Collective Bosonization for the Mean-Field Fermi Gas

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Quantum System of N Fermions

Hamilton operator of N identical spinless particles on the (fixed size) 3D torus:

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

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

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

For reasonable potentials, the Hamiltonian is self–adjoint.

The spectrum $\sigma(H_N)$ is interpreted as excitation energies measurable in experiments.

Ground State Energy

The ground state energy is defined as

$$E_N := \inf \sigma(H_N) = \inf_{\substack{\psi \in L^2_a(\mathbb{T}^{3N}) \\ \|\psi\|=1}} \langle \psi, H_N \psi \rangle \,.$$

How to compute E_N? Define the reduced density matrices

$$\gamma^{(2)} := \frac{N!}{(N-2)!} \operatorname{tr}_{3,4,\dots N} |\psi\rangle\langle\psi| \,, \qquad \gamma^{(1)} := \frac{1}{N-1} \operatorname{tr}_2 \gamma^{(2)} \,.$$

Then

$$\langle \psi, H_N \psi \rangle = \operatorname{tr}\left(-\Delta \gamma^{(1)}\right) + \frac{1}{2} \iint V(x_1 - x_2) \gamma^{(2)}(x_1, x_2; x_1, x_2) \, \mathrm{d}x_1 \mathrm{d}x_2 \,.$$

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So we simply minimize over $\gamma^{(2)}$?

The set of all 2-particle rdm is hard to characterize: N-representability problem.

Mean–Field Regime

This problem cannot be solved in full generality: H_N describes almost the entire variety of our daily lives, superconductors, neutron stars, our bodies...

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Mathematical Model: Mean–Field Scaling Regime

- high density: fixed volume (torus) and N particles, $N \to \infty$.
- weak interation: $\lambda = N^{-1/3}$ because

$$\left\langle \sum_{i=1}^{N} (-\Delta_i) \right\rangle \sim N^{5/3} \quad \text{(antisymmetry!)}\,, \qquad \left\langle \lambda \sum_{1\leq i<j\leq N} V(x_i - x_j) \right\rangle \sim \lambda N^2\,.$$

Leading Order Approximation:
Hartree–Fock Theory

Hartree–Fock Theory = Restriction to Slater Determinants

Multiply the entire Hamiltonian by $\times\hbar^2$, with $\hbar := N^{-1/3}$:

$$H_N = \sum_{i=1}^{N} \left(-\hbar^2 \Delta_i\right) + \frac{1}{N} \sum_{1 \leq i < j \leq N} V(x_i - x_j) \,.$$

Convergence to the Hartree–Fock energy [Bach '92, Graf–Solovej '94]:

$$\left|E_N - E_N^{\mathrm{HF}}\right| = o(N)\,, \qquad \text{where } E_N^{\mathrm{HF}} := \inf_{\substack{\psi \text{ is Slater} \\ \text{determinant}}} \langle \psi, H_N \psi \rangle \,.$$

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Furthermore, if we consider a Slater determinant and evolve it in time, it stays close to a Slater determinant, but with evolved "orbitals" $f_{j,t}$.

Stability of the Hartree–Fock Approximation

Theorem: [B–Porta–Schlein '14]

Let $\psi_N = \bigwedge_{j=1}^N f_j$ and $i\hbar\partial_t\psi_{N,t} := H_N\psi_{N,t}$.

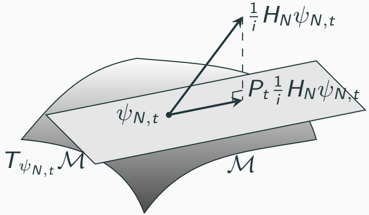
Assume $\|[\hat{x},\gamma^{(1)}]\|_{\mathrm{tr}}\,,\ \|[\hat{p},\gamma^{(1)}]\|_{\mathrm{tr}} \leq CN\hbar.$ $(*)$

