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Correlation energy of weakly interacting fermions

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In many-body QM, two types of particles

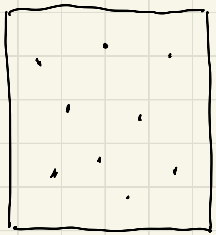
- bosons: described by symmetric wave-functions, ie.

$$\Psi_N(x_{\pi 1}, \dots, x_{\pi N}) = \Psi_N(x_1, \dots, x_N) \quad \forall \pi \in S_N$$

- fermions: described by antisymmetric wave-functions,

$$\Psi_N(x_{\pi 1}, \dots, x_{\pi N}) = \sigma_\pi \cdot \Psi_N(x_1, \dots, x_N)$$

Bosonic systems



$\Lambda = [0; 2\pi]^3$

Consider N bosons, trapped in torus Λ, interacting through mean-field potential.

Hamilton operator:

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \frac{1}{N} \sum_{i<j}^{N} V(x_i - x_j)$$

acting on $L^2_s(\Lambda^N)$.

Goal: compute ground-state energy and excitations.

BEC: most particle in state $\varphi_0(x) \equiv 1 \quad \forall x \in \Lambda$, ie.

$$\langle \Psi, \sum_{j=1}^{N} |\varphi_0\rangle\langle\varphi_0|_j \, \Psi \rangle \geq N - C$$

Bogoliubov theory

Describe Bose gas on Fock space

$$\mathcal{F}_s := \bigoplus_{n\geq 0} L^2_s(\Lambda^n)$$

with creation and annihilation ops. $a_p^*, a_p, p \in \mathbb{Z}^3$.

We have CCR:

$$[a_p, a_q^*] = \delta_{pq}, \quad [a_p, a_q] = [a_p^*, a_q^*] = 0$$

Observe: $a_p^* a_p = \#$ particles with momentum p.

In particular:

$$\sigma(a_p^* a_p) = \mathbb{N}$$

We write

$$H_N = \sum_{p \in \mathbb{Z}^3} p^2 a_p^* a_p + \frac{1}{2N} \sum_{p,q,r \in \mathbb{Z}^3} \hat{V}(r) a_{p+r}^* a_q^* a_{q+r} a_p$$

C-number substitution: $a_0, a_0^* \sim \sqrt{N} \gg 1 = [a_0, a_0^*]$

$$\Rightarrow H_N \simeq \frac{(N-1)\hat{V}(0)}{2}$$

$$+ \sum_{p \neq 0} (p^2 + \hat{V}(p)) a_p^* a_p + \frac{1}{2} \sum_{p \neq 0} \hat{V}(p) \left[a_p^* a_{-p}^* + a_p a_{-p} \right]$$

$$+ \frac{1}{\sqrt{N}} \sum_{p,r \neq 0} \hat{V}(r) \left[a_{p+r}^* a_{-r}^* a_p + h.c. \right]$$

$$+ \frac{1}{2N} \sum_{p,r,q \neq 0} \hat{V}(r) a_{p+r}^* a_q^* a_{q+r} a_p$$

Neglect cubic, quartic terms: we find

$$H_N \cong \frac{(N-1)\hat{V}(0)}{2} + \sum_{p\neq 0} (p^2 + \hat{V}(p))\, a_p^* a_p + \frac{1}{2}\sum_{p\neq 0} \hat{V}(p)\left[a_p^* a_{-p}^* + a_p a_{-p}\right]$$

Diagonalize quadratic Hamiltonian: with

$$T = \exp\left[\frac{1}{2}\sum_{p\neq 0} \tau_p \left(a_p^* a_{-p}^* - a_p a_{-p}\right)\right],$$

we find

$$T^* a_p^* T = \cosh \tau_p \cdot a_p^* + \sinh \tau_p \cdot a_{-p}$$

$$T^* a_p T = \cosh \tau_p \, a_p + \sinh \tau_p \, a_{-p}^*$$

Choosing τ_p s.t. : $\tanh(2\tau_p) = \dfrac{\hat{V}(p)}{p^2 + \hat{V}(p)}$

we obtain

$$T^* H_N T \cong \frac{(N-1)\hat{V}(0)}{2} - \frac{1}{2}\sum_{p \neq 0}\left[p^2 + \hat{V}(p) - \sqrt{|p|^4 + 2p^2\hat{V}(p)}\right]$$

