Hilbert-Schmidt norm estimates for fermionic reduced density matrices

Quantissima sur Oise, CY Advanced Studies 2025

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Fermionic reduced density matrices

Let $(\mathcal{H}, \langle\cdot,\cdot\rangle)$ be a separable Hilbert space. Consider N-body fermionic wavefunctions $\Psi \in \mathcal{H}_N$:

$$U_\sigma \Psi = \mathrm{sgn}(\sigma)\Psi, \tag{1}$$

for any permutation σ of $\{1, \ldots, N\}$. The permutation operator U_σ is defined by

$$U_\sigma u_1 \otimes \cdots \otimes u_N = u_{\sigma(1)} \otimes \cdots \otimes u_{\sigma(N)}, \tag{2}$$

for all $u_1, \ldots, u_N \in \mathcal{H}$.

Given $\Psi \in \mathcal{H}_N$, define the k-particle reduced density matrix

$$\Gamma^{(k)} = \binom{N}{k} \mathrm{Tr}_{k+1\to N} |\Psi\rangle\langle\Psi|.$$

This is a nonnegative trace-class operator that satisfies

$$\mathrm{Tr}\,\Gamma^{(k)} = \binom{N}{k}. \tag{3}$$

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Estimates on the operator norm

As a consequence of the normalisation

$$\operatorname{Tr}\Gamma^{(k)} = \binom{N}{k},$$

we have the trivial bound

$$\|\Gamma^{(k)}\|_{\mathrm{op}} \leq \binom{N}{k}. \tag{4}$$

Optimal for bosons, but not at all for fermions. For $\Gamma^{(1)}$, the **Pauli exclusion principle** implies

$$\|\Gamma^{(1)}\|_{\mathrm{op}} \leq 1, \tag{5}$$

which is optimised by Slater determinants. For $\Gamma^{(2)}$, Yang '62 proved

$$\|\Gamma^{(2)}\|_{\mathrm{op}} \leq N/2, \tag{6}$$

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Estimates on the operator norm II

For $\Gamma^{(1)}$ and $\Gamma^{(2)}$,

$$\|\Gamma^{(1)}\|_{\mathrm{op}} \leq 1 \quad \text{and} \quad \|\Gamma^{(2)}\|_{\mathrm{op}} \leq N/2.$$

More generally, Bell '62 (k odd) and Yang '63 (k even) proved the bound

$$\|\Gamma^{(k)}\|_{\mathrm{op}} \leq C_k N^{\lfloor k/2 \rfloor}. \tag{7}$$

The optimal constant is conjectured to be given by Yang pairing states (see Carlen-Lieb-Reuvers '16).

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Bell's argument

Let $(u_i)_i$ be an ONB of $\mathcal{H}$. Denote by a_i^* and a_i the operators that create and annihilate a particle in state u_i. Let $f \in \mathcal{H}_k$ and write

$$\langle f, \Gamma^{(k)} f \rangle = \sum_{i_1 < \cdots < i_k} \sum_{j_1 < \cdots < j_k} \overline{f_{i_1 \ldots i_k}} f_{j_1 \ldots j_k} \langle a_{i_1}^* \ldots a_{i_k}^* a_{j_k} \ldots a_{j_1} \rangle_\Psi .$$

Define

$$F = \sum_{i_1 < \cdots < i_k} f_{i_1 \ldots i_k} a_{i_k} \ldots a_{i_1} .$$

Then,

$$\langle f, \Gamma^{(k)} f \rangle = \langle F^* F \rangle_\Psi \leq \langle F^* F + F F^* \rangle_\Psi .$$

Using the CAR

$$\{a_i, a_j\} = \{a_i^*, a_j^*\} = 0 \quad \text{and} \quad \{a_i, a_j^*\} = \delta_{ij},$$

we see that

$$a_{i_1}^* \ldots a_{i_k}^* a_{j_k} \ldots a_{j_1} = (-1)^k a_{j_k} \ldots a_{j_1} a_{i_1}^* \ldots a_{i_k}^* + \text{lower order terms}.$$

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Hilbert–Schmidt norm

Consider

$$\|\Gamma^{(k)}\|_{\mathrm{HS}}^2 = \operatorname{Tr}\left[(\Gamma^{(k)})^2\right].$$

The estimate $\|\Gamma^{(1)}\|_{\mathrm{op}} \leq 1$ implies

$$\|\Gamma^{(1)}\|_{\mathrm{HS}}^2 \leq \operatorname{Tr}\Gamma^{(1)} = N, \tag{8}$$

which is optimised by Slater determinants. More generally, the estimate $\|\Gamma^{(k)}\|_{\mathrm{op}} \leq C_k N^{\lfloor k/2 \rfloor}$ implies

$$\|\Gamma^{(k)}\|_{\mathrm{HS}}^2 \leq C_k N^{\lfloor k/2 \rfloor} \operatorname{Tr}\Gamma^{(k)} \leq C_k N^{\lfloor k/2 \rfloor} N^k. \tag{9}$$

