Yuya Dan 11 March 2017

The N-Representability Problem for Reduced Density Operators

$$H = -\frac{1}{2}\sum_{j=1}^{N} \Delta_{x_j} + V(\underline{x})$$

$$\underline{x} = (x_1, \dots, x_N) \in \mathbb{R}^{3N}$$

$$\psi \in \mathcal{H} := L^2(\mathbb{R}^{3N})$$

$$\|\psi\|^2 = \int_{\mathbb{R}^{3N}} |\psi(x_1, \dots, x_N)|^2 \underbrace{dx_1 \cdots dx_N}_{d\underline{x}} = 1$$

Statistics $\pi \in S_N$, $\pi : \{1, \dots, N\} \to \{1, \dots, N\}$

Boson $\psi(x_{\pi(1)}, \dots, x_{\pi(N)}) = \begin{cases} \psi(x_1, \dots, x_N) \\ (-1)^{|\pi|}\psi(x_1, \dots, x_N) \end{cases}$

Fermion ~~ψ~~

Density Matrices

$\Gamma : \mathcal{H}^N \to \mathcal{H}^N$

- self-adjoint $(\phi', \Gamma\phi) = (\Gamma\phi', \phi)$ $\forall \phi, \phi' \in \mathcal{H}^N$
- positive semidefinite $(\phi, \Gamma\phi) \geq 0$ $\forall \phi \in \mathcal{H}^N$
- trace class $\mathrm{Tr}\,\Gamma = 1$

$$\Gamma\psi_j = \lambda_j \psi_j$$

$$\Gamma = \sum_{j=1}^{\infty} \lambda_j \Gamma_{\psi_j}, \quad \Gamma_\psi = (\psi, \cdot)\psi$$

$$(\Gamma\phi)(\underline{x}) = \int_{\mathbb{R}^{3N}} \Gamma(\underline{x},\underline{x}')\,\phi(\underline{x}')\,d\underline{x}'$$

$$\begin{cases} \Gamma_\psi \ : \ \Gamma_\psi(\underline{x},\underline{x}') = \psi(\underline{x})\,\overline{\psi(\underline{x}')} \\ \Gamma \ : \ \Gamma(\underline{x},\underline{x}') = \sum_{j=1}^{\infty} \lambda_j \psi_j(\underline{x})\,\overline{\psi_j(\underline{x}')} \end{cases}$$

$$\mathcal{E}(\psi) := (\psi, H\psi)$$

$$\mathcal{E}(\Gamma) := \operatorname{Tr} H\Gamma = \sum_{j=1}^{\infty} \lambda_j\, \mathcal{E}(\psi_j)$$

Reduced Density Matrices (RDM)

$$\gamma^{(k)} : \mathcal{H}^k \to \mathcal{H}^k$$

$$\gamma^{(k)}(\underline{x}^{(k)}; \underline{x}'^{(k)}) = \frac{N!}{(N-k)!}\int \Gamma(\underline{x}^{(k)}, \underline{x}^{(N-k)}; \underline{x}'^{(k)}, \underline{x}^{(N-k)})\ d\underline{x}^{(N-k)}$$

$$\gamma^{(k)} = \frac{N!}{(N-k)!} \operatorname{Tr}^{(N-k)} \Gamma$$

N-representability problem

$$\begin{tikzcd}
\Gamma \arrow[rr, "\text{reduced}"'] & & \gamma^{(k)} \\
 & & \begin{cases} (\phi', \gamma\phi) = (\gamma\phi', \phi) \\ (\phi, \gamma\phi) \geq 0 \\ \operatorname{Tr}\gamma = \frac{N!}{(N-k)!} \end{cases} \arrow[llu, bend left, "\text{reprentable}"]
\end{tikzcd}$$

Theorem (Coleman, 1963)

$\gamma : \mathcal{H} \to \mathcal{H}$, RDM

$\boxed{\gamma \leq \mathbb{1}} \iff \gamma$ is admissible

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

- ☐ Kuhn (1960)
- ☐ Watanabe (1939)

$k \geq 2$ ... open

Application

$$H = \sum_j h_j + \sum_{j,k} w_{jk}$$

$$h_j = -\Delta_j + V(x)$$

$$\mathcal{E}(\Gamma) = \mathrm{Tr}\, H \Gamma = \mathrm{Tr}\, h \gamma^{(1)} + \frac{1}{2} \mathrm{Tr}\, W \gamma^{(2)}$$

