Momentum distribution of a high density Fermi gas in Random Phase Approximation

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Setting

Consider N spinless fermions on a torus $\mathbb{T}^3 := [0, 2\pi]^3$.

Hilbert Space: $\mathcal{H}^{(N)} := L^2_a(\mathbb{T}^{3N}) \cong \bigwedge_{i=1}^{N} L^2(\mathbb{T}^3)$

$$\forall \psi \in \mathcal{H}^{(N)}, \psi(\dots, x_{\pi(i)}, x_{\pi(j)}, x_{\pi(k)}, \dots) = (-1)^{\pi} \psi(\dots, x_i, x_j, x_k, \dots)$$

Hamilton operator:

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

Mean-field Scaling regime: $N \to \infty$, weak interaction potential, mean particle distance $\ll$ interaction range
$\Rightarrow$ Balance kinetic energy and interaction energy

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Mean-field Scaling regime: $N \to \infty$, weak interaction potential, mean particle distance $\ll$ interaction range

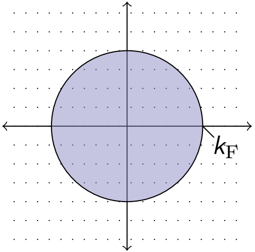
$$\Rightarrow \lambda \sim N^{-\frac{1}{3}}$$

For $V = 0$,

$$\psi_{\mathrm{GS}}(x_1, x_2, \ldots, x_N) = \bigwedge_{j=1}^{N} \left((2\pi)^{-3/2} e^{ik_j \cdot x} \right)$$
$$= \frac{1}{\sqrt{N!}} \det \left((2\pi)^{-3/2} e^{ik_j \cdot x_i} \right)_{j,i=1}^{N} \quad \text{with} \quad k_j \in \mathbb{Z}^3$$

Fermi ball:

$$B_{\mathrm{F}} := \left\{ k \in \mathbb{Z}^3 : |k| \leq k_{\mathrm{F}} \right\} \quad \text{with } N = |B_{\mathrm{F}}| \quad \text{and} \quad k_{\mathrm{F}} \sim N^{\frac{1}{3}}$$



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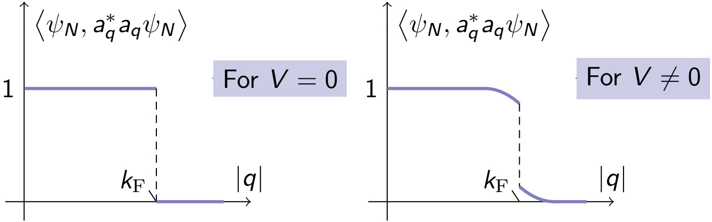
For $V \neq 0$, in Hartree-Fock approximation, we have

$$\psi = \frac{1}{\sqrt{N!}} \det \left(\phi_j(x_i) \right)_{j,i=1}^{N},$$

for N orthonormal functions $\{\phi_j : j = 1, \ldots, N\} \subset L^2(\mathbb{T}^3)$, which minimizes $\langle \psi, H_N \psi \rangle$ in our setting.

Momentum Distribution: $n_q = \langle \psi, a_q^* a_q \psi \rangle$, for $q \in \mathbb{Z}^3$, with a_q^*, a_q fermionic creation and annihilation operators on $\mathcal{F} := \bigoplus_{n=0}^{N} L_a^2(\mathbb{T}^{3n})$ with $\Omega = (1, 0, 0, \ldots)$ the vacuum state.



In the Hartree-Fock approximation too,

$$\langle \psi, a_q^* a_q \psi \rangle = \begin{cases} 0 & \text{for } q \in B_{\mathrm{F}}^c \\ 1 & \text{for } q \in B_{\mathrm{F}} \end{cases}$$

And beyond Hartee-Fock?

Main Result

Theorem [Benedikter, Lill, N. (about to appear)]
For interaction potential satisfying $\hat{V} \in \ell^1(\mathbb{Z}^3)$, $\hat{V} \geq 0$, $\hat{V}(0) = 0$ and $\hat{V}(k) = \hat{V}(-k)$. Then, for any sequence of k_{F} with $k_{\mathrm{F}} \to \infty$ and $N = N(k_{\mathrm{F}}) := |B_{k_{\mathrm{F}}}(0)|$, $\exists$ a sequence of trial states $(\Psi_{N(k_{\mathrm{F}})})_{k_{\mathrm{F}}}$ with $\Psi_N \in L^2_{\mathrm{a}}(\mathbb{T}^{3N})$ such that

- Ψ_N is energetically close to the ground state in the sense that for any $\varepsilon > 0$ there exists a $C_\varepsilon > 0$ such that $\forall\, k_{\mathrm{F}}$ we have

$$\langle \Psi_N, H_N \Psi_N \rangle - E_{\mathrm{GS}} \leq C_\varepsilon k_{\mathrm{F}}^{1-\frac{1}{6}+\varepsilon} \;,$$