Then

$$\|\gamma_t^{(1)} - \gamma_t^{\mathrm{HF}}\|_{\mathrm{tr}} \leq N^{1/6} C_t$$

for $i\hbar\partial_t\gamma_t^{\mathrm{HF}} = [h(\gamma_t^{\mathrm{HF}}), \gamma_t^{\mathrm{HF}}]$. (HF)

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



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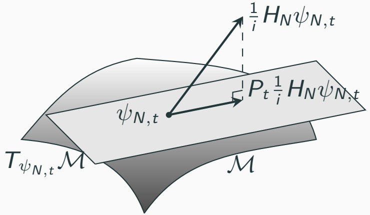

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- $(*)$ can be directly verified for non–interacting fermions on torus/in harmonic trap; using semiclassical analysis also for arbitrary traps [Fournais–Mikkelsen '19].
- γ_t^{HF} is the 1-particle rdm of a Slater determinant $\bigwedge_{j=1}^N f_{j,t}$ with evolved orbitals; (HF) is a system of coupled non–linear equations for the orbitals $f_{j,t}$.
- Dirac–Frenkel principle shows that (HF) is optimal choice [B–Sok–Solovej '18].

Beyond Hartree–Fock Theory

Conclusion: Hartree–Fock theory (Slater determinants) is a good description of many quantities at leading order, for fermions in the mean–field regime.

However: HF theory produces some unphysical predictions, e. g., vanishing density of states at the Fermi energy (contradicting specific heat measurements in metals)!

$\rightsquigarrow$ We need to go to the next order. We need to do better than just Slater determinants and include non–trivial quantum correlations.

> [Wigner ’34]: Next order of the ground state energy (correlation energy)?

We accomplish a description of quantum correlations by bosonizing collective particle–hole excitations.

Next Order:
Bosonization of Collective Excitations

The Almost–Optimal Slater Determinant

Hamiltonian in momentum representation, written with anti-commuting operators:

$$H_N := \hbar^2 \sum_{k\in\mathbb{Z}^3} |k|^2 a_k^* a_k + \frac{1}{N} \sum_{q,s,k\in\mathbb{Z}^3} \hat{V}(k) a_{q+k}^* a_{s-k}^* a_s a_q \,, \qquad \hbar = N^{-1/3} \,.$$

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Introduce the Slater determinant of N plane waves

$$\Psi_N := \bigwedge_{k \in \mathcal{B}_F} f_k \,, \qquad \mathcal{B}_F = \text{Fermi ball} := \left\{ k \in \mathbb{Z}^3 \mid |k| \leq N^{1/3} \left(\frac{3}{4\pi} \right)^{1/3} \right\} .$$

Its energy is almost exactly the Hartree–Fock energy [Gontier–Hainzl–Lewin '18]:

$$\langle \Psi_N, H_N \Psi_N \rangle = E_N^{\mathrm{HF}} + \mathcal{O}(e^{-N^{1/3}}) \,.$$

(The optimal Slater determinant probably develops weak density waves.)

Separating the Slater Determinant: Particle–Hole Transformation R

Define the unitary map R on fermionic Fock space by

$$R\,\Omega := \Psi_N \;, \qquad\qquad R\, a_k^*\, R^* := \begin{cases} a_k^* & k \in \mathcal{B}_F^c \\ a_k & k \in \mathcal{B}_F \end{cases}$$

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Write $\tilde{\Psi}_N = R\xi$. Expand $R^* H_N R$ and normal–order

$$\langle \tilde{\Psi}_N, H_N \tilde{\Psi}_N \rangle = E_N^{\mathrm{HF}} + \langle \xi, \Bigg(\underbrace{\hbar^2 \sum_{p \in \mathcal{B}_F^c} p^2 a_p^* a_p - \hbar^2 \sum_{h \in \mathcal{B}_F} h^2 a_h^* a_h}_{=:\ H^{\mathrm{kin}}} + \underbrace{Q}_{\substack{\text{quartic in} \\ \text{operators } a^*,\, a}} \Bigg) \xi \rangle$$

For $\xi = \Omega$: $\big(H^{\mathrm{kin}} + Q\big)\,\Omega = 0$.