- ☐ Frank, Lieb, Seiringer, and Siedentop (2007)
  $\gamma = \gamma^{(1)} \longrightarrow \gamma^{1/2}$ (Müller)
- ☐ Frank, et. al. (2016)
  ionization conjecture $\gamma^{1/2}$
- ☐ Kehle (2017)
  $\gamma^{p} \left(\frac{1}{2} \leq p \leq 1 \right)$

Lemma

$$\boxed{\begin{array}{l} 0 \le \varepsilon_j \le 1, \qquad M \in \mathbb{N} \cup \{\infty\} \\ \displaystyle\sum_{k=1}^{M} \varepsilon_k \prod_{j=1}^{k-1} (1-\varepsilon_j) = 1 - \prod_{j=1}^{M} (1-\varepsilon_j) \end{array}}$$

Proof.

$$\sum_{k=1}^{M} (\alpha_{k-1} - \alpha_k) = \alpha_0 - \alpha_M$$

$$\alpha_k = \begin{cases} \displaystyle\prod_{j=1}^{k} (1-\varepsilon_j) & k = 1, \dots, M \\ 0 & k = 0 \end{cases}$$

$$\begin{aligned} \alpha_{k-1} - \alpha_k &= \prod_{j=1}^{k-1} (1-\varepsilon_j) - \prod_{j=1}^{k} (1-\varepsilon_j) \\ &= \underbrace{\{1 - (1-\varepsilon_k)\}}_{\overset{\shortparallel}{\varepsilon_k}} \prod_{j=1}^{k-1} (1-\varepsilon_j) \qquad (k \ge 2) \end{aligned}$$

$$\alpha_0 - \alpha_1 = 1 - (1-\varepsilon_1) = \varepsilon_1 \qquad (k=1)$$

$(M = \infty)$

$$\sum_{k=1}^{M} \underbrace{\varepsilon_k \prod_{j=1}^{k-1} (1-\varepsilon_j)}_{\ge 0} \le 1 \qquad //$$

Proof.

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

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

$$0 \leq \lambda_j \leq 1, \quad \sum_{j=1}^{\infty} \lambda_j = N$$

$$\lambda_1 \geq \lambda_2 \geq \dots$$

$$\lambda_{N+1} = 0 \quad \Rightarrow \quad \lambda_1 = \cdots = \lambda_N = 1$$

Slater $\psi(\underline{x}) = \frac{1}{\sqrt{N!}} \det \{ u_i(x_j) \}_{i,j=1}^{N} \quad \in \mathcal{H}^N$

$$\sum_{\pi \in S_N} (-1)^{|\pi|} \prod_{i=1}^{N} u_i(x_{\pi(i)})$$

$$\begin{array}{ccc} \Gamma_\psi : \mathcal{H}^N & \longrightarrow & \mathcal{H}^N \\ \psi & & \psi \\ \phi & \longmapsto & (\psi, \phi)\psi \end{array}$$

$$\Gamma_\psi(\underline{x}, \underline{x}') = \psi(\underline{x}) \overline{\psi(\underline{x}')}$$

$$\left(\mathrm{Tr}^{(N-1)} \Gamma_\psi \right) (x, x')$$

$$= \int \psi(x, \underline{x}^{(N-1)}) \overline{\psi(x', \underline{x}^{(N-1)})} \quad d\underline{x}^{(N-1)}$$

$$= \frac{1}{N!} \int \sum_{\pi} (-1)^{|\pi|} u_1(x_{\pi(1)}) \prod_{i=2}^{N} u_i(x_{\pi(i)}) \cdot \sum_{\pi'} (-1)^{|\pi'|} \overline{u_1(x'_{\pi'(1)})}$$

$$\times \prod_{i=2}^{N} \overline{u_i(x_{\pi'(i)})} \quad d\underline{x}^{(N-1)}$$

$$= \frac{1}{N!}\int \sum_{\pi}(-1)^{|\pi|} u_{\pi^{-1}(1)}(x_1) \prod_{i=2}^{N} u_{\pi^{-1}(i)}(x_i)$$

$$\times \sum_{\pi'}(-1)^{|\pi'|} \overline{u_{\pi'^{-1}(1)}(x_1')} \prod_{i=2}^{N} \overline{u_{\pi'^{-1}(i)}(x_i)} \quad d\underline{x}^{(N-1)}$$

