Fermion Correlation Inequalities Derived from G- and P-Conditions

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Abstract. It is shown in this paper that the G-Condition and the P-Condition from representability imply the fermion correlation estimate from [1] which, in turn, is known to yield a nontrivial bound on the accuracy of the Hartree–Fock approximation for large Coulomb systems.

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1 Introduction

The dynamics of N electrons in an atom ($K = 1$) or molecule ($K \geq 2$) with K nuclei of charges $\underline{Z} := (Z_1, Z_2, \ldots, Z_K)$, fixed at positions $\underline{R} := (R_1, R_2, \ldots, R_K)$, is generated by the Hamiltonian

$$H^{(N)}(\underline{Z}, \underline{R}) := \sum_{n=1}^{N} \left(-\Delta_{x_n} - \sum_{j=1}^{K} \frac{Z_j}{|x_n - R_j|} \right) + \sum_{1 \leq n < m \leq N} \frac{1}{|x_n - x_m|} \quad (1)$$

to lowest order in the Born–Oppenheimer approximation. $H^{(N)}(\underline{Z}, \underline{R}) \equiv H^{(N)}$ is a semibounded, self-adjoint operator defined on a suitable dense domain

$\mathcal{D}^{(N)}$ in the Hilbert space $\mathcal{F}_{\mathrm{f}}^{(N)}[\mathfrak{h}]$ of antisymmetric N-electron wave functions, cf. (18) below.
Basic quantities of interest are the ground state energy

$$E_{\mathrm{gs}}^{(N)}(\underline{Z},\underline{R}) \;:=\; \inf\left\{\sigma\left\{H^{(N)}(\underline{Z},\underline{R})\right\}\right\},$$

whose variational characterization

$$E_{\mathrm{gs}}^{(N)}(\underline{Z},\underline{R}) = \inf\left\{\left\langle\Psi^{(N)}\middle|\, H^{(N)}\Psi^{(N)}\right\rangle\,\middle|\; \Psi^{(N)}\in\mathcal{D}^{(N)}\cap\mathcal{F}_{\mathrm{f}}^{(N)}[\mathfrak{h}],\ \|\Psi^{(N)}\|=1\right\} \tag{2}$$

is given by the Rayleigh–Ritz principle, and corresponding ground states $\Psi_{\mathrm{gs}}^{(N)}$, i.e., normalized solutions of the stationary Schrödinger equation

$$H^{(N)}(\underline{Z},\underline{R})\Psi_{\mathrm{gs}}^{(N)} \;=\; E_{\mathrm{gs}}^{(N)}(\underline{Z},\underline{R})\Psi_{\mathrm{gs}}^{(N)}.$$

The Hartree–Fock (HF) variational principle is an important method to obtain approximations to both, the ground state energy and ground states. The HF energy $E_{\mathrm{hf}}^{(N)}(\underline{Z},\underline{R})$ is defined by restricting the variation in (2) to $\mathcal{SD}^{(N)}[\mathfrak{h}]$,

$$\begin{aligned}&E_{\mathrm{hf}}^{(N)}(\underline{Z},\underline{R})\\ &\quad=\inf\left\{\left\langle\Phi^{(N)}\middle|\, H^{(N)}\Phi^{(N)}\right\rangle\,\middle|\; \Phi^{(N)}\in\mathcal{D}^{(N)}\cap\mathcal{SD}^{(N)}[\mathfrak{h}],\ \|\Phi^{(N)}\|=1\right\},\end{aligned} \tag{3}$$

where $\mathcal{SD}^{(N)}[\mathfrak{h}]\subseteq\mathcal{F}_{\mathrm{f}}^{(N)}[\mathfrak{h}]$ denotes the set of Slater determinants, i.e., the set of all antisymmetrized product vectors $\varphi_1\wedge\cdots\wedge\varphi_N$. Since the variation in (3), compared to (2), is restricted, we clearly have

$$E_{\mathrm{hf}}^{(N)}(\underline{Z},\underline{R}) \;\geq\; E_{\mathrm{gs}}^{(N)}(\underline{Z},\underline{R}).$$

A lower bound to the ground state energy by the HF energy minus an error which is small in the large-Z limit was obtained by one of us in [1, 2]. In the case of a neutral atom, i.e., $N=Z:=Z_1$ and $R_1=0$, the resulting estimate was

$$E_{\mathrm{gs}}^{(Z)}(Z) \;\geq\; E_{\mathrm{hf}}^{(Z)}(Z) - \mathcal{O}\big(Z^{(5/3)-\varepsilon}\big), \tag{4}$$

for some $\varepsilon>0$. The error term $\mathcal{O}(Z^{(5/3)-\varepsilon})$ is small compared to all three contributions to $E_{\mathrm{hf}}^{(Z)}(Z)$, namely, the kinetic, the classical electrostatic, and the exchange energy which are at least of size $cZ^{5/3}$ in magnitude for some constant $c>0$.
A key inequality derived in [1] that eventually lead to (4) is the fermion correlation estimate

$$\mathrm{tr}_2\left\{(X\otimes X)\Gamma^{(\mathrm{T})}\right\} \;\geq\; -\,\mathrm{tr}_1\left\{X\gamma\right\}\min\left\{1;\ \mathrm{const}\cdot\sqrt{\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}}\right\} \tag{5}$$

where $X = X^* = X^2$ is an orthogonal projection, $\Gamma^{(\mathrm{T})} := \Gamma - (1 - \mathrm{Ex})(\gamma \otimes \gamma)$, $\Gamma \equiv \Gamma_{\Phi^{(N)}}$ is the two-particle- and $\gamma \equiv \gamma_{\Phi^{(N)}}$ the one-particle density matrix of a normalized N-electron state $\Phi^{(N)} \in \mathcal{F}_{\mathrm{f}}^{(N)}[\mathfrak{h}]$.
The purpose of the present paper is to give an alternative derivation of (5) by using ideas originating from the theory of N-representability. More precisely, we show that (5) follows already from the G-Condition and the P-Condition specified by Garrod and Percus [8] and Coleman [4].
Observing that the Rayleigh–Ritz principle (2) can be rewritten as a variation over all N-representable two-particle density matrices Γ, we consequently obtain (4) from relaxing the requirement of N-representability of Γ to merely requiring Γ to fulfill the G-Condition and the P-Condition:

Theorem 1.1. *The G-Condition and the P-Condition imply* (5).