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Goal: a quadratic approximation to the excitation Hamiltonian $H^{\mathrm{kin}} + Q$.
(Quadratic Hamiltonians can be diagonalized by Bogoliubov transformations.)

Collective Particle–Hole Pairs

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

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

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

$$[b^*_k, b^*_l] = 0 \quad , \qquad [b_l, b^*_k] = \delta_{k,l} n^2_k + \xcancel{\mathcal{E}(k,l)}\,.$$

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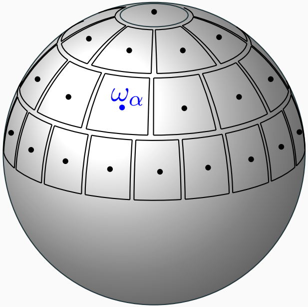
But how to express H^{kin} through pair operators?

Localization to Patches – Linearizing the Kinetic Energy

Fermi ball $\mathcal{B}_F$



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

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

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

where $n_{\alpha,k}$ is for normalization such that $\|b^*_{\alpha,k}\Omega\| = 1$.

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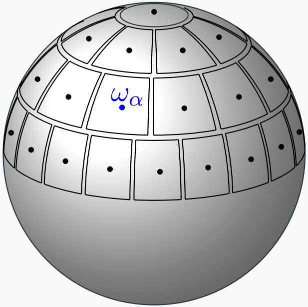

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Linearize kinetic energy around patch center ω_α:

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

as if $b^*_{\alpha,k}$ was a mode of a harmonic oscillator.
(c. f., [Lieb–Mattis '65] for the 1D Luttinger model)

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

Quadratic Effective Hamiltonian

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

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

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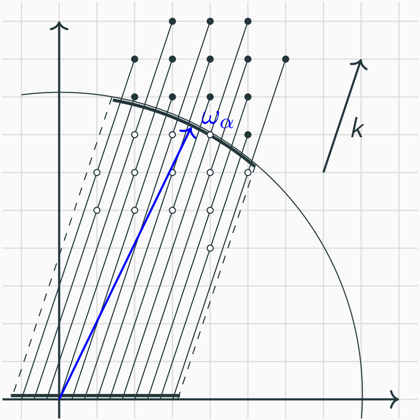
Normalization:

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

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



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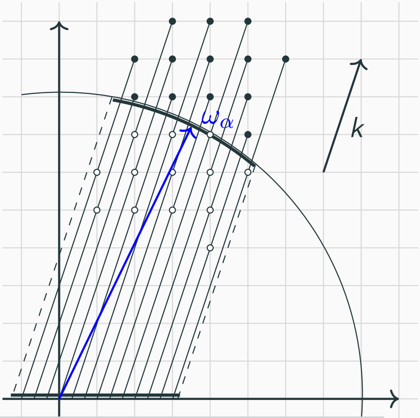


Effective Bosonic Hamiltonian

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

Diagonalization of the Bosonic Hamiltonian

We can write

$$H^{\text{eff}} = \hbar \sum_{k\in\mathbb{Z}^3} \left[h^{\text{eff}}(k) - \frac{1}{2}\,\text{tr}(D+W) \right]$$

where (with k–dependence suppressed)

$$h^{\text{eff}} = \frac{1}{2} \begin{pmatrix} (b^*)^T & b^T \end{pmatrix} \begin{pmatrix} D+W & \widetilde{W} \\ \widetilde{W} & D+W \end{pmatrix} \begin{pmatrix} b \\ b^* \end{pmatrix}, \qquad b = \begin{pmatrix} \vdots \\ b_\alpha \\ \vdots \end{pmatrix},$$

$$D = \begin{pmatrix} \text{diag}(u_\alpha^2) & 0 \\ 0 & \text{diag}(u_\alpha^2) \end{pmatrix}, \quad W = \hat{V} \begin{pmatrix} |u\rangle\langle u| & 0 \\ 0 & |u\rangle\langle u| \end{pmatrix}, \quad \widetilde{W} = \hat{V} \begin{pmatrix} 0 & |u\rangle\langle u| \\ |u\rangle\langle u| & 0 \end{pmatrix}.$$

