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Hilbert–Schmidt Estimates for Fermionic 2-Body Operators

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Abstract: We prove that the 2-body operator γ_2^{Ψ} of a fermionic N-particle state Ψ obeys $\|\gamma_2^{\Psi}\|_{\mathrm{HS}} \leq \sqrt{5}N$, which complements the bound of Yang (Rev Mod Phys 34:694, 1962) that $\|\gamma_2^{\Psi}\|_{\mathrm{op}} \leq N$. This estimate furthermore resolves a conjecture of Carlen–Lieb–Reuvers (Commun Math Phys 344:655–671, 2016) concerning the entropy of the normalized 2-body operator. We also prove that the Hilbert–Schmidt norm of the truncated 2-body operator $\gamma_2^{\Psi,T}$ obeys the inequality $\|\gamma_2^{\Psi,T}\|_{\mathrm{HS}} \leq \sqrt{5N \,\mathrm{tr}\,(\gamma_1^{\Psi}(1-\gamma_1^{\Psi}))}$.

1. Introduction

Let $(\mathfrak{h}, \langle\cdot,\cdot\rangle)$ be a (separable) Hilbert space and consider the space of fermionic N-particle states, $\bigwedge^N \mathfrak{h}$. Given a normalized state $\Psi \in \bigwedge^N \mathfrak{h}$, one defines *the 1- and 2-body operators associated to* Ψ, $\gamma_1^{\Psi} : \mathfrak{h} \to \mathfrak{h}$ and $\gamma_2^{\Psi} : \mathfrak{h}\otimes\mathfrak{h} \to \mathfrak{h}\otimes\mathfrak{h}$, by

$$\left\langle \varphi_1, \gamma_1^{\Psi} \psi_1 \right\rangle = \left\langle \Psi, c^*(\psi_1)\, c(\varphi_1)\, \Psi \right\rangle \tag{1.1}$$

and

$$\left\langle (\varphi_1\otimes\varphi_2), \gamma_2^{\Psi}(\psi_1\otimes\psi_2) \right\rangle = \left\langle \Psi, c^*(\psi_1)\, c^*(\psi_2)\, c(\varphi_2)\, c(\varphi_1)\, \Psi \right\rangle \tag{1.2}$$

for any $\varphi_1, \varphi_2, \psi_1, \psi_2 \in \mathfrak{h}$. Here $c^*(\cdot)$ and $c(\cdot)$ denote the fermionic creation and annihilation operators, which obey the canonical anticommutation relations (CAR)

$$\left\{ c(\varphi), c^*(\psi) \right\} = \langle \varphi, \psi \rangle, \quad \{ c(\varphi), c(\psi) \} = 0 = \left\{ c^*(\varphi), c^*(\psi) \right\}. \tag{1.3}$$

We recall some well-known properties of γ_1^{Ψ} and γ_2^{Ψ}: Firstly, they are non-negative. This is obvious in the case of γ_1^{Ψ}, and for γ_2^{Ψ} this follows by noting that if $(u_k)_{k=1}^{\infty}$ is an orthonormal basis for $\mathfrak{h}$, then a general tensor $\Phi \in \mathfrak{h}\otimes\mathfrak{h}$ can be written as

$$\Phi = \sum_{k,l=1}^{\infty} \overline{\Phi_{k,l}}\, (u_k \otimes u_l) \tag{1.4}$$

for $\Phi_{k,l} = \langle \Phi, u_k \otimes u_l \rangle$, from which it readily follows that the inner product $\langle \Phi, \gamma_2^{\Psi} \Phi \rangle$ is given by

$$\langle \Phi, \gamma_2^{\Psi} \Phi \rangle = \left\| \sum_{k,l=1}^{\infty} \Phi_{k,l} c_l c_k \Psi \right\|^2 \tag{1.5}$$

where $c_k^* = c^*(u_k)$ and $c_k = c(u_k)$ denotes the creation and annihilation operators associated to the basis $(u_k)_{k=1}^{\infty}$.

Secondly, they are trace-class, with

$$\operatorname{tr}\left(\gamma_1^{\Psi}\right) = N, \quad \operatorname{tr}\left(\gamma_2^{\Psi}\right) = N(N-1), \tag{1.6}$$

which follows from the identity $\sum_{k=1}^{\infty} c_k^* c_k = M \, \mathrm{id}_{\bigwedge^M \mathfrak{h}}$, which holds on $\bigwedge^M \mathfrak{h}$ for any $M \in \mathbb{N}$.

