Theorem 3.2
(Admissible One-Body Density Matrices for Fermions)

$\gamma : L^2(\mathbb{R}^3; \mathbb{C}^q) \to L^2(\mathbb{R}^3; \mathbb{C}^q)$
self-adjoint, positive semidefenite

$\mathrm{Tr}\,\gamma = N \quad (N \geq 1, \text{ integer})$

$\Longrightarrow \exists \Gamma$: fermionic N-particle density matrix

s.t. $\gamma = N \cdot \mathrm{Tr}^{(N-1)} \Gamma$

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

Moreover, we cannot expect $\Gamma = \Gamma_\psi$.

Proof

Step 1. To show $\gamma \leq \mathbb{1} \Rightarrow \exists \Gamma$

$\gamma \leq \mathbb{1} \iff (\phi, \gamma\phi) \leq (\phi, \phi) \quad \forall \phi \in \mathcal{H}$

$\lambda_1 \geq \lambda_2 \geq \cdots \geq 0$

$\gamma u_j = \lambda_j u_j \quad (j = 1, 2, \cdots)$

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

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

$\leq (u_j, u_j) = 1.$

$0 \leq \lambda_j \leq 1 \quad (j = 1, 2, \ldots)$

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

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

$$\lambda_1 = 1, \ \dots, \ \lambda_N = 1$$

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

$$\Longrightarrow \Gamma = \Gamma_\psi, \text{ fermionic.}$$

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

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

$$0 < \lambda_N < 1 \quad (\because \lambda_N = 1 \Rightarrow \lambda_{N+1} = 0)$$

$$\varepsilon_1 := \min\{\lambda_N, 1 - \lambda_{N+1}\}$$

$$\chi_1 = \chi_{S_1}, \quad S_1 = \{1, \dots, N\}$$

$$\chi_1(j) = \begin{cases} 1 & (j \in S_1) \\ 0 & (j \notin S_1) \end{cases}$$

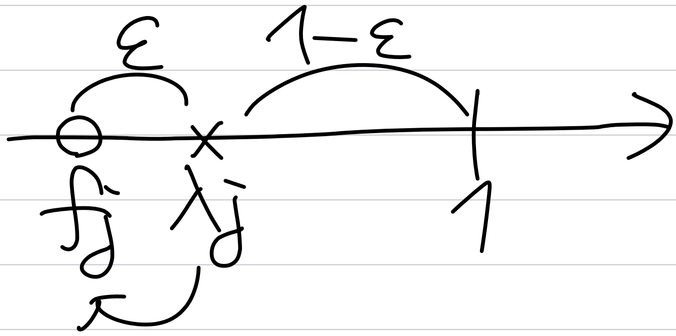
$$\lambda_j = \varepsilon_1 \chi_1(j) + (1 - \varepsilon_1) f_j$$

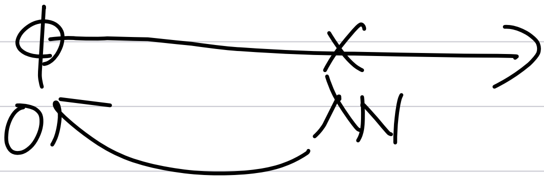
$$f_j = \frac{\lambda_j - \varepsilon_1 \chi_1(j)}{1 - \varepsilon_1}$$

$$\begin{cases} 0 \leq f_j \leq 1 & (\forall j = 1, 2, \dots) \\ \sum_{j=1}^{\infty} f_j = N \end{cases}$$

