Optimal Upper Bound for the Correlation Energy of the Mean-Field Fermi Gas

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Many-Body Systems

General Hamiltonian of N identical spinless particles

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

on the bosonic Hilbert space

$$L^2_{\text{symm}}(\mathbb{R}^{3N}) = \left\{ \psi \in L^2(\mathbb{R}^{3N}) \mid \psi(x_{\sigma(1)}, x_{\sigma(2)}, \dots) = \psi(x_1, x_2, \dots) \quad \forall \sigma \in S_N \right\}$$

or on the fermionic Hilbert space

$$L^2_{\text{antisymm}}(\mathbb{R}^{3N}) = \left\{ \psi \in L^2(\mathbb{R}^{3N}) \mid \psi(x_{\sigma(1)}, x_{\sigma(2)}, \dots) = \text{sgn}(\sigma)\psi(x_1, x_2, \dots) \quad \forall \sigma \in S_N \right\} .$$

Ground State Energy

What is the ground state energy

$$E_N := \inf_{\|\psi\|=1} \langle \psi, H\psi \rangle \,?$$

We always have

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

in terms of the two- and one-particle reduced density matrices

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

So we simply minimize over $\gamma^{(2)}$? Unfortunately not: the set of all two-particle rdm is hard to characterize: N-representability problem.

Bosonic Mean-Field Limit

The way out: restrict to specific physical regimes.
Simplest: high density & weak interaction, s. th. we expect approximate mean-field behaviour:

$$H^{\mathrm{mf}} = \sum_{i=1}^{N} (-\Delta_i + V_{\mathrm{ext}}(x_i)) + \frac{1}{N} \sum_{1 \le i < j \le N} V(x_i - x_j)\,, \quad \text{particle number } N \to \infty\,.$$

As $N \to \infty$, the set of two-particle rdm is characterized by Quantum de-Finetti theorem, see e. g., [Størmer '69, Hudson–Moody '75, Christandl–König–Mitchison–Renner '07]:

$$\frac{(N-k)!}{N!}\gamma^{(k)} \to \int |u^{\otimes k}\rangle\langle u^{\otimes k}| \mathrm{d}\mu(u)\,, \quad \mu = \text{probability measure on } \left\{ u \in L^2(\mathbb{R}^3) \mid \|u\| = 1 \right\}.$$

Implies convergence to Hartree functional [Lewin–Nam–Rougerie '13]

$$E_N^{\mathrm{mf}} \to N \inf_{\substack{u \in L^2(\mathbb{R}^3) \\ \|u\|=1}} \left[\int \overline{u(x)}\,(-\Delta_x + V_{\mathrm{ext}}(x))\,u(x)\mathrm{d}x + \frac{1}{N} \int |u(x)|^2 V(x-y) |u(y)|^2 \,\mathrm{d}x\mathrm{d}y \right].$$

Next smaller term due to quantum correlations? Bogoliubov correction [Grech–Seiringer '13].

Fermionic Mean-Field Limit

Fermions have high kinetic energy (Fermi energy), to be tamed down in mean-field limit

$$H^{\mathrm{mf}} = \sum_{i=1}^{N} \Big(-\hbar^2 \Delta_i + V_{\mathrm{ext}}(x_i) \Big) + \frac{1}{N} \sum_{1 \leq i < j \leq N} V(x_i - x_j) \,, \quad \hbar = N^{-1/3} \,.$$

There is no Quantum de-Finetti for fermions.
The set of two-particle rdm is complicated, see e. g., [Klyachko '06].

But by specialized methods [Graf–Solovej '94] one can show that correlations are small, implying convergence to the Hartree–Fock functional

$$E_N^{\mathrm{mf}} \to \inf_{\substack{\omega^2 = \omega \text{ on } L^2(\mathbb{R}^3) \\ \operatorname{tr}\omega = N}} \underbrace{\left[\operatorname{tr}(-\Delta + V_{\mathrm{ext}})\omega + \iint \omega(x,x) V(x-y) \omega(y,y) - \iint |\omega(x,y)|^2 V(x-y) \right]}_{=: \mathcal{E}_{\mathrm{HF}}(\omega)} .$$

What is the next order term, due to quantum correlations?