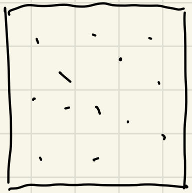
$$+ \sum_{p\neq 0} \sqrt{|p|^4 + 2p^2 \hat{V}(p)} \cdot a_p^* a_p$$

$\rightsquigarrow$ ground-state energy + low-energy spectrum, up to $o(1)$.

Rigorous results: Seiringer, Grech-Seiringer, Lewin-Nam-Serfaty-Solovej, Derezinski-Napiorkowski, Pizzo, Bossmann-Petrat-Seiringer, ...

Extension to GP limit: Boccato-Brennecke-Cenatiempo-S

Mean-field fermions



$\Lambda = [0;2\pi]^3$

Consider N fermions, trapped in torus Λ.

Because of statistics, kinetic energy is of order $N^{5/3}$.

We consider therefore the Hamilton operator

$$H_N = \sum_{j=1}^{N} -\varepsilon^2 \Delta_{x_j} + \frac{1}{N} \sum_{i<j}^{N} V(x_i - x_j) \quad \text{on } L^2_a(\Lambda^N)$$

Here, we set $\varepsilon = N^{-1/3}$.

$\rightsquigarrow$ Mean-field limit is linked with semiclassical limit, with $\varepsilon = N^{-1/3}$ playing role of Planck's constant.

Hartree-Fock theory

For $\{f_j\}_{j=1,\dots,N}$ an ONS on $L^2(\Lambda)$, consider Slater det.

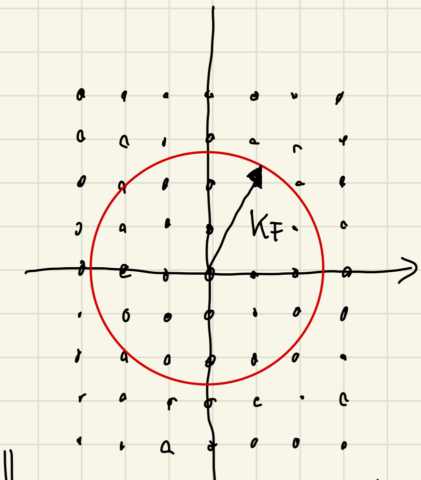
$$\Psi(x_1\dots x_N) = \bigwedge_{j=1}^{N} f_j \,(x_1\dots x_N) = \frac{1}{\sqrt{N!}} \det\left(f_i(x_j)\right)_{1\le i,j\le N}$$

We define

$$E_N^{HF} = \inf\left\{ \langle \Psi, H_N \Psi\rangle \;:\; \Psi = \bigwedge_{j=1}^{N} f_j \right\}$$

If $V=0$, E_N^{HF} attained by Fermi sea

$$\Psi_F = \bigwedge_{\substack{p\in\mathbb{Z}^3:\\ |p|\le k_F}} f_p \,, \quad \text{with } f_p(x) = e^{-ip\cdot x}/(2\pi)^{3/2}$$



If $\hat V \geq 0$ and Fermi ball filled, we find

$$E_N^{HF} = \langle \Psi_F, H_N \Psi_F \rangle \quad \text{even if } V \neq 0$$

$k_F = \varkappa \cdot N^{1/3}$

$\varkappa \cong (3/4\pi)^{1/3}$

Let $E_N = \inf \{ \langle \Psi, H_N \Psi \rangle : \Psi \in L^2_a(\Lambda^N) \}$

Interested in correlation energy : $E_{corr} = E_N - E_N^{HF} \leq 0$.