This combined with their non-negativity implies the trivial estimates $\left\| \gamma_1^{\Psi} \right\|_{\mathrm{op}} \leq N$ and $\left\| \gamma_2^{\Psi} \right\|_{\mathrm{op}} \leq N(N-1)$. In the *bosonic* case these are in fact optimal, but this is not so for the fermionic case: For γ_1^{Ψ} one may note that

$$\langle \varphi, \gamma_1^{\Psi} \varphi \rangle = \langle \Psi, c^*(\varphi) c(\varphi) \Psi \rangle \leq \langle \Psi, \{c^*(\varphi), c(\varphi)\} \Psi \rangle = \langle \varphi, \varphi \rangle, \quad \varphi \in \mathfrak{h}, \tag{1.7}$$

where we simply added the non-negative quantity $\|c^*(\varphi)\Psi\|^2$ and applied the CAR. This shows that $\left\| \gamma_1^{\Psi} \right\|_{\mathrm{op}} \leq 1$, which is usually described as a consequence of the *Fermi exclusion principle*, which informally speaking prohibits more than one fermion from occupying any given one-particle state.

In terms of the operators c_k this bound can equivalently be phrased as

$$\left\| \sum_{k=1}^{\infty} \alpha_k c_k \right\|_{\mathrm{op}} \leq \sqrt{\sum_{k=1}^{\infty} |\alpha_k|^2} \tag{1.8}$$

which we can also use to improve our bound on $\left\| \gamma_2^{\Psi} \right\|_{\mathrm{op}}$ as follows: By the triangle and Cauchy–Schwarz inequalities, we can apply this to equation (1.5) for

$$\sqrt{\langle \Phi, \gamma_2^{\Psi} \Phi \rangle} \leq \sum_{k=1}^{\infty} \left\| \left(\sum_{l=1}^{\infty} \Phi_{k,l} c_l \right) c_k \Psi \right\| \leq \sqrt{\sum_{k,l=1}^{\infty} \left| \Phi_{k,l} \right|^2} \sqrt{\sum_{k=1}^{\infty} \|c_k \Psi\|^2} = \sqrt{N} \, \|\Phi\| \tag{1.9}$$

which implies that $\left\| \gamma_2^{\Psi} \right\|_{\mathrm{op}} \leq N$ - a bound which Yang proved was optimal[1] in the classic paper [7].

[1] In fact he proved the stronger statement that $\left\| \gamma_2^{\Psi} \right\|_{\mathrm{op}} \leq \frac{M-N+2}{M} N$ when $M = \dim(\mathfrak{h}) < \infty$ and M and N are even, and characterized the optimizers in this case.

1.1. Main results. In this paper we present two results on γ_2^Ψ. The first result concerns $\|\gamma_2^\Psi\|_{\mathrm{HS}}$: Given the identity $\|\gamma_2^\Psi\|_{\mathrm{tr}} = \mathrm{tr}\left(\gamma_2^\Psi\right) = N(N-1)$ and the general inequality $\|\gamma_2^\Psi\|_{\mathrm{op}} \leq N$, one can deduce that the Hilbert–Schmidt norm of γ_2^Ψ must obey

$$\|\gamma_2^\Psi\|_{\mathrm{HS}} \leq \sqrt{\|\gamma_2^\Psi\|_{\mathrm{tr}}\|\gamma_2^\Psi\|_{\mathrm{op}}} \leq N\sqrt{N-1} = O\left(N^{\frac{3}{2}}\right), \tag{1.10}$$

and since $\|\gamma_2^\Psi\|_{\mathrm{tr}} = N(N-1)$ is an identity and $\|\gamma_2^\Psi\|_{\mathrm{op}} \leq N$ is optimal, one might suppose that this is at least nearly optimal. Below we will however prove that this is far from the case, as the following holds:

Theorem 1. *For any $N \in \mathbb{N}$ and normalized $\Psi \in \bigwedge^N \mathfrak{h}$ it holds that*

$$\|\gamma_2^\Psi\|_{\mathrm{HS}} \leq \sqrt{5}N.$$

This result is interesting in two respects: Firstly, it is of the same order (with respect to N) as the optimal bound $\|\gamma_2^\Psi\|_{\mathrm{op}} \leq N$, even though $\|\gamma_2^\Psi\|_{\mathrm{tr}} = N(N-1)$. This informally implies that although it is possible for γ_2^Ψ to have eigenvalues of order N, it can not have "too many" large eigenvalues.

Secondly, it is easy to compute that for a Slater state $\Psi = u_1 \wedge \cdots \wedge u_N$, $\|\gamma_2^\Psi\|_{\mathrm{HS}} = \sqrt{2N(N-1)}$, which is also $O(N)$. This suggests that an $O(N)$ behavior of the Hilbert–Schmidt norm of fermionic 2-body operators might be a general feature.

