§3.1.5 Reduced Density Matrices (p. 41~)

Γ : <u>physical</u> N-particle density matrix
(only bosons or only fermions)

$\Gamma(\underline{z}, \underline{z}')$: its kernel

kernel of the k-particle <u>reduced</u> density matrix
$(1 \leq k < N)$

$$\gamma^{(k)}(z_1, \dots, z_k ; z_1', \dots, z_k')$$

$$:= \frac{N!}{(N-k)!} \int \Gamma(\underbrace{z_1, \dots, z_k}_{\underline{z}^{(k)}}, \underbrace{z_{k+1}, \dots, z_N}_{\underline{z}^{(N-k)}} ; z_1', \dots, z_k', z_{k+1}, \dots, z_N) \underbrace{dz_{k+1} \cdots dz_N}_{d\underline{z}^{(N-1)}}$$

Remarks

(1) We can give

$$\Gamma(z, z') = \sum_{j=1}^{\infty} \lambda_j \psi_j(\underline{z}) \overline{\psi_j(\underline{z}')} \quad \text{with } \Gamma\psi_j = \lambda_j \psi_j$$

$$\because) \ |\Gamma(z, z')| \leq \sum_j \lambda_j |\psi_j(\underline{z}) \overline{\psi_j(\underline{z}')}|$$

$$\leq \frac{1}{2} \sum_j \lambda_j \left(|\psi_j(\underline{z})|^2 + |\psi_j(\underline{z}')|^2 \right)$$

$$\int |\psi_j(\underline{z})|^2 d\underline{z}^{(N-k)} = \Psi(\underline{z}^{(k)}) \text{ a.e. in } L^2(\mathbb{R}^k)$$

$$\int |\psi_j(\underline{z}^{(k)\prime}, \underline{z}^{(N-k)})|^2 d\underline{z}^{(N-k)} = \Phi(\underline{z}^{(k)}) \text{ a.e. in } L^2(\mathbb{R}^k)$$

(2) $\operatorname{Tr}\gamma^{(k)} = \int \gamma^{k}(\underline{z}^{(k)}, \underline{z}^{(k)})\, d\underline{z}^{(k)}$

$$= \frac{N!}{(N-k)!} \iint \Gamma(\underline{z}^{(k)}, \underline{z}^{(N-k)}; \underline{z}^{(k)}, \underline{z}^{(N-k)})\, d\underline{z}^{(N-k)} d\underline{z}^{(k)}$$

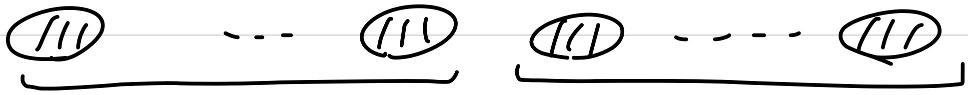
$$= \frac{N!}{(N-k)!} \int \Gamma(\underline{z}, \underline{z})\, d\underline{z}$$

$$= \frac{N!}{(N-k)!} \neq 1.$$

(3) • different nuclei

$\cdots \quad \rightarrow C_{N,k} = 1$

• $N \in 2\mathbb{Z}$



$N/2 \longleftrightarrow N/2$
different species of particles

$$\tau : \{1, \dots, N\} \hookrightarrow \{\tau_1, \dots, \tau_k\}$$

$$C_{N,k} = \sum_{\tau} \sum_{k_1 + k_2 = k} k_1!\, k_2! \binom{N}{k} \qquad \text{etc.}$$

Example (Slater determinant)

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

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

$$(u_i, u_j) = \delta_{ij}$$

$$\Longrightarrow \Gamma_\psi(z, z') = \psi(z) \overline{\psi(z')}$$

$$\gamma^{(k)}(z_1, \dots, z_k; z_1', \dots, z_k')$$

$$= k! \sum_{\tau} \frac{1}{\sqrt{k!}} \det\{ u_{\tau_i}(z_j) \}_{i,j=1}^{k} \cdot \frac{1}{\sqrt{k}} \det\{ \overline{u_{\tau_i}(z_j)} \}_{i,j=1}^{k}$$

$$\tau : \{1, \dots, N\} \mapsto \{\tau_1, \dots, \tau_k\}$$

$\binom{N}{k} = \frac{N!}{k!(N-k)!}$ possible combination

In particular,

$$\gamma^{(1)}(z, z') = \sum_{i=1}^{N} u_i(z) \overline{u_i(z')}$$

$$\gamma^{(2)}(z_1,z_2;z_1,z_2)=\gamma^{(1)}(z_1,z_1)\gamma^{(1)}(z_2,z_2)-|\gamma^{1}(z_1,z_2)|^2$$

Proof.