$$= \frac{1}{N!}\sum_{\pi}\sum_{\pi'}(-1)^{|\pi|+|\pi'|} u_{\pi^{-1}(1)}(x)\, \overline{u_{\pi'^{-1}(1)}(x')} \prod_{i=2}^{N} \left(u_{\pi^{-1}(i)}, u_{\pi'^{-1}(i)}\right)$$

$$\pi^{-1}(i) = \pi'^{-1}(i) \quad i = 2, \ldots, N$$

$$\Longrightarrow \pi = \pi'$$

$$= \frac{1}{N!} \underset{(N-1)!}{\sum_{\substack{\pi=\pi' \\ \pi(j)=1}}} \sum_{j=1}^{N} u_{\underbrace{\pi^{-1}(1)}_{\substack{\shortparallel \\ j}}}(x)\, \overline{u_{\underbrace{\pi^{-1}(1)}_{\substack{\shortparallel \\ j}}}(x')}$$

$$= \frac{1}{N}\sum_{j=1}^{N} u_j(x)\overline{u_j(x')}$$

$$\therefore N \cdot \left(\mathrm{Tr}^{(N-1)} \Gamma_{\psi}\right)(x, x') = \gamma(x, x') \quad //$$

$\lambda_{N+1} > 0$

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

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

$\varepsilon = \min\{\lambda_N, 1-\lambda_{N+1}\} \quad \Rightarrow \quad 0 < \varepsilon < 1$

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

$$\chi_{[1,N]}(j) = \begin{cases} 1 & j = 1, \dots, N \\ 0 & \text{otherwise} \end{cases}$$

$\Rightarrow \quad f_j = \frac{\lambda_j - \varepsilon \chi_{[1,N]}(j)}{1-\varepsilon} \qquad (\lambda \overset{T}{\longmapsto} f)$

$0 \leq f_j \leq 1, \quad \sum_{j=1}^{\infty} f_j = N.$

$\because)$ $\underline{j = 1, \dots, N\,\rfloor}$

$$f_j = \frac{\lambda_j - \varepsilon}{1-\varepsilon} \underset{(\varepsilon \leq \lambda_N)}{\geq} \frac{\lambda_j - \lambda_N}{1-\varepsilon} \geq 0$$

$\underline{j \geq N+1\,\rfloor}$

$$f_j = \frac{\lambda_j}{1-\varepsilon} \leq \frac{\lambda_{N+1}}{1-\varepsilon} \leq 1$$

$$\sum_{j=1}^{\infty} f_j = \frac{N - \varepsilon N}{1-\varepsilon} = N \quad //$$

$\tilde{f}_1 \geq \tilde{f}_2 \geq \cdots$

$\tilde{f}_j := f_{\tau(j)}, \quad \tau : \mathbb{N} \to \mathbb{N}$

$$\begin{tikzcd}
\lambda \arrow[r, mapsto, "T_\varepsilon"] \arrow[d, phantom, sloped, "\in"] & f \arrow[r, mapsto, "\tau"] \arrow[d, phantom, sloped, "\in"] & \tilde{f} \arrow[d, phantom, sloped, "\in"] \\
\widetilde{\mathcal{F}} & \mathcal{F} & \widetilde{\mathcal{F}}
\end{tikzcd}$$

$\varepsilon_2 = \min\{\tilde{f}_N, 1-\tilde{f}_{N+1}\} \qquad 0 < \varepsilon_2 < 1$

$\tilde{f}_j = \varepsilon_2 \chi_{[1,N]}(j) + (1-\varepsilon_2) f_j^{(2)}$

$\underline{\varepsilon = 1-\lambda_{N+1}}$ $f_j = \tilde{f}_{\sigma(j)} \qquad \sigma : \mathbb{N} \to \mathbb{N}$

$\underline{\varepsilon = \lambda_N}$

$$f_j = \begin{cases} \tilde{f}_{\sigma(j)} & j \neq N \qquad \sigma : \mathbb{N}\setminus\{N\} \to \mathbb{N} \\ 0 & j = N \end{cases}$$

$$\lambda_j = \varepsilon \underbrace{\chi_{[1,N]}(j)}_{\chi_1(j)} + (1-\varepsilon) \underbrace{\tilde{f}_{\sigma(j)}}_{\varepsilon_2 \underbrace{\chi_{[1,N]}(\sigma(j))}_{\chi_2(j)} + (1-\varepsilon_2) f^{(2)}_{\sigma(j)}}$$

$$= \sum_{k=1}^{2} \varepsilon_k \prod_{i=1}^{k-1} (1-\varepsilon_i) \cdot \chi_k(j) + f^{(2)}_{\sigma(j)} \prod_{i=1}^{2} (1-\varepsilon_i)$$