This bound also resolves a conjecture of Carlen–Lieb–Reuvers concerning the entropy of the trace-normalized 2-body operator $\overline{\gamma}_2 = \frac{1}{N(N-1)}\gamma_2^\Psi$. In [4] they conjectured (Conjecture 2.6) that the entropy of this should always obey a bound of the form

$$S\left(\overline{\gamma}_2\right) := -\mathrm{tr}\left(\overline{\gamma}_2 \log\left(\overline{\gamma}_2\right)\right) \geq 2\log(N) + O(1). \tag{1.11}$$

As noted in [4], Jensen's inequality for the convex function $x \mapsto -\log(x)$ implies that

$$S(\overline{\gamma}) \geq -\log\left(\mathrm{tr}\left(\overline{\gamma}^2\right)\right) = -\log\left(\|\overline{\gamma}\|_{\mathrm{HS}}^2\right) \tag{1.12}$$

for any density operator $\overline{\gamma}$, so as a consequence of Theorem 1 we find that

$$S\left(\overline{\gamma}_2\right) \geq -\log\left(\frac{5N^2}{(N(N-1))^2}\right) = 2\log(N) - \log\left(5\left(1 + \frac{2N-1}{(N-1)^2}\right)\right) \tag{1.13}$$

for any $N \geq 2$, which is to say $S\left(\overline{\gamma}_2\right) \geq 2\log(N) - \log(5) + o(1)$ as $N \to \infty$.

Truncated 2-Body Operators Our second result concerns the *truncated* 2-body operator: It is well-known that Ψ is a Slater state if and only if γ_1^Ψ is a projection, i.e. $\left(\gamma_1^\Psi\right)^2 = \gamma_1^\Psi$, and that in this case the 2-body operator can be expressed in terms of γ_1^Ψ as

$$\gamma_2^\Psi = (1 - \mathrm{Ex})\, \gamma_1^\Psi \otimes \gamma_1^\Psi \tag{1.14}$$

where $\mathrm{Ex} : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h}$ acts according to $\mathrm{Ex}(\varphi \otimes \psi) = \psi \otimes \varphi$.

For a general state Ψ one would expect that if Ψ is "nearly Slater", in an appropriate sense, then the same expression should be approximately valid for γ_2^Ψ - this leads to the

Hartree-Fock functional as an approximation to the energy of a fermionic system, for instance.

A way to make this precise is to consider the truncated 2-body operator $\gamma_2^{\Psi,T} : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h}$, defined by

$$\gamma_2^{\Psi,T} = \gamma_2^{\Psi} - (1 - \mathrm{Ex})\, \gamma_1^{\Psi} \otimes \gamma_1^{\Psi}, \tag{1.15}$$

and establish that this can be controlled in terms of $\mathrm{tr}\left(\gamma_1^{\Psi}\left(1 - \gamma_1^{\Psi}\right)\right) = \mathrm{tr}\left(\gamma_1^{\Psi} - \left(\gamma_1^{\Psi}\right)^2\right)$, which can be viewed as a measure of the "Slaterness" of the state Ψ. A result of this form was first derived by Bach in [1], where he proved the following (see also Bach's paper [2] and Graf–Solovej's paper [6] for related generalizations):

Theorem (Bach [1]). *Let $X : \mathfrak{h} \to \mathfrak{h}$ be an orthogonal projection. Then for any normalized $\Psi \in \bigwedge^N \mathfrak{h}$ it holds that*

$$\mathrm{tr}\left((X \otimes X)\, \gamma_2^{\Psi,T}\right) \geq -\,\mathrm{tr}\left(X\gamma_1^{\Psi}\right) \cdot \min\left\{1, 7.554\sqrt{\mathrm{tr}\left(X\left(\gamma_1^{\Psi}\left(1 - \gamma_1^{\Psi}\right)\right)\right)}\right\}.$$

This can be seen as a sort of lower bound for $\gamma_2^{\Psi,T}$. Below we will complement this result by proving the following Hilbert-Schmidt bound for $\gamma_2^{\Psi,T}$:

Theorem 2. *For any $N \in \mathbb{N}$ and $\Psi \in \bigwedge^N \mathfrak{h}$ it holds that*

$$\left\| \gamma_2^{\Psi,T} \right\|_{\mathrm{HS}} \leq \sqrt{5N\, \mathrm{tr}\left(\gamma_1^{\Psi}\left(1 - \gamma_1^{\Psi}\right)\right)}.$$

We remark that at worst $\mathrm{tr}\left(\gamma_1^{\Psi}\left(1 - \gamma_1^{\Psi}\right)\right) \leq \mathrm{tr}\left(\gamma_1^{\Psi}\right) = N$, in which case this bound essentially reduces to that of Theorem 1 (up to the quantity $\left\|(1 - \mathrm{Ex})\, \gamma_1^{\Psi} \otimes \gamma_1^{\Psi}\right\|_{\mathrm{HS}}$), but in view of that theorem this bound is non-trivial for any Ψ with $\mathrm{tr}\left(\gamma_1^{\Psi}\left(1 - \gamma_1^{\Psi}\right)\right) \ll N$.

