Correlation Energy of the Mean-Field Fermi Gas as an Upper Bound

Niels Benedikter

joint work with

Phan Thành Nam, Marcello Porta, Benjamin Schlein, and Robert Seiringer

IST AUSTRIA

Institute of Science and Technology

What is the Mean-Field Fermi Gas?

$N \gg 1$ fermions without spin in the box $[0, 2\pi]^3$ with periodic boundary conditions

$$H := \hbar^2 \sum_{k \in \mathbb{Z}^3} |k|^2 a_k^* a_k + \lambda \sum_{q,s,k \in \mathbb{Z}^3} \hat{V}(k) a_{q+k}^* a_{s-k}^* a_s a_q$$

Mean-field scaling: $\hbar := N^{-1/3}$, $\lambda := N^{-1}$

Ground state energy $\quad E_N := \inf_{\substack{\psi \text{ has } N \text{ particles} \\ \|\psi\|=1}} \langle \psi, H\psi \rangle$

What is the Correlation Energy?

Correlation energy := deviation from Hartree–Fock energy

$$E_N = \underbrace{E_{\text{kin+direct}} + E_{\text{exchange}}}_{\substack{= \inf \mathcal{E}_{\text{HF}} \\ \text{Hartree-Fock functional}}} + \underbrace{E_{\text{GMB}} + \dots}_{\text{correlation energy}}$$

with $\quad E_{\text{kin+direct}} \sim N, \qquad E_{\text{exchange}} \sim 1, \qquad E_{\text{GMB}} \sim \hbar = N^{-1/3}.$

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[Bohm–Pines '53, Gell-Mann–Brueckner '57, Sawada–Brueckner–Fukuda–Brout '57]:

Random Phase Approximation

$$E_{\text{GMB}} = \hbar \sum_{k \in \mathbb{Z}^3} |k| \left[\int_0^\infty \log\left(1 + \hat{V}(k)\left(1 - v \arctan v^{-1}\right)\right) \mathrm{d}v - \frac{1}{4}\hat{V}(k)\,. \right]$$

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All orders of perturbation theory in $\hat{V}$

Emergence of bosonic collective modes

Our Result: Optimal Upper Bound

Theorem: Let $\hat{V}(k) \geq 0$, $\hat{V}$ bounded and compactly supported. Then

$$E_N \leq \mathcal{E}_{\text{HF}}(\text{plane waves}) + E_{\text{GMB}} + \mathcal{O}(\hbar N^{-1/27})\,.$$

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- [Hainzl-Porta-Rexze '18]: 2nd order in $\hat{V}$ as lower bound

Particle-Hole Transformation

Unitary map R on fermionic Fock space such that

$$R\Omega = \psi_{\text{Slater, Fermi ball}} \qquad R a_k^* R^* = \begin{cases} a_k & k \in B_F \\ a_k^* & k \in B_F^c \end{cases}$$

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Write $\psi = R\xi$ and transform H to get

$$\langle \psi, H\psi \rangle = \mathcal{E}_{\text{HF}}(\text{plane waves}) + \langle \xi, \Big(\underbrace{\hbar^2 \sum_{p \in B_F^c} p^2 a_p^* a_p - \hbar^2 \sum_{h \in B_F} h^2 a_h^* a_h}_{=: \, \mathbb{H}_{\text{kin}}} + Q \Big) \xi \rangle + \mathcal{O}(N^{-1})\,.$$

We “only” need to pick ξ.

Collective Particle-Hole Pairs

The interaction Q can be expressed through pair operators

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

as

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

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- ground state of quadratic Hamiltonians given by Bogoliubov transformations

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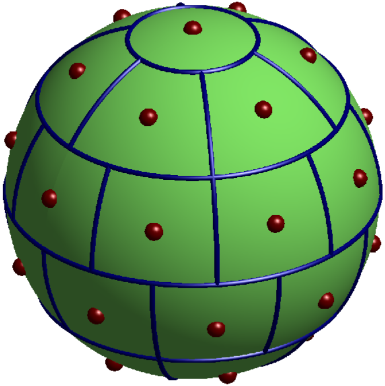
How to express $\mathbb{H}_{\mathrm{kin}}$ through pair operators?

Localization to Patches



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

$$b^*_{\alpha,k} := \sum_{\substack{h \in B_F \cap B_\alpha \\ p \in B_F^C \cap B_\alpha}} \delta_{p-h,k} a^*_p a^*_h$$

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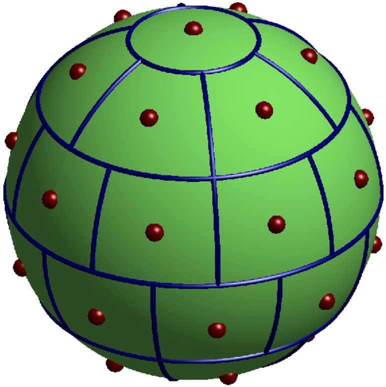

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If $M \gg N^{1/3}$ we can linearize around centers ω_α:

$$\mathbb{H}_{\text{kin}} b^*_{\alpha,k} \Omega \simeq \hbar^2 k \cdot 2\omega_\alpha \, b^*_{\alpha,k} \Omega \,.$$

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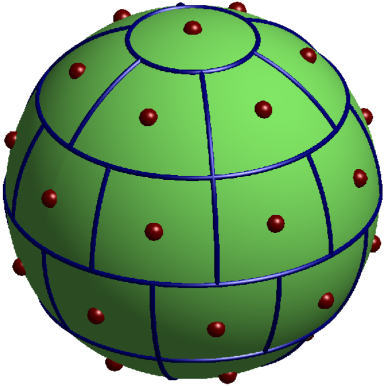

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Quadratic Effective Hamiltonian:

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

Bosonic Approximation

For this slide: Assume $b^*_{\alpha,k}$, $b_{\alpha,k}$ are *exactly bosonic* operators.

Then the ground state of $\mathbb{H}_{\text{eff}}$ is given by a Bogoliubov transformation:

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

$K(k)$ is an explicit $M \times M$-matrix

and

$$\langle \xi_{\text{gs}}, \mathbb{H}_{\text{eff}} \xi_{\text{gs}} \rangle = E_{\text{GMB}} \,.$$

Turn this into a rigorous upper bound for the fermionic system

Convergence to Bosonic Approximation

Lemma: We have approximate CCR

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

where for all ξ in fermionic Fock space

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

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Lemma: If $M \ll N^{2/3}$ then typically $n_{\alpha,k} \to \infty$ as $N \to \infty$.

Proof of Main Theorem

Proposition: With $K(k)$ from the bosonic approximation, let in fermionic Fock space

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

Then T acts as an approximate Bogoliubov transformation on $b^*_{\alpha,k}$ and $b_{\alpha,k}$.

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Proof of Main Theorem. Calculate $\langle T\Omega, (\mathbb{H}_{\text{kin}} + Q)\, T\Omega \rangle$. □