

- Minimize $\mathcal{E}_{\text{HF}}(\varphi_1, \ldots, \varphi_N) \rightsquigarrow$ Approximation to ground state.

Hartree-Fock Evolution Equation

- Start with (approximate) ground state ψ_0 in a trap V_{trap}.
- Switch off $V_{\text{trap}} \rightsquigarrow$ Evolution by Schrödinger equation.
- Restricted to Slater determinants:

$$\psi_\tau \simeq \mathcal{A}(\varphi_{1,\tau} \otimes \ldots \otimes \varphi_{N,\tau}).$$

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- Evolution of the orbitals deduced from HF energy functional:

$$i\varepsilon\partial_\tau \varphi_{i,\tau} = -\varepsilon^2 \Delta\varphi_{i,\tau} + \frac{1}{N}\sum_{j=1}^{N}\left(V * |\varphi_{j,\tau}|^2\right)\varphi_{i,\tau} - \frac{1}{N}\sum_{j=1}^{N}\left(V * (\varphi_{i,\tau}\overline{\varphi_{j,\tau}})\right)\varphi_{j,\tau}.$$

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- Reduced density of Slater determinant: $\omega_\tau = \frac{1}{N}\sum_{j=1}^{N}|\varphi_{j,\tau}\rangle\langle\varphi_{j,\tau}|$.

Hartree-Fock equation for reduced density:

$$i\varepsilon\partial_\tau\omega_\tau = [-\varepsilon^2\Delta + V * \rho_\tau - X_\tau, \omega_\tau], \qquad \omega_0 = \gamma_0.$$

where $\rho_\tau(x) = \omega_\tau(x;x)$, X_τ integral op. with kernel $X_\tau(x;y) = V(x-y)\omega_\tau(x;y)$.

Accuracy of Hartree-Fock Dynamics

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

- *Erdős, Elgart, Schlein, Yau* '04: Convergence to HF. Short times. Analytic V.
- *B, Porta, Schlein* '13: Convergence to HF. Weaker assumptions: $V \in L^1(\mathbb{R}^3)$ with $\int |\hat{V}(p)|(1+|p|)^2 \mathrm{d}p < \infty$. Quantitative bounds on rate of convergence. Arbitrary times.

Without semiclassical scaling:

- *Bardos, Golse, Gottlieb, Mauser* '03: Short times, bounded V.
- *Fröhlich, Knowles* '11: Short times, Coulomb potential.

Theorem (B-Porta-Schlein '13)

Let $\{\varphi_j\}_{j=1}^{\infty}$ be an orthonormal basis in $L^2(\mathbb{R}^3)$.
Consider the Slater determinant $\psi_0 = \mathcal{A}(\varphi_1 \otimes \ldots \otimes \varphi_N)$.
Assume that its reduced density γ_0 satisfies the semiclassical commutator bounds

$$\mathrm{tr}|[\hat{x}, \gamma_0]| \leq \varepsilon C, \qquad \mathrm{tr}|[\varepsilon\nabla, \gamma_0]| \leq \varepsilon C.$$

Let ψ_τ be the solution to the Schrödinger equation with initial data ψ_0 and γ_τ its reduced density.
Let ω_τ be solution to the Hartree-Fock equation with initial data $= \gamma_0$.

Then there exist constants C, c such that for all times $\tau \in \mathbb{R}$

$$\mathrm{tr}|\gamma_\tau - \omega_\tau| \leq \frac{C}{N^{5/6}} \exp(c \exp(c|\tau|)).$$

(arXiv:1305.2768)

Extensions of the theorem

We can also treat

- more general initial data with a small number of extra particles that can carry arbitrary correlations,
- relativistic kinetic energy $\sqrt{-\varepsilon^2\Delta + m^2}$,
- k-particle reduced densities,
- Hilbert-Schmidt norm (rate $N^{-1/2}$).
- There is a subclass of observables ('semiclassical' observables), with expectation values converging at rate N^{-1}.