2. Proof of the Theorems

To prove Theorem 1 we first observe that by the characterization $\|T\|_{\mathrm{HS}} = \sup_A |\mathrm{tr}\,(AT)|$, where the supremum is over all Hilbert–Schmidt operators A with $\|A\|_{\mathrm{HS}} = 1$, it suffices to estimate a quantity of the form $\left|\mathrm{tr}\left(A\gamma_2^{\Psi}\right)\right|$. To do this we begin by writing

$$\begin{aligned}\mathrm{tr}\left(A\gamma_2^{\Psi}\right) &= \sum_{k,l,m,n=1}^{\infty} \langle (u_k \otimes u_l), A\,(u_m \otimes u_n)\rangle \left\langle \Psi, c_k^* c_l^* c_n c_m \Psi\right\rangle \\ &= -\sum_{n=1}^{\infty} \left\langle \sum_{k,l,m=1}^{\infty} \overline{A_{k,l,m,n}}\, c_m^* c_l c_k \Psi, c_n \Psi \right\rangle\end{aligned} \tag{2.1}$$

where $A_{k,l,m,n} = \langle (u_k \otimes u_l), A\,(u_m \otimes u_n)\rangle$. The Cauchy–Schwarz inequality thus allows us to estimate

$$\left|\mathrm{tr}\left(A\gamma_2^{\Psi}\right)\right| \leq \sum_{n=1}^{\infty} \left\| \sum_{k,l,m=1}^{\infty} \overline{A_{k,l,m,n}}\, c_m^* c_l c_k \Psi \right\| \|c_n \Psi\|$$

$$\leq \sqrt{\sum_{n=1}^{\infty} \left\| \sum_{k,l,m=1}^{\infty} \overline{A_{k,l,m,n}} c_m^* c_l c_k \Psi \right\|^2} \sqrt{\sum_{n=1}^{\infty} \|c_n \Psi\|^2}$$

$$\leq \sqrt{N \sum_{n=1}^{\infty} \left\langle \Psi, \left\{ \left(\sum_{k,l,m=1}^{\infty} \overline{A_{k,l,m,n}} c_m^* c_l c_k \right)^*, \sum_{k,l,m=1}^{\infty} \overline{A_{k,l,m,n}} c_m^* c_l c_k \right\} \Psi \right\rangle} \tag{2.2}$$

where we recognized that $\sum_{n=1}^{\infty} \|c_n \Psi\|^2 = \langle \Psi, \mathcal{N} \Psi \rangle = N$, and used that as in the proof of the inequality $\gamma_1^\Psi \leq 1$, we are free to add the quantity $\left\| \left(\sum_{k,l,m=1}^{\infty} \overline{A_{k,l,m,n}} c_m^* c_l c_k \right)^* \Psi \right\|^2$ to obtain the anticommutator of $\sum_{k,l,m=1}^{\infty} \overline{A_{k,l,m,n}} c_m^* c_l c_k$ with its adjoint.

The reason for this last step is an argument which was recently used in the study of the correlation energy of Fermi gases in [5], although it has since been learned this was first used by Bell in [3]: Although the CAR does not imply a useful anticommutator identity for sums of an *even* number of creation and annihilation operators, it does for sums of an *odd* number of such operators.

In the present case we note the following identity:

Proposition 3. *Let* $A_{k,l,m,n} \in \mathbb{C}$ *for* $k, l, m, n \in \mathbb{N}$ *obey* $A_{l,k,m,n} = -A_{k,l,m,n}$. *Then it holds for any* $n \in \mathbb{N}$ *that* $T_n = \left\{ \left(\sum_{k,l,m=1}^{\infty} \overline{A_{k,l,m,n}} c_m^* c_l c_k \right)^*, \sum_{k,l,m=1}^{\infty} \overline{A_{k,l,m,n}} c_m^* c_l c_k \right\}$ *is given by*

$$T_n = \sum_{m=1}^{\infty} \left| \sum_{k,l=1}^{\infty} \overline{A_{k,l,m,n}} c_l c_k \right|^2 + 4 \sum_{k=1}^{\infty} \left| \sum_{l,m=1}^{\infty} A_{k,l,m,n} c_l^* c_m \right|^2 - 2 \sum_{k,l=1}^{\infty} \left| \sum_{m=1}^{\infty} A_{k,l,m,n} c_m \right|^2 .$$

