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Correlation energy of Fermi gases

Martin R. Christiansen [1, 2] Emanuela Giacomelli [1]
Christian Hainzl [1] Phan Thành Nam [1] Robert Seiringer [2]
[1]LMU Munich [2]IST Austria

Fermionic correlations

A long-standing challenge in mathematical physics is the rigorous understanding of **quantum correlations** from microscopic principles. In the context of interacting Fermi gases, this question goes back to Wigner (1934) and Heisenberg (1947), who recognized the difficulty of solving this task using a perturbation method.

The goal of **Project A5** is to develop a unified mathematical approach to compute the fermionic correlation energy in different regimes, from high-density systems with long-range interactions to low-density systems with short-range interactions.

A many-body quantum problem

Consider a Hamiltonian of N fermions in a torus $\Lambda = [0, L]^3 \subset \mathbb{R}^3$ with an interaction potential $V : \Lambda \to \mathbb{R}$

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \sum_{1\le j<k\le N} V(x_j - x_k)$$

acting on the Hilbert space $L^2_s(\Lambda^N)$ of **anti-symmetric** functions

$$\Psi(..., x_i, ..., x_j, ...) = -\Psi(...x_j, ..., x_i, ...).$$

In second quantization, this Hamiltonian can be written as

$$H_N = \sum_{p\in\Lambda^*} |p|^2 a_p^* a_p + \frac{1}{2|\Lambda|} \sum_{k,p,q\in\Lambda^*} \hat{V}_k a^*_{p+k} a^*_{q-k} a_q a_p.$$

Here a_p^*, a_p are the fermionic creation and annihilation operators of momentum $p \in \Lambda^*$, which satisfy the **anti-canonical commutator relations** (CAR)

$$\{a_p, a_q^*\} = a_p a_q^* + a_q^* a_p = \delta_{p,q}, \quad \{a_p, a_q\} = 0 = \{a_p^*, a_q^*\}$$

For the non-interacting system ($V = 0$), the ground state is simply the Slater determinant associated with all momenta in the **Fermi ball** $B_F = B(0, k_F) \cap \Lambda^*$ with $|B_F| = N$. The central task is to understand how excitations around the Fermi ball emerge in the ground state(s) for the interacting system ($V \neq 0$).

Bosonization method

Our approach is based on an adaptation of the **bosonic Bogoliubov theory** to Fermi systems, where suitable pairs of fermions are interpreted as virtual bosons. More precisely, we consider certain pairs of fermions, one inside and one outside the Fermi ball, described by the **excitation operators**

$$b_{k,p}^* = a_p^* a_{p-k}, \quad p \in L_k = B_F^c \backslash (B_F + k).$$

Historically, in 1957, in an attempt to explain the **random phase approximation** of Bohm and Pines, Sawada [13] suggested the following heuristic arguments:

- The excitation operators $b_{k,p}$ are quasi-bosonic, namely they satisfy the (approximate) **canonical commutator relations** (CCR)

$$[b_{k,p}, b_{\ell,q}^*] = b_{k,p} b_{\ell,q}^* - b_{\ell,q}^* b_{k,p} \approx \delta_{k,\ell}\delta_{p,q}, \quad [b_{k,p}, b_{\ell,q}] = [b_{k,p}^*, b_{\ell,q}^*] = 0$$

- The main contribution of the interaction only comes from the **bosonizable terms**

$$\sum_{k\neq 0} \hat{V}_k (2B_k^* B_k + B_k B_{-k} + B_{-k}^* B_k^*), \quad B_k = \sum_{p\in L_k} b_{k,p}$$

- The fermionic kinetic operator can be replaced by a bosonic operator via the **dispersion relations**

$$\Big[\sum_q |q|^2 a_q^* a_q, b_{k,p}\Big] = \underbrace{(|p|^2 - |p-k|^2)}_{2\lambda_{k,p}} b_{k,p} \approx \Big[\sum_{k,q} 2\lambda_{k,q} b_{k,q}^* b_{k,q}, b_{k,p}\Big].$$

All this results in the **quadratic Hamiltonian**

$$\sum 2\lambda_{k,q} b_{k,q}^* b_{k,q}, + \frac{1}{2|\Lambda|}\sum_{k\neq 0} \hat{V}_k (2B_k^* B_k + B_k B_{-k} + B_{-k}^* B_k^*)$$

which is explicitly solvable in the bosonic picture, leading to a prediction of the correlation energy

$$E_{\text{corr,bo}} = \frac{1}{\pi}\int_0^\infty F\left(\frac{\hat{V}_k}{|\Lambda|}\sum_{p\in L_k} \frac{\lambda_{k,p}}{\lambda_{k,p}^2 + t^2}\right) dt, \quad F(x) = \log(1+x) - x.$$

However, Sawada also realized that this method is insufficient to reproduce the Gell-Mann–Brueckner formula for the correlation energy of Jellium [10]. Thus our task is to understand the **validity of the bosonization method** and to derive the **necessary correction**.

