

Theorem 3.2

(Admissible One-Body Density Matrices for Fermions)

γ on $\mathcal{H} = L^2(\mathbb{R}^3; \mathbb{C}^4)$
 γ as in Theorem 3.1.

$$\left(\begin{array}{l} \text{i.e. } (\phi', \gamma \phi) = (\gamma \phi', \phi) \quad \text{self-adjoint} \\ \quad \quad \quad \forall \phi, \phi' \in \mathcal{H} \\ (\phi, \gamma \phi) \geq 0 \quad \text{positive semidefinite} \\ \quad \quad \quad \forall \phi \in \mathcal{H} \\ \text{Tr } \gamma = N, \quad N \geq 1 \text{ integer} \end{array} \right.$$

$$\Rightarrow \exists \Gamma : \text{fermionic } N\text{-particle density matrix} \\ \text{s.t. } \gamma = N \cdot \text{Tr}(N-1) \Gamma$$

$$\Leftrightarrow \gamma \leq \mathbb{1}.$$

Proof.

To ~~show~~ prove

$$\gamma \leq \mathbb{I} \Rightarrow \exists \Gamma$$

$1 \geq \lambda_1 \geq \lambda_2 \geq \dots \geq 0$ in decreasing order

$$\gamma u_j = \lambda_j u_j \text{ for } j=1, 2, \dots$$

$$(u_j, u_k) = \delta_{jk}$$

$$\lambda_j = \lambda_j(u_j, u_j) = (u_j, \lambda_j u_j) = (u_j, \gamma u_j) \geq 0$$

$$\lambda_1 = (u_1, \gamma u_1) \leq 1$$

$$\sum_{j=1}^{\infty} \lambda_j = \text{Tr } \gamma = N.$$

Case I. $\lambda_{N+1} = 0$

$$\Rightarrow \lambda_1 = \lambda_2 = \dots = \lambda_N = 1, \lambda_j = 0 \text{ for } j \geq N+1$$

Slater determinant

$$\psi(\underline{z}) = (N!)^{1/2} \det \{u_i(z_j)\}_{i,j=1}^N$$

with $u_1, \dots, u_N$

$$\Gamma = \Gamma_\psi \text{ with } \gamma = N \cdot \text{Tr}(N^{-1}) \Gamma$$

$$\Gamma \psi(\underline{z}; \underline{z}') = \psi(\underline{z}) \overline{\psi(\underline{z}')}$$

$$\begin{aligned} \Gamma \psi \phi &= (\psi, \phi) \psi = \int \overline{\psi(\underline{z}')} \phi(\underline{z}') \psi(\underline{z}) d\underline{z}' \\ &= \int \underbrace{\psi(\underline{z}) \overline{\psi(\underline{z}')}}_{\Gamma(\underline{z}; \underline{z}')} \cdot \phi(\underline{z}') d\underline{z}' \end{aligned}$$

$$f^{(1)}(\underline{z}; \underline{z}') = N \cdot \int \psi(\underline{z}_1, \underline{z}^{(N-1)}) \overline{\psi(\underline{z}'_1, \underline{z}^{(N-1)})} d\underline{z}^{(N-1)}$$

$$\begin{aligned} \psi(\underline{z}_1, \underline{z}^{(N-1)}) &= (N!)^{-1/2} \sum_{\pi \in S_N} \epsilon_\pi \prod_{\bar{c}=1}^N u_{\pi(\bar{c})}(z_{\pi(\bar{c})}) \\ &\downarrow \\ &= (N!)^{1/2} \sum_{\pi \in S_N} \epsilon_\pi u_{\pi(1)}(z_1) \prod_{\bar{c}=2}^N u_{\pi(\bar{c})}(z_{\bar{c}}) \end{aligned}$$