Notice:

- Exchange term $-X_\tau$ is of subleading order
  $\rightsquigarrow$ the Hartree equation is just as good as Hartree-Fock.

Justification of Semiclassical Commutator Bounds

- Consider as initial data the ground state of non-interacting fermions in a box $[0, 2\pi]^3$ with periodic boundary conditions:

$$\text{one-particle orbitals} = \text{plane waves:} \quad \varphi_j(x) = e^{ik_j x}, \quad k_j \in \mathbb{Z}^3.$$

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  Reduced density of $\psi_0 = \mathcal{A}(\varphi_1 \otimes \ldots \otimes \varphi_N)$ is

$$\gamma_0(x; y) = \frac{1}{N} \sum_{j=1}^{N} \varphi_j(x) \overline{\varphi_j}(y) = \frac{1}{N} \sum_{|k| \leq cN^{1/3}} e^{ik(x-y)}$$

$$\stackrel{q=\varepsilon k}{=} \frac{1}{N} \frac{1}{\varepsilon^3} \sum_{|q| \leq c} \varepsilon^3 e^{iq(x-y)/\varepsilon} \simeq \int_{|q| \leq 1} \mathrm{d}q \, e^{iq(x-y)/\varepsilon} = \varphi\left(\frac{x-y}{\varepsilon}\right).$$

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- In more realistic trap, we expect non-trivial configuration space density χ:

$$\gamma_0(x; y) \simeq \varphi\left(\frac{x-y}{\varepsilon}\right) \chi\left(\frac{x+y}{2}\right), \quad \varphi, \chi : \mathbb{R}^3 \to \mathbb{C}.$$

Justification of Semiclassical Commutator Bounds

- First semiclassical estimate:

$$[\hat{x}, \gamma_0](x; y) \simeq (x-y)\varphi\left(\frac{x-y}{\varepsilon}\right)\chi\left(\frac{x+y}{2}\right) \lesssim \varepsilon\varphi\left(\frac{x-y}{\varepsilon}\right)\chi\left(\frac{x+y}{2}\right).$$

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- Second semiclassical estimate:

$$[\varepsilon\nabla, \gamma_0](x; y) = \varepsilon(\nabla_x + \nabla_y)\gamma_0(x, y) \simeq \varepsilon\varphi\left(\frac{x-y}{\varepsilon}\right)\nabla\chi\left(\frac{x+y}{2}\right).$$

(Compare to $\varepsilon\nabla_x\gamma_0(x; y) = \varepsilon\frac{1}{\varepsilon}\nabla\varphi\left(\frac{x-y}{\varepsilon}\right)\chi\left(\frac{x+y}{2}\right) + \ldots$.)

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Proposition

The semiclassical commutator bounds are stable w. r. t. the Hartree-Fock equation: If initial data satisfies the semiclassical commutator bounds, then

$$\mathrm{tr}|[\hat{x},\omega_\tau]| \leq \varepsilon C e^{K|\tau|}, \qquad \mathrm{tr}|[\varepsilon\nabla,\omega_\tau]| \leq \varepsilon C e^{K|\tau|}.$$

Strategy of Proof

Outline:

1. Lift theory to Fock space (second quantization).
2. Particle-hole transformation $\rightsquigarrow$ Slater determinant = transformed vacuum (Fermi sea).
3. Reduced problem: Bound creation of excitations over the Fermi sea.
4. By Grönwall, it is sufficient to prove

$$\varepsilon \frac{\mathrm{d}}{\mathrm{d}\tau} \langle U(\tau)\Omega, \mathcal{N} U(\tau)\Omega \rangle \leq \varepsilon C(\tau) \langle U(\tau)\Omega, \mathcal{N} U(\tau)\Omega \rangle .$$

   $U(\tau)$: dynamics of excitatons.

