Effective Dynamics of Interacting Fermions

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2014–2022 joint work with Vojkan Jakšić, Phan Thành Nam, Marcello Porta, Chiara Saffirio, Benjamin Schlein, Robert Seiringer, Jan Philip Solovej, and Jérémy Sok

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Quantum System of N Fermions

Hamilton operator of N identical spinless fermions:

$$H_N := \sum_{i=1}^{N}(-\Delta_i) + \lambda \sum_{1\le i<j\le N} V(x_i - x_j) \qquad \text{with } V : \mathbb{R}^3 \to \mathbb{R}\,.$$

Acts on the L^2–subspace of antisymmetric wave functions of $3N$ variables

$$\psi(x_{\sigma(1)}, x_{\sigma(2)}, \ldots, x_{\sigma(N)}) = \operatorname{sgn}(\sigma)\psi(x_1, x_2, \ldots, x_N) \qquad \forall \sigma \in S_N\,.$$

Time evolution is described by Schrödinger equation:

$$\left.\begin{array}{l} i\partial_t\psi_t = H_N\psi_t \\ \text{initial data } \psi_0 \end{array}\right\} \quad \Leftrightarrow \quad \psi_t = e^{-iH_N t}\psi_0\,.$$

Mean–Field Scaling Limit = High Density & Weak Interaction

- **High density:** N fermions, (at least initially) confined by external trapping potential or fixed–size torus and $N \to +\infty$

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- **High density:** N fermions, (at least initially) confined by external trapping potential or fixed–size torus and $N \to +\infty$

- **Weak interaction?** For simplicity consider antisymmetrized elementary tensors

$$\psi = \frac{1}{N!} \sum_{\sigma \in S_N} \operatorname{sgn}(\sigma)\, \varphi_{\sigma(1)} \otimes \cdots \otimes \varphi_{\sigma(N)}$$

of plane waves $\varphi_j(x) := \frac{1}{(2\pi)^{3/2}} \exp\left(ik_j \cdot x\right)$ with momenta $k_j \in \mathbb{Z}^3$:

$$\langle \psi, \sum_{j=1}^{N} (-\Delta_j) \psi \rangle = \sum_{|k| \leq cN^{1/3}} |k|^2 \sim N^{5/3} \qquad \text{c. f.} \qquad \langle \psi, \lambda \sum_{1 \leq i < j \leq N} V(x_i - x_j) \psi \rangle \sim \lambda N^2 \,.$$

fermionic mean–field scaling: $\lambda = N^{-1/3}$ (bosons: $\lambda = N^{-1}$)

Semiclassical Time Scale

- Velocity $\sim$ highest momenta $k \sim N^{1/3}$.
  A particle traverses the torus in a time of order $N^{-1/3}$.
  We consider $t = N^{-1/3}\tau$, where $\tau \sim 1$:

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

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- Convention: define effective Planck constant $\hbar := N^{-1/3}$ and multiply by $\hbar^2$

Fermionic mean–field scaling is naturally a semiclassical scaling:

$$i\hbar\partial_\tau \psi_\tau = \left[\sum_{j=1}^{N} -\hbar^2\Delta_{x_j} + \frac{1}{N} \sum_{1\leq i<j\leq N} V(x_i - x_j)\right] \psi_\tau \qquad \text{with } \hbar = N^{-1/3} \ .$$

Goal: Approximate ψ_τ by simpler initial value problems (effective theories)

- **Vlasov equation:**
  on classical phase space, no quantum effects retained, "semiclassical"
- **Hartree–Fock equation:**
  quantum, only the unavoidable minimum of entanglement due to the antisymmetry requirement (kinematic entanglement)
- **Random Phase Approximation:**
  quantum, entanglement of particle–hole pairs (leading order of the dynamical entanglement, i. e., due to the many–body interaction)

$\{\text{Vlasov}, \text{HF}, \text{RPA}\}$ is not an ordered set (no transitive or antisymmetric relation):

- Simpler equations may permit more precision in computations!
- Do we enlarge or restrict the set of permitted initial data?
- More effects neglected — more mathematical work to estimate them?

