Theorem 3.1
(Admissible One-Body Density Matrices for Bosons)

γ : self-adjoint, positive semidefinite op. on $L^2(\mathbb{R}^3;\mathbb{C}^q)$

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

$\Longrightarrow \exists \Gamma$: bosonic N-particle density matrix on $L^2(\mathbb{R}^{3N};\mathbb{C}^{q^N})$

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

Moreover, $N \geq 2 \Longrightarrow \exists \psi$: pure state
s.t. $\Gamma = \Gamma_\psi$

Proof.

$N=1$. $\qquad \mathrm{Tr}\,\gamma = N = 1 \qquad \therefore\ \Gamma = \gamma.$

$N \geq 2$. $\qquad \gamma f_j = \lambda_j f_j, \quad j = 1, 2, \ldots$

$$(f_j, f_k) = \delta_{jk}$$

$$\psi(\underline{z}) := N^{-1/2} \sum_{j=1}^{\infty} \lambda_j^{1/2} \prod_{i=1}^{N} f_j(z_i) \leftarrow \text{bosonic}$$

$$(\psi,\psi) = N^{-1} \int \sum_{j=1}^{\infty} \lambda_j^{1/2} \prod_{i=1}^{N} \overline{f_j(z_i)} \cdot \sum_{j'=1}^{\infty} \lambda_{j'}^{1/2} \prod_{i=1}^{N} f_{j'}(z_i)\, d\underline{z}$$

$$= N^{-1} \int \lim_{M,M'\to\infty} \sum_{j=1}^{M} \sum_{j'=1}^{M'} \lambda_j^{1/2} \lambda_{j'}^{1/2} \prod_{i=1}^{N} \overline{f_j(z_i)} f_{j'}(z_i)\, d\underline{z}$$

$$\int \sum_{j=1}^{M} \sum_{j'=1}^{M'} \lambda_j^{1/2} \lambda_{j'}^{1/2} \prod_{i=1}^{N} | f_j(z_i) f_{j'}(z_i) | \, d\underline{z}$$

$$= \sum_j \sum_{j'} \lambda_j^{1/2} \lambda_{j'}^{1/2} \int \prod_{i=1}^{N} | f_j(z_i) f_{j'}(z_i) | \, d\underline{z}$$

$$= \sum_j \sum_{j'} \lambda_j^{1/2} \lambda_{j'}^{1/2} \prod_{i=1}^{N} \int | f_j(z_i) f_{j'}(z_i) | \, dz_i$$

$f_j, f_{j'} \in L^2(\mathbb{R}^3; \mathbb{C}^q)$

$$\Rightarrow \int | f_j(z_i) f_{j'}(z_i) | \, dz_i$$

$$\leq \frac{1}{2} \int \left(|f_j(z_i)|^2 + |f_{j'}(z_i)|^2 \right) dz_i$$

$$= \frac{1}{2} \left(\|f_j\|^2 + \|f_{j'}\|^2 \right) < \infty$$

$\therefore (\Psi, \Psi)$

$$= N^{-1} \lim_{M, M' \to \infty} \sum_{j=1}^{M} \sum_{j'=1}^{M'} \lambda_j^{1/2} \lambda_{j'}^{1/2} \prod_{i=1}^{N} \underbrace{\int \overline{f_j(z_i)} \, f_{j'}(z_i) \, dz_i}_{= (f_j, f_{j'})}$$

$$= N^{-1} \lim \sum_{\substack{j \\ (j'=j)}} \lambda_j = N^{-1} \cdot \operatorname{Tr} \gamma = 1.$$

$\therefore \Psi$ is normalised!

$$\Gamma_\psi(\underline{z};\underline{z}') = \psi(\underline{z})\overline{\psi(\underline{z}')} \qquad \because \text{pure state}$$

$$N\cdot \mathrm{Tr}^{(N-1)}\Gamma_\psi\,\phi(z)$$

$$= N\int\left(\int \Gamma_\psi(z, \underline{z}^{(N-1)}; z', \underline{z}^{(N-1)})\, d\underline{z}^{(N-1)}\right)\phi(z')\,dz'$$

$$= \iint \sum_{j=1}^{\infty}\lambda_j^{1/2} f_j(z)\prod_{i=2}^{N} f_j(z_i)\cdot \sum_{j'=1}^{\infty}\lambda_{j'}^{1/2}\overline{f_{j'}(z')}\prod_{i=2}^{N}\overline{f_j(z_i)}\,d\underline{z}^{(N-1)}\cdot\phi(z')\,dz'$$