Case (i) $\varepsilon = \lambda_N$ or $\lambda_N \leq 1 - \lambda_{N+1}$

<u>$j \in S_1$</u>



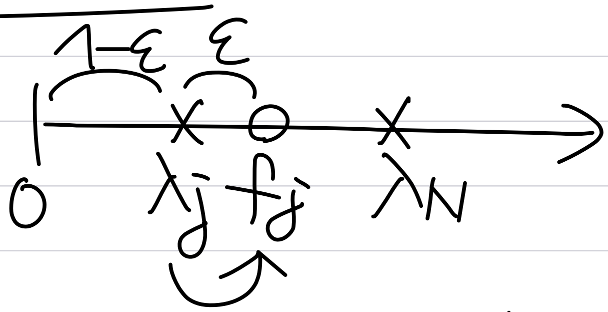


$f_N = 0$

$f_j \leq \lambda_j$, $\lambda_j = 1 \Rightarrow f_j = 1$

$f_1 \geq f_2 \geq \cdots \geq f_N = 0$

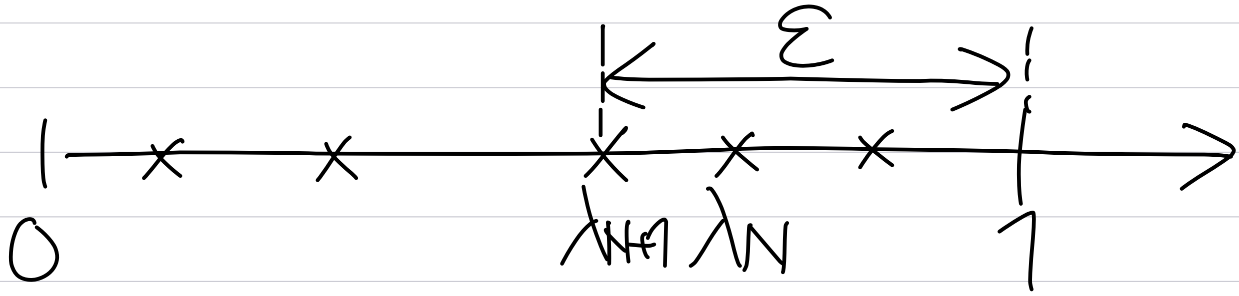
<u>$j \notin S_1$</u>



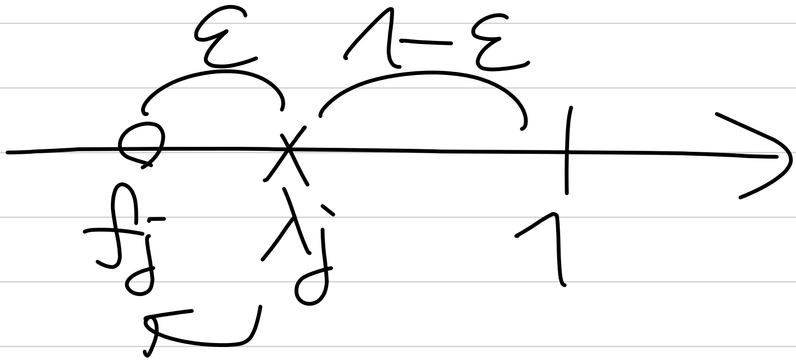
$\lambda_j \leq f_j$, $\lambda_j = 0 \Rightarrow f_j = 0$