We note that (5) was also derived by Graf and Solovej in [13] by a different method that, in retrospective, resembles the application of Garrod and Percus' G-Condition. In fact, one part of the derivation in [13] follows already from the G-Condition. A main difference to using representability methods, however, lies in the use of operator inequalities in [13] which are necessarily formulated on the N-particle Hilbert space, as opposed to the one- or two-particle Hilbert spaces in the presented work.

In future work we plan to sharpen this result by making additional use of Erdahl's T_1- and T_2-Conditions [6, 5] which have recently lead to very good numerical results in quantum chemistry computations [3, 10, 11], as well as Coleman's Q-Condition which was also given in [4] but is not necessary for the derivation of our present result. Furthermore, similar representability conditions also exist for bosons [10]. There we like to adress the question whether analogous results can also be obtained.

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2 Density Matrices and Reduced Density Matrices

2.1 Fock space, Creation and Annihilation Operators

Let $\mathfrak{h}$ be a separable complex Hilbert space which we henceforth refer to as the one-particle Hilbert space. The fermion Fock space $\mathcal{F} \equiv \mathcal{F}_{\mathrm{f}}[\mathfrak{h}]$ is defined to be the orthogonal sum

$$\mathcal{F}_{\mathrm{f}}[\mathfrak{h}] := \bigoplus_{N=0}^{\infty} \mathcal{F}_{\mathrm{f}}^{(N)}[\mathfrak{h}],$$

where

$$\mathcal{F}_{\mathrm{f}}^{(N)}[\mathfrak{h}] := \bigwedge^N \mathfrak{h} := \mathcal{A}_N\Big(\bigotimes^N \mathfrak{h}\Big)$$

is the antisymmetric tensor product of N copies of $\mathfrak{h}$, for $N \geq 1$, and $\mathcal{F}_{\mathrm{f}}^{(0)}[\mathfrak{h}] := \mathbb{C}\cdot\Omega$, with Ω being the normalized vacuum vector. Here, $\mathcal{A}_N$ is the orthogonal projection from $\bigotimes^N \mathfrak{h}$ onto $\bigwedge^N \mathfrak{h}$ uniquely defined by

$$\begin{aligned}\mathcal{A}_N\left(\varphi_1 \otimes \cdots \otimes \varphi_N\right) &:= \frac{1}{N!}\sum_{\pi\in\mathcal{S}_N} (-1)^{\pi}\, \varphi_{\pi(1)} \otimes \cdots \otimes \varphi_{\pi(N)} \\ &=: \frac{1}{\sqrt{N!}}\varphi_1 \wedge \cdots \wedge \varphi_N,\end{aligned}$$

for $\varphi_1, \ldots, \varphi_N \in \mathfrak{h}$. It is convenient to introduce creation operators $c^*(f) \in \mathcal{B}(\mathcal{F})$ for any $f \in \mathfrak{h}$ by

$$c^*(f)\Omega := f, \tag{6}$$

$$c^*(f)\left(\varphi_1 \wedge \cdots \wedge \varphi_N\right) := f \wedge \varphi_1 \wedge \cdots \wedge \varphi_N \tag{7}$$

for $\varphi_1, \ldots, \varphi_N \in \mathfrak{h}$, and extension by linearity and continuity. By induction and (6)-(7)

$$\varphi_1 \wedge \varphi_2 \wedge \cdots \wedge \varphi_N = c^*(\varphi_1)c^*(\varphi_2)\cdots c^*(\varphi_N)\Omega \tag{8}$$

for all $\varphi_1, \varphi_2, \ldots, \varphi_N \in \mathfrak{h}$. If $\{\varphi_k\}_{k=1}^{\infty} \subseteq \mathfrak{h}$ is an orthonormal basis (ONB) of $\mathfrak{h}$, then for any $N \in \mathbb{N}$

$$\{c^*(\varphi_{k_1})\cdots c^*(\varphi_{k_N})\Omega|\ 1 \leq k_1 < k_2 < \cdots < k_N\} \subseteq \mathcal{F}_{\mathrm{f}}^{(N)}[\mathfrak{h}] \tag{9}$$

is an ONB of $\mathcal{F}_{\mathrm{f}}^{(N)}[\mathfrak{h}]$, and

$$\{c^*(\varphi_{k_1})\cdots c^*(\varphi_{k_N})\Omega|\ N \in \mathbb{N}_0,\ 1 \leq k_1 < k_2 < \cdots < k_N\} \subseteq \mathcal{F} \tag{10}$$

is an ONB of $\mathcal{F}$.
The adjoint operators $c(f) := \left(c^*(f)\right)^* \in \mathcal{B}(\mathcal{F})$, with $f \in \mathfrak{h}$, are the annihilation operators. Note that, while $f \mapsto c^*(f)$ is linear, $f \mapsto c(f)$ is antilinear. Together with the creation operators they fulfill the canonical anticommutation relations (CAR), i.e.,

$$\forall f, g \in \mathfrak{h}:\ \{c(f), c^*(g)\} = \langle f|g\rangle_{\mathfrak{h}}\cdot \mathbb{1}_{\mathcal{F}}, \quad \{c^*(f), c^*(g)\} = 0, \tag{11}$$