$$= \iint \lim_{M,M'\to\infty}\sum_{j=1}^{M}\sum_{j'=1}^{M'}\lambda_j^{1/2}\lambda_{j'}^{1/2} f_j(z)\overline{f_{j'}(z')}\prod_{i=2}^{N} f_j(z_i)\overline{f_{j'}(z_i)}\,d\underline{z}^{(N-1)}\cdot\phi(z')\,dz'$$

$$\left(\lim_{M\to\infty}\lim_{M'\to\infty}\right)\sum_{j=1}^{M}\sum_{j'=1}^{M'}\lambda_j^{1/2}\lambda_{j'}^{1/2} f_j(z)\overline{f_{j'}(z')}\prod_{i=2}^{N} f_j(z_i)\overline{f_{j'}(z_i)}$$

$$\in L^2(\mathbb{R}^{3(N-1)}; \mathbb{C}^{q^{N-1}})$$

$$\text{a.e. } z, z' \in (\mathbb{R}^3;\sigma)$$

$$\therefore N\cdot \mathrm{Tr}^{(N-1)}\Gamma_\psi\,\phi(z)$$

$$= \int \lim_{M,M'\to\infty}\sum_{j=1}^{M}\sum_{j'=1}^{M'}\lambda_j^{1/2}\lambda_{j'}^{1/2} f_j(z)\overline{f_{j'}(z')}\prod_{i=2}^{N}\underbrace{\int f_j(z_i)\overline{f_{j'}(z_i)}\,dz_i}_{=(f_j, f_{j'})}\cdot\phi(z')\,dz'$$

$$= \int \underbrace{\lim \sum_{j\,(j'=j)}\lambda_j f_j(z)\overline{f_j(z')}}_{=\gamma(z,z')}\cdot\phi(z')\,dz' = (\gamma\phi)(z) \quad //$$

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

γ as in Theorem 3.1

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

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

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

Proof.

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

$\gamma u_j = \lambda_j u_j$, $\quad j = 1, 2, \ldots \quad (u_j, u_k) = \delta_{jk}$

$\lambda_1 \geq \lambda_2 \geq \cdots$ decreasing order

$\gamma \leq \mathbb{1} \Longrightarrow \lambda_j \leq 1$

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

$= (u_j, \gamma u_j) \leq (u_j, u_j) = 1$ //

$\therefore$ $0 \leq \lambda_j \leq 1$ and $\sum_{j=1}^{\infty} \lambda_j = \mathrm{Tr}\,\gamma = N$

$(\lambda_{N+1} = 0$ or $\lambda_{N+1} > 0)$

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

$$\lambda_1 = \cdots = \lambda_N = 1$$

$\Longrightarrow$ Slater det.

$$\psi(\underline{z}) = (N!)^{-1/2} \det\{u_i(z_j)\}_{i,j=1}^{N}$$
$$= (N!)^{-1/2} \sum_{\pi \in S_N} \varepsilon_\pi \prod_{i=1}^{N} u_i(z_{\pi(i)})$$

$\longrightarrow$ fermionic

$N \cdot \mathrm{Tr}^{(N-1)} \Gamma \phi(z)$

$$= N \int \left(\int \psi(z, \underline{z}^{(N-1)}) \overline{\psi(z', \underline{z}^{(N-1)})} \, d\underline{z}^{(N-1)} \right) \phi(z') \, dz'$$

$$= ((N-1)!)^{-1} \iint \sum_{\pi \in S_N} \varepsilon_\pi \prod_{i=1}^{N} u_i(z_{\pi(i)}) \cdot \sum_{\pi' \in S_N} \varepsilon_{\pi'} \prod_{i=1}^{N} \overline{u_i(z_{\pi'(i)})} \, d\underline{z}^{(N-1)} \cdot \phi(z') \, dz'$$

$$= \frac{1}{(N-1)!} \iint \sum_{\pi} \sum_{\pi'} \varepsilon_\pi \varepsilon_{\pi'} u_{\pi(1)}(z) \overline{u_{\pi'(1)}(\overline{z})} \prod_{i=2}^{N} u_{\pi(i)}(z_i) \overline{u_{\pi'(i)}(z_i)} \, d\underline{z}^{(N-1)} \cdot \phi(z') \, dz'$$