This is however **not** optimal at all. In fact, Carlen–Lieb–Reuvers '16 conjectured that the Hilbert–Schmidt norm is maximised by Slater determinants. Namely,

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Estimates on the Hilbert–Schmidt norm

Theorem (Christiansen'24)

Let $\Psi \in \mathcal{H}_N$ be normalised and denote its 2-particle reduced density matrix by $\Gamma^{(2)}$. Then

$$\|\Gamma^{(2)}\|_{\mathrm{HS}} \leq \sqrt{5}N/2. \tag{11}$$

Idea: use the characterisation $\|\Gamma^{(2)}\|_{\mathrm{HS}} = \sup_A \mathrm{Tr}(A\Gamma^{(2)})$ over all A such that $\|A\|_{\mathrm{HS}} = 1$. Write

$$4\,\mathrm{Tr}(A\Gamma^{(2)}) = \sum_{i,j,k,\ell} A_{ijk\ell}\langle\Psi, a_i^* a_j^* a_\ell a_k \Psi\rangle = \sum_k \Big\langle \sum_{i,j,\ell} A_{ijk\ell} a_\ell^* a_j a_i \Psi, a_k \Psi \Big\rangle.$$

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Estimates on the Hilbert–Schmidt norm II

Theorem (V.'25)

Let $\Psi \in \mathcal{H}_N$ be normalised and denote its k-particle reduced density matrix by $\Gamma^{(k)}$. Then

$$\|\Gamma^{(k)}\|_{\mathrm{HS}} \leq C_k N^{k/2}, \tag{12}$$

for some C_k depending only on k.

Idea: expand Ψ into Slater determinants built from $(u_i)_i$:

$$\Psi = \sum_{\mathrm{I}} c_{\mathrm{I}} u_{\mathrm{I}},$$

where $\mathrm{I} = (i_1, \ldots, i_N)$ with $i_1 < \cdots < i_N$ and

$$u_{\mathrm{I}} = u_{i_1} \wedge \cdots \wedge u_{i_N}.$$

This gives

$$\|\Gamma^{(k)}\|_{\mathrm{HS}}^2 = \sum_{\substack{\mathrm{I},\mathrm{J} \\ \mathrm{I}',\mathrm{J}'}} c_{\mathrm{I}} c_{\mathrm{J}} c_{\mathrm{I}'} c_{\mathrm{J}'} \operatorname{Tr}(\operatorname{Tr}_{k+1\to N} |u_{\mathrm{I}}\rangle\langle u_{\mathrm{J}}| \operatorname{Tr}_{k+1\to N} |u_{\mathrm{J}'}\rangle\langle u_{\mathrm{I}'}|). \tag{13}$$

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Entropy

Given $\Psi \in \mathcal{H}_N$, let $\gamma^{(k)}$ denote its **trace normalised** k-particle reduced density matrix:

$$\gamma^{(k)} = \mathrm{Tr}_{k+1 \to N} |\Psi\rangle\langle\Psi|.$$

The von Neumann entropy of $\gamma^{(k)}$ is defined as

$$\mathcal{S}(\gamma^{(k)}) = -\mathrm{Tr}(\gamma^{(k)} \log \gamma^{(k)}).$$

Jensen's inequality implies

$$\mathcal{S}(\gamma^{(k)}) \geq -\log(\|\gamma^{(k)}\|_{\mathrm{HS}}^2).$$

Then, the bound $\|\gamma^{(k)}\|_{\mathrm{HS}}^2 \leq C_k N^{-k}$ yields

$$\mathcal{S}(\gamma^{(k)}) \geq k \log N + \mathcal{O}(1). \tag{14}$$

This was conjectured by Lemm '17 and proven by himself for $k = 2$ and $\mathcal{H}$ of dimension not much larger than N.

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Thank you for your attention!

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Bibliography II

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Yang pairing states

Take $\mathcal{H} = \mathbb{C}^M$ and assume $N = 2n$ and $M = 2m$. Let $(u_i)_i$ be an ONB of $\mathcal{H}$. Define $p_i = (2i-1, 2i)$ and $u_{p_i} = u_{2i-1} \wedge u_{2i}$. Define also

$$\Phi_{i_1 \ldots i_m} = u_{p_{i_1}} \wedge \cdots \wedge u_{p_{i_m}}.$$

Then, the Yang pairing state $\Psi_{N,M}$ is given by

$$\Psi_{N,M} = \binom{m}{n}^{-1/2} \sum_{i_1 < \cdots < i_m} \Phi_{i_1 \ldots i_m}.$$

Proposition (Carlen–Lieb–Reuvers '16)

Let $\Gamma^{(2)}$ denote the 2-particle reduced density matrix of $\Psi_{N,M}$. Then, $\Gamma^{(2)}$ has eigenvalues

$$\Lambda_2^{N,M} = \frac{N}{2} \frac{m-n+1}{m} \quad \textit{and} \quad \lambda_2^{N,M} = \frac{N}{2} \frac{n-1}{m(m-1)},$$

with respective multiplicities 1 *and* $2m^2 - m - 1$.