$$f^{(1)}(\underline{z}_1; \underline{z}'_1)$$

$$\begin{aligned} &= \frac{1}{(N-1)!} \sum_{\pi \in S_N} \sum_{\pi' \in S_N} \epsilon_\pi \epsilon_{\pi'} \int u_{\pi(1)}(z_1) \overline{u_{\pi'(1)}(z'_1)} \\ &\quad \times \int \prod_{\bar{c}=2}^N u_{\pi(\bar{c})}(z_{\bar{c}}) \overline{u_{\pi'(\bar{c})}(z'_{\bar{c}})} d\underline{z}^{(N-1)} \end{aligned}$$

$$\prod_{\bar{c}=2}^N \int u_{\pi(\bar{c})}(z_{\bar{c}}) \overline{u_{\pi'(\bar{c})}(z'_{\bar{c}})} dz_{\bar{c}}$$

$$\prod_{\bar{c}=2}^N (u_{\pi(\bar{c})}, u_{\pi'(\bar{c})}) = 1$$

$$\text{if } \pi(\bar{c}) = \pi'(\bar{c}), \text{ for } \bar{c}=2, \dots, N \\ \Rightarrow \pi(1) = \pi'(1)$$

$$\therefore \pi = \pi'$$

$$\therefore f^{(1)}(z; z')$$

$$= \frac{1}{(N-1)!} \sum_{\substack{\pi \in S_N \\ \pi(1) = \pi'}} \varepsilon_{\pi}^2 u_{\pi(1)}(z) \overline{u_{\pi(1)}(z')}$$

$$\sum_{\pi \in S_N} = \sum_{j=1}^N \sum_{\pi(1)=j}$$

$$= \frac{1}{(N-1)!} \sum_{j=1}^N \sum_{\pi(1)=j} u_j(z) \overline{u_j(z')}$$

$$= \frac{1}{(N-1)!} \underbrace{\#\{\pi \in S_N; \pi(1)=j\}}_{(N-1)!} \left(\sum_{j=1}^N u_j(z) \overline{u_j(z')} \right)$$

$$= \sum_{j=1}^N u_j(z) \overline{u_j(z')}. //$$

Case II. $\lambda_{N+1} > 0$

$$\lambda_{N+1} \leq \frac{N}{N+1} < 1 \quad \boxed{0 < \lambda_{N+1} < 1}$$

$$\therefore N = \sum_{j=1}^{\infty} \lambda_j \geq \sum_{j=1}^{N+1} \lambda_j \geq (N+1) \lambda_{N+1} //$$

$$\boxed{0 < \lambda_N < 1} \quad \therefore \lambda_{N+1} \leq \frac{N}{N+1}$$

$$1 \geq \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_N$$

$$\lambda_N = 0 \Rightarrow \begin{aligned} &\lambda_j = 0 \text{ for } j \geq N+1 \\ &\sum_{j=1}^{\infty} \lambda_j = \sum_{j=1}^{N-1} \lambda_j \leq N-1 \neq N \\ &\text{Contradiction!} \end{aligned}$$

$$\begin{aligned} \lambda_N = 1 &\Rightarrow 1 \geq \lambda_1 \geq \dots \geq \lambda_N = 1 \\ &\therefore \lambda_1 = \dots = \lambda_N = 1 \\ &\Rightarrow \lambda_{N+1} = 0 \text{ contradiction!} \end{aligned}$$

$$\chi_{[1, N]}(j) = \begin{cases} 1 & (1 \leq j \leq N) \\ 0 & (j > N) \end{cases}$$