The model is solved (i. e., all excitation energies are known) if we can find linear combinations of b– and b^*–operators with unchanged commutator relations such that

$$h^{\text{eff}} = \sum_{\gamma=1}^{M} e_\gamma \left(\tilde{b}_\gamma^* \, \tilde{b}_\gamma + \frac{1}{2} \right), \quad e_\gamma \in \mathbb{R}.$$

Bogoliubov Transformation

Linear transformations of the operators that leave the commutator relations invariant are called Bogoliubov transformations. They can be written as

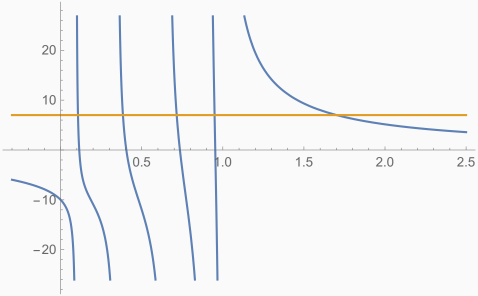
$$b = \frac{1}{2}(S_1 + S_2)\tilde{b} + \frac{1}{2}(S_1 - S_2)\tilde{b}^* \quad , \qquad S = \begin{pmatrix} S_1 & 0 \\ 0 & S_2 \end{pmatrix} \text{ a symplectic matrix .}$$

We construct [B '19] S such that

$$h^{\text{eff}} = \sum_{\gamma,\delta=1}^{M} E_{\gamma,\delta}\, \tilde{b}^*_\gamma\, \tilde{b}_\delta + \frac{1}{2}\operatorname{tr} E \ ,$$

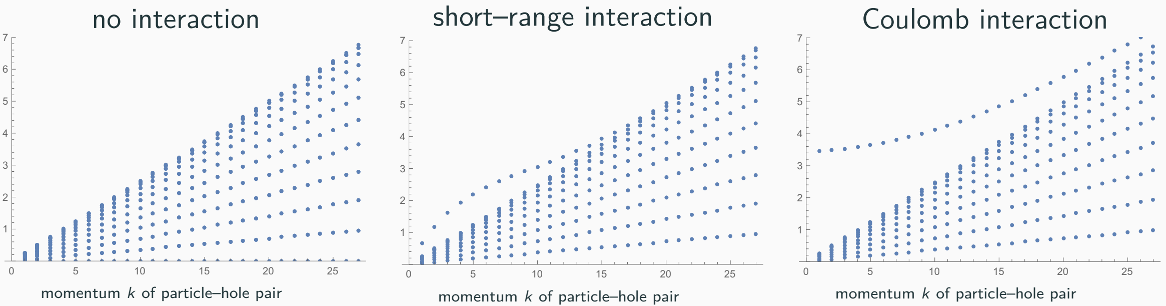
$$E \simeq \sqrt{\operatorname{diag}(u_\alpha^2) + \hat{V}|u\rangle\langle u|} \ .$$

The eigenvalues of "diagonal + rank–one" matrices can be found graphically.



Orange: $y = \frac{1}{\hat{V}(k)}$. Qualitative change for Coulomb singularity $\hat{V}(k) = \frac{1}{|k|^2}$ at $k \to 0$.

Spectrum



- plasmon mode (collective oscillation) emerges
- continuous spectrum qualitatively unchanged

A non–perturbative approach to screening and Fermi liquid theory?