- and $\exists$ constants $C_1, C_2 > 0$, depending on $\|\hat{V}\|_1$, s.t. $\forall\, k_{\mathrm{F}}$ and $q \in \mathbb{Z}^3$,

$$n(q) = \left\langle \Psi_N, a_q^* a_q \Psi_N \right\rangle = \begin{cases} n_q^{\mathrm{b}} + \mathcal{E}_q & \text{for } |q| \geq k_{\mathrm{F}} \\ 1 - n_q^{\mathrm{b}} + \mathcal{E}_q & \text{for } |q| < k_{\mathrm{F}} \end{cases} ,$$

where n_q^{b}, the bosonized excitation density, satisfying $|n_q^{\mathrm{b}}| \leq C_1 k_{\mathrm{F}}^{-1} e(q)^{-1}$ and the error $|\mathcal{E}_q| \leq C_2 k_{\mathrm{F}}^{-\frac{7}{4}} e(q)^{-1}$, with $e(q)$ being the excitation energy.

Consider $\psi_N \in \mathcal{H}^{(N)}$ such that

$$\langle \psi_N, H_N \psi_N \rangle = c_{\mathrm{KE}} k_{\mathrm{F}}^5 + c_{\mathrm{DI}} k_{\mathrm{F}}^5 + c_{\mathrm{EI}} k_{\mathrm{F}}^3 + c_{\mathrm{RPA}} k_{\mathrm{F}} + o(k_{\mathrm{F}}), \quad \text{as} \quad N \to \infty$$

where $c_{\mathrm{RPA}} k_{\mathrm{F}}$ is energy of the Random Phase approximation.
Construction of such ψ_N: We use
1. Particle-Hole transformation: $R : \mathcal{F} \to \mathcal{F}$, a unitary transformation acting as

$$R^* a_q^* R := \begin{cases} a_q^* & \text{if } q \in B_{\mathrm{F}}^c \\ a_q & \text{if } q \in B_{\mathrm{F}} \end{cases}$$

2. An almost-bosonic Bogoliubov transformation: $T : \mathcal{F} \to \mathcal{F}$, a unitary operator defined explicitly as $T = e^{\mathcal{K}}$,

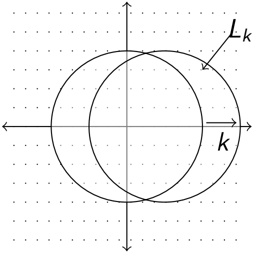
$$\mathcal{K} = \frac{1}{2} \sum_{\ell \in \mathbb{Z}_*^3} \sum_{r,s \in L_\ell} K(\ell)_{r,s} \left(b_r(\ell) b_{-s}(-\ell) - b_{-s}^*(-\ell) b_r^*(\ell) \right)$$

We defined our T using b, b^*, the quasi-bosonic pair operators, defined as

$$b_q(k) = a_{q-k} a_q \ , \quad b_q^*(k) = a_q^* a_{q-k}^* \quad \forall q \in L_k$$

where $L_k := \{q : q \in B_{\mathrm{F}}^c \cap (B_{\mathrm{F}} + k)\}$.
These pair operators follow the Quasi-bosonic canonical commutation relation **(QBCCR)**

$$[b_p(k), b_q(\ell)] = [b_p^*(k), b_q^*(\ell)] = 0 \,,$$
$$[b_p(k), b_q^*(\ell)] = \delta_{p,q}\delta_{k,\ell} + \epsilon_{p,q}(k,\ell),$$



where

$$\epsilon_{p,q}(k,\ell) = -\left(\delta_{p,q} a_{q-\ell}^* a_{p-k} + \delta_{p-k,q-\ell} a_q^* a_p\right)$$

Then the **momentum distribution** of the trial state ψ_N is

$$n_q = \left\langle \psi_N, a_q^* a_q \psi_N \right\rangle = \begin{cases} \left\langle \Omega, T^* a_q^* a_q T\Omega \right\rangle & \text{if } q \in B_{\mathrm{F}}^c \\ 1 - \left\langle \Omega, T^* a_q^* a_q T\Omega \right\rangle & \text{if } q \in B_{\mathrm{F}} \end{cases} .$$

We do an iterated Duhamel expansion .

Definition Let A be a family of symmetric operators $A(\ell)$, for any $\ell \in \mathbb{Z}^3_*$, with $A(\ell) : \ell^2(L_\ell) \to \ell^2(L_\ell)$. We define the quadratic operators for A as

$$Q_1(A) \coloneqq \sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} A(\ell)_{r,s} \left(b_r^*(\ell) b_s(\ell) + b_s^*(\ell) b_r(\ell) \right)$$

$$Q_2(A) \coloneqq \sum_{\ell \in \mathbb{Z}^3_*} \sum_{r,s \in L_\ell} A(\ell)_{r,s} \left(b_r(\ell) b_{-s}(-\ell) + b_{-s}^*(-\ell) b_r^*(\ell) \right) .$$

Then write the expansion in terms of these quadratic operators.

