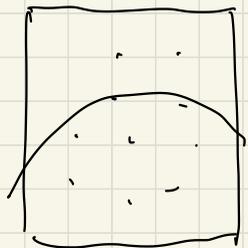


Bozolinov theory for
many-body quantum
systems.



III. Correlation energy for trapped weakly interacting fermions

Joint work with N. Benedikter, P.T. Nam, M. Porta,
R. Seiringer



$$\Lambda = [-1/2; 1/2]^3$$

$$\Psi_N \in L^2(\Lambda^N), \quad \Psi_N(x_{\pi_1}, \dots, x_{\pi_N}) = \delta_{\pi} \Psi_N(x_1, \dots, x_N)$$

$$\sum_{j=1}^N -\Delta x_j \sim N^{5/3}$$

$$\sum_{i < j}^N V(x_i - x_j) \sim N^2$$

Hence, we consider the Hamiltonian operator:

$$H_N = \sum_{j=1}^N -\varepsilon^2 \Delta x_j + \frac{1}{N} \sum_{i < j} V(x_i - x_j), \quad \varepsilon = N^{-1/3}$$

We will assume that $\hat{V} \geq 0$, and \hat{V} has compact support.

Slater determinants are states of the form

$$\Psi_{\text{Slater}}(x_1, \dots, x_N) = C \cdot \det (f_i(x_j))_{1 \leq i, j \leq N}$$

where $\{f_1, \dots, f_N\}$ is orthonormal system on $L^2(\Lambda)$

$$\begin{aligned} \omega &= N \operatorname{tr}_{2, \dots, N} |\Psi_{\text{Slater}}\rangle \langle \Psi_{\text{Slater}}| \\ &= \sum_{j=1}^N |f_j\rangle \langle f_j| \end{aligned}$$

$$\langle \Psi_{\text{Slater}}, H_N \Psi_{\text{Slater}} \rangle =$$

$$= \text{tr}(-\epsilon^2 \Delta \omega) + \frac{1}{2N} \int dx dy V(x-y) \left[\omega(x,x) \omega(y,y) - |\omega(x,y)|^2 \right]$$

(remark

$$\omega(x,y) = \sum_{j=1}^N f_j(x) \overline{f_j(y)}$$

$$\parallel \omega \parallel_{\text{HF}}^2 = E_{\text{HF}}(\omega)$$

$$E_{\text{HF}} = \inf_{\substack{\omega \text{ w/ th. prop.} \\ \text{on } L^2(\Lambda) \text{ with} \\ \text{tr } \omega = N}} E_{\text{HF}}(\omega)$$

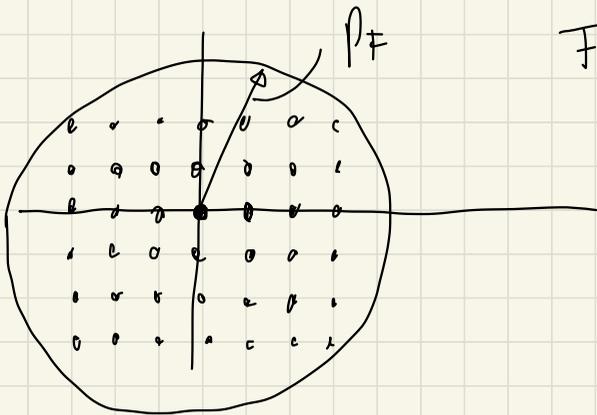
What can we say about E_{HF} ?

For free particles

$$E_{\text{WF}}(\omega) = \text{tr} - E^2 \Delta \omega$$

$$-\Delta e^{ip \cdot x} = p^2 e^{ip \cdot x}$$

$$p \in 2\pi \mathbb{Z}^3 =: \Lambda^*$$



Find $p_F > 0$ s.t. ball

B_F ~~is~~ of radius p_F
contains exactly N points

$$\rightarrow \frac{4\pi}{3} p_F^3 = (2\pi)^3 \cdot N$$

Minimizer of E_{WF} is: $\rightarrow p_F = \alpha_F \cdot N^{1/3}$

$$\omega_F = \sum_{p \in 2\pi \mathbb{Z}^3 : |p| < p_F} |e^{ip \cdot x} \rangle \langle e^{ip \cdot x}|$$