$$\gamma^{(2)}(z_1,z_2;z_1',z_2')$$

$$=\sum_{\tau}\det\{u_{\tau_i}(z_j)\}_{i,j=1}^{2}\det\{\overline{u_{\tau_i}(z_j')}\}_{i,j=1}^{2}$$

$$=\sum_{\tau}\begin{vmatrix} u_{\tau_1}(z_1) & u_{\tau_1}(z_2)\\ u_{\tau_2}(z_1) & u_{\tau_2}(z_2)\end{vmatrix}\cdot\begin{vmatrix} \overline{u_{\tau_1}(z_1')} & \overline{u_{\tau_1}(z_2')}\\ \overline{u_{\tau_2}(z_1')} & \overline{u_{\tau_2}(z_2')}\end{vmatrix}$$

$$=\sum_{\tau}\Big(u_{\tau_1}(z_1)u_{\tau_2}(z_2)-u_{\tau_2}(z_1)u_{\tau_1}(z_2)\Big)$$
$$\times\Big(\overline{u_{\tau_1}(z_1')}\,\overline{u_{\tau_2}(z_2')}-\overline{u_{\tau_2}(z_1')}\,\overline{u_{\tau_1}(z_2')}\Big)$$

$$=\sum_{\tau}\Big(u_{\tau_1}(z_1)\overline{u_{\tau_1}(z_1')}\,u_{\tau_2}(z_2)\overline{u_{\tau_2}(z_2')}$$
$$+u_{\tau_2}(z_1)\overline{u_{\tau_2}(z_1')}\,u_{\tau_1}(z_2)\overline{u_{\tau_1}(z_2')}$$
$$-u_{\tau_1}(z_1)\overline{u_{\tau_2}(z_2')}\,u_{\tau_2}(z_2)\overline{u_{\tau_2}(z_2')}$$
$$-u_{\tau_2}(z_1)\overline{u_{\tau_1}(z_2')}\,u_{\tau_1}(z_2)\overline{u_{\tau_2}(z_1')}\Big)+0$$

$$=\frac{1}{2}\sum_{i}\sum_{j}\Big(\cdots\tau_1\to i,\ \tau_2\to j\cdots\Big)\qquad \sum_{\tau_1=\tau_2}$$

$$=\gamma^{(1)}(z_1,z_1')\gamma^{1}(z_2,z_2')-\gamma^{(1)}(z_1,z_2')\gamma^{(1)}(z_2,z_1')$$

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partial trace $\mathrm{Tr}^{(N-k)}$

$\psi \in L^2(\mathbb{R}^{3k}; \mathbb{C}^{2k})$

$(\gamma^{(k)}\psi)(z_1, \dots, z_k)$

$= \int \gamma^{(k)}(z_1, \dots, z_k; z_1', \dots, z_k')\, \psi(z_1', \dots, z_k')\, dz_1' \cdots dz_k'$

$= \frac{N!}{(N-k)!} \iint \Gamma(\underline{z}^{(k)}, \underline{z}^{(N-k)}; \underline{z}^{(k)'}, \underline{z}^{(N-k)})\, \psi(\underline{z}^{(k)'})\, d\underline{z}^{(N-k)}\, d\underline{z}^{(k)}$

$= \frac{N!}{(N-k)!} \left(\mathrm{Tr}^{(N-k)} \Gamma \psi \right)(\underline{z}^{(k)})$

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

Is $\gamma^{(k)}$ a k-particle density matrix?

$$\mathrm{Tr}\,\gamma^{(k)} = \frac{N!}{(N-k)!} \neq 1$$

$\forall \phi \in L^2(\mathbb{R}^{3k}; \mathbb{C}^{qk})$, $\quad z^{(k)} = (z_1, \dots, z_k) \in (X,\sigma)^k$

$$(\phi, \gamma^{(k)} \phi)$$

$$= \int \overline{\phi(\underline{z}^{(k)})} \left(\int \gamma^{(k)}(\underline{z}^{(k)}; \underline{z}^{(k)'}) \phi(\underline{z}^{(k)'}) \, d\underline{z}^{(k)'} \right) d\underline{z}^{(k)}$$

$$= \iint \overline{\phi(\underline{z}^{(k)})} \phi(\underline{z}^{(k)'}) \gamma^{(k)}(\underline{z}^{(k)}; \underline{z}^{(k)'}) \, d\underline{z}^{(k)} d\underline{z}^{(k)'}$$

$$\gamma^{(k)}(\underline{z}^{(k)}; \underline{z}^{(k)'}) = \sum_{j=1}^{\infty} \lambda_j \int \psi_j(\underline{z}^{(k)}; \underline{z}^{(N-k)}) \psi_j(\underline{z}^{(k)'}, \underline{z}^{(N-k)}) \, d\underline{z}^{(N-k)}$$