where $\{A, B\} := AB + BA$ denotes the anticommutator.
Moreover,

$$\forall f \in \mathfrak{h}:\ c(f)\Omega = 0, \tag{12}$$

and $\{c^*(f), c(f)|\ f \in \mathfrak{h}\}$ is completely determined by (6), (11) and (12), i.e., (7)-(10) follow from (6), (11) and (12). The creation and annihilation operators introduced here are a specific representation of the (abstract) CAR (11), namely the Fock representation. For φ_k being any element of a given ONB $\{\varphi_k\}_{k=1}^{\infty} \subseteq \mathfrak{h}$, we write

$$c_k^* \equiv c^*(\varphi_k),\ c_k \equiv c(\varphi_k).$$

An important unbounded, self-adjoint and positive operator on $\mathcal{F}$ is the number operator $\widehat{\mathbb{N}}$ defined by

$$\widehat{\mathbb{N}}\,(c^*(f_1)\cdots c^*(f_N)\Omega) := N \cdot c^*(f_1)\cdots c^*(f_N)\Omega$$

for any $f_1, \ldots, f_N \in \mathfrak{h}$. It is not difficult to see that

$$\widehat{\mathbb{N}} = \sum_{k=1}^{\infty} c_k^* c_k$$

as a quadratic form, for any ONB $\{\varphi_k\}_{k=1}^{\infty} \subseteq \mathfrak{h}$.

2.2 Density Matrices

A positive trace class operator $\rho \in \mathcal{L}_+^1(\mathcal{F})$ of unit trace, $\mathrm{tr}_{\mathcal{F}}\{\rho\} = 1$, is called density matrix. Given a density matrix ρ, the map $A \mapsto \mathrm{tr}_{\mathcal{F}}\{\rho\, A\}$ defines a state, i.e., a normalized, linear, and positive functional on $\mathcal{B}(\mathcal{F}) \ni A$. If $\Psi \in \mathcal{F}$ is a normalized vector, then $|\Psi\rangle\langle\Psi|$ is a density matrix (of rank one) called pure state. In this paper we study fermion systems with a repulsive interaction and whose dynamics preserve the particle number. For this reason we restrict our attention to density matrices which commute with the particle number operator and have a finite squared particle number expectation value,

$$\rho = \bigoplus_{N=0}^{\infty} \rho^{(N)}, \quad \text{and} \quad \left\langle \widehat{\mathbb{N}}^2 \right\rangle_{\rho} < \infty, \tag{13}$$

where here and henceforth we denote for any $A \in \mathcal{B}(\mathfrak{h})$

$$\langle A \rangle_{\rho} := \mathrm{tr}_{\mathcal{F}} \left\{ \rho^{\frac{1}{2}} A \rho^{\frac{1}{2}} \right\}.$$

Note that, if $m \neq n,\ m, n \geq 0$, then $\mathrm{tr}_{\mathcal{F}}\{\rho\, c^*(f_1)\cdots c^*(f_m) c(g_1)\cdots c(g_n)\} = 0$ for any choice of $f_1, \ldots, f_m, g_1, \ldots, g_n \in \mathfrak{h}$, due to (13).

2.3 Reduced Density Matrices

Given a density matrix $\rho \in \mathcal{L}_+^1(\mathcal{F})$ subject to (13), we introduce two bounded operators, $\gamma_\rho \in \mathcal{B}(\mathfrak{h})$ and $\Gamma_\rho \in \mathcal{B}(\mathfrak{h} \otimes \mathfrak{h})$, by

$$\forall f, g \in \mathfrak{h}:\ \langle f|\, \gamma_\rho g\rangle := \mathrm{tr}_{\mathcal{F}}\{\rho\, c^*(g) c(f)\} \tag{14}$$

and

$$\forall f_1, f_2, g_1, g_2 \in \mathfrak{h}: \ \langle f_1 \otimes f_2 | \, \Gamma_\rho(g_1 \otimes g_2) \rangle := \mathrm{tr}_{\mathcal{F}} \{ \rho \, c^*(g_2) c^*(g_1) c(f_1) c(f_2) \} \, . \tag{15}$$

γ_ρ is called the one-particle density matrix (1-pdm) and Γ_ρ the two-particle density matrix (2-pdm) corresponding to ρ. For any ONB $\{\varphi_k\}_{k=1}^\infty \subseteq \mathfrak{h}$ we define the exchange operator $\mathrm{Ex} \in \mathcal{B}(\mathfrak{h} \otimes \mathfrak{h})$ by

$$\mathrm{Ex} := \sum_{k,l=1}^{\infty} |\varphi_k \otimes \varphi_l\rangle \langle \varphi_l \otimes \varphi_k| \, , \tag{16}$$

such that $\mathrm{Ex}(f \otimes g) = g \otimes f$. Then the CAR leads to the antisymmetry property of Γ_ρ:

$$\mathrm{Ex}\, \Gamma_\rho = -\Gamma_\rho = \Gamma_\rho \, \mathrm{Ex}. \tag{17}$$

The following properties of the 1-pdm and the 2-pdm are easily proven (we denote $\mathrm{tr}_1 := \mathrm{tr}_{\mathfrak{h}}$ and $\mathrm{tr}_2 := \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}$):

LEMMA 2.1. *Let $\rho \in \mathcal{L}^1_+(\mathcal{F})$ be a density matrix obeying (13). Then the following assertions hold true:*

i) $\gamma_\rho \in \mathcal{L}^1_+(\mathfrak{h})$, $0 \leq \gamma_\rho \leq \mathbb{1}$, $\mathrm{tr}_1\{\gamma_\rho\} = \langle \widehat{\mathbb{N}} \rangle_\rho$, $\Gamma_\rho \in \mathcal{L}^1_+(\mathfrak{h} \otimes \mathfrak{h})$, $0 \leq \Gamma_\rho \leq \langle \widehat{\mathbb{N}} \rangle_\rho$, *and* $\mathrm{tr}_2\{\Gamma_\rho\} = \langle \widehat{\mathbb{N}}(\widehat{\mathbb{N}} - 1) \rangle_\rho$.