Vlasov Equation

Classical Approximation

- In classical mechanics a system is described by a particle density on phase phase:

$$f : \mathbb{R}^3 \times \mathbb{R}^3 \to [0, \infty) \,, \qquad \int f(x,p)\mathrm{d}x\mathrm{d}p = 1 \,.$$

- Classical mean–field evolution for f_τ: Vlasov equation

$$\underbrace{\frac{\partial f_\tau}{\partial \tau} + 2p \cdot \nabla_x f_\tau}_{\text{free transport}} = - \underbrace{F(f_\tau) \cdot \nabla_p f_\tau}_{\text{mean–field force}}$$

where

$$F(f_\tau) := -\nabla(V * \rho_{f_\tau}) \,, \qquad \rho_{f_\tau}(x) := \int f_\tau(x,p)\mathrm{d}p \,.$$

From Quantum to Classical

- **From quantum mechanics to phase space:**
  For $\psi \in L^2(\mathbb{R}^3)^{\otimes N}$, define the one–particle reduced density matrix

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

  and then the Wigner transform

$$W_\psi(x,p) := \frac{1}{(2\pi)^3} \int e^{-ip\cdot y/\hbar}\, \gamma_\psi\left(x + \frac{y}{2}; x - \frac{y}{2}\right) \mathrm{d}y\ .$$

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- *Narnhofer–Sewell* '81: W_{ψ_τ} converges to solution of Vlasov equation for analytic V,
- *Spohn* '81: generalization to twice differentiable V,
- *B–Porta–Saffirio–Schlein* '16: with explicit rate estimates,
- *Chong–Lafleche–Saffirio* '20–'22: singular V for mixed states as initial data,
- *Chen–Lee–Liew 19–'22*: Husimi function, mixed norm of two–particle r. d. m.

Hartree–Fock Approximation

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Restrict to antisymmetrized elementary tensors (Slater determinants) $\psi = \mathcal{A}(\varphi_1 \otimes \ldots \otimes \varphi_N)$ and optimize the choice of the $\varphi_j \in L^2(\mathbb{R}^3)$.

- Approximate time evolution

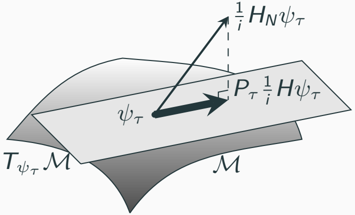
$$e^{-iH_N\tau/\hbar}\mathcal{A}(\varphi_{1,0} \otimes \ldots \otimes \varphi_{N,0}) \simeq \mathcal{A}(\varphi_{1,\tau} \otimes \ldots \otimes \varphi_{N,\tau})$$

- Hartree-Fock equations, for $i = 1, 2, \ldots N$:

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

Dirac–Frenkel principle:

Submanifold $\mathcal{M} \subset \mathcal{H}$



P_τ = orthog. projection on $T_{\psi_\tau}\mathcal{M}$

[Lubich '08, B–Sok–Solovej '18]

Rigorous Error Estimates

- *Erdős–Elgart–Schlein–Yau* '04: Convergence from Schrödinger equation to Hartree–Fock equation for short times, $\tau < \tau_0$. Analytic V.
- Hartree–Fock equation for scalings with weaker interaction or shorter time scale:
  - *Bardos–Golse–Gottlieb–Mauser* '03
  - *Fröhlich–Knowles* '11
  - *Pickl–Petrat '14*
  - *Bach–Breteaux–Petrat–Pickl–Tzaneteas '16*.
- *B–Porta–Schlein* '14: $V \in L^1(\mathbb{R}^3)$ with $\int |\hat{V}(p)|(1+|p|)^2 \mathrm{d}p < \infty$, arbitrary τ.
- generalizations: mixed states *B–Jakšić–Porta–Saffirio–Schlein* '16, singular interactions: *Porta–Rademacher–Saffirio–Schlein* '17, *Chong–Lafleche–Saffirio* '21–'22

Theorem (B–Porta–Schlein '14)

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

Let $\{\varphi_j\}_{j=1}^{\infty}$ *be an orthonormal basis in* $L^2(\mathbb{R}^3)$.
Let $\psi_0 = \mathcal{A}(\varphi_1 \otimes \ldots \otimes \varphi_N)$. *Assume semiclassical commutator bounds*

$$\|[x_i, \gamma_{\psi_0}]\|_{\mathrm{tr}} \le CN\hbar\,, \qquad \|[i\hbar\partial_i, \gamma_{\psi_0}]\|_{\mathrm{tr}} \le CN\hbar\,, \qquad \forall i = 1,2,3.$$

Let

- γ_{ψ_t}: *one–particle reduced density matrix of the solution of the Schrödinger equation with initial data* ψ_0,
- γ_t^{HF}: *solution of the Hartree–Fock equation with initial data* γ_{ψ_0}.