$f_{N+1} \geq f_{N+2} \geq \cdots \geq 0$

Case (ii) $\varepsilon = 1-\lambda_{N+1}$ or $1-\lambda_{N+1} \le \lambda_N$



<u>$j \in S_1$</u>

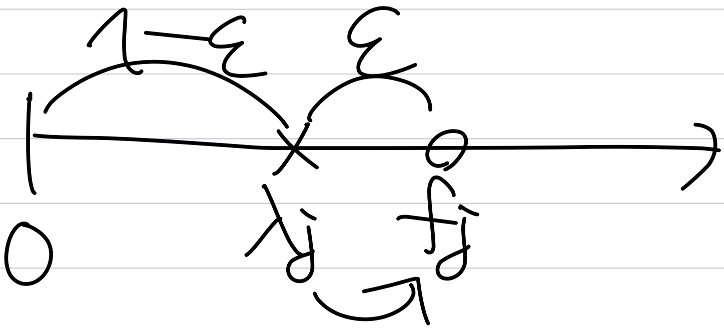


$f_j \le \lambda_j$

$\lambda_j = 1 \Rightarrow f_j = 1$

$f_1 \ge f_2 \ge \cdots \ge f_N \ge 0$

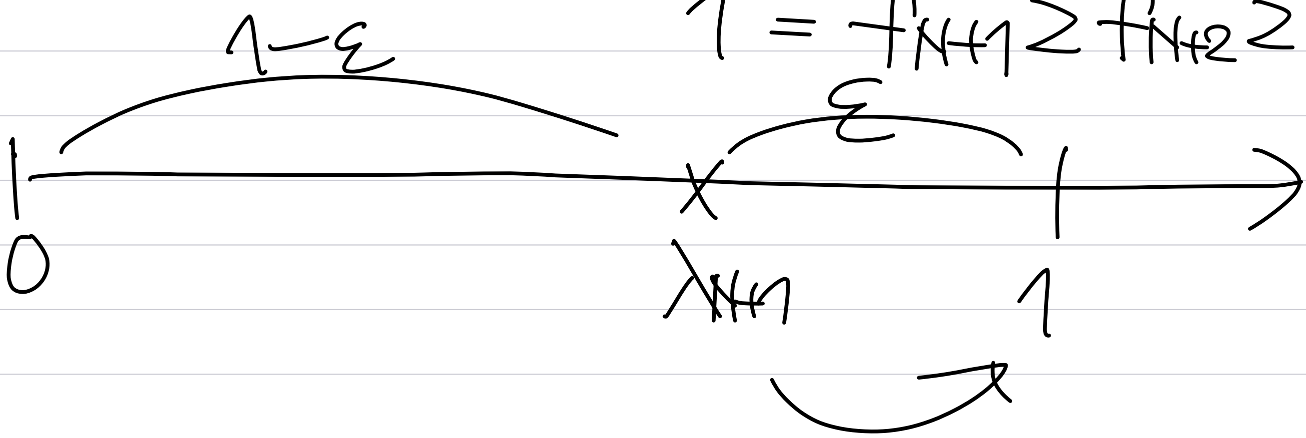
<u>$j \notin S_1$</u>



$\lambda_j \le f_j$

$\lambda_j = 0 \Rightarrow f_j = 0$

$1 = f_{N+1} \ge f_{N+2} \ge \cdots \ge 0$



Iteration

$$\{\lambda_1, \lambda_2, \dots\} \longmapsto \{f_1, f_2, \dots\}$$

$$\tilde{f}_1 \geq \tilde{f}_2 \geq \cdots \geq 0 \quad \text{(rearranged)}$$

$$\tilde{f}_j = f_{\sigma_1(j)} \iff f_i = \tilde{f}_{\sigma_1^{-1}(i)}$$

$$\sigma_1 : \{1, 2, \dots\} \to \{1, 2, \dots\}$$

$$\lambda_j = \varepsilon_1 \chi_1(j) + (1-\varepsilon_1)\tilde{f}_j$$

$$\varepsilon_2 = \min\{\tilde{f}_N, 1-\tilde{f}_{N+1}\}$$

$$\tilde{f}_j = \varepsilon_2 \chi_2(j) + (1-\varepsilon_2) f_j^{(2)}$$

$$\chi_2 = \chi_{S_2}$$

$$S_2 = \{\sigma_1(1), \dots, \sigma_1(N)\}$$

$$\{\tilde{f}_j\} \longmapsto \{f_j^{(2)}\}$$

$$\tilde{f}_1^{(2)} \geq \tilde{f}_2^{(2)} \geq \cdots \geq 0 \quad \text{(rearranged)}$$

$$\tilde{f}_j^{(2)} = f^{(2)}_{\sigma_2(j)} \iff f_i^{(2)} = \tilde{f}_{\sigma_2^{-1}(i)}$$

after M-iteration

$$\varepsilon_M = \min\{ \tilde{f}_N^{(M)}, 1 - \tilde{f}_{N+1}^{(M)} \}$$

$$f_j^{(M-1)} = \varepsilon_M x_M(j) + (1-\varepsilon_M) f_j^{(M)}$$

$$x_M = x_{S_M}$$

$$S_M = \{ \sigma_M \cdots \sigma_2 \sigma_1(1), \dots, \sigma_M \cdots \sigma_2 \sigma_1(N) \}$$