ii) If $\mathrm{Ran}\{\rho\} \subseteq \mathcal{F}_{\mathrm{f}}^{(N)}$, *then, for all* $f, g \in \mathfrak{h}$,

$$\langle f | \, \gamma_\rho g \rangle = \frac{1}{N-1} \sum_{k=1}^{\infty} \langle f \otimes \varphi_k | \, \Gamma_\rho(g \otimes \varphi_k) \rangle \, ,$$

where $\{\varphi_k\}_{k=1}^\infty \subseteq \mathfrak{h}$ *is an ONB.*

iii) Furthermore,

$$\rho = |c^*(\varphi_1) \cdots c^*(\varphi_N)\Omega\rangle \langle c^*(\varphi_1) \cdots c^*(\varphi_N)\Omega| \quad \Leftrightarrow \quad \gamma_\rho = \sum_{i=1}^{N} |\varphi_i\rangle \langle \varphi_i|$$

and, in this case,

$$\Gamma_\rho = (1 - \mathrm{Ex})(\gamma_\rho \otimes \gamma_\rho) \, .$$

2.4 Hamiltonian and Ground State Energy

Recall from (1) that the Hamiltonian of an atom or molecule is given by

$$H^{(N)}(\underline{Z},\underline{R}) := \sum_{n=1}^{N}\left(-\Delta_{x_n} - \sum_{k=1}^{K}\frac{Z_k}{|x_n - R_k|}\right) + \sum_{1\leq n<m\leq N}\frac{1}{|x_n - x_m|}. \quad (18)$$

Choosing an ONB $\{\varphi_k\}_{k=1}^{\infty} \subseteq \mathfrak{h} = \mathrm{L}^2\left(\mathbb{R}^3\times\mathbb{Z}_2\right)$ such that $\{\varphi_k\}_{k=1}^{\infty} \subseteq \mathrm{H}^2\left(\mathbb{R}^3\times\mathbb{Z}_2\right)$, where $\mathrm{H}^2\left(\mathbb{R}^3\times\mathbb{Z}_2\right)$ denotes the Sobolev space, we define

$$h_{kl} := \left\langle \varphi_k \middle| \left(-\Delta_x - \sum_{k=1}^{K}\frac{Z_k}{|x-R_k|}\right)\varphi_l \right\rangle,$$
$$V_{kl;mn} := \left\langle \varphi_k\otimes\varphi_l \middle| \frac{1}{|x-y|}\left(\varphi_m\otimes\varphi_n\right)\right\rangle,$$

and

$$\widehat{\mathbb{H}} := \sum_{k,l=1}^{\infty} h_{kl}\, c_k^* c_l + \sum_{k,l,m,n=1}^{\infty} V_{kl;mn}\, c_l^* c_k^* c_m c_n.$$

Stability of matter ensures that $\widehat{\mathbb{H}}+\mu\widehat{\mathbb{N}}$ is a semibounded self-adjoint operator, provided $\mu<\infty$ is sufficiently large. Moreover, the Hamiltonian of an atom or molecule can be viewed as

$$H^{(N)}(\underline{Z},\underline{R}) = \widehat{\mathbb{H}}\big|_{\mathcal{F}_{\mathrm{f}}^{(N)}[\mathfrak{h}]},$$

i.e., $H^{(N)}(\underline{Z},\underline{R})$ is the restriction of $\widehat{\mathbb{H}}$ to $\mathcal{F}_{\mathrm{f}}^{(N)}[\mathfrak{h}]$.
The ground state energy can now be reexpressed as

$$\begin{aligned} E_{\mathrm{gs}}^{(N)}(\underline{Z},\underline{R}) &= \inf\left\{\mathrm{tr}_{\mathcal{F}}\left\{\rho^{\frac{1}{2}}\widehat{\mathbb{H}}\rho^{\frac{1}{2}}\right\}\,\middle|\, \rho\in\mathcal{L}_+^1(\mathcal{F}),\ \widehat{\mathbb{N}}\,\rho = N\rho,\ \mathrm{tr}_{\mathcal{F}}\{\rho\}=1\right\} \\ &= \inf\left\{\mathcal{E}\left(\gamma_\rho,\Gamma_\rho\right)\,\middle|\, \rho\in\mathcal{L}_+^1(\mathcal{F}),\ \widehat{\mathbb{N}}\,\rho = N\rho,\ \mathrm{tr}_{\mathcal{F}}\{\rho\}=1\right\}, \end{aligned}$$

where the energy functional is defined as

$$\mathcal{E}\left(\gamma_\rho,\Gamma_\rho\right) := \mathrm{tr}_1\{h\gamma_\rho\} + \frac{1}{2}\,\mathrm{tr}_2\{V\Gamma_\rho\}.$$

We call $(\gamma,\Gamma)\in\mathcal{B}(\mathfrak{h})\times\mathcal{B}(\mathfrak{h}\otimes\mathfrak{h})$ N-representable if there exists a density matrix $\rho\in\mathcal{L}_+^1(\mathcal{F})$ with $\widehat{\mathbb{N}}\,\rho = N\rho$ and $\mathrm{tr}_{\mathcal{F}}\{\rho\}=1$ such that $\gamma=\gamma_\rho$ and $\Gamma=\Gamma_\rho$. Using the notion of N-representability, the ground state energy can be rewritten as

$$E_{\mathrm{gs}}^{(N)} = \inf\left\{\mathcal{E}\left(\gamma,\Gamma\right)\,\middle|\, (\gamma,\Gamma) \text{ is } N\text{-representable}\right\}.$$