Then

$$\|\gamma_{\psi_t} - \gamma_t^{HF}\|_{\mathrm{tr}} \le CN^{1/6} e^{ce^{c|t|}} \qquad (\text{compare to } \operatorname{tr}\gamma_{\psi_t} = N = \operatorname{tr}\gamma_t^{HF})\,.$$

Construction of Semiclassical Initial Data

We require an $\hbar$–gain in commutators with position and momentum:

$$\|[x_i, \gamma_{\psi_0}]\|_{\mathrm{tr}} \leq CN\hbar \,, \qquad \|[i\hbar\partial_i, \gamma_{\psi_0}]\|_{\mathrm{tr}} \leq CN\hbar \,.$$

Verified for non–interacting fermions in different situations:

- translation invariant state: plane waves on torus (stationary under the HF evolution even when the interaction is switched on)
- in general trapping potentials [Fournais–Mikkelsen '19]: by semiclassical analysis
- in a harmonic oscillator: by explicit computation [B' 22]

Experimentally: quantum quench, i. e., prepare non–interacting trapped fermions in ground state, than switch on the interaction (and optionally switch off the trap).

Random Phase Approximation

Excitations over the Fermi ball

Start from the Fermi ball of the Hamiltonian on the torus. The Fermi ball is stationary under HF evolution. We study the evolution of its b excitations.

Split off the stationary Fermi ball by a particle–hole transformation:

$$R\, a_k^*\, R^* := \begin{cases} a_k^* & |k| > (\frac{3}{4\pi})^{1/3} N^{1/3} \\ a_k & |k| \leq (\frac{3}{4\pi})^{1/3} N^{1/3}\,. \end{cases}$$

Expand $R^* H_N R$ and normal–order

$$R^* H_N R = E_N^{\mathrm{pw}} + \underbrace{\hbar^2 \sum_{p \in \mathcal{B}_F^c} p^2 a_p^* a_p - \hbar^2 \sum_{h \in \mathcal{B}_F} h^2 a_h^* a_h}_{=:\; H^{\mathrm{kin}}} + \underbrace{X}_{\substack{\text{exchange term,}\\ \text{negligible}}} + \underbrace{Q}_{\substack{\text{interaction, quartic in}\\ \text{operators } a^* \text{ and } a}}$$

Try to find a quadratic approximation to the excitation Hamiltonian $H^{\mathrm{kin}} + Q$.

(Quadratic Hamiltonians can be diagonalized by Bogoliubov transformations.)

Bosonization of the Interaction

Observe: if we introduce collective pair operators

$$b_k^* := \sum_{\substack{p \in \mathcal{B}_F^c \\ h \in \mathcal{B}_F}} \delta_{p-h,k} a_p^* a_h^*$$

p "particle" outside the Fermi ball

h "hole" inside the Fermi ball

then

$$Q = \frac{1}{N} \sum_{k \in \mathbb{Z}^3} \hat{V}(k) \Big(2 b_k^* b_k + b_k^* b_{-k}^* + b_{-k} b_k \Big) + \mathcal{O}\Big(\frac{\mathcal{N}^2}{N} \Big) .$$

This is convenient because the b_k^* and b_k have approximately bosonic commutators:

$$[b_k^*, b_l^*] = 0 \quad , \qquad [b_l, b_k^*] = \delta_{k,l} n_k^2 + \mathcal{E}(k, l) .$$

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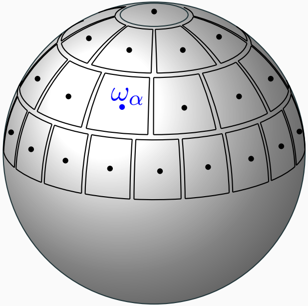
But how to express H^{kin} through pair operators?

Bosonization of the Kinetic Energy

Fermi ball $\mathcal{B}_F$



[Benfatto–Gallavotti '90]
[Haldane '94]
[Fröhlich–Götschmann–Marchetti '95]
[Kopietz et al. '95]

Localize to $M = M(N)$ patches near the Fermi surface,

$$b^*_{\alpha,k} := \frac{1}{n_{\alpha,k}} \sum_{\substack{p \in \mathcal{B}_F^c \cap B_\alpha \\ h \in \mathcal{B}_F \cap B_\alpha}} \delta_{p-h,k} a^*_p a^*_h$$

with $n_{\alpha,k}$ chosen to normalize $\|b^*_{\alpha,k}\Omega\| = 1$.