$$\iint \lim_{M\to\infty} \sum_{j=1}^{M} \lambda_j \overline{\phi(\underline{z}^{(k)})} \psi_j(\underline{z}^{(k)}) \cdot \phi(\underline{z}^{(k)'}) \overline{\psi_j(\underline{z}^{(k)})} \, dz^{(k)} dz^{(k)'}$$

$$\left| \overline{\phi(\underline{z}^{(k)})} \psi_j(\underline{z}^{(k)}) \right| \leq \frac{1}{2}\left(|\phi(\underline{z}^{(k)})|^2 + |\psi_j(\underline{z}^{(k)})|^2 \right)$$

$$\Longrightarrow \int \left| \overline{\phi(\underline{z}^{(k)})} \psi_j(\underline{z}^{(k)}) \right| d\underline{z}^{(k)} \leq \frac{1}{2}\left(\int |\phi(\underline{z}^{(k)})|^2 d\underline{z}^{(k)} + \int |\psi_j(\underline{z}^{(k)})|^2 d\underline{z}^{(k)} \right)$$

$$= \lim_{M\to\infty} \sum_{j=1}^{M} \lambda_j \left| \int \overline{\phi(\underline{z}^{(k)})} \psi_j(\underline{z}^{(k)}) \, d\underline{z}^{(k)} \right|^2$$

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eigenfunction expansion

$$\gamma^{(k)}(\underline{z}^{(k)}, \underline{z}^{(k)\prime}) = \sum_{j=1}^{\infty} \lambda_j^{(k)} f_j(\underline{z}^{(k)}) \overline{f_j(\underline{z}^{(k)\prime})}$$

$$\gamma^{(k)} f_j = \lambda_j^{(k)} f_j$$

$$(f_j, f_k) = \delta_{jk}, \quad \lambda_j^{(k)} \geq 0 \quad (\Leftarrow \gamma^{(k)} \geq 0)$$

$$\sum_{j=1}^{\infty} \lambda_j^{(k)} = \mathrm{Tr}\,\gamma^{(k)} = \frac{N!}{(N-k)!}$$

<u>Def.</u> $\frac{(N-k)!}{N!}\gamma^{(k)}$ is an H^1 density matrix if Γ is one.

one-particle density

$$\rho_\psi = \sum_{i=1}^{N} \rho_\psi^i = \gamma^{(1)}(z, z)$$

$$\rho_\psi^i = \int_{\mathbb{R}^{3(N-1)}} |\psi(x_1, \dots, \underset{\hat{i}}{x_i}, \dots, x_N)|^2 \, dx_1 \cdots \widehat{dx_i} \cdots dx_N.$$

Spin-summed density matrix

$\gamma^{(1)}$ on $L^2(\mathbb{R}^3; \mathbb{C}^q) \cong L^2(\mathbb{R}^3) \otimes \mathbb{C}^q$

$$\mathring{\gamma}^{(1)}(x, x') = \sum_{\sigma=1}^{q} \gamma^{(1)}(x, \sigma; x', \sigma)$$

$$\begin{aligned} \operatorname{Tr} \mathring{\gamma}^{(1)} &:= \int_{\mathbb{R}^3} \mathring{\gamma}(x, x)\, dx \\ &= \sum_{\sigma} \int_{\mathbb{R}^3} \gamma^{(1)}(x, \sigma; x, \sigma)\, dx \\ &= \int \gamma^{(1)}(\underline{z}, \underline{z})\, d\underline{z} = \operatorname{Tr} \gamma^{(1)}. \end{aligned}$$

$\|\gamma\|_\infty$ the largest eigenvalue of γ

$$\|\gamma^{(1)}\|_\infty \leq \|\mathring{\gamma}^{(1)}\|_\infty \leq q \|\gamma^{(1)}\|_\infty$$

Application of $\gamma^{(1)}$ and $\gamma^{(2)}$

$$H = \sum_{i=1}^{N} h_i + \sum_{1 \le i < j \le N} W_{ij}$$

e.g. $h_i = -\Delta_{x_i} + V(x_i)$

on $L^2(\mathbb{R}^3; \mathbb{C}^q)$

$$\mathcal{E}(\psi) = \int \left(\sum_i |\nabla_{x_i} \psi|^2 + \sum_i V(x_i) |\psi|^2 \right) d\underline{x}$$

W_{ij} : Coulomb

on $L^2(\mathbb{R}^3; \mathbb{C}^q) \otimes L^2(\mathbb{R}^3; \mathbb{C}^q)$

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

$$\gamma^{(1)} = \frac{1}{N-1} \mathrm{Tr}^{(1)} \gamma^{(2)}$$

$$\gamma^{(2)} \longrightarrow \gamma^{(1)} \longrightarrow \mathcal{E}(\Gamma) \ ??$$