The Fermi sea has energy

$$\text{tr} (-\varepsilon^2 \Delta \omega_F) = \sum_{\substack{p \in \pi \mathbb{Z}^3: \\ |p| < p_F}} \varepsilon^2 p^2 \sim N$$

Interestingly: ω_F also minimizes E_{HF} , if B_F is completely filled. If not $E_{HF}(\omega_F)$ is anyway exponentially close to E_{HF} .

$$\Rightarrow E_{HF} = E_{HF}(\omega_F)$$

What is relation between E_{HF} and

$$E_N = \inf_{\Psi_N \in L^2_a(\Lambda^N)} \langle \Psi_N, H_N \Psi_N \rangle$$

Clearly: $E_N \leq E_{HF} = E_{HF}(W_F)$

We define the correlation energy as

$$E_{\text{corr}} = E_N - E_{HF} \leq 0$$

Fock space representation:

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

On \mathcal{F}_a , we introduce creation/annihilation ops.

$a_p^*, a_p \quad \forall p \in \mathbb{R}^3$. These satisfy: (CAR)

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

On \mathcal{F}_a , we find a unitary operator R
(particle-hole transf.) s.t.:

$$R \Omega = \prod_{\substack{p \in \mathcal{N}: \\ |p| \leq p_F}} a_p^* \Omega \quad (= \text{Fermi sea})$$

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



For $|p| > p_F$, a_p^* now creates a part.
For $|p| < p_F$, a_p^* " " a hole

Goal: $R: \mathcal{X}(N_n = N_p) \xrightarrow{\sim} \mathcal{L}_a(\Lambda^N)$

where
$$N_n = \sum_{|p| \leq p_F} a_p^* a_p$$

$$N_p = \sum_{|p| > p_F} a_p^* a_p$$

We find the excitation Hamiltonian:

$$L = R^* H_N R$$

Let's compute L :

What happens with kinetic energy?

$$\mathcal{N}^* \sum_{p \in \Lambda^*} \varepsilon_p^2 a_p^\dagger a_p \mathcal{N} =$$

$$= \sum_{|p| \leq p_F} \varepsilon_p^2 a_p a_p^\dagger + \sum_{|p| > p_F} \varepsilon_p^2 a_p^\dagger a_p$$

$$= - \sum_{|p| \leq p_F} \varepsilon_p^2 a_p^\dagger a_p + \sum_{|p| \leq p_F} \varepsilon_p^2 + \sum_{|p| > p_F} \varepsilon_p^2 a_p^\dagger a_p$$

$$= \sum_{|p| \leq p_F} (\varepsilon_{p_F}^2 - \varepsilon_p^2) a_p^\dagger a_p + \sum_{|p| \leq p_F} \varepsilon_p^2$$

$$+ \sum_{|p| > p_F} (\varepsilon_p^2 - \varepsilon_{p_F}^2) a_p^\dagger a_p = \text{tr}(-\varepsilon^2 \Delta \omega_F) + \sum_{p \in \Lambda^*} |\varepsilon_p^2 - \varepsilon_{p_F}^2| a_p^\dagger a_p$$

From pert. energy, we get two types of terms:

$$\left| \frac{1}{N} \sum_{\substack{|k+r| > p_F \\ |q+r| > p_F \\ |p, q| > p_F}} \hat{V}(r) \langle \xi, a_{p+r}^* a_q^* a_{q+r} a_p \xi \rangle \right|$$

$$\leq \frac{1}{N} \sum \hat{V}(r) \| a_{p+r} a_q \xi \| \| a_{q+r} a_p \xi \|$$

$$\leq \frac{1}{N} \left[\sum |\hat{V}(r)| \| a_{p+r} a_q \xi \|^2 \right]^{1/2} \left[\sum |\hat{V}(r)| \| a_{q+r} a_p \xi \|^2 \right]^{1/2}$$

$$\leq \frac{C}{N} \| N_+ \xi \|^2 \rightarrow$$

small on
states with
few excit.