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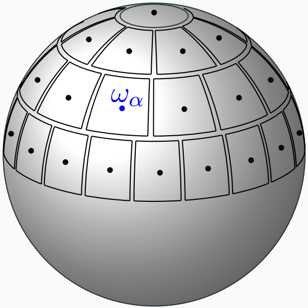

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Linearize kinetic energy around patch center ω_α:

$$[H^{\text{kin}}, b^*_{\alpha,k}] \simeq 2\hbar|k\cdot\hat{\omega}_\alpha| b^*_{\alpha,k}\ .$$

We approximate

$$H^{\text{kin}} \simeq \sum_{k\in\mathbb{Z}^3} \sum_{\alpha=1}^{M} 2\hbar u_\alpha(k)^2 b^*_{\alpha,k} b_{\alpha,k}\,, \quad u_\alpha(k)^2 := |k\cdot\hat{\omega}_\alpha|\,.$$

Decomposing the Interaction over Patches

Recall

$$Q = \frac{1}{N} \sum_{k \in \mathbb{Z}^3} \hat{V}(k) \left(2 b_k^* b_k + b_k^* b_{-k}^* + b_{-k} b_k \right)$$

Decompose

$$b_k^* = \sum_{\alpha=1}^{M} n_{\alpha,k} b_{\alpha,k}^* + \text{lower order} \; .$$

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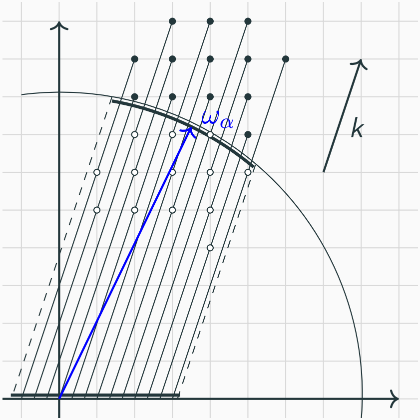
Normalization:

$$n_{\alpha,k}^2 = \#\text{p-h pairs in patch } B_\alpha \text{ with momentum } k$$

$$\simeq \frac{4\pi N^{2/3}}{M} |k \cdot \hat{\omega}_\alpha| = \frac{4\pi N^{2/3}}{M} u_\alpha(k)^2 .$$



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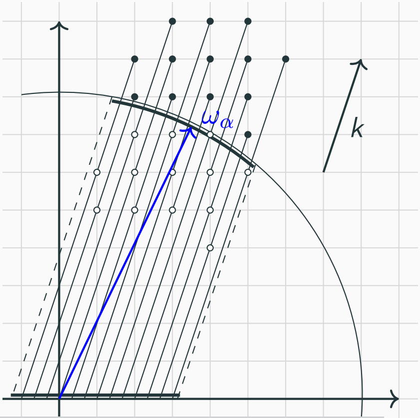


Effective Quadratic Bosonic Hamiltonian

$$H^{\text{eff}} = \hbar \sum_{k \in \mathbb{Z}^3} \left[\sum_{\alpha} u_\alpha(k)^2 b_{\alpha,k}^* b_{\alpha,k} + \frac{\hat{V}(k)}{M} \sum_{\alpha,\beta} \left(u_\alpha(k) u_\beta(k) b_{\alpha,k}^* b_{\beta,k} + u_\alpha(k) u_\beta(k) b_{\alpha,k}^* b_{\beta,-k}^* + \text{h.c.} \right) \right]$$

Bogoliubov Diagonalization

Quadratic Hamiltonians can be diagonalized by a Bogoliubov transformation

$$T = \exp\left(\sum_{k \in \mathbb{Z}^3} \sum_{\alpha,\beta=1}^{M} K(k)_{\alpha,\beta} b^*_{\alpha,k} b^*_{\beta,-k} - \text{h.c.} \right) .$$

Expanding into commutators we find

$$T^* b_{\alpha,k} T \simeq \sum_{\beta=1}^{M} \cosh(K(k))_{\alpha,\beta} b_{\beta,k} + \sum_{\beta=1}^{M} \sinh(K(k))_{\alpha,\beta} b^*_{\beta,-k} .$$

Choose the $M \times M$–matrix $K(k)$ to make $b^* b^*$– and bb–terms vanish from $T^* H^{\text{eff}} T$:

$$T^* H^{\text{eff}} T \simeq E_N^{\text{RPA}} + \hbar \sum_{k \in \mathbb{Z}^3} \sum_{\alpha,\beta=1}^{M} E(k)_{\alpha,\beta} b^*_{\alpha,k} b_{\beta,k} .$$

In particular, the ground state of H^{eff} is $\xi_{\text{gs}} \simeq T\Omega$, and therefore the ground state of H_N is approximately $RT\Omega$. Now add bosonic excitations and follow their evolution!

