

Last time we introduced the reduced one-particle density matrix $\gamma_{\Psi_N}: \mathcal{L}^2 \rightarrow \mathcal{L}^2$ via its kernel

$$\gamma_{\Psi_N}(x, y) := \int dx_2 \dots dx_N \overline{\Psi_N(y, x_2, \dots, x_N)} \Psi_N(x, x_2, \dots, x_N).$$

We had also defined the expected number of particles not in the product state Π_φ as

$$\alpha(\Psi_N, \varphi) = \sum_{k=0}^N \frac{k}{N} \langle \Psi_N, P_{Nk}^\varphi \Psi_N \rangle = \langle \Psi_N, q_1^\varphi \Psi_N \rangle.$$

Next, we establish a relation between $\gamma_{\Psi_N} - \overbrace{\gamma_{\Pi_\varphi}^\varphi}^{= P^\varphi}$ and $\alpha(\Psi_N, \varphi)$:

Lemma 4.10: For any symmetric $\Psi_N \in \mathcal{L}^2(\mathbb{R}^{3N})$, $\varphi \in \mathcal{L}^2(\mathbb{R}^3)$ with $\|\Psi_N\| = 1 = \|\varphi\|$, we have

$$(a) \quad \alpha(\Psi_N, \varphi) \leq \|\gamma_{\Psi_N} - P^\varphi\|_{\mathcal{S}} \leq 4\sqrt{\alpha(\Psi_N, \varphi)},$$

$$(b) \quad |\langle \Psi_N, A \Psi_N \rangle - \langle \varphi, A \varphi \rangle| \leq \|A\| \cdot 4\sqrt{\alpha(\Psi_N, \varphi)} \quad \text{for any } A \in \mathcal{S}(\mathcal{L}^2(\mathbb{R}^3)).$$

Proof: (a) Note that $p^\varphi + q^\varphi = \mathbb{1}$ by def., so we can decompose

$$\gamma_{\Psi_N} = (p^\varphi + q^\varphi) \gamma_{\Psi_N} (p^\varphi + q^\varphi)$$

$$= \underbrace{p^\varphi \gamma_{\Psi_N} p^\varphi}_{= p^\varphi \langle \varphi, \gamma_{\Psi_N} \varphi \rangle} + p^\varphi \gamma_{\Psi_N} q^\varphi + q^\varphi \gamma_{\Psi_N} p^\varphi + q^\varphi \gamma_{\Psi_N} q^\varphi$$

$$= p^\varphi \langle \varphi, \gamma_{\Psi_N} \varphi \rangle$$

$$= p^\varphi \langle \Psi_N, p_1^\varphi \Psi_N \rangle = p^\varphi - p^\varphi \langle \Psi_N, q_1^\varphi \Psi_N \rangle$$

$$\begin{aligned}
\Rightarrow \|\chi_{\psi_N} - p^\varphi\|_{\mathcal{D}} &= \left\| -p^\varphi \langle \psi_N, q_1^\varphi \psi_N \rangle + p^\varphi \chi_{\psi_N} q_1^\varphi + q_1^\varphi \chi_{\psi_N} p^\varphi + q_1^\varphi \chi_{\psi_N} q_1^\varphi \right\|_{\mathcal{D}} \\
&\leq \underbrace{\|p^\varphi\|_{\mathcal{D}}}_{\leq 1} \underbrace{\langle \psi_N, q_1^\varphi \psi_N \rangle}_{= \|\psi_N\|_{q_1^\varphi}^2 = \alpha(\psi_N, \varphi)} + \underbrace{\|p^\varphi \chi_{\psi_N} q_1^\varphi\|_{\mathcal{D}}}_{\leq \|p^\varphi\|_{\mathcal{D}} \|\psi_N\|_{q_1^\varphi}} + \underbrace{\|q_1^\varphi \chi_{\psi_N} p^\varphi\|_{\mathcal{D}}}_{\leq 1} + \underbrace{\|q_1^\varphi \chi_{\psi_N} q_1^\varphi\|_{\mathcal{D}}}_{= \sqrt{\alpha(\psi_N, \varphi)}} \\
&\leq 2 \underbrace{\alpha(\psi_N, \varphi)}_{\leq \sqrt{\alpha(\psi_N, \varphi)} \text{ since } 0 \leq \alpha(\psi_N, \varphi) \leq 1} + 2 \sqrt{\alpha(\psi_N, \varphi)} \\
&\leq 4 \sqrt{\alpha(\psi_N, \varphi)}
\end{aligned}$$

Also:

$$\alpha(\psi_N, \varphi) = \|\psi_N\|_{q_1^\varphi}^2 = 1 - \|\psi_N\|_{p_1^\varphi}^2 = 1 - \langle \varphi, \chi_{\psi_N} \varphi \rangle = \langle \varphi, (p^\varphi - \chi_{\psi_N}) \varphi \rangle \leq \|p^\varphi - \chi_{\psi_N}\|_{\mathcal{D}}.$$

(b) Similarly, we find for any $A \in \mathcal{D}(L^2(\mathbb{R}^3))$:

$$\begin{aligned}
&\langle \psi_N, A_1 \psi_N \rangle - \langle \varphi, A \varphi \rangle \\
&= \langle \psi_N, \underbrace{(p_1^\varphi + q_1^\varphi)}_{= 1} A_1 (p_1^\varphi + q_1^\varphi) \psi_N \rangle - \langle \varphi, A \varphi \rangle \\
&= \underbrace{\langle \psi_N, p_1^\varphi A_1 p_1^\varphi \psi_N \rangle - \langle \varphi, A \varphi \rangle}_{= |\varphi\rangle\langle\varphi| A |\varphi\rangle\langle\varphi| = \langle \varphi, A \varphi \rangle p_1^\varphi} + \underbrace{\langle \psi_N, p_1^\varphi A_1 q_1^\varphi \psi_N \rangle}_{\leq \|A\| \|\psi_N\|_{p_1^\varphi} \|\psi_N\|_{q_1^\varphi} \leftarrow \text{Cauchy-Schwarz}} + \underbrace{\langle \psi_N, q_1^\varphi A_1 p_1^\varphi \psi_N \rangle}_{\leq \|A\| \alpha(\psi_N, \varphi)} + \underbrace{\langle \psi_N, q_1^\varphi A_1 q_1^\varphi \psi_N \rangle}_{\leq \|A\| \alpha(\psi_N, \varphi)} \\
&\leq \|A\| \sqrt{\alpha(\psi_N, \varphi)} \\
&= \langle \varphi, A \varphi \rangle (\langle \psi_N, p_1^\varphi \psi_N \rangle - 1) \\
&= -\langle \varphi, A \varphi \rangle \alpha_N(\psi_N, \varphi)
\end{aligned}$$

$$\Rightarrow |\langle \psi_N, A_1 \psi_N \rangle - \langle \varphi, A \varphi \rangle| \leq \|A\| 4 \sqrt{\alpha(\psi_N, \varphi)}$$

□

Conclusion: If we can show that $\alpha(\psi_N(t), \varphi(t)) \xrightarrow{N \rightarrow \infty} 0$, then also $\chi_{\psi_N} \xrightarrow{N \rightarrow \infty} p^\varphi$ and $\langle \psi_N, A_1 \psi_N \rangle \xrightarrow{N \rightarrow \infty} \langle \varphi, A \varphi \rangle \forall A \in \mathcal{D}$.