By Lemma 2.1, we have that

$$E_{\mathrm{hf}}^{(N)} = \inf\left\{\mathcal{E}\Big(\gamma, (1-\mathrm{Ex})(\gamma\otimes\gamma)\Big)\,\Big|\, \gamma=\gamma^*=\gamma^2,\ \mathrm{tr}_1\{\gamma\}=N\right\},$$

and Lieb's variational principle [9, 1] ensures that actually

$$E_{\mathrm{hf}}^{(N)} = \inf\left\{\mathcal{E}\Big(\gamma, (1-\mathrm{Ex})(\gamma\otimes\gamma)\Big)\,\Big|\, 0\le\gamma\le 1,\ \mathrm{tr}_1\{\gamma\}=N\right\}.$$

3 G-, P- and Q-Conditions

In this section we derive necessary conditions on (γ,Γ) to be N-representable. To this end, we assume $N\in\mathbb{N}$, $\gamma\in\mathcal{L}^1(\mathfrak{h})$ with $0\le\gamma\le 1$ and $\mathrm{tr}_1\{\gamma\}=N$, $\Gamma\in\mathcal{L}^1(\mathfrak{h}\otimes\mathfrak{h})$, $\mathrm{Ex}\,\Gamma=\Gamma\,\mathrm{Ex}=-\Gamma$, and we call (γ,Γ) admissible in this case.

(P) (γ,Γ) fulfills the P-Condition

$$:\Leftrightarrow \Gamma\ge 0. \tag{19}$$

(G) (γ,Γ) fulfills the G-Condition

$$:\Leftrightarrow \forall A\in\mathcal{B}(\mathfrak{h}):\ \mathrm{tr}_2\{(A^*\otimes A)(\Gamma+\mathrm{Ex}(\gamma\otimes\mathbb{1}))\}\ge|\mathrm{tr}_1\{A\gamma\}|^2. \tag{20}$$

(Q) (γ,Γ) fulfills the Q-Condition

$$:\Leftrightarrow \Gamma+(1-\mathrm{Ex})(\mathbb{1}\otimes\mathbb{1}-\gamma\otimes\mathbb{1}-\mathbb{1}\otimes\gamma)\ge 0. \tag{21}$$

Our main result of this section is

Theorem 3.1. *Let $\rho\in\mathcal{L}^1(\mathcal{F})$ (not necessarily positive) such that $\mathrm{tr}_{\mathcal{F}}\{\rho\}=1$, $\mathrm{tr}_{\mathcal{F}}\left\{|\rho|^{\frac12}\widehat{\mathbb{N}}^2|\rho|^{\frac12}\right\}<\infty$, and that ρ preserves the particle number, i.e., $\left[\widehat{\mathbb{N}},\rho\right]=0$. Define γ_ρ and Γ_ρ by (14) and (15), respectively, and let $\{\varphi_k\}_{k=1}^\infty\subseteq\mathfrak{h}$ be an ONB. Then the following two statements are equivalent.*

(i) If $\mathcal{P}_r\in\mathcal{B}(\mathcal{F})$ is a polynomial in $\{c_k^*,c_k\}_{k=1}^\infty$ of degree $r\le 2$, then

$$\mathrm{tr}_{\mathcal{F}}\{\rho\,\mathcal{P}_r^*\mathcal{P}_r\}\ge 0. \tag{22}$$

(ii) $(\gamma_\rho,\Gamma_\rho)$ is admissible and fulfills the G-, P- and Q-Conditions.

Before we turn to the proof of Theorem 3.1, we establish its finite-dimensional analogue in Lemma 3.2 below. Theorem 3.1 then follows from Lemma 3.2 by a limiting argument.

Lemma 3.2. *Let $\rho\in\mathcal{L}^1(\mathcal{F})$ (not necessarily positive) such that $\mathrm{tr}_{\mathcal{F}}\{\rho\}=1$, $\mathrm{tr}_{\mathcal{F}}\left\{|\rho|^{\frac12}\widehat{\mathbb{N}}^2|\rho|^{\frac12}\right\}<\infty$, and that ρ preserves the particle number, i.e., $\left[\widehat{\mathbb{N}},\rho\right]=0$. Define γ_ρ and Γ_ρ by (14) and (15), respectively, and let $\{\varphi_k\}_{k=1}^\infty\subseteq\mathfrak{h}$ be an ONB. Then the following statements are equivalent.*

(i) If $\mathcal{P}_r \in \mathcal{B}(\mathcal{F})$ is a polynomial in $\{c_k^*, c_k\}_{k=1}^{\infty}$ of degree $r \leq 2$, then

$$\mathrm{tr}_{\mathcal{F}}\left\{\rho\, \mathcal{P}_r^* \mathcal{P}_r\right\} \geq 0. \tag{23}$$

(ii) For any $\phi \in \mathrm{span}\,\{\varphi_k|\ k \in \mathbb{N}\}$, $\Psi \in \mathrm{span}\,\{\varphi_k \otimes \varphi_l|\ k,l \in \mathbb{N}\}$, we have

$$0 \leq \langle \phi|\, \gamma_\rho \phi\rangle \leq 1, \tag{24}$$

$$\langle \Psi|\, \Gamma_\rho \Psi\rangle \geq 0, \tag{25}$$

$$\langle \Psi|\, (\Gamma_\rho + (1-\mathrm{Ex})(\mathbb{1}\otimes\mathbb{1} - \gamma_\rho \otimes \mathbb{1} - \mathbb{1}\otimes\gamma_\rho))\, \Psi\rangle \geq 0, \tag{26}$$

and, for all $A := \sum_{k,l=1}^{M} \alpha_{kl}\, |\varphi_k\rangle\langle\varphi_l|$, $M < \infty$, $(\alpha_{kl})_{k,l=1}^{M} \in \mathbb{C}^{M\times M}$,

$$\mathrm{tr}_2\left\{(A^* \otimes A)\,(\Gamma_\rho + \mathrm{Ex}\,(\gamma_\rho \otimes \mathbb{1}))\right\} \geq \left|\mathrm{tr}_1\left\{A\gamma_\rho\right\}\right|^2. \tag{27}$$