Effective Bosonic Evolution

Note that this is an (approximately) bosonic second quantization:

$$
\begin{aligned}
T^* H^{\text{eff}} T &\simeq E_N^{\text{RPA}} + \hbar \sum_{k \in \mathbb{Z}^3} \sum_{\alpha,\beta=1}^{M} E(k)_{\alpha,\beta} b^*_{\alpha,k} b_{\beta,k} \\
&\simeq E_N^{\text{RPA}} + \mathrm{d}\Gamma_{\text{bosonic}} \underbrace{\Big(\hbar \bigoplus_{k \in \mathbb{Z}^3} E(k) \Big)}_{=:\, H_{\mathrm{B}}} .
\end{aligned}
$$

Consider a one–boson state

$$
\eta \in \bigoplus_{k \in \mathbb{Z}^3} \mathbb{C}^M \qquad (M \text{ was the number of patches}) .
$$

The time–evolution in the (first quantized) one–boson space is

$$
\eta_t := e^{-iH_B \tau/\hbar} \eta_0 .
$$

For a one–boson state $\eta \in \bigoplus_{k\in\mathbb{Z}^3} \mathbb{C}^M$ define: $\quad b^*(\eta) := \sum_{k\in\mathbb{Z}^3} \sum_{\alpha=1}^{M} b^*_{\alpha,k}\eta(k)_\alpha$.

Theorem (B–Nam–Porta–Schlein–Seiringer '21)

Assume that $\hat{V}(p)$ is compactly supported and non–negative. Let

$$\xi_0 := \frac{1}{Z_m} b^*(\eta_1)\cdots b^*(\eta_m)\Omega\,, \qquad \xi_t := \frac{1}{Z_m} b^*(\eta_{1,\tau})\cdots b^*(\eta_{m,\tau})\Omega\,.$$

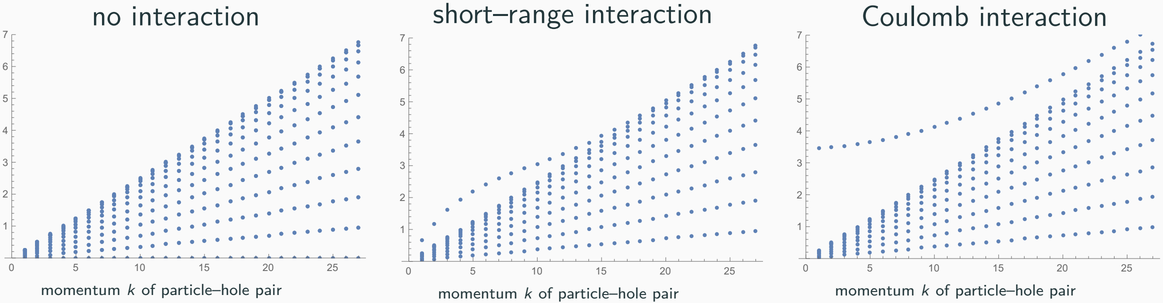
Then

$$\| e^{-iH_N\tau/\hbar} RT\xi_0 - e^{-i(E_N^{\mathrm{pw}}+E_N^{\mathrm{RPA}})\tau/\hbar} RT\xi_\tau \| \leq C_{m,V}\hbar^{1/15}|\tau|\,.$$

If $H_{\mathrm{B}}\eta_i = e_i\eta_i$ ($e_i \in \mathbb{R}$) then we have constructed an approximate eigenstate of the many–body Hamiltonian, evolving up to times $|\tau| \ll N^{1/45}$ just with a phase:

$$e^{-iH_N\tau/\hbar} RT\xi_0 \simeq e^{-i\left(E_N^{\mathrm{pw}}+E_N^{\mathrm{RPA}}+\sum_{j=1}^{m} e_j\right)\tau/\hbar} RT\xi_0\,.$$

Spectrum of the bosonic effective theory [B ’20, Christiansen–Hainzl–Nam ’22]



- plasmon mode (collective oscillation) emerges for long–range interaction
- bulk of the spectrum almost unchanged

Robustness of the bulk of the spectrum as an indicator of Fermi liquid behavior?