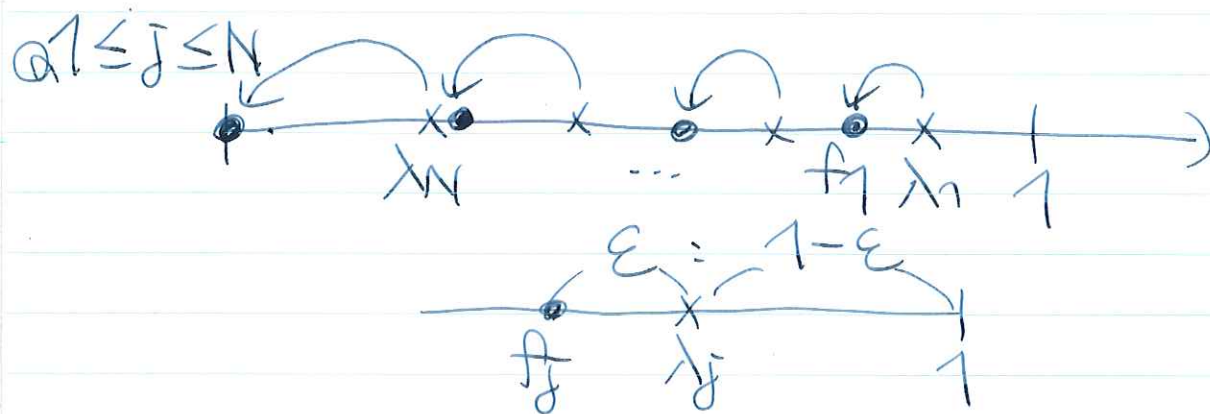
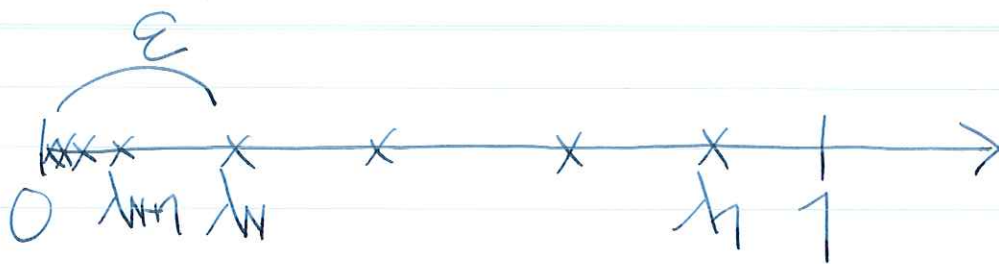
$$\varepsilon = \min\{\lambda_N, 1 - \lambda_{N+1}\}$$

$$0 < \varepsilon < 1.$$

$$\lambda_j = \varepsilon \chi_{[1, N]}(j) + (1 - \varepsilon) f_j$$

$$\text{with } f_j = \frac{1}{1 - \varepsilon} (\lambda_j - \varepsilon \chi_{[1, N]}(j))$$

$$\Rightarrow 0 \leq f_j \leq 1 \text{ and } \sum_{j=1}^{\infty} f_j = N.$$

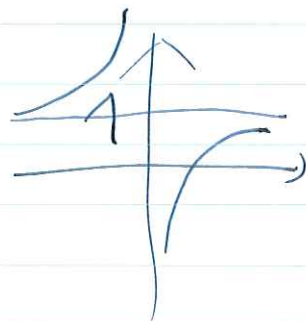


$$0 \leq f_j = \frac{\lambda_j - \varepsilon}{1 - \varepsilon} \leq \lambda_j$$

$$\begin{aligned} \lambda_j &= \varepsilon + (1 - \varepsilon) f_j \\ &\leq \varepsilon f_j + (1 - \varepsilon) f_j \\ &= f_j \end{aligned}$$

$$\begin{aligned} \frac{b+x}{a+x} &= \frac{(a+x) - (a-b+x)}{a+x} = 1 - \frac{a-b}{a+x} \\ &= 1 - \frac{a-b}{a+x} \end{aligned}$$