Proof. First we show *(i) ⇒ (ii)*. The properties (24)-(27) of $(\gamma_\rho, \Gamma_\rho)$ can be checked by suitable choices of $\mathcal{P}_r$.

a) The first inequality of (24) follows by choosing $\mathcal{P}_1 := \sum_{i=1}^{M} \overline{\alpha}_i c_i$, where $\alpha_i \in \mathbb{C}$ and $M < \infty$:

$$\begin{aligned} 0 \leq \mathrm{tr}_{\mathcal{F}}\left\{\rho\, \mathcal{P}_1^* \mathcal{P}_1\right\} &= \sum_{i,j=1}^{M} \alpha_i \overline{\alpha}_j \mathrm{tr}_{\mathcal{F}}\left\{\rho\, c_i^* c_j\right\} \\ &= \sum_{j=1}^{M}\sum_{i=1}^{M} \langle \alpha_j\varphi_j|\, \gamma_\rho(\alpha_i\varphi_i)\rangle = \left\langle \phi_M\right|\gamma_\rho\phi_M\left\rangle\right., \end{aligned} \tag{28}$$

with $\phi_M := \sum_{i=1}^{M} \alpha_i\varphi_i \in \mathrm{span}\,\{\varphi_k|\ k \in \mathbb{N}\}$. The second inequality derives from the CAR and $\mathcal{P}_1 := \sum_{i=1}^{M} \alpha_i c_i^*$:

$$\begin{aligned} 0 \leq \mathrm{tr}_{\mathcal{F}}\left\{\rho\, \mathcal{P}_1^* \mathcal{P}_1\right\} &= \sum_{i,j=1}^{M} \overline{\alpha}_i \alpha_j \mathrm{tr}_{\mathcal{F}}\left\{\rho\, c_i c_j^*\right\} \\ &= \sum_{i,j=1}^{M} \overline{\alpha}_i \alpha_j \mathrm{tr}_{\mathcal{F}}\left\{\rho\,(\delta_{ij} - c_j^* c_i)\right\} \\ &= \sum_{i=1}^{M}\sum_{j=1}^{M} \langle \alpha_i\varphi_i|\, (\mathbb{1}-\gamma_\rho)(\alpha_j\varphi_j)\rangle \\ &= \left\langle \phi_M\right|(\mathbb{1}-\gamma_\rho)\phi_M\left\rangle\right.. \end{aligned} \tag{29}$$

b) Property (27) is obtained by choosing $\mathcal{P}_2 := \mu + \frac{1}{2}\sum_{k,l=1}^{M} \alpha_{kl}\,(c_k^* c_l - c_l c_k^*)$ with $\mu, \alpha_{kl} \in \mathbb{C},\ M < \infty$ and calculating $\mathrm{tr}_{\mathcal{F}}\{\rho\,\mathcal{P}_2^*\mathcal{P}_2\}$:

$$\begin{aligned}
0 \leq \mathrm{tr}_{\mathcal{F}}\Big\{\rho\Big(\mu + \frac{1}{2}\sum_{k,l=1}^{M} \alpha_{kl}(c_k^* c_l - c_l c_k^*)\Big)^* \\
\times \Big(\mu + \frac{1}{2}\sum_{m,n=1}^{M} \alpha_{mn}(c_m^* c_n - c_n c_m^*)\Big)\Big\} \\
= \mathrm{tr}_{\mathcal{F}}\Big\{\rho\Big(\frac{1}{2}\sum_{k,l=1}^{M} \alpha_{kl}(c_k^* c_l - c_l c_k^*)\Big)^* \Big(\frac{1}{2}\sum_{m,n=1}^{M} \alpha_{mn}(c_m^* c_n - c_n c_m^*)\Big)\Big\} \\
+ 2\,\mathfrak{Re}\Big\{\overline{\mu}\,\mathrm{tr}_{\mathcal{F}}\Big\{\frac{1}{2}\,\rho\sum_{k,l=1}^{M} \alpha_{kl}(c_k^* c_l - c_l c_k^*)\Big\}\Big\} + |\mu|^2\,.
\end{aligned}$$

Now we expand the brackets and use the CAR to reorder the annihilation and creation operators:

$$\begin{aligned}
0 \leq \sum_{k,l,m,n=1}^{M} \overline{\alpha}_{kl}\alpha_{mn}\mathrm{tr}_{\mathcal{F}}\Big\{\rho\Big(- c_l^* c_m^* c_k c_n + \delta_{km} c_l^* c_n - \frac{1}{2}\delta_{kl} c_m^* c_n \\
- \frac{1}{2}\delta_{mn} c_l^* c_k + \frac{1}{4}\delta_{kl}\delta_{mn}\Big)\Big\} \\
+ 2\,\mathfrak{Re}\Big\{\overline{\mu}\sum_{k,l=1}^{M} \alpha_{kl}\mathrm{tr}_{\mathcal{F}}\Big\{\rho\Big(c_k^* c_l - \frac{1}{2}\delta_{kl}\Big)\Big\}\Big\} + |\mu|^2\,.
\end{aligned}$$