Correlation Energy in the Fermionic Jellium Model

The non-rigorous solution of this problem, by [Bohm–Pines '53, Gell-Mann–Brueckner '57, Sawada et al. '57], established theoretical condensed matter physics as a field.

They considered the jellium model: no scaling of constants, thermodynamic limit, Coulomb interaction, and density $\rho \to \infty$.

Random Phase Approximation

$$E^{\mathrm{jellium}}(\rho) = \underbrace{C_{\mathrm{TF}} \rho^{5/3} - C_{\mathrm{D}} \rho^{4/3}}_{\substack{\text{Hartree-Fock energy} \\ \text{of non-interacting Fermi ball}}} + C_{\mathrm{BP}} \rho \log(\rho) + C_{\mathrm{GB}} \rho + o(\rho) \qquad \text{as } \rho \to \infty \,.$$

Mean-field scaling is slightly different:

$$E^{\mathrm{mf}} = \underbrace{E_{\mathrm{kin}} + E_{\mathrm{direct}} + E_{\mathrm{exchange}}}_{\substack{\text{Hartree-Fock energy} \\ \text{of non-interacting Fermi ball}}} + E_{\mathrm{BP}} + E_{\mathrm{GB},1} + E_{\mathrm{GB},2}$$

$$E_{\mathrm{kin}}, E_{\mathrm{direct}} \sim N, \quad E_{\mathrm{exchange}} \sim 1, \quad E_{\mathrm{BP}}, E_{\mathrm{GB},1} \sim N^{-1/3}, \quad E_{\mathrm{GB},2} \sim N^{-2/3} \,.$$

The Gell-Mann–Brueckner Formula

[Gell-Mann–Brueckner '57] proposed that (here rewritten in the mean-field case)

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

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

GB collect the dominant terms at all order of perturbation theory. For Coulomb interaction, $\hat{V}(k) = 1/|k|^2$, high orders are badly IR divergent, $\sim |k|^{-2n+1}$ for $k \to 0$.
By summing the series first, as for $\hat{V}(k)$ small, they get (1), which is regularized to $\log(\rho)$.

Much simpler, $E_{\mathrm{GB},2}$ is just the second-order perturbation of exchange type.

[Sawada et al '75]: "Think of $a_p^* a_h^*$ as bosonic." — But: $(a_p^* a_h^*)^2 = 0$ ↯

Momentum Representation in Fock Space

The mean-field Fermi gas in the box $[0, 2\pi]^3$ with periodic boundary conditions

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

Non-interacting system: Fermi ball

$$B_F := \left\{ k \in \mathbb{Z}^3 \mid |k| \leq N^{1/3} \left(\frac{3}{4\pi}\right)^{1/3} \right\}$$

Associated one-particle density matrix constructed from plane waves

$$\omega_0 = (2\pi)^{-3} \sum_{k \in B_F} |e^{ipx}\rangle\langle e^{ipx}| \,.$$

Our Result: Optimal Upper Bound

Theorem: [B-Nam-Porta-Schlein-Seiringer, arXiv:1809.01902]

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

$$E_N \leq \mathcal{E}_{\mathrm{HF}}(\omega_0) + E_{\mathrm{BP}} + E_{\mathrm{GB},1} + \mathcal{O}(\hbar N^{-1/27})\,.$$

Remarks:

- Slightly earlier [Hainzl-Porta-Rexze '18] obtained an upper and also lower bound, but only to second order in $\hat{V}$.
- We use a trial state which in principle also captures $E_{\mathrm{GB},2}$, but in the mean-field scaling this contribution is too small to be seen.