$$\{ f_j^{(M-1)} \} \longmapsto \{ f_j^{(M)} \}$$

$$\tilde{f}_1^{(M)} \geq \tilde{f}_2^{(M)} \geq \cdots \geq 0$$

$$\tilde{f}_j^{(M)} = f_{\sigma_M(j)}^{(M)} \Longleftrightarrow f_i^{(M)} = \tilde{f}_{\sigma_M^{-1}(i)}^{(M)}$$

$$\lambda_j = \sum_{k=1}^{M} \underbrace{\varepsilon_k \prod_{i=1}^{k-1}(1-\varepsilon_i)}_{c_k} x_k(j) + \underbrace{f_j^{(M)} \prod_{i=1}^{M}(1-\varepsilon_i)}_{R_j^{(M)}}$$

$$= \sum_{k=1}^{M} c_k x_k(j) + R_j^{(M)}$$

Example $(N=2)$

$$\{\lambda_j\} = \{1, \tfrac{1}{2}, \tfrac{1}{3}, \tfrac{1}{6}, 0, \dots\}$$

$$\lambda_N = \frac{1}{2},\quad 1-\lambda_{N+1} = 1-\frac{1}{3} = \frac{2}{3}$$

$$\varepsilon_1 = \min\left\{\frac{1}{2}, \frac{2}{3}\right\} = \frac{1}{2}$$

$$1 \overset{T}{\longmapsto} 1 =: f_1$$

$$\lambda_N = \frac{1}{2} \longmapsto \frac{\frac{1}{2}-\frac{1}{2}}{1-\frac{1}{2}} = 0 =: f_2$$

$$\frac{1}{3} \longmapsto \frac{\frac{1}{3}}{\frac{1}{2}} = \frac{2}{3} =: f_3$$

$$\frac{1}{6} \longmapsto \frac{\frac{1}{6}}{\frac{1}{2}} = \frac{1}{3} =: f_4$$

$$\xrightarrow{I} \begin{array}{cccccc} \{1, & \frac{2}{3}, & \frac{1}{3}, & 0, & 0, & \dots\} \\ \| & \| & \| & \| & & \\ f_1^{(1)} & f_2^{(1)} & f_3^{(1)} & f_2 & & \\ \| & \| & \| & & & \\ f_1 & f_3 & f_4 & & & \end{array}$$

j	1	2	3	4
$\sigma_1(j)$	1	3	4	2

$$\varepsilon_2 = \min\left\{\frac{2}{3}, \frac{2}{3}\right\} = \frac{2}{3}$$

$$1 \xmapsto{T} 1 =: f_1^{(2)}$$

$$\lambda_N = \frac{2}{3} \longmapsto \frac{\frac{2}{3} - \frac{2}{3}}{1 - \frac{2}{3}} = 0 =: f_2^{(2)}$$

$$\lambda_{N+1} = \frac{1}{3} \longmapsto \frac{\cancel{\frac{1}{3}}}{\cancel{\frac{1}{3}}} = 1 =: f_3^{(2)}$$

$$\xrightarrow{T} \{\underset{f_1^{(2)}}{\underset{\|}{1}}, \underset{\underset{f_3^{(2)}}{\underset{\|}{f_2^{(2)}}}}{\underset{\|}{1}}, 0, 0, 0, \dots\}$$

j	1	2	3	4	$\cdots$
$\sigma_2(j)$	1	3	2	4	$\cdots$

$$\varepsilon_3 = \min\{1, 1-0\} = 1 \quad \text{Stop!}$$

$$\lambda_j = \sum_k c_k \chi_k(j)$$

$$c_k = \varepsilon_k \prod_{i=1}^{k-1} (1-\varepsilon_i)$$

$$\begin{cases} c_1 = \varepsilon_1 = \frac{1}{2} \\ c_2 = \varepsilon_2(1-\varepsilon_1) = \frac{2}{3}\cdot\frac{1}{2} = \frac{1}{3} \\ c_3 = \varepsilon_3(1-\varepsilon_2)(1-\varepsilon_1) = 1\cdot\frac{1}{3}\cdot\frac{1}{2} = \frac{1}{6} \\ c_4 = 0 \end{cases}$$