$(\lambda_N = \varepsilon \cdot 1 \quad \text{if } \varepsilon = \lambda_N)$

$$\begin{tikzcd} f^{(2)} \arrow[r, mapsto, "\tau_2"] \arrow[d, phantom, "\rotatebox{90}{$\in$}"] & \tilde{f}^{(2)} \arrow[d, phantom, "\rotatebox{90}{$\in$}"] \\ \mathcal{F} & \mathcal{F} \end{tikzcd}$$

$$\tilde{f}^{(2)}_j := f^{(2)}_{\tau_2(j)}, \quad \tau_2 : \mathbb{N} \to \mathbb{N}$$

$$\varepsilon_3 = \min\{\tilde{f}^{(2)}_N, 1-\tilde{f}^{(2)}_{N+1}\} \qquad 0<\varepsilon_3<1$$

$$\tilde{f}^{(2)}_j = \varepsilon_3 \chi_{[1,N]}(j) + (1-\varepsilon_3) f^{(3)}_j$$

$$T_{\varepsilon_3} : \tilde{f}^{(2)} \longmapsto f^{(3)}$$

$$\left(\varepsilon_2 = \tilde{f}^{(1)}_N \right)$$

$$f^{(2)}_j = \begin{cases} \tilde{f}^{(2)}_{\sigma_2(j)} & j \neq N \\ 0 & j = N \end{cases}$$

$$\lambda_j = \sum_{k=1}^{2} \varepsilon_k \prod_{i=1}^{k-1}(1-\varepsilon_i)\cdot\chi_k(j) + \underbrace{\tilde{f}^{(2)}_{\sigma_1\sigma_2(j)}}_{} \prod_{i=1}^{2}(1-\varepsilon_i)$$

$$\varepsilon_3 \underbrace{\chi_{[1,N]}(\sigma_2(j))}_{\chi_3(j)} + (1-\varepsilon_3) f^{(3)}_{\sigma_1\sigma_2(j)}$$

$$= \sum_{k=1}^{3} \varepsilon_k \prod_{i=1}^{k-1}(1-\varepsilon_i)\cdot\chi_k(j) + f^{(3)}_{\sigma_1\sigma_2(j)} \prod_{i=1}^{3}(1-\varepsilon_i)$$

$$\lambda_j = \sum_{k=1}^{m} \underbrace{\varepsilon_k \prod_{i=1}^{k-1} (1-\varepsilon_i)}_{\substack{\shortparallel \\ c_k}} \cdot x_k(j) + \underbrace{\overbrace{f^{(m)}\sigma_1\cdots\sigma_{m-1}(j)}^{r_j^{(m)}} \prod_{i=1}^{m} (1-\varepsilon_i)}_{\substack{\shortparallel \\ R_j^{(m)}}}$$

Lemma $\Rightarrow \sum_{k=1}^{\infty} c_k =: d \leq 1.$

$$\boxed{\exists R = \{R_j\} \ \text{s.t.} \ \lim_{M\to\infty} \sum_{j=1}^{\infty} \left| R_j^{(M)} - R_j \right| = 0}$$

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

$$R_j^{(M)} - R_j^{(M+1)} = c_{M+1} x_{M+1}(j) \geq 0$$

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

$$\exists R_j \geq 0 \ \text{s.t.} \ R_j^{(M)} \xrightarrow[(M\to\infty)]{} R_j \geq 0$$

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

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

$$= \sum_{k=M+1}^{\infty} c_k x_k(j) \quad (\geq 0)$$

$$\therefore \ \sum_{j=1}^{\infty} \left| R_j^{(M)} - R_j \right|$$

$$= \cancel{\lim} \ \sum_{j} \sum_{k=M+1} c_k x_k(j)$$

$$\sum_{k} \sum_{j} c_k x_k(j) = \sum_{k} c_k \underbrace{\sum_{j} x_k(j)}_{\overset{\shortparallel}{N}}$$