Particle-Hole Transformation

Unitary map R on fermionic Fock space such that

$$R\Omega = (N!)^{-1/2} \bigwedge_{k \in B_F} e^{ikx}\,, \qquad R a_k^* R^* = \begin{cases} a_k & k \in B_F \\ a_k^* & k \in B_F^c \end{cases}$$

Write $\psi = R\xi$. Calculate $R^* H R$ to get

$$\langle \psi, H\psi \rangle = \mathcal{E}_{\mathrm{HF}}(\omega_0) + \langle \xi, \Big(\underbrace{\hbar^2 \sum_{p \in B_F^c} p^2 a_p^* a_p - \hbar^2 \sum_{h \in B_F} h^2 a_h^* a_h}_{=:\, \mathbb{H}_{\mathrm{kin}}} + Q \Big) \xi \rangle + \mathcal{O}(N^{-1})$$

where Q is quartic in fermionic operators.

We "only" need to pick ξ.

Collective Particle-Hole Pairs

The dominant part Q of the interaction can be expressed through collective pair operators

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

as

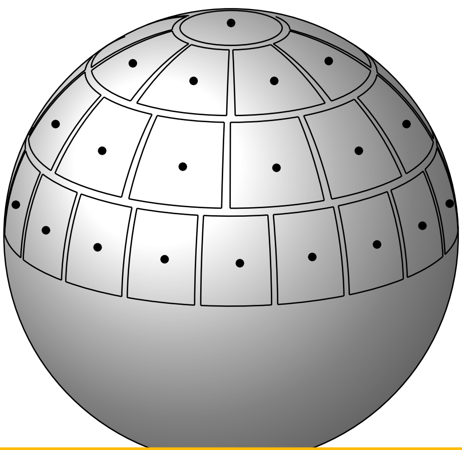
$$Q = \frac{1}{N} \sum_{k \in \mathbb{Z}^3} \hat{V}(k) \left(2 b_k^* b_k + b_k^* b_{-k}^* + b_{-k} b_k \right) .$$

This is convenient because

- The b^* and b have approximately bosonic commutators; summation over many modes relaxes the Pauli principle
- ground state of quadratic Hamiltonians explicitly given by Bogoliubov transformations.

But how to express $\mathbb{H}_{\text{kin}}$ through pair operators?

Localization to Patches



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

$$b_{\alpha,k}^* := \frac{1}{n_{\alpha,k}} \sum_{\substack{h \in B_F \cap B_\alpha \\ p \in B_F^c \cap B_\alpha}} \delta_{p-h,k} a_p^* a_h^*$$

where $n_{\alpha,k} = \#$p-h pairs in α with momentum k.

Linearize kinetic energy around centers ω_α:

$$\mathbb{H}_{\text{kin}} b_{\alpha,k}^* \Omega \simeq 2\hbar \underbrace{|k \cdot \hat{\omega}_\alpha|}_{=: u_\alpha(k)} b_{\alpha,k}^* \Omega .$$

suggests the quadratic effective Hamiltonian

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

Heuristics: Bosonic Approximation

For this slide only: 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:

$$\xi_{\text{gs}} = T\Omega, \quad T = \exp\left(\sum_{k\in\mathbb{Z}^3} \sum_{\alpha,\beta} K(k)_{\alpha,\beta} b^*_{\alpha,k} b^*_{\beta,-k} - \text{h.c.} \right) \tag{2}$$

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

and

$$\langle \xi_{\text{gs}}, \mathbb{H}_{\text{eff}} \xi_{\text{gs}} \rangle \to E_{\text{BP}} + E_{\text{GB},1} \qquad \text{as } M \to \infty\,.$$

Use formula (2) to define a trial state in fermionic Fock space, thus get 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 the error is bounded by

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

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

Remark: To be precise, $b^*_{\alpha,k} = 0$ for $k \cdot \hat{\omega}_\alpha < 0$. We replace such $b^*_{\alpha,k}$ by $b^*_{\alpha,-k}$, reducing the number of pair creation operators by half.