Rewriting of the Hilbert–Schmidt norm

Define

$$\Lambda(\mathrm{D};\boldsymbol{\alpha},\boldsymbol{\beta};\boldsymbol{\varepsilon},\boldsymbol{\eta}) = \mathrm{sgn}(\boldsymbol{\alpha}\cup\boldsymbol{\beta},\boldsymbol{\varepsilon}\cup\boldsymbol{\eta})c_{\mathrm{D}\cup\boldsymbol{\alpha}\cup\boldsymbol{\varepsilon}}c_{\mathrm{D}\cup\boldsymbol{\alpha}\cup\boldsymbol{\eta}}c_{\mathrm{D}\cup\boldsymbol{\beta}\cup\boldsymbol{\varepsilon}}c_{\mathrm{D}\cup\boldsymbol{\beta}\cup\boldsymbol{\eta}}.$$

Then,

$$\begin{aligned}\|\Gamma^{(k)}\|_{\mathrm{HS}}^2 &= \sum_{\substack{\mathrm{I},\mathrm{J}\\ \mathrm{I}',\mathrm{J}'}} c_{\mathrm{I}}c_{\mathrm{J}}c_{\mathrm{I}'}c_{\mathrm{J}'}\,\mathrm{Tr}(\mathrm{Tr}_{k+1\to N}|u_{\mathrm{I}}\rangle\langle u_{\mathrm{J}}|\,\mathrm{Tr}_{k+1\to N}|u_{\mathrm{J}'}\rangle\langle u_{\mathrm{I}'}|)\\ &= \sum_{s=0}^{k}\sum_{r=0}^{N}\binom{N-r}{k-s}\sum_{|\mathrm{D}|=N-r}\ \sum_{|\boldsymbol{\varepsilon}|,|\boldsymbol{\eta}|=r-s}\ \sum_{|\boldsymbol{\alpha}|,|\boldsymbol{\beta}|=s}\Lambda(\mathrm{D};\boldsymbol{\alpha},\boldsymbol{\beta};\boldsymbol{\varepsilon},\boldsymbol{\eta}) \qquad (15)\end{aligned}$$

The multi-indices $\mathrm{I}, \mathrm{J}, \mathrm{I}'$ and J' can be related to the indices in (15) as follows:

- D is the set of indices that $\mathrm{I}, \mathrm{J}, \mathrm{I}'$ and J' all have in common;
- $\boldsymbol{\varepsilon}$ is the set of indices that only I and J have in common;
- $\boldsymbol{\eta}$ is the set of indices that only I' and J' have in common;
- $\boldsymbol{\alpha}$ is the set of indices that only I and I' have in common;
- $\boldsymbol{\beta}$ is the set of indices that only J' and J' have in common.

Rewriting of the Hilbert–Schmidt norm II

$$\|\Gamma^{(k)}\|_{\mathrm{HS}}^2 = \sum_{s=0}^{k}\sum_{r=0}^{N}\binom{N-r}{k-s}\sum_{|\mathsf{D}|=N-r}\ \sum_{|\boldsymbol{\varepsilon}|,|\boldsymbol{\eta}|=r-s}\ \sum_{|\boldsymbol{\alpha}|,|\boldsymbol{\beta}|=s}\Lambda(\mathsf{D};\boldsymbol{\alpha},\boldsymbol{\beta};\boldsymbol{\varepsilon},\boldsymbol{\eta})$$

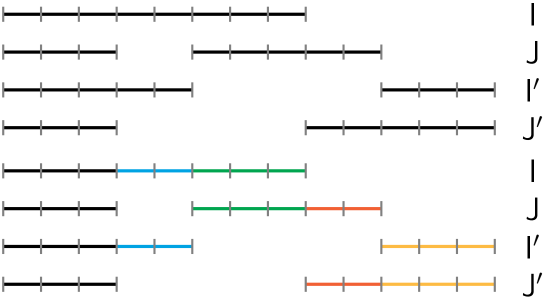

Figure: The multi-indices in (15) are colour coded in the right-hand side as follows: D, $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, $\boldsymbol{\varepsilon}$, $\boldsymbol{\eta}$.