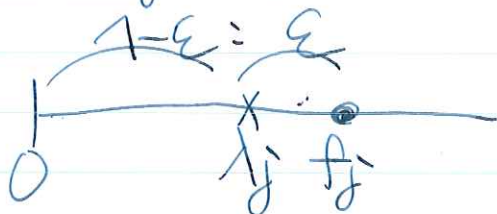
$$\frac{a-b}{(a+x)^2} \geq 0$$



$$f_N = \frac{\lambda_N - \varepsilon}{1 - \varepsilon} = \frac{\lambda_N - \lambda_N}{1 - \lambda_N} = 0$$

$$\begin{aligned} &0 \leq f_j < \lambda_j \\ &0 = f_N \leq f_{N-1} \leq \dots \leq f_1. \end{aligned}$$

$$0 \leq \lambda_j \leq 1$$



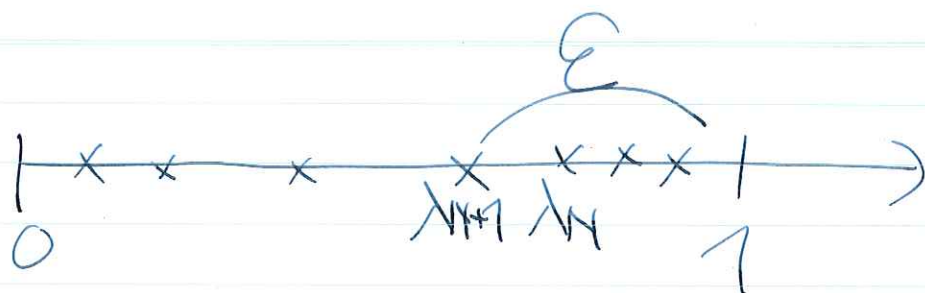
$$\lambda_j = (1 - \epsilon) \lambda_{j+1}, \quad \lambda_{j+1} = \frac{\lambda_j}{1 - \epsilon} \geq \frac{\lambda_j}{1 - \epsilon + \epsilon} = \lambda_j$$

$$\lambda_j = 0 \Rightarrow \lambda_{j+1} = 0$$

$$\lambda_{N+1} \geq \lambda_{N+2} \geq \dots \geq 0$$

$\downarrow$ $\downarrow$
 λ_N λ_{N+1}

$$\lambda_j = \frac{\lambda_j}{1 - \epsilon} \leq \frac{\lambda_j}{1 - (1 - \lambda_N)} = \frac{\lambda_j}{\lambda_N} \leq 1.$$



① $1 \leq j \leq N$



$$f_j = \frac{\lambda_j - \varepsilon}{1 - \varepsilon}$$

$$\cancel{\lambda_j} \leq f_j \leq 1.$$

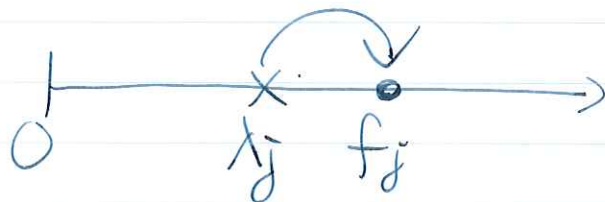
$$\therefore f_j = \frac{\lambda_j - \varepsilon}{1 - \varepsilon} \leq \frac{1 - \varepsilon}{1 - \varepsilon} = 1$$

$$1 \geq f_1 \geq f_2 \geq \dots \geq f_N$$

$$0 \leq f_j < \lambda_j \leq 1$$

$$\begin{aligned} \lambda_j &= \varepsilon + (1 - \varepsilon)f_j \\ &> \varepsilon f_j + (1 - \varepsilon)f_j \\ &\Rightarrow f_j \end{aligned}$$

② $j \geq N+1$



$$f_j = \frac{\lambda_j}{1 - \varepsilon}$$

$$0 \leq \lambda_j \leq f_j \leq 1$$

$$f_j = \frac{\lambda_j}{1 - \varepsilon} = \frac{\lambda_j}{1 - (1 - \lambda_N)} = \frac{\lambda_j}{\lambda_N} \leq 1$$

$$\lambda_j = (1 - \varepsilon)f_j \leq f_j$$

$$f_{N+1} = \frac{\lambda_{N+1}}{1 - (1 - \lambda_{N+1})} = 1.$$

$$1 = f_{N+1} \geq f_{N+2} \geq \dots \geq 0$$