Proof. By applying the CAR we find that for any $k, l, m, k', l', m' \in \mathbb{N}$

$$\begin{aligned} \left\{ c_k^* c_l^* c_m, c_{m'}^* c_{l'} c_{k'} \right\} &= -c_k^* c_l^* c_{m'}^* c_m c_{l'} c_{k'} + \delta_{m,m'} c_k^* c_l^* c_{l'} c_{k'} + c_{m'}^* c_{l'} c_{k'} c_k^* c_l^* c_m \\ &= -c_{m'}^* c_k^* c_l^* c_{l'} c_{k'} c_m + \delta_{m,m'} c_k^* c_l^* c_{l'} c_{k'} + c_{m'}^* c_{l'} c_{k'} c_k^* c_l^* c_m \\ &= -c_{m'}^* \left[c_k^* c_l^*, c_{l'} c_{k'} \right] c_m + \delta_{m,m'} c_k^* c_l^* c_{l'} c_{k'}, \end{aligned} \tag{2.3}$$

and by standard commutator identities

$$\begin{aligned} \left[c_k^* c_l^*, c_{l'} c_{k'} \right] &= c_k^* \left[c_l^*, c_{l'} c_{k'} \right] + \left[c_k^*, c_{l'} c_{k'} \right] c_l^* \\ &= c_k^* \left(\left\{ c_l^*, c_{l'} \right\} c_{k'} - c_{l'} \left\{ c_l^*, c_{k'} \right\} \right) + \left(\left\{ c_k^*, c_{l'} \right\} c_{k'} - c_{l'} \left\{ c_k^*, c_{k'} \right\} \right) c_l^* \\ &= \delta_{l,l'} c_k^* c_{k'} - \delta_{l,k'} c_k^* c_{l'} + \delta_{k,l'} c_{k'} c_l^* - \delta_{k,k'} c_{l'} c_l^* \\ &= -\delta_{k,k'} c_{l'} c_l^* - \delta_{l,l'} c_{k'} c_k^* + \delta_{k,l'} c_{k'} c_l^* + \delta_{l,k'} c_{l'} c_k^* + \delta_{k,k'} \delta_{l,l'} - \delta_{k,l'} \delta_{l,k'}, \end{aligned} \tag{2.4}$$

so

$$\begin{aligned} \left\{ c_k^* c_l^* c_m, c_{m'}^* c_{l'} c_{k'} \right\} = {} & \delta_{m,m'} c_k^* c_l^* c_{l'} c_{k'} + \delta_{k,k'} c_{m'}^* c_{l'} c_l^* c_m + \delta_{l,l'} c_{m'}^* c_{k'} c_k^* c_m \\ & - \delta_{k,l'} c_{m'}^* c_{k'} c_l^* c_m - \delta_{l,k'} c_{m'}^* c_{l'} c_k^* c_m - \delta_{k,k'} \delta_{l,l'} c_{m'}^* c_m + \delta_{k,l'} \delta_{l,k'} c_{m'}^* c_m . \end{aligned} \tag{2.5}$$

Consequently T_n is given by

$$
\begin{aligned}
T_n = & \sum_{k,l,m=1}^{\infty}\sum_{k',l',m'=1}^{\infty} A_{k,l,m,n}\overline{A_{k',l',m',n}}\left\{c_k^* c_l^* c_m, c_{m'}^* c_{l'} c_{k'}\right\} \\
= & \sum_{m=1}^{\infty}\left|\sum_{k',l'=1}^{\infty}\overline{A_{k',l',m,n}} c_{l'} c_{k'}\right|^2 + \sum_{k=1}^{\infty}\left|\sum_{l,m=1}^{\infty} A_{k,l,m,n} c_l^* c_m\right|^2 + \sum_{l=1}^{\infty}\left|\sum_{k,m=1}^{\infty} A_{k,l,m,n} c_k^* c_m\right|^2 \\
& - \sum_{k=1}^{\infty}\left(\sum_{k',m'=1}^{\infty} A_{k',k,m',n} c_{k'}^* c_{m'}\right)^*\left(\sum_{l,m=1}^{\infty} A_{k,l,m,n} c_l^* c_m\right) \\
& - \sum_{l=1}^{\infty}\left(\sum_{l',m'=1}^{\infty} A_{l,l',m',n} c_{l'}^* c_{m'}\right)^*\left(\sum_{k,m=1}^{\infty} A_{k,l,m,n} c_k^* c_m\right) \\
& - \sum_{k,l=1}^{\infty}\left|\sum_{m=1}^{\infty} A_{k,l,m,n} c_m\right|^2 + \sum_{k,l=1}^{\infty}\left(\sum_{m'=1}^{\infty} A_{l,k,m',n} c_{m'}\right)^*\left(\sum_{m=1}^{\infty} A_{k,l,m,n} c_m\right). \qquad (2.6)
\end{aligned}
$$