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

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

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

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

where the error is bounded by

$$\left[\sum_{\alpha=1}^{M} \|\mathfrak{E}_{\alpha,k}\psi\|^2\right]^{1/2} \leq \frac{C}{\min_\alpha n^2_{\alpha,k}} \|(\mathcal{N}+2)^{3/2} T_\lambda \psi\| \quad \text{for all } \psi \text{ in fermionic Fock space}\,.$$

Remark: To be precise, we need a cutoff excluding patches with $|k\cdot\hat{\omega}_\alpha| \leq N^{-\delta}$, otherwise the $\min_\alpha n^2_{\alpha,k}$ may vanish. The parameter δ can be optimized at the end.

Lemma: (Self-Consistency of the Bosonic Approximation)

The particle number on our trial state $\xi_{\text{trial}} := T_{\lambda=1}\Omega$ is bounded by

$$\langle \xi_{\text{trial}}, (\mathcal{N}+1)^n \xi_{\text{trial}}\rangle \leq C_n \quad \text{independent of } N\,.$$

Proof: Show that for some $D_n = D_n\Big(\sum_k \|K(k)\|_{\text{HS}}\Big) < \infty$ we have

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle T_\lambda\Omega, (\mathcal{N}+5)^n T_\lambda\Omega\rangle \leq D_n \langle T_\lambda\Omega, (\mathcal{N}+5)^n T_\lambda\Omega\rangle\,.$$

Then by Grönwall's lemma

$$\langle T_\lambda\Omega, (\mathcal{N}+5)^n T_\lambda\Omega\rangle \leq e^{\lambda D_n}\langle T_{\lambda=0}\Omega, (\mathcal{N}+5)^n T_{\lambda=0}\Omega\rangle\,.$$

Set $\lambda = 1$ and $C_n := e^{D_n}$. □

Lemma: The kinetic energy can be linearized as $H_{\text{kin}} = H_{\text{linear}} + \mathfrak{E}$, where

$$H_{\text{linear}} = \hbar \sum_{\alpha=1}^{M} \left[\sum_{p \in B_F^c \cap B_\alpha} |p \cdot \hat{\omega}_\alpha| a_p^* a_p - \sum_{h \in B_F \cap B_\alpha} |h \cdot \hat{\omega}_\alpha| a_h^* a_h \right]$$

and the error operator $\mathfrak{E}$ is small compared to $\hbar = N^{-1/3}$ if $M(N) \gg N^{1/3}$; namely

$$|\langle \xi, \mathfrak{E} \xi \rangle| \leq \frac{C}{M} \langle \xi, \mathcal{N} \xi \rangle \qquad \text{for all } \xi \text{ in fermionic Fock space}.$$

Lemma: We have

$$[H_{\text{linear}}, b^*_{\alpha,k}] = 2\hbar |k \cdot \hat{\omega}_\alpha| b^*_{\alpha,k} ,$$

exactly as for the effective Hamiltonian and exactly bosonic b^*-operators.

Proof of Main Theorem

Proof: We just have to calculate $\langle \xi_{\text{trial}}, H \xi_{\text{trial}} \rangle$.

- Expand into commutators by applying once the Duhamel formula

$$\langle \xi_{\text{trial}}, H \xi_{\text{trial}} \rangle = \int_0^1 \langle \Omega, T_\lambda^* [H, B] T_\lambda \Omega \rangle \, \mathrm{d}\lambda \,.$$

- Now use the kinetic energy commutator.
  The resulting expression for $[H, B]$ is quadratic in b^*- and b-operators.
- Calculate explicitly $\langle \Omega, T_\lambda^* (\text{quadratic}) T_\lambda \Omega \rangle$ using the approximate Bogoliubov transformation property, then integrate over λ to find $E_{\text{BP}} + E_{\text{GB},1}$.
- Optimize over $M(N)$ to see that all errors are smaller than $\hbar N^{-1/27}$ times $\langle \xi_{\text{trial}} \mathcal{N} \xi_{\text{trial}} \rangle \leq \text{const}$.

□