$$\chi_k = \chi_{S_k}$$

$$\begin{cases} S_1 = \{1, 2\} \\ S_2 = \{\sigma_1(1), \sigma_1(2)\} = \{1, 3\} \\ S_3 = \{\sigma_2\sigma_1(1), \sigma_2\sigma_1(2)\} \\ \quad = \{\sigma_2(1), \sigma_2(4)\} \\ \quad = \{1, 4\} \end{cases}$$

$$\lambda_1 = \sum_k c_k \chi_k(1) = \frac{1}{2} + \frac{1}{3} + \frac{1}{6} = 1$$

$$\lambda_2 = \frac{1}{2}$$

$$\lambda_3 = \frac{1}{3}$$

$$\lambda_4 = \frac{1}{6}$$

$$\sum_{k=1}^{M} c_k = \sum_{k=1}^{M} \varepsilon_k \prod_{i=1}^{k-1} (1-\varepsilon_i) = 1 - \prod_{i=1}^{M} (1-\varepsilon_i)$$

$$\therefore \sum_{k=1}^{M} c_k \leq 1.$$

$$\lim_{M\to\infty} \sum_{k=1}^{M} c_k = 1 \quad \text{or} \quad \lim_{M\to\infty} \sum_{k=1}^{M} c_k < 1$$

$$\boxed{\sum_{k=1}^{\infty} c_k = 1}$$

$$\lambda_j = \sum_{k=1}^{M} c_k x_k(j) + R_j^{(M)}$$

$$\sum_{j=1}^{\infty} \lambda_j = \sum_{j=1}^{\infty} \sum_{k=1}^{M} c_k x_k(j) + \sum_{j=1}^{\infty} R_j^{(M)}$$

$$\sum_{k=1}^{M} \sum_{j=1}^{\infty} |c_k x_k(j)|$$

$$= \sum_{k} c_k \underbrace{\sum_{j} x_k(j))}_{\substack{\| \\ N}} = N \sum_{k=1}^{M} c_k < \infty$$

$$N = N \underbrace{\sum_{k=1}^{M} c_k}_{\substack{\downarrow \text{ as } M\to\infty \\ 1}} + \sum_{j=1}^{\infty} R_j^{(M)}$$

$$\therefore \sum_{j=1}^{\infty} R_j^{(M)} \longrightarrow 0 \quad (\text{as } M \to \infty)$$

$$\Rightarrow R_j^{(M)} \longrightarrow 0 \quad (\text{as } M \to \infty)$$

$$\therefore \lambda_j = \sum_{k=1}^{\infty} c_k \chi_k(j)$$

$\longrightarrow$ Slater determinants (rank N projections)

$$\boxed{\sum_{k=1}^{\infty} c_k =: d < 1}$$

j : fixed

$R_j^{(M)} \longrightarrow R_j$ strongly as $M \to \infty$

$\because$) $R_j^{(M)} = \lambda_j - \sum_{k=1}^{M} c_k x_k(j)$

$$R_j^{(1)} \geq R_j^{(2)} \geq \cdots \geq R_j^{(M)} \geq \cdots \geq 0$$

$\therefore \exists R_j \geq 0$ s.t. $R_j^{(M)} \longrightarrow R_j \geq 0$

(as $M \to \infty$)

$$R_j = \lim_{M \to \infty} R_j^{(M)} = \lambda_j - \sum_{k=1}^{\infty} c_k x_k(j)$$

$$R_j^{(M)} - R_j = \sum_{k=1}^{\infty} c_k x_k(j) - \sum_{k=1}^{M} c_k x_k(j)$$

$$= \sum_{k=M+1}^{\infty}$$

$$\because \sum_{j=1}^{\infty} |R_j^{(M)} - R_j| = \sum_{j=1}^{\infty} \sum_{k=M+1}^{\infty} c_k \chi_k(j)$$