Theorem: Assume $\hat{V} \geq 0$, compactly supported, small enough. Then:

$$E_{corr} = \varepsilon \varkappa \cdot \sum_{k \in \mathbb{Z}^3} |k| \cdot \left[\frac{1}{\pi} \int_0^\infty \log\left[1 + 2\pi\varkappa \hat{V}(k) \cdot \left(1 - \lambda \arctan\left(\tfrac{1}{\lambda}\right)\right)\right] d\lambda - \frac{\pi}{2} \varkappa \hat{V}(k) \right] + \mathcal{O}(\varepsilon^{1+\frac{1}{16}})$$

Remarks: • to second order in V, we find:

$E_{corr}/\varepsilon \simeq \pi/2 \, (1 - \log 2) \cdot \sum_{k \in \mathbb{Z}^3} |k| \, |\hat{V}(k)|^2 \cdot (1 + \mathcal{O}(\hat{V}))$,

as previously shown by Hainzl-Porta-Rexze.

- result consistent with formula derived in physics through random-phase-approximation by Gell-Mann – Brückner and others...

To estimate correlation energy, it's convenient to factor out Fermi sea and focus on excitations.

Fock space: we define fermionic Fock space

$$\mathcal{F}_a = \bigoplus_{n \geq 0} L^2_a(\Lambda^n)$$

Creation and annihilation operators satisfy CAR

$$\{a_p, a_q^*\} = a_p a_q^* + a_q^* a_p = \delta_{pq}$$

$$\{a_p, a_q\} = \{a_p^*, a_q^*\} = 0$$

We write: $H_N = \sum_{p \in \mathbb{Z}^3} \varepsilon^2 p^2 a_p^* a_p + \frac{1}{2N} \sum_{p,q,r \in \mathbb{Z}^3} \hat{V}(r) a_{p+r}^* a_q^* a_{q+r} a_p$

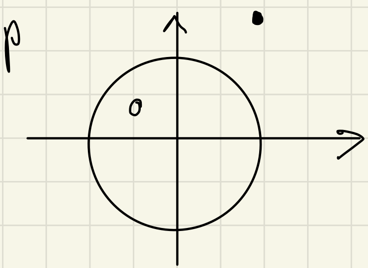
On $\mathcal{F}_a$, we find a unitary map R s.t.

- $R\Omega = \prod_{|p|\leq k_F} a_p^* \Omega = \Psi_F$ ($\Omega = \{1, 0, 0, \dots\}$ is vacuum on $\mathcal{F}_a$)

and

- $R a_p^* R^* = \begin{cases} a_p^* & \text{if } |p| > k_F \\ a_p & \text{if } |p| \leq k_F \end{cases}$

After conjugation with R, Ω represents Fermi sea, a_p^* creates an excitation with momentum p (a particle if $|p| > k_F$, a hole if $|p| \leq k_F$).



With R, we can define <u>excitation Hamiltonian</u>

$$\mathcal{L} = R H_N R^*$$

We compute:

$$R \sum_{p\in\mathbb{Z}^3} \varepsilon^2 p^2 a_p^* a_p R^* = \sum_{|p|\le k_F} \varepsilon^2 p^2 a_p a_p^* + \sum_{|p|>k_F} \varepsilon^2 p^2 a_p^* a_p$$

$$= \sum_{|p|\le k_F} \varepsilon^2 p^2 - \sum_{|p|\le \varepsilon^2 p^2} \varepsilon^2 p^2 a_p^* a_p + \sum_{|p|>k_F} \varepsilon^2 p^2 a_p^* a_p$$

$$= \underbrace{\sum_{|p|\le k_F} \varepsilon^2 p^2}_{\text{kinetic energy of Fermi sea}} + \underbrace{\sum_{p\in\mathbb{Z}^3} |\varepsilon^2 p^2 - \varepsilon^2 k_F^2| a_p^* a_p}_{\text{kin. energy of excitations}}$$