$$= \frac{1}{(N-1)!} \int \sum_{\pi} \sum_{\pi'} \varepsilon_\pi \varepsilon_{\pi'} u_{\pi(1)}(z) u_{\pi'(1)}(\overline{z}) \times \prod_{i=2}^{N} \underbrace{\int u_{\pi(i)}(z_i) \overline{u_{\pi'(i)}(z_i)} \, dz_i}_{= (u_{\pi(i)},\, u_{\pi'(i)})} \cdot \phi(z') \, dz'$$

$$\begin{cases} \pi(i) = \pi'(i) & \forall i = 2, \dots, N \\ \pi(1) = \pi'(1) & \end{cases}$$
$$\Longrightarrow \pi = \pi'$$

$$N \cdot \mathrm{Tr}^{(N-1)} \Gamma \phi(z)$$

$$= \frac{1}{(N-1)!} \int \sum_{\substack{\pi \\ (\pi'=\pi)}} (\varepsilon_\pi)^2 u_{\pi(1)}(z) \overline{u_{\pi(1)}(z')} \cdot \phi(z')\, dz'$$

$$= \frac{1}{\cancel{(N-1)!}} \int \cancel{(N-1)!} \sum_{j=1}^{N} u_j(z) \overline{u_j(z')} \cdot \phi(z')\, dz'$$

$$= \int \underbrace{\sum_{j=1} u_j(z) \overline{u_j(z')}}_{\gamma(z, z')} \cdot \phi(z')\, dz' = (\gamma \phi)(z) \quad //$$

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

$$N = \mathrm{Tr}\gamma = \sum_{j=1}^{\infty} \lambda_j \geq \sum_{j=1}^{N+1} \lambda_j \geq (N+1) \lambda_{N+1}$$

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

$$\begin{cases} \chi_{[1,N]}(j) = \begin{cases} 1 & (1 \leq j \leq N) \\ 0 & (j > N) \end{cases} \\ \varepsilon = \min\{\lambda_N, 1 - \lambda_{N+1}\} \end{cases}$$

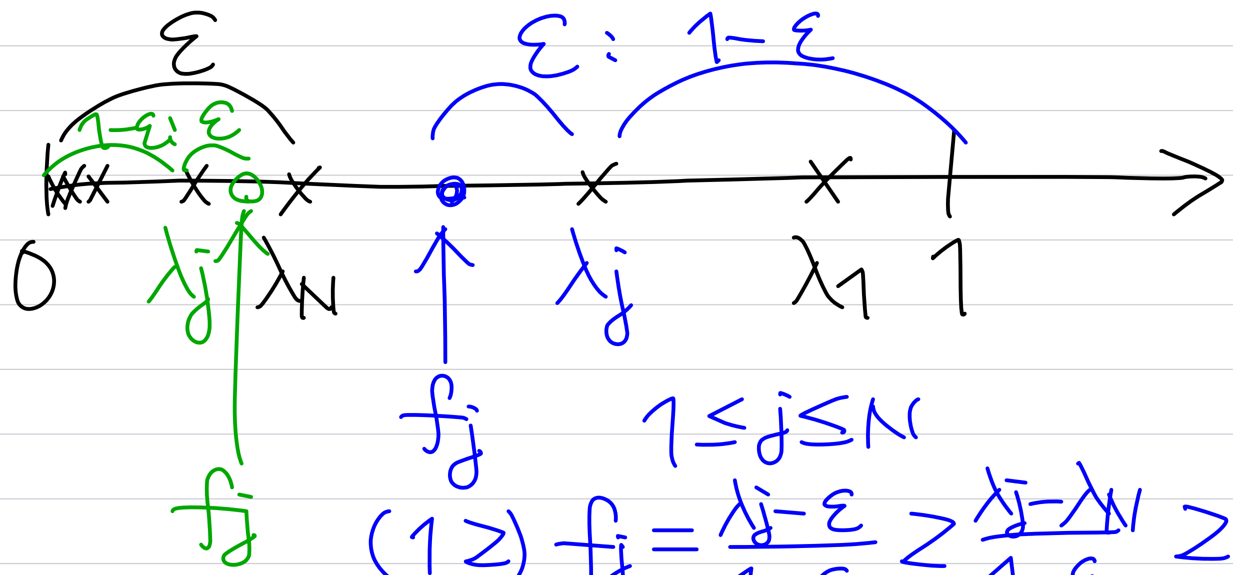
$$\lambda_j = \varepsilon \chi_{[1,N]}(j) + \lambda_j - \varepsilon \chi_{[1,N]}(j)$$