Rigorous Result:
Upper Bound on the Ground State Energy

Upper Bound on Correlation Energy

Theorem: [B–Nam–Porta–Schlein–Seiringer '19]

Let $\hat{V}(k)$ be non-negative, bounded, and compactly supported. Then

$$E_N \leq E_N^{\mathrm{HF}} + \hbar \sum_{k \in \mathbb{Z}^3} |k| \left[\int_0^\infty \log \Big(1 + \hat{V}(k)\Big(1 - \lambda \arctan \lambda^{-1}\Big)\Big) \, \mathrm{d}\lambda - \frac{1}{4} \hat{V}(k) \right] + \mathcal{O}(\hbar N^{-1/27}) \,.$$

This is $\frac{1}{2} \operatorname{tr} [E - (D + W)]$ as in the bosonic H^{eff}.

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- Non–rigorously obtained by [Macke '50, Bohm–Pines '53, Gell-Mann–Brueckner '57, Sawada et al. '57]. Historical breakthrough!
- [Hainzl–Porta–Rexze '18] obtained a rigorous lower bound to second order in $\hat{V}$,

$$E_N \geq E^{\mathrm{HF}} - \hbar\frac{\pi}{2}(1 - \log 2) \sum_{k\in\mathbb{Z}^3} |k| \hat{V}(k)^2 + \mathcal{O}(\hat{V}^3)\,.$$

Proof:
Justification of the Bosonic Approximation

Ground State in the Bosonic Picture

The previously introduced Bogoliubov transformation has an explicit formula:

$$T = \exp\left(\sum_{k \in \mathbb{Z}^3} \sum_{\alpha,\beta=1}^{M} K(k)_{\alpha,\beta} b^*_{\alpha,k} b^*_{\beta,-k} - \text{h.c.} \right) , \quad K(k) = \log|S_1|$$

and thus, in the bosonic picture, the ground state of H^{eff} is given by

$$\xi_{\text{gs}} = T\Omega \, .$$

Makes sense even if the b^*–operators are actually pairs of fermionic operators.

Maybe not optimal, but we can still use it as a trial state.

Convergence to Bosonic Approximation

General idea: bosonic approximation is good if the number of occupied fermionic modes is much smaller than the number of available fermionic modes (per patch).

Lemma: We have approximately bosonic commutators:

$$[b^*_{\alpha,k}, b^*_{\beta,l}] = 0 = [b_{\alpha,k}, b_{\beta,l}] \qquad \text{and} \qquad [b_{\alpha,k}, b^*_{\beta,l}] = \delta_{\alpha,\beta}\Big(\delta_{k,l} + \mathcal{E}_\alpha(k,l)\Big)\,,$$

where for all ψ in fermionic Fock space the error operator $\mathcal{E}_\alpha(k,l)$ is bounded by

$$\|\mathcal{E}_\alpha(k,l)\psi\| \leq \frac{2}{n_{\alpha,k} n_{\alpha,l}} \|\mathcal{N}\psi\| \qquad (\mathcal{N} = \text{fermionic number operator})\,.$$

Approximate Bogoliubov Transformation

Lemma: T acts as an approximate Bogoliubov transformation, i. e.,

$$T^* b_{\alpha,k} T = \sum_{\beta=1}^{M} \frac{1}{2}(S_1 + S_2)_{\alpha,\beta} b_{\beta,k} + \sum_{\beta=1}^{M} \frac{1}{2}(S_1 - S_2)_{\alpha,\beta} b^*_{\beta,-k} + \mathfrak{E}_{\alpha,k}$$

where for all ψ in fermionic Fock space the error operator $\mathfrak{E}_{\alpha,k}$ is bounded by

$$\left[\sum_{\alpha} \|\mathfrak{E}_{\alpha,k}\psi\|^2\right]^{1/2} \leq \frac{C}{\min_{\alpha} n^2_{\alpha,k}} \|(\mathcal{N} + 2)^{3/2}\psi\| \,.$$

Lemma: The number of fermions is uniformly bounded (Grönwall argument):

$$\langle \xi_{\mathrm{gs}}, (\mathcal{N} + 1)^3 \, \xi_{\mathrm{gs}} \rangle \leq C \,.$$

QED