Bearing $\alpha_{kl} = \langle\varphi_k|\,A\varphi_l\rangle$ and $\mathrm{tr}_{\mathcal{F}}\{\rho\} = 1$ in mind, we derive from the definitions of Γ_ρ and γ_ρ that

$$\begin{aligned}
0 \leq \sum_{k,l,m,n=1}^{M} \Big\langle \varphi_k \otimes \varphi_n \Big|\Big(- \Gamma_\rho + \mathbb{1}\otimes\gamma_\rho - \frac{1}{2}\mathrm{Ex}\,(\gamma_\rho\otimes\mathbb{1}) - \frac{1}{2}\mathrm{Ex}\,(\mathbb{1}\otimes\gamma_\rho) \\
+ \frac{1}{4}\mathrm{Ex}\,(\mathbb{1}\otimes\mathbb{1})\Big)(\varphi_m\otimes\varphi_l)\Big\rangle \\
\times \big\langle \varphi_l\otimes\varphi_m\big|\,(A^*\otimes A)\,(\varphi_k\otimes\varphi_n)\big\rangle \\
+ 2\,\mathfrak{Re}\left\{\overline{\mu}\sum_{k,l=1}^{M} \langle\varphi_k|\,A\varphi_l\rangle\,\langle\varphi_l|\,\gamma_\rho\varphi_k\rangle - \frac{\overline{\mu}}{2}\sum_{k=1}^{M}\langle\varphi_k|\,A\varphi_k\rangle\right\} + |\mu|^2\,.
\end{aligned}$$

We can now perform the summations and arrive at

$$\begin{aligned}
0 \le \mathrm{tr}_2\Big\{ & \mathrm{Ex}\,(A^*\otimes A)\,\Big(-\Gamma_\rho + \mathbb{1}\otimes\gamma_\rho \\
& \qquad + \frac{1}{2}\mathrm{Ex}\Big(\frac{1}{2}\mathbb{1}\otimes\mathbb{1} - \mathbb{1}\otimes\gamma_\rho - \gamma_\rho\otimes\mathbb{1}\Big)\Big)\Big\} \\
& + 2\,\mathfrak{Re}\left\{\overline{\mu}\,\mathrm{tr}_1\,\{A\gamma_\rho\} - \frac{\overline{\mu}}{2}\,\mathrm{tr}_1\,\{A\}\right\} + |\mu|^2 \\
= \mathrm{tr}_2\Big\{ & (A^*\otimes A)\Big(\Gamma_\rho + (\mathbb{1}\otimes\gamma_\rho)\mathrm{Ex} + \frac{1}{4}\mathbb{1}\otimes\mathbb{1} - \frac{1}{2}(\mathbb{1}\otimes\gamma_\rho + \gamma_\rho\otimes\mathbb{1})\Big)\Big\} \\
& + 2\,\mathfrak{Re}\left\{\overline{\mu}\,\mathrm{tr}_1\,\{A\gamma_\rho\} - \frac{\overline{\mu}}{2}\,\mathrm{tr}_1\,\{A\}\right\} + |\mu|^2\,. \qquad (30)
\end{aligned}$$

Defining $s \in \mathbb{C}$ by $\mu =: \left(s + \frac{1}{2}\right)\mathrm{tr}_1\,\{A\}$, the inequality can be rewritten as

$$\begin{aligned}
0 \le \mathrm{tr}_{\mathcal{F}}\Big\{ & \rho\Big(\mu + \frac{1}{2}\sum_{k,l=1}^{M}\alpha_{kl}(c_k^*c_l - c_lc_k^*)\Big)^* \\
& \qquad \times\left(\mu + \frac{1}{2}\sum_{m,n=1}^{M}\alpha_{mn}(c_m^*c_n - c_nc_m^*)\right)\Big\} \\
= \mathrm{tr}_2\Big\{ & (A^*\otimes A)\Big(\Gamma_\rho + |s|^2\,\mathbb{1}\otimes\mathbb{1} + \overline{s}\,\mathbb{1}\otimes\gamma_\rho + s\,\gamma_\rho\otimes\mathbb{1} + (\mathbb{1}\otimes\gamma_\rho)\mathrm{Ex}\Big)\Big\}. \qquad (31)
\end{aligned}$$

This inequality is valid for all s. We first assume that $\mathrm{tr}_1\,\{A\} = \sum_{i=1}^{M}\alpha_{ii} \neq 0$, then the choice $s := -\frac{\mathrm{tr}_1\{A\gamma\}}{\mathrm{tr}_1\{A\}}$ optimizes the inequality. The conclusion is (27):

$$\mathrm{tr}_2\,\{(A^*\otimes A)\,(\Gamma_\rho + \mathrm{Ex}\,(\gamma_\rho\otimes\mathbb{1}))\} - |\mathrm{tr}_1\,\{A\gamma_\rho\}|^2 \ge 0. \qquad (32)$$

Note that (31) and (32) are equivalent because (32) implies (31) by

$$\begin{aligned}
\mathrm{tr}_2\,\{(A^*\otimes A)\,(\Gamma_\rho + \mathrm{Ex}\,(\gamma_\rho\otimes\mathbb{1}))\} & \ge |\mathrm{tr}_1\,\{A\gamma_\rho\}|^2 \\
& \ge -\mathrm{tr}_2\left\{(A^*\otimes A)\left(|s|^2\,\mathbb{1}\otimes\mathbb{1} + \overline{s}\,\mathbb{1}\otimes\gamma_\rho + s\,\gamma_\rho\otimes\mathbb{1}\right)\right\}.
\end{aligned}$$

Conversely, if $\mathrm{tr}_1\,\{A\} = 0$, the choice $\mu = -\,\mathrm{tr}_1\,\{A\gamma\}$ in (30) leads directly to (32).