$$= \sum_{k=M+1}^{\infty} c_k \underbrace{\sum_{j=1}^{\infty} \chi_k(j)}_{= N}$$

$$= N \sum_{k=M+1}^{\infty} c_k$$

$$= N\Big(\underbrace{\sum_{k=1}^{\infty} c_k}_{= d} - \underbrace{\sum_{k=1}^{M} c_k}_{\downarrow\, d}\Big) \to 0 \quad (M \to \infty) \quad //$$

$$\boxed{R_j^{(M)} \le 1 - \sum_{k=1}^{M} c_k}$$

$$\because)\ R_j^{M} + \sum_{k=1}^{M} c_k = f_j^{(M)} \prod_{i=1}^{M} (1-\varepsilon_i) + \sum_{k=1}^{M} \varepsilon_k \prod_{i=1}^{k-1} (1-\varepsilon_i)$$

$$= f_j^{(M)} \prod_{i=1}^{M} (1-\varepsilon_i) + 1 - \prod_{i=1}^{M} (1-\varepsilon_i)$$

$$= 1 - (1 - f_j^{(M)}) \prod_i (1-\varepsilon_i)$$

$$\le 1 \qquad (\because 0 \le f_j^{(M)} \le 1)$$

$$\therefore R_j = \lim_{M\to\infty} R_j^{(M)} \le 1 - d \quad //$$

$$\boxed{\sum_{j=1}^{\infty} R_j = N(1-d)}$$

$$\sum_{j=1}^{\infty} R_j^{(n)} = \sum_{j=1}^{\infty} 1_j - \sum_{j=1}^{\infty}\sum_{k=1}^{\infty} c_k \chi_k(j)$$

$$\sum_{k=1}^{\infty}\sum_{j=1}^{\infty} \Big| c_k \underbrace{\chi_k(j)}_{=1} \Big| = Nd < \infty \qquad (j \in S_k)$$

$$= N - Nd \quad //$$

$$\boxed{\lim_{k\to\infty} \varepsilon_k > 0}$$

$$r_j^{(M)} = \frac{R_j^{(M)}}{1-\sum_{k=1}^{M} c_k}$$

$$\begin{cases} R_j^{(M)} = f_j^{(M)} \prod_{i=1}^{M} (1-\varepsilon_i) \\ \sum_{k=1}^{M} c_k = 1 - \prod_{i=1}^{M} (1-\varepsilon_i) \end{cases}$$

$$\Rightarrow r_j^{(M)} = f_j^{(M)}$$

$$\hat{r}_1^{(M)} \geq \hat{r}_2^{(M)} \geq \cdots$$

$$\hat{r}_j^{(M)} = r^{(M)}_{\sigma_M(j)} = f^{(M)}_{\sigma_M \cdots \sigma_2 \sigma_1(j)}$$

$$0 \leq \hat{r}_{N+1}^{(M)} \leq \frac{N}{N+1} \Rightarrow 1 - \hat{r}_{N+1}^{(M)} \geq \frac{1}{N+1} > 0$$

$$\therefore 1 - \hat{r}_{N+1} \geq \frac{1}{N+1} > 0$$

$$r_j = \lim_{M\to\infty} \hat{r}_j^{(M)} = \frac{R_j}{1-d} > 0$$

$$\therefore \hat{r}_N > 0$$

$$\lim_{M\to\infty} \varepsilon_M = \min\{\hat{r}_N, 1 - r_{N+1}\} > 0 \quad //$$

$$\sum_{k=1}^{M} \varepsilon_k \prod_{i=1}^{k-1} (1-\varepsilon_i) = 1 - \prod_{i=1}^{M} (1-\varepsilon_i)$$

$$(\mathrm{LHS}) = \sum_{k=1}^{M} c_k \to d < 1$$

$$\lim_{M\to\infty} \varepsilon_M > 0 \Rightarrow \prod_{i=1}^{M} (1-\varepsilon_i) \to 0 \quad (M \to \infty)$$

$$d = 1 \qquad \text{contradiction!}$$