The claim now follows by renaming indices and using the assumed antisymmetry of $A_{k,l,m,n}$. □

With this identity we now obtain the central estimate of this paper:

Proposition 4. *For any Hilbert–Schmidt operator* $A : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h}$ *and* $N \in \mathbb{N}$ *it holds that with respect to* $\bigwedge^N \mathfrak{h}$

$$
\sum_{n=1}^{\infty}\left\{\left(\sum_{k,l,m=1}^{\infty}\overline{A_{k,l,m,n}} c_m^* c_l c_k\right)^*, \sum_{k,l,m=1}^{\infty}\overline{A_{k,l,m,n}} c_m^* c_l c_k\right\} \leq 5N \|A\|_{\mathrm{HS}}^2 .
$$

Proof. We begin by noting that as

$$
\begin{aligned}
\sum_{k,l,m=1}^{\infty}\overline{A_{k,l,m,n}} c_m^* c_l c_k &= \frac{1}{2}\sum_{k,l,m=1}^{\infty}\overline{A_{k,l,m,n}} c_m^*\left(c_l c_k - c_k c_l\right) \\
&= \sum_{k,l,m=1}^{\infty}\overline{\frac{A_{k,l,m,n} - A_{l,k,m,n}}{2}} c_m^* c_l c_k \qquad (2.7)
\end{aligned}
$$

and $\sum_{k,l,m,n}\left|A_{k,l,m,n} - A_{l,k,m,n}\right|^2 \leq 4\sum_{k,l,m,n}\left|A_{k,l,m,n}\right|^2$, we can assume without loss of generality that $A_{l,k,m,n} = -A_{k,l,m,n}$.

It then follows from the previous proposition that

$$
\begin{aligned}
T := & \sum_{n=1}^{\infty}\left\{\left(\sum_{k,l,m=1}^{\infty}\overline{A_{k,l,m,n}} c_m^* c_l c_k\right)^*, \sum_{k,l,m=1}^{\infty}\overline{A_{k,l,m,n}} c_m^* c_l c_k\right\} \\
\leq & \sum_{m,n=1}^{\infty}\left|\sum_{k,l=1}^{\infty}\overline{A_{k,l,m,n}} c_l c_k\right|^2 + 4\sum_{k,n=1}^{\infty}\left|\sum_{l,m=1}^{\infty} A_{k,l,m,n} c_l^* c_m\right|^2, \qquad (2.8)
\end{aligned}
$$

and the same argument we applied in equation (1.9) now shows that for any $\Psi \in \bigwedge^N \mathfrak{h}$

$$\begin{aligned}\sum_{m,n=1}^{\infty} \left\| \sum_{k,l=1}^{\infty} \overline{A_{k,l,m,n}} c_l c_k \Psi \right\|^2 &\leq \sum_{m,n=1}^{\infty} \left(\sum_{k=1}^{\infty} \left\| \sum_{l=1}^{\infty} \overline{A_{k,l,m,n}} c_l c_k \Psi \right\| \right)^2 \\ \leq \sum_{m,n=1}^{\infty} \left(\sum_{k=1}^{\infty} \sqrt{\sum_{l=1}^{\infty} \left| A_{k,l,m,n} \right|^2} \left\| c_k \Psi \right\| \right)^2 &\leq \left(\sum_{k,l,m,n=1}^{\infty} \left| A_{k,l,m,n} \right|^2 \right) \left(\sum_{k=1}^{\infty} \left\| c_k \Psi \right\|^2 \right) \\ = N \left\| A \right\|_{\mathrm{HS}}^2 \left\| \Psi \right\|^2, \end{aligned} \tag{2.9}$$

i.e. $\sum_{m,n=1}^{\infty} \left| \sum_{k,l=1}^{\infty} \overline{A_{k,l,m,n}} c_l c_k \right|^2 \leq N \left\| A \right\|_{\mathrm{HS}}^2$, and as also $\left\| \sum_k \alpha_k c_k^* \right\|_{\mathrm{op}} \leq \sqrt{\sum_k |\alpha_k|^2}$, it similarly holds that

$$\sum_{k,n=1}^{\infty} \left\| \sum_{l,m=1}^{\infty} A_{k,l,m,n} c_l^* c_m \Psi \right\|^2 \leq N \left\| A \right\|_{\mathrm{HS}}^2 . \tag{2.10}$$