5. In time derivative: Quadratic terms $\sim a^\# a^\#$ completely cancel against the Hartree-Fock equation.
6. Quartic terms $\sim a^\# a^\# a^\# a^\#$ remain.
7. To bound quartics with $\varepsilon\mathcal{N}$, use semiclassical commutator bounds.

Conclusions

Second Quantization

- Fermionic Fock space

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

$$\psi = (\psi^{(0)}, \psi^{(1)}, \ldots, \psi^{(n)}, \ldots) \in \mathcal{F}$$

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- Creation/annihilation operators $a(f)$, $a^*(f)$, where $f \in L^2(\mathbb{R}^3)$:

$$[a^*(f)\psi]^{(n)}(x_1, \dots, x_n) = \frac{1}{n}\sum_{j=1}^{n}(-1)^{j-1}\sqrt{n}\, f(x_j)\psi^{(n-1)}(x_1, \dots, \widehat{x_j}, \dots, x_n)$$

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$$[a(f)\psi]^{(n)}(x_1, \dots, x_n) = \sqrt{n+1}\int dx\, \overline{f}(x)\psi^{(n+1)}(x, x_1, \dots, x_n).$$

- Canonical anticommutation relations ($\{A, B\} = AB + BA$):

$$\{a(f), a^*(g)\} = \langle f, g\rangle_{L^2(\mathbb{R}^3)}, \quad \{a(f), a(g)\} = \{a^*(f), a^*(g)\} = 0.$$

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- Hamiltonian extended to act on Fock space $\mathcal{F}$:

$$\mathcal{H} = \varepsilon^2 \int dx\, \nabla a_x^* \nabla a_x + \frac{1}{2N} \int dxdy\, V(x-y) a_x^* a_y^* a_y a_x$$

On $\psi^{(N)}$ with exactly N particles $\mathcal{H} = H$.

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  On $\psi^{(N)}$ with exactly N particles $\mathcal{H} = H$.
- A product of a^*'s and a's is called normal-ordered, if the a^* are to the left of the a, e. g. $a^* a^* \cdots a^* a a \cdots a$.
- Rule of thumb: Normal-ordered products can be estimated with number-of-particles operator

$$\mathcal{N} = \int \mathrm{d}x \, a_x^* a_x \quad \text{(or powers of it).}$$

Particle-Hole Transformation

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- Extend $\varphi_1, \ldots, \varphi_N$ to o. n. b. $\{\varphi_j\}_{j\in\mathbb{N}}$ of $L^2(\mathbb{R}^3)$.
- Introduce a Bogoliubov transformation R:

$$R\, a_x\, R^* = a(u_x) + a^*(v_x),$$

where $u_x(y) = \delta(y-x) - \sum_{j=1}^{N} \varphi_j(y)\overline{\varphi}_j(x)$ and $v_x(y) = \sum_{j=1}^{N} \varphi_j(y)\varphi_j(x)$.

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$$R\, a_x\, R^* = a(u_x) + a^*(v_x),$$

where $u_x(y) = \delta(y-x) - \sum_{j=1}^{N} \varphi_j(y)\overline{\varphi}_j(x)$ and $v_x(y) = \sum_{j=1}^{N} \varphi_j(y)\varphi_j(x)$.

- Transformed vacuum is Slater determinant (Fermi sea):

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Particle-Hole Transformation

Redefine notion of particle s. th. "particle = excitation over Slater determinant". Implement as a unitary $R : \mathcal{F} \to \mathcal{F}$.