(on states with # holes = # particles)

Similarly, we can compute

$$R \frac{1}{2N} \sum_{p,q,r \in \mathbb{Z}^3} \hat{V}(r)\, a^*_{p+r}\, a^*_q\, a_{q+r}\, a_p\, R^*$$

This generates many terms. Some of them, like

$$\Bigg| \frac{1}{2N} \sum_{\substack{|p|, |q| > k_F \\ |p+r|, |q+r| > k_F}} \hat{V}(r) \langle \Psi, a^*_{p+r}\, a^*_q\, a_{q+r}\, a_p \Psi \rangle \Bigg|$$

$$\lesssim \frac{1}{2N} \sum \hat{V}(r) \| a_{p+r}\, a_q \Psi \| \, \| a_{q+r}\, a_p \Psi \|$$

$$\lesssim C/N \cdot \| \mathcal{N} \Psi \|^2$$

are small, on states with few excitations.
($\mathcal{N} = \sum_{p \in \mathbb{Z}^3} a^*_p a_p$ measures # of excitations).

We find

$$h = E_N^{HF} + \mathbb{H}_0 + Q_B + \text{small}$$

with

$$\mathbb{H}_0 = \sum_{p \in \mathbb{Z}^3} \left| \varepsilon^2 p^2 - \varepsilon^2 k_F^2 \right| a_p^* a_p$$

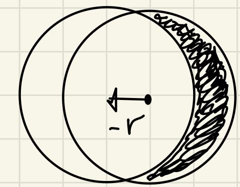
$$Q_B = \frac{1}{2N} \sum_{\substack{|p+r|, |q| > k_F \\ |q+r|, |p| \leq k_F}} \hat{V}(r) \left[a^*_{p+r} a^*_q a^*_{q+r} a^*_p + h.c. \right]$$

$$+ \frac{1}{N} \sum_{\substack{|p+r|, |q+r| > k_F \\ |p|, |q| \leq k_F}} \hat{V}(r) \cdot a^*_{p+r} a^*_p a_q a_{q+r}$$

↳ Terms involve two particles and two holes

Define particle-hole pair operators

$$b_r^* = \sum_{\substack{|p| \le k_F \\ |p+r| > k_F}} a_{p+r}^* a_p^*$$



Then:

$$Q_B = \frac{1}{N} \sum_{r \in \mathbb{Z}^3} \hat{V}(r) \left[b_r^* b_r + \frac{1}{2} \left(b_r^* b_{-r}^* + b_r b_{-r} \right) \right]$$

Furthermore:

$$[b_r, b_k] = [b_r^*, b_k^*] = 0 \quad \forall r, k \in \mathbb{Z}^3$$

$$[b_r, b_k^*] \simeq C \cdot \delta_{r,k} \,, \quad \text{on states with few excitations}$$

normalization constant

Problem:

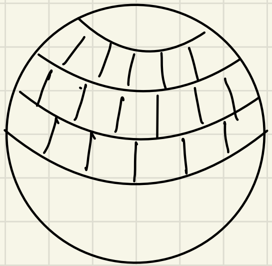
$$\mathbb{H}_0 b_k^* \Omega = \sum_{p\in\mathbb{Z}^3} \sum_{\substack{|q|\leq k_F \\ |q+k|>k_F}} |\varepsilon^2 p^2 - k_F^2| \, a_p^* a_p a_{q+k}^* a_q^* \Omega$$

$$= \sum_{\substack{|q|\leq k_F \\ |q+k|>k_F}} \varepsilon^2 \left[(q+k)^2 - q^2\right] a_{q+k}^* a_q^* \Omega$$

$$\simeq 2\varepsilon^2 \sum_{\substack{|q|\leq k_F \\ |q+k|>k_F}} q\cdot k \; a_{q+k}^* a_q^* \Omega$$

$\hookrightarrow$ cannot be expressed in terms of b_k^*

To solve problem, we need to **localize** pairs operators.