Doing n Duhamel steps we arrive at

$$\left\langle \Omega, T_1^* a_q^* a_q T_1 \Omega \right\rangle = \frac{1}{2} \sum_{\ell \in \mathbb{Z}^3_*} \mathbb{1}_{L_\ell}(q) \sum_{\substack{m=2, \\ m: even}}^{n+1} \frac{((2K(\ell))^m)_{q,q}}{(2m)!}$$

$$- \frac{1}{2} \left\langle \Omega, \sum_{m=1}^{n} \tilde{E}_m(\Theta_K^n(P^q)) \Omega \right\rangle$$

$$- \frac{1}{2} \int_{\Delta^n} \mathrm{d}^n \underline{\lambda} (-1)^n \left\langle \Omega, \left(T_{\lambda_n}^* Q_{\sigma(n)}(\Theta_K^{n+1}(P^q) T_{\lambda_n} \right) \Omega \right\rangle$$

where, $\Theta_K^n(P^q) = \underbrace{\{K, \dots \{K}_{n \text{times}}, P^q\} \dots\}$ and $\sigma(n) = \begin{cases} 1 & \text{for } n \text{ odd} \\ 2 & \text{for } n \text{ even} \end{cases}$

$$\tilde{E}_m(P^q) := - \int_{\Delta^m} \mathrm{d}^m \underline{\lambda} \, T_{\lambda_m}^* E_{Q_{\sigma(m-1)}} \left(\Theta_K^{m-1}(P^q) \right) T_{\lambda_m}. \quad (1)$$

Then in the limit $n \to \infty$ we get

$$\left\langle \Omega, T_1^* a_q^* a_q T_1 \Omega \right\rangle = \frac{1}{2} \sum_{\ell \in \mathbb{Z}^3_*} \mathbb{1}_{L_\ell}(q) \big(\cosh(2K(\ell)) - 1 \big)_{q,q}$$
$$- \frac{1}{2} \left\langle \Omega, \sum_{m=1}^{\infty} \tilde{E}_m(\Theta_K^n(P^q)) \Omega \right\rangle .$$

1. First term gives us leading order term n_q^{b} with

$$n_q^{\mathrm{b}} := \sum_{\ell \in \mathbb{Z}^3_*} \mathbb{1}_{L_\ell}(q) \, \frac{1}{\pi} \int_0^\infty \frac{g_\ell (t^2 - \lambda_{\ell,q}^2)(t^2 + \lambda_{\ell,q}^2)^{-2}}{1 + 2 g_\ell \sum_{p \in L_\ell} \lambda_{\ell,p} (t^2 + \lambda_{\ell,p}^2)^{-1}} \mathrm{d}t \, ,$$

   where the relative excitation energy $\lambda_{\ell,p} > 0$, and $g_\ell > 0$ are defined by

$$\lambda_{\ell,p} := \frac{1}{2}(|p|^2 - |p - \ell|^2) \, , \qquad g_\ell := \frac{\hat{V}(\ell) k_{\mathrm{F}}^{-1}}{2(2\pi)^3} \, .$$

2. Second term is the error term.
3. Last term tends to 0 in the $n \to \infty$.

A comment on the error estimation.

We estimate the $\left\langle \Omega, \sum_{m=1}^{n} E_m(A)\Omega \right\rangle$: in terms of k_{F} and the bootstrap quantity $\Xi := \sup_{q\in\mathbb{Z}^3} n_q$

$$n_q = I_q(\ell, \hat{V}_\ell) k_{\mathrm{F}}^{-1} e(q)^{-1} + C' k_{\mathrm{F}}^{-2} e(q)^{-2} + C \left(k_{\mathrm{F}}^{-\frac{3}{2}} \Xi^{\frac{1}{2}} + k_{\mathrm{F}}^{-1} \Xi^{\frac{3}{4}} \right) e(q)^{-1} .$$

Bootstrap estimates:

1. We know $n_q \leq 1$ and $e(q) \leq \frac{1}{2}$.
2. We also proved that the leading order $|n_q^{\mathrm{b}}| \leq C_1 k_{\mathrm{F}}^{-1} e(q)^{-1}$.
3. Then the bootstrap quantity is controlled by

$$\Xi \leq \sup_{q\in\mathbb{Z}^3} n_q^{\mathrm{b}} + C \left(k_{\mathrm{F}}^{-\frac{3}{2}} \Xi^{\frac{1}{2}} + k_{\mathrm{F}}^{-1} \Xi^{\frac{3}{4}} \right) \leq C k_{\mathrm{F}}^{-1} .$$

4. Then we do one bootstrap step and the error becomes $|\mathcal{E}_q| \leq C_2 k_{\mathrm{F}}^{-\frac{7}{4}} e(q)^{-1}$.

And we have the result.

Thank you for the attention!