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

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

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

$$\Longrightarrow \quad 0 \le f_j \le 1 \quad \text{and} \quad \sum_{j=1}^{\infty} f_j = N$$



$1 \le j \le N$

$$(1 \ge)\ f_j = \frac{\lambda_j - \varepsilon}{1-\varepsilon} \ge \frac{\lambda_j - \lambda_N}{1-\varepsilon} \ge 0$$

$j > N$

$$(0 \le)\ f_j = \frac{\lambda_j}{1-\varepsilon} \le \frac{\lambda_j}{1-(1-\lambda_{N+1})} = \frac{\lambda_j}{\lambda_{N+1}} \le 1$$

$$\because \quad \sum_{j=1}^{\infty} f_j = \sum_{j=1}^{\infty} \frac{\lambda_j - \varepsilon \chi_{[1,N]}(j)}{1-\varepsilon}$$

$$= \frac{1}{1-\varepsilon}\Bigg(\underbrace{\sum_{j=1}^{\infty} \lambda_j}_{= N} - \underbrace{\sum_{j=1}^{N} \varepsilon}_{= N\varepsilon} \Bigg) = \frac{N - N\varepsilon}{1-\varepsilon} = N$$

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

$$= \varepsilon_1 \chi_1(j) + (1-\varepsilon_1)\left\{\varepsilon_2 \chi_2(j) + (1-\varepsilon_2) f_j'\right\}$$

$$= \varepsilon_1 \chi_1(j) + \varepsilon_2(1-\varepsilon_1)\chi_2(j) + (1-\varepsilon_1)(1-\varepsilon_2) f_j'$$

$$\vdots$$

$$= \sum_{k=1}^{M} \underbrace{\boxed{\varepsilon_k \prod_{j=1}^{k-1}(1-\varepsilon_j)}}_{= C_k} \chi_k(j) + R_j^M$$

after M-iteration

Here, we have

$$\sum_{k=1}^{M} \varepsilon_k \prod_{j=1}^{k-1}(1-\varepsilon_j) = 1 - \prod_{j=1}^{M}(1-\varepsilon_j)$$

for $0 \leq {}^\forall \varepsilon_j \leq 1,\ M \in \mathbb{N} \cup \{\infty\}$

$$\because)\ \sum_{k=1}^{M}(\alpha_{k-1} - \alpha_k) = \alpha_0 - \alpha_1 + \alpha_1 - \alpha_2 + \cdots + \alpha_{M-1} - \alpha_M$$

$$= \alpha_0 - \alpha_M \quad \text{(telescopic sum)}$$

$$\alpha_0 = 1, \quad \alpha_k = \prod_{j=1}^{k}(1-\varepsilon_j) \quad \text{for } k = 1, 2, \ldots$$

$$\alpha_{k-1} - \alpha_k = \prod_{j=1}^{k-1}(1-\varepsilon_j) - \prod_{j=1}^{k}(1-\varepsilon_j)$$

$$= \prod_{j=1}^{k-1}(1-\varepsilon_j) \cdot \{1 - (1-\varepsilon_k)\} = \varepsilon_k \prod_{j=1}^{k-1}(1-\varepsilon_j) \quad //$$

$$\therefore \sum_{k=1}^{M} C_k = \sum_{k=1}^{M} \varepsilon_k \prod_{j=1}^{k-1} (1-\varepsilon_j) = 1 - \prod_{j=1}^{M} (1-\varepsilon_j)$$
$$\leq 1$$

$$\sum_{k=1}^{\infty} C_k = 1 \quad \text{or} \quad \sum_{k=1}^{\infty} C_k < 1$$

When $\sum_{k=1}^{\infty} C_k = 1$.

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

$$\underbrace{\sum_{j=1}^{\infty} \lambda_j}_{= N} = \sum_{j=1}^{\infty} \sum_{k=1}^{M} C_k X_k(j) + \sum_{j=1}^{\infty} R_j^M$$

$$\sum_{k=1}^{M} C_k \underbrace{\sum_{j=1}^{\infty} X_k(j)}_{= N}$$

$$\therefore \sum_{j=1}^{\infty} R_j^M = 0$$

$$\therefore \lambda_j = \sum_{k=1}^{\infty} C_k X_k(j)$$

Rank $N \Longrightarrow$ Slater det.

to be continued...