□

As noted at the beginning of this section, Theorem 1 immediately follows since we now have from equation (2.2) that

$$\left| \mathrm{tr} \left(A \gamma_2^{\Psi} \right) \right| \leq \sqrt{5} N \left\| A \right\|_{\mathrm{HS}} . \tag{2.11}$$

Proof of Theorem 2. We note the following identity for $\gamma_2^{\Psi,T}$:

Proposition 5. *For any $\varphi_1, \varphi_2, \psi_1, \psi_2 \in \mathfrak{h}$ it holds that*

$$\begin{aligned}\left\langle (\varphi_1 \otimes \varphi_2), \gamma_2^{\Psi,T} (\psi_1 \otimes \psi_2) \right\rangle &= \left\langle \Psi, c \left(\gamma_1^{\Psi} \varphi_2 \right) c^* (\psi_1) c^* (\psi_2) c (\varphi_1) \Psi \right\rangle \\ &\quad - \left\langle \Psi, c^* (\psi_1) c^* (\psi_2) c (\varphi_1) c \left(\left(1 - \gamma_1^{\Psi} \right) \varphi_2 \right) \Psi \right\rangle .\end{aligned}$$

Proof. By the CAR we have that

$$\begin{aligned} c^* (\psi_1) c^* (\psi_2) c (\varphi_2) c (\varphi_1) &= -c^* (\psi_1) c (\varphi_2) c^* (\psi_2) c (\varphi_1) + \langle \varphi_2, \psi_2 \rangle c^* (\psi_1) c (\varphi_1) \\ &= c (\varphi_2) c^* (\psi_1) c^* (\psi_2) c (\varphi_1) \\ &\quad + \langle \varphi_2, \psi_2 \rangle c^* (\psi_1) c (\varphi_1) - \langle \varphi_2, \psi_1 \rangle c^* (\psi_2) c (\varphi_1) , \end{aligned} \tag{2.12}$$

which by applying $\langle \Psi, (\cdot) \Psi \rangle$ yields

$$\begin{aligned}\left\langle (\varphi_1 \otimes \varphi_2), \gamma_2^{\Psi} (\psi_1 \otimes \psi_2) \right\rangle &= \left\langle \Psi, c (\varphi_2) c^* (\psi_1) c^* (\psi_2) c (\varphi_1) \Psi \right\rangle \\ &\quad + \left\langle (\varphi_1 \otimes \varphi_2), \left(\gamma_1^{\Psi} \otimes 1 \right) (1 - \mathrm{Ex}) (\psi_1 \otimes \psi_2) \right\rangle . \end{aligned} \tag{2.13}$$

Consequently

$$\begin{aligned}\left\langle (\varphi_1 \otimes \varphi_2), \gamma_2^{\Psi} (\psi_1 \otimes \psi_2) \right\rangle &= \left\langle \left(\varphi_1 \otimes \gamma_1^{\Psi} \varphi_2 \right), \gamma_2^{\Psi} (\psi_1 \otimes \psi_2) \right\rangle \\ &\quad + \left\langle \left(\varphi_1 \otimes \left(1 - \gamma_1^{\Psi} \right) \varphi_2 \right), \gamma_2^{\Psi} (\psi_1 \otimes \psi_2) \right\rangle\end{aligned}$$

$$
\begin{aligned}
&= \left\langle \Psi, c\left(\gamma_1^{\Psi}\varphi_2\right) c^*\left(\psi_1\right) c^*\left(\psi_2\right) c\left(\varphi_1\right) \Psi\right\rangle \\
&- \left\langle \Psi, c^*\left(\psi_1\right) c^*\left(\psi_2\right) c\left(\varphi_1\right) c\left(\left(1-\gamma_1^{\Psi}\right)\varphi_2\right) \Psi\right\rangle \\
&+ \left\langle \left(\varphi_1 \otimes \varphi_2\right), \left(1 \otimes \gamma_1^{\Psi}\right)\left(\gamma_1^{\Psi} \otimes 1\right)(1-\mathrm{Ex})\left(\psi_1 \otimes \psi_2\right)\right\rangle
\end{aligned} \tag{2.14}
$$

which implies the claim since $\left(1 \otimes \gamma_1^{\Psi}\right)\left(\gamma_1^{\Psi} \otimes 1\right)(1-\mathrm{Ex}) = (1-\mathrm{Ex})\left(\gamma_1^{\Psi} \otimes \gamma_1^{\Psi}\right)$. □

Theorem 2 can now be concluded in the following form:

Proposition 6. *For any Hilbert–Schmidt operator $A : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h}$, $N \in \mathbb{N}$ and normalized $\Psi \in \bigwedge^N \mathfrak{h}$ it holds that*

$$
\left|\operatorname{tr}\left(A\gamma_2^{\Psi,T}\right)\right| \leq \sqrt{5N \operatorname{tr}\left(\gamma_1^{\Psi}\left(1-\gamma_1^{\Psi}\right)\right)}\, \|A\|_{\mathrm{HS}}\,.
$$

Proof. By the previous proposition we can write the trace as

$$
\begin{aligned}
\operatorname{tr}\left(A\gamma_2^{\Psi,T}\right) &= \sum_{k,l,m,n=1}^{\infty} \left\langle \left(u_k \otimes u_l\right), A\left(u_m \otimes u_n\right)\right\rangle \left\langle \left(u_m \otimes u_n\right), \gamma_2^{\Psi,T}\left(u_k \otimes u_l\right)\right\rangle \\
&= \sum_{n=1}^{\infty} \left\langle c^*\left(\gamma_1^{\Psi} u_n\right)\Psi, \left(\sum_{k,l,m=1}^{\infty} \overline{A_{k,l,m,n}} c_m^* c_l c_k\right)^* \Psi\right\rangle \\
&\quad - \sum_{n=1}^{\infty} \left\langle \left(\sum_{k,l,m=1}^{\infty} \overline{A_{k,l,m,n}} c_m^* c_l c_k \Psi\right), c\left(\left(1-\gamma_1^{\Psi}\right)u_n\right)\Psi\right\rangle,
\end{aligned} \tag{2.15}
$$

so by Cauchy–Schwarz and Proposition 4

$$
\begin{aligned}
\left|\operatorname{tr}\left(A\gamma_2^{\Psi,T}\right)\right| &\leq \sqrt{\sum_{n=1}^{\infty}\left\langle \Psi, \sum_{n=1}^{\infty}\left\{\left(\sum_{k,l,m=1}^{\infty} \overline{A_{k,l,m,n}} c_m^* c_l c_k\right)^*, \sum_{k,l,m=1}^{\infty} \overline{A_{k,l,m,n}} c_m^* c_l c_k\right\}\Psi\right\rangle} \\
&\quad \cdot \sqrt{\sum_{n=1}^{\infty}\left(\left\|c^*\left(\gamma_1^{\Psi}u_n\right)\Psi\right\|^2 + \left\|c\left(\left(1-\gamma_1^{\Psi}\right)u_n\right)\Psi\right\|^2\right)} \\
&\leq \sqrt{5N \sum_{n=1}^{\infty}\left(\left\|c^*\left(\gamma_1^{\Psi}u_n\right)\Psi\right\|^2 + \left\|c\left(\left(1-\gamma_1^{\Psi}\right)u_n\right)\Psi\right\|^2\right)}\, \|A\|_{\mathrm{HS}}\,.
\end{aligned} \tag{2.16}
$$

Now we note that by the CAR

$$
\begin{aligned}
\sum_{n=1}^{\infty}\left\|c^*\left(\gamma_1^{\Psi}u_n\right)\Psi\right\|^2 &= \sum_{n=1}^{\infty}\left\langle \Psi, \left(\left\|\gamma_1^{\Psi}u_n\right\|^2 - c^*\left(\gamma_1^{\Psi}u_n\right)c\left(\gamma_1^{\Psi}u_n\right)\right)\Psi\right\rangle \\
&= \operatorname{tr}\left(\left(\gamma_1^{\Psi}\right)^2 - \left(\gamma_1^{\Psi}\right)^3\right) = \operatorname{tr}\left(\gamma_1^{\Psi}\left(\gamma_1^{\Psi} - \left(\gamma_1^{\Psi}\right)^2\right)\right)
\end{aligned} \tag{2.17}
$$

and

$$
\sum_{n=1}^{\infty}\left\|c\left(\left(1-\gamma_1^{\Psi}\right)u_n\right)\Psi\right\|^2 = \sum_{n=1}^{\infty}\left\langle \Psi, c^*\left(\left(1-\gamma_1^{\Psi}\right)u_n\right)c\left(\left(1-\gamma_1^{\Psi}\right)u_n\right)\Psi\right\rangle
$$

$$= \operatorname{tr}\left(\gamma_1^\Psi \left(1-\gamma_1^\Psi\right)^2\right) = \operatorname{tr}\left(\gamma_1^\Psi \left(1-2\gamma_1^\Psi + \left(\gamma_1^\Psi\right)^2\right)\right) \tag{2.18}$$

for the claim. □

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