We decompose a thin shell around Fermi sphere in patches

$$\{B_\alpha\}_{\alpha=1,\dots,M}, \quad \text{for } M = N^\delta$$

We define corresponding local particle-holes pairs operators

$$b^*_{\alpha,k} = \frac{1}{n_\alpha(k)} \cdot \sum_{\substack{p\in B_\alpha, \\ |p|\leq k_F \\ |p+k|>k_F}} a^*_{p+k} a^*_p$$

Advantage:

$$\mathbb{H}_0 b^*_{\alpha,k} \Omega \simeq 2\varepsilon^2 \underbrace{\omega_\alpha}_{\text{center of } B_\alpha} \cdot k \; b^*_{\alpha,k} \Omega$$

$$\Longrightarrow \quad \mathbb{H}_0 \simeq 2\varepsilon^2 \sum_{k,\alpha} \omega_\alpha \cdot k \; b^*_{\alpha,k} b_{\alpha,k}$$

We conclude that

$$\mathcal{L} - E_N^{HF}$$

$$= 2\varepsilon\varkappa \sum_{k\in\mathbb{Z}^3} |k| \sum_{\alpha,\beta=1}^{M} \Big[\big(D(k)+W(k)\big)_{\alpha\beta}\, b^*_{\alpha,k} b_{\beta,k} + \frac{1}{2} W(k)_{\alpha\beta} \big(b^*_{\alpha,k} b^*_{\beta,k} + b_{\alpha,k} b_{\beta,k} \big) \Big]$$

$$+ \text{small}$$

Hence: leading contributions to correlation energy arise from a quadratic Hamiltonian in approximately bosonic fields $b^*_{\alpha,k}$, $b_{\alpha,k}$.

For appropriate kernel K, we consider the approximate Bogoliubov transformation:

$$T = \exp\Big[\frac{1}{2} \sum_{k} \sum_{\alpha,\beta} K(k)_{\alpha\beta} \big(b^*_{\alpha,k} b^*_{\beta,k} - b_{\alpha,k} b_{\beta,k} \big) \Big]$$

Then:

$$T^* b^*_{\alpha,k} T = \cosh(K(k))_{\alpha\beta}\, b^*_{\beta,k} + \sinh(K(k))_{\alpha,\beta}\, b_{\beta,k} + \text{small}$$

and:

$$T^* \mathcal{L} T - E_N^{HF}$$

Gell-Mann - Brückner formula

$$= \varepsilon\kappa \cdot \sum_{k \in \mathbb{Z}^3} |k| \cdot \Big[\frac{1}{\pi} \int_0^\infty \log\Big[1 + 2\pi\kappa \hat{V}(k) \cdot \big(1 - \lambda \operatorname{arctg}(1/\lambda)\big)\Big] d\lambda - \frac{\pi}{2} \kappa \hat{V}(k) \Big] + \text{small}$$

Appendix: how do we know there are only few excitations of Fermi sea?

$$0 \leq \int V(x-y) \left[\sum_{j=1}^{N} \delta(x-x_j) - N \right] \left[\sum_{j=1}^{N} \delta(y-x_j) - N \right] dx\, dy$$

$$= 2 \cdot \sum_{i<j}^{N} V(x_i - x_j) + N V(0) - N^2 \hat{V}(0)$$

$$\Rightarrow H_N \geq \frac{N \hat{V}(0)}{2} - \frac{V(0)}{2} + \sum_{p \in \mathbb{Z}^3} p^2 a_p^* a_p$$

$$\mathcal{L} = R H_N R^* \geq E_N^{HF} + \mathbb{H}_0 - C \cdot \varepsilon$$

$$\left.\begin{aligned} &\Rightarrow \langle \Psi, \mathbb{H}_0 \Psi \rangle \leq C \cdot \varepsilon \\ &\Rightarrow \langle \Psi, \mathcal{N} \Psi \rangle \leq C \cdot N^{1/3} \end{aligned}\right\}$$ on states with small excess energy.