High-density regime

Theorem [5,6]: In mean-field regime $\Lambda = [0, 2\pi]^3$ and $\hat{V}(k) \sim k_F^{-1}|k|^{-2}$, the correlation energy of H_N is

$$E_{\text{corr}} = E_N - E_{\text{HF}} = \underbrace{E_{\text{corr,bo}}}_{\sim k_F \log k_F} + \underbrace{E_{\text{corr,ex}}}_{\sim k_F} + o(k_F)_{k_F\to\infty}$$

with the bosonic correlation $E_{\text{corr,bo}}$ predicted by Sawada's picture and the exchange correlation

$$E_{\text{corr,ex}} = \frac{1}{4(2\pi)^6}\sum_{k\neq 0}\sum_{p,q\in L_k} \frac{\hat{V}_k \hat{V}_{p+q-k}}{\lambda_{k,p} + \lambda_{k,q}}.$$

Remarks:

- By formally removing the mean-field scaling $\hat{V}_k \mapsto |k|^{-2}$ and taking the thermodynamic limit $|\Lambda| \to \infty$, we reproduce exactly the **Gell-Mann–Brueckner formula** $c_1\rho\log\rho + c_2\rho$ for Jellium [10].
- Theorem 1 applies equally well to less singular potentials $\sum \hat{V}_k^2 |k| < \infty$. In this case, $E_{\text{corr,bo}} \sim k_F$ and $E_{\text{corr,ex}} = o(k_F)$, namely Sawada's picture is sufficient to understand the correlation energy. This case was first understood for $\|\hat{V}\|_{\ell^1}$ small in [1], and extended to $\sum \hat{V}_k |k| < \infty$ in [2,4].
- The Coulomb potential is critical since the exchange correlation becomes important. This requires a rigorous bosonization method to correct Sawada's purely bosonic picture.

Low-density regime

Consider N fermions with spin $1/2$ ($\sigma \in \{\uparrow, \downarrow\}$) in a torus $\Lambda = [0, L]^3$, described by the Hamiltonian

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \sum_{1\le j<k\le N} V(x_j - x_k) \quad \text{on} \quad \mathfrak{h}(N_\uparrow, N_\downarrow) \subset \bigwedge^N L^2_a(\Lambda, \mathbb{C}^2)$$

We are interested in the ground state energy density in thermodynamic limit

$$e(\rho_\uparrow, \rho_\downarrow) = \lim_{N_\sigma = \rho_\sigma L^3 \to\infty} \frac{1}{L^3} \inf_{\psi\in\mathfrak{h}(N_\uparrow, N_\downarrow)} \frac{\langle\psi, H_N\psi\rangle}{\langle\psi,\psi\rangle}$$

Theorem [8]: Let $0 \le V \in L^2(\mathbb{R}^3)$ be radial, compactly supported, $\rho_\uparrow = \rho_\downarrow = \rho/2 \to 0$. Then

$$e(\rho_\uparrow, \rho_\downarrow) \le \frac{3}{5}(3\pi^2)^{2/3}\rho^{5/3} + 2\pi a\rho^2 + \frac{4}{35}(11 - 2\log 2)(9\pi)^{2/3} a^2 \rho^{7/3} + o(\rho^{7/3})_{\rho\to 0}$$

with $a = (8\pi)^{-1}\int_{\mathbb{R}^3} V(1-\varphi)$, the **scattering length** of V defined by equation

$$2\Delta\varphi + V(1-\varphi) = 0 \text{ in } \mathbb{R}^3, \quad \lim_{|x|\to\infty}\varphi(x) = 0.$$

Remarks:

- The Huang-Yang formula [11] suggests that the matching lower bound holds.
- The second order term, with both upper and lower bounds, was first proved in [9], and recently reproduced in [7]. An optimal bound for the third order term was proved in [8].

Some ideas of the proofs

For the upper bound:

- In the high-density regime, the trial state has the form

$$\Psi_{\text{trial}} = e^{\mathcal{K}} \bigwedge_{p\in B_F} u_p, \quad \mathcal{K} = \sum_{k,p,q} K_{k,p,q} b_{k,p}^* b_{k,q}^* - \text{h.c.}$$

where $K_{k,p,q}$ is chosen **exactly from the bosonic Bogoliubov method**. By Duhamel's expansion

$$e^{-\mathcal{K}} H_N e^{\mathcal{K}} = H_N + \int_0^1 e^{-t\mathcal{K}}[H, \mathcal{K}]e^{t\mathcal{K}} = E_{\text{HF}} + E_{\text{corr,bo}} + \int_0^1 e^{-t\mathcal{K}}\mathcal{E}_{\text{ex}}(t)e^{t\mathcal{K}}$$

where the exchange contribution $\mathcal{E}_{\text{ex}}(t)$ comes from the CCR-corrector $[b_{k,p}, b_{k,q}^*] - \delta_{p,q} \neq 0$.

- In the low density regime, the Bogoliubov kernel is essentially chosen as

$$\mathcal{K} = \frac{1}{L^3}\sum_{p,r,r'} \hat{\varphi}_{r,r'}(p) b_{p,r,\uparrow} b_{-p,-r',\downarrow} - \text{h.c.}$$

where $\varphi_{r,r'}$ solves the **Bethe–Goldstone equation**

$$(2\widetilde{\lambda}_{p,r} + 2\widetilde{\lambda}_{p,r'})\widehat{\phi}_{r,r'}(p) = \widehat{V}(p) - \widehat{V\phi_{r,r'}}(p), \quad 2\widetilde{\lambda}_{p,r} = |p-r|^2 - |r|^2$$

Rigorously, it is possible to decompose $T \approx T_1 T_2$ where the **high-momentum** part T_1 reconstructs $2\pi a\rho^2$ and the **low-momentum** part T_2 gives the Huang–Yang contribution.

For the lower bound in the high-density regime, **'undoing' the Bogoliubov transformation** suggests to complete a suitable square, which can be modified to take the exchange contribution into account. New correlation estimates based on **Bell's odd commutator argument**, in the spirit of [3], are crucial to control the error. A similar strategy is expected to work in the low-density regime.

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