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- Transformed creation operators:

$$Ra^*(\varphi_i)R^* = \begin{cases} a(\varphi_i) & \text{for } i \leq N \quad \text{(creates hole)} \\ a^*(\varphi_i) & \text{for } i > N \quad \text{(creates particle).} \end{cases}$$

Excitation Dynamics

- General identity:

$$\gamma_\tau(y;x) = \frac{1}{N}\langle \psi_\tau, a_x^* a_y \psi_\tau \rangle = \frac{1}{N}\langle e^{-i\mathcal{H}\tau/\varepsilon} R\Omega, a_x^* a_y e^{-i\mathcal{H}\tau/\varepsilon} R\Omega \rangle.$$

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Error $\lesssim$ Number of Excitations

- $\rightsquigarrow$ Identity:

$$\gamma_\tau(y;x) - \omega_\tau(y;x)$$
$$= \frac{1}{N}\langle U(\tau)\Omega, \big(a^*(u_{\tau,x})a(u_{\tau,y}) + a(v_{\tau,x})a(u_{\tau,y}) + a^*(u_{\tau,x})a^*(v_{\tau,y})$$
$$- a^*(v_{\tau,y})a(v_{\tau,x})\big)\, U(\tau)\Omega\rangle.$$

- Operators are normal-ordered $\rightsquigarrow$ can be bounded with the number-of-particles operator $\mathcal{N} = \int \mathrm{d}x\, a_x^* a_x$.

$$\mathrm{tr}|\gamma_\tau - \omega_\tau| \lesssim \frac{C}{N^{5/6}}\langle U(\tau)\Omega, \mathcal{N} U(\tau)\Omega\rangle.$$

- To show: $\varepsilon \frac{\mathrm{d}}{\mathrm{d}\tau}\langle U(\tau)\Omega, \mathcal{N} U(\tau)\Omega\rangle \leq \varepsilon C(\tau)\langle U(\tau)\Omega, (\mathcal{N}+1) U(\tau)\Omega\rangle$.

  (Then by Grönwall's lemma $\langle U(\tau)\Omega, \mathcal{N} U(\tau)\Omega\rangle \leq \tilde{C}(\tau)$.)

Cancellations against Hartree-Fock Equation

- Time derivative:

$$i\varepsilon \frac{\mathrm{d}}{\mathrm{d}\tau} U^*(\tau)\mathcal{N} U(\tau) = U^*(\tau) R_\tau^* \Big(\mathrm{d}\Gamma(i\varepsilon \partial_\tau \omega_\tau) - [\mathcal{H}_N, \mathrm{d}\Gamma(\omega_\tau)] \Big) R_\tau U(\tau),$$

where $\mathrm{d}\Gamma(O) = \int \mathrm{d}x\, O(x;y) a_x^* a_y$.

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  By normal-ordering: quadratic + quartic terms.
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- Remaining:

$$\varepsilon \frac{\mathrm{d}}{\mathrm{d}\tau}\langle U(\tau)\Omega, \mathcal{N}U(\tau)\Omega\rangle$$
$$\simeq \frac{1}{N}\int \mathrm{d}x\mathrm{d}y\, V(x-y)\langle U(\tau)\Omega, a(u_{\tau,x})a(v_{\tau,x})a(v_{\tau,y})a(u_{\tau,y})U(\tau)\Omega\rangle.$$

Using the Semiclassical Commutator Bounds

- Have to extract a factor ε from the last expression,

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

$$\int \mathrm{d}x\, v_{\tau,x}e^{ip\cdot x}u_{\tau,x} = \int \mathrm{d}x\, v_{\tau,x}[e^{ip\cdot\hat{x}}, u_{\tau,x}] = \int \mathrm{d}x\, v_{\tau,x}\underbrace{[e^{ip\cdot\hat{x}}, N\omega_\tau](.,x)}_{\text{extract } \sqrt{\varepsilon}}.$$

□

Conclusions

- Hartree-Fock theory $\sim$ Restriction to Slater determinants.
- Fermionic mean-field scaling is coupled to semiclassical scaling.
- Controlling arbitrary times uses semiclassical commutator bounds, which hold for examples of initial data.
- Convenient language: particle-hole transformations.

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- Stationary properties: Semiclassical commutator bounds in general initial data? Excitation spectrum?
- Dynamical properties: Coulomb interaction? Gravitational collapse of stars? BCS theory of superconductivity/atomic nuclei?