$$= dN < \infty$$

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

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

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

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

$$\sum_{j=1}^{\infty} R_j^{(M)} = \underbrace{\sum_{j=1}^{\infty} \lambda_j}_{\overset{\shortparallel}{N}} - \underbrace{\sum_{j=1}^{\infty}\sum_{k=1}^{M} c_k x_k(j)}_{\overset{\shortparallel}{N \sum_{k=1}^{M} c_k}}$$

$$\therefore\ \sum_{j=1}^{\infty} R_j = \lim_{M\to\infty} \sum_{j=1}^{\infty} R_j^{(M)} \qquad \left(\because R_j^{(M)} \xrightarrow[\text{strong}]{} R_j\right)$$

$$= \lim_{M\to\infty}\left(N - N\sum_{k=1}^{M} c_k\right)$$

$$= N(1-d) \ //$$

Cor. $d = 1 \Rightarrow \lambda_j = \sum_{k=1}^{\infty} c_k x_k(j)$

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

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

$$= 1 - (1 - r_j^{(M)}) \prod_{i=1}^{M}(1-\varepsilon_i) \quad \leq 1 \ //$$

Cor. $R_j = \lim_{M\to\infty} R_j^{(M)} \leq 1 - d \ //$

$$\boxed{d < 1 \Rightarrow \lim_{M \to \infty} \varepsilon_M > 0}$$

$\because$) $R_j^{(M)} \longrightarrow \exists R_j$

$$r_j := \frac{R_j}{1-d} \in \mathcal{F}$$

$$\tau \downarrow$$

$$\widetilde{r_j} \in \widetilde{\mathcal{F}}$$

$$r_j^{(M)}$$

$$\tau \downarrow$$

$$\widetilde{r}_j^{(M)} := r^{(M)}_{\tau(j)} \notin \widetilde{\mathcal{F}}_N \text{ in general}$$

$$\downarrow (M \to \infty)$$

$$\widetilde{r_j}$$

$$\forall M \geq M_0 \quad \widetilde{r}_j^{(M)} \geq \frac{\widetilde{r_j}}{2}$$

$$\therefore \quad \widetilde{r}_N^{(M)} \geq \frac{\widetilde{r_N}}{2} > 0$$

$$\varepsilon_M = \min\left\{\widetilde{r}_N^{(M)}, 1 - \widetilde{r}_{N+1}^{(M)}\right\}$$

$$\geq \min\left\{\frac{\widetilde{r_N}}{2}, \frac{1}{N+1}\right\}$$

$$\lim_{M \to \infty} \varepsilon_M \geq \min\left\{\frac{\widetilde{r_N}}{2}, \frac{1}{N+1}\right\} > 0 \quad //$$

Cor. contradiction!

$d = 1.$

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

$$\gamma = \sum_{j=1}^{\infty} \lambda_j \gamma_{u_j} \qquad \gamma_{u_j} = (u_j, \cdot\,) u_j$$

$$= \sum_j \Big(\sum_k c_k x_k(j) \Big) \gamma_{u_j}$$

$$= \sum_k c_k \underbrace{\sum_j x_k(j) \gamma_{u_j}}_{\gamma_k}$$

$\psi_k \leftarrow \{u_j\}$ rank N

Slater

$$\gamma = \sum_k c_k \overset{\text{proj.}}{\gamma_k}$$

$$\downarrow$$

$$\sum_k c_k \Gamma_{\psi_k} =: \Gamma$$

$$\therefore \quad \gamma = N \cdot \mathrm{Tr}^{(N-1)} \Gamma$$

Q.E.D

Example

$$\lambda = \left\{1, \underline{\frac{1}{2}}, \underline{\frac{1}{3}}, \frac{1}{6}, 0, \dots \right\} \qquad N = 2$$

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

$$f^{(1)} = \left\{1, 0, \frac{2}{3}, \frac{1}{3}, 0, \dots \right\}$$

$$\tau_1 \quad \tilde{f}^{(1)} = \left\{1, \frac{2}{3}, \frac{1}{3}, 0, 0, \dots \right\} \qquad \tau_1 = \begin{pmatrix} 1 & 2 & 3 & (4) & \cdots \\ 1 & 3 & 4 & (5) & \cdots \end{pmatrix}$$

$$\varepsilon_2 = \frac{2}{3}$$

$$f^{(2)} = \{1, 1, 0, 0, 0, \dots\} \qquad //$$

$$\lambda = \left\{\underbrace{1, \dots, 1}_{N-1}, \frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \dots \right\}$$