On the other hand

$$\left| \frac{1}{N} \sum_{\substack{|p+r|, |q| > p \\ |q+r|, |p| \leq p}} \hat{V}(r) \langle \xi, a_{p+r}^* a_q a_{q+r} a_p^* \rangle \right|$$

$$\leq \frac{1}{N} \sum |\hat{V}(r)| \| a_{p+r} a_q a_{q+r} a_p N_+^{-1} \xi \| \| N_+ \xi \|$$

$$\leq \frac{1}{N} \left[\sum |\hat{V}(r)| \| a_{p+r} a_q a_{q+r} a_p N_+^{-1} \xi \|^2 \right]^{1/2}$$

$$\left[\sum |\hat{V}(r)| \| N_+ \xi \|^2 \right]^{1/2}$$

$$\leq C N_+ \|\xi\|^2 \leq C \cdot \| N_+ \xi \|^2$$

Defining:

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

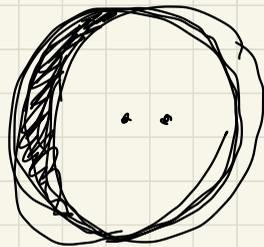
⇒ The previous term
has term

$$\frac{1}{N} \sum_{r \in \Lambda^*} \hat{V}(r) b_r^* b_{-r}^*$$

Remark: $[b_r, b_k] = 0,$

$$[b_r, b_k^*] = \text{const. } \delta_{kr}$$

+ const. (small on lattice with low exc.)



We find:

$$\mathcal{L} = E_{H\neq}(\omega_{\neq}) + \sum_{p \in \Lambda^{\neq}} \underbrace{|\underbrace{E_{p\neq}^2 - E_{p^2}^2}_{\omega_{\neq}^2}|}_{H|_0} a_p^\dagger a_p$$

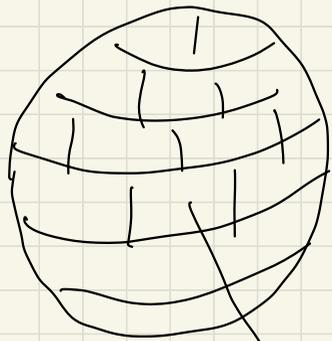
+ Q_B + errors small on states with few particles

$$Q_B = \frac{1}{2N} \sum_r \hat{V}(r) \left[b_r^\dagger b_r + \frac{1}{2} (b_r^\dagger b_{-r}^\dagger + b_r b_{-r}) \right]$$

Problem kinetic energy:

$$H_0 b_u^\dagger \Omega = H_0 \sum_{\substack{|\mathbf{l}| \leq p \neq \\ |\mathbf{l}+\mathbf{u}| > p \neq}} a_{p+\mathbf{l}}^\dagger a_p^\dagger \Omega = \sum_{|\mathbf{l}| \dots} [E^2(p+\mathbf{l}) - E_{p^2}^2] a_{p+\mathbf{l}}^\dagger a_p^\dagger \Omega$$

$$= \sum_p \varepsilon \varepsilon^2 p \cdot k a_{p+u}^* \cdot a_p^* \Omega \neq C \cdot b_u^* \Omega$$



Divide B_F in M patches,
and define new modes

$$b_{k,\alpha}^* = \sum_{\substack{|p| \leq p_F \\ |p+u| > p_F, p \in B_\alpha}} a_{p+u}^* a_p^* \Omega$$

Thm: if $\|V\|$ is small enough, then

$$E_{\text{can}} = E_N - \varepsilon_{N_F} (w_F) \omega$$

$$= -\varepsilon_{N_F} \sum_{u \in \Lambda^N} |u| \left[\frac{1}{\varepsilon} \int_0^{\varepsilon} \log \left[1 + 2\varepsilon \hat{V}(u) (1 - \lambda \text{ardg}(\frac{1}{\lambda})) \right] d\lambda \right. \\ \left. - \varepsilon/2 \varepsilon \hat{V}(u) \right]$$

$+ O(\varepsilon^{1+1/16})$