c) Inserting $\mathcal{P}_2 := \sum_{k,l=1}^{M} \overline{\alpha}_{kl} c_k c_l$ into (23) yields inequality (25):

$$\begin{aligned} 0 &\leq \mathrm{tr}_{\mathcal{F}}\Big\{\rho\Big(\sum_{k,l=1}^{M} \overline{\alpha}_{kl} c_k c_l\Big)^* \Big(\sum_{m,n=1}^{M} \overline{\alpha}_{mn} c_m c_n\Big)\Big\} \\ &= \sum_{k,l,m,n=1}^{M} \alpha_{kl}\overline{\alpha}_{mn} \mathrm{tr}_{\mathcal{F}}\left\{\rho\, c_l^* c_k^* c_m c_n\right\}. \end{aligned}$$

By the definition of Γ_ρ one finds

$$\begin{aligned} 0 &\leq \sum_{k,l,m,n=1}^{M} \alpha_{kl}\overline{\alpha}_{mn} \left\langle \varphi_m \otimes \varphi_n \middle| \Gamma_\rho(\varphi_k \otimes \varphi_l)\right\rangle \\ &= \left\langle \Psi_M \middle| \Gamma_\rho \Psi_M \right\rangle, \end{aligned} \tag{33}$$

where $\Psi_M := \sum_{i,j=1}^{M} \alpha_{ij} (\varphi_i \otimes \varphi_j) \in \mathrm{span}\{\varphi_k \otimes \varphi_l |\ k,l \in \mathbb{N}\}$.

d) Inequality (26) follows from (23) by choosing $\mathcal{P}_2 := \sum_{k,l=1}^{M} \alpha_{kl} c_k^* c_l^*$:

$$\begin{aligned} 0 &\leq \mathrm{tr}_{\mathcal{F}}\Big\{\rho\Big(\sum_{k,l=1}^{M} \alpha_{kl} c_k^* c_l^*\Big)^* \Big(\sum_{m,n=1}^{M} \alpha_{mn} c_m^* c_n^*\Big)\Big\} \\ &= \sum_{k,l,m,n=1}^{M} \overline{\alpha}_{kl}\alpha_{mn} \mathrm{tr}_{\mathcal{F}}\left\{\rho\, c_l c_k c_m^* c_n^*\right\}. \end{aligned}$$

By normal-ordering using the CAR, one establishes the required relationship to Γ_ρ and γ_ρ:

$$\begin{aligned} 0 \leq \sum_{k,l,m,n=1}^{M} & \overline{\alpha}_{kl}\alpha_{mn} \mathrm{tr}_{\mathcal{F}}\big\{\rho\,\big(c_m^* c_n^* c_l c_k - \delta_{ln} c_m^* c_k + \delta_{kn} c_m^* c_l + \delta_{lm} c_n^* c_k \\ & - \delta_{km} c_n^* c_l - \delta_{lm}\delta_{kn} + \delta_{km}\delta_{ln}\big)\big\} \\ = \Bigg\langle \sum_{k,l=1}^{M} \alpha_{kl}(\varphi_l \otimes \varphi_k) \Bigg| & \Big(\Gamma_\rho + (1-\mathrm{Ex})(\mathbb{1}\otimes\mathbb{1} - \gamma_\rho \otimes \mathbb{1} - \mathbb{1}\otimes\gamma_\rho)\Big) \\ & \times \Bigg(\sum_{m,n=1}^{M} \alpha_{mn}(\varphi_n \otimes \varphi_m)\Bigg)\Bigg\rangle \\ = \Big\langle \Psi_M \Big| & \Big(\Gamma_\rho + (1-\mathrm{Ex})(\mathbb{1}\otimes\mathbb{1} - \gamma_\rho \otimes \mathbb{1} - \mathbb{1}\otimes\gamma_\rho)\Big)\Psi_M\Big\rangle. \end{aligned} \tag{34}$$

Next we prove *(ii)* ⇒ *(i)*. Thus, we assume (24)-(27).

e) A general polynomial of degree $r \leq 1$ is of the form $\mathcal{P}_1 = \sum_{k=1}^{M} (\alpha_k c_k^* + \beta_k c_k) + \mu$ with $\mu, \alpha_k, \beta_k \in \mathbb{C}$. This means we have to consider

$$\mathrm{tr}_{\mathcal{F}} \{\rho \mathcal{P}_1^* \mathcal{P}_1\} = \sum_{k,l=1}^{M} \mathrm{tr}_{\mathcal{F}} \{\rho (\alpha_k c_k^* + \beta_k c_k + \mu)^* (\alpha_l c_l^* + \beta_l c_l + \mu)\}. \quad (35)$$

We expand the product on the right side of (35) and compute the traces, taking into account that $\mathrm{tr}_{\mathcal{F}} \{\rho c_i^*\} = \mathrm{tr}_{\mathcal{F}} \{\rho c_i\} = \mathrm{tr}_{\mathcal{F}} \{\rho c_i^* c_j^*\} = \mathrm{tr}_{\mathcal{F}} \{\rho c_i c_j\} = 0$ for every i, j since ρ preserves the particle number. Therefore, only three terms in (35) are non-vanishing,

$$\mathrm{tr}_{\mathcal{F}} \{\rho \mathcal{P}_1^* \mathcal{P}_1\} = \sum_{k,l=1}^{M} \mathrm{tr}_{\mathcal{F}} \left\{\rho \left((\alpha_k c_k^*)^* (\alpha_l c_l^*) + (\beta_k c_k)^* (\beta_k c_k)\right)\right\} + |\mu|^2,$$

where we additionally use $\mathrm{tr}_{\mathcal{F}} \{\rho\} = 1$. The sum over the terms in braces is non-negative due to (28) and (29). The conclusion is $\mathrm{tr}_{\mathcal{F}} \{\rho \mathcal{P}_1^* \mathcal{P}_1\} \geq 0$.

f) For $r \leq 2$ we have a general polynomial given by

$$\mathcal{P}_2 = \nu + \sum_{k=1}^{M} (\alpha_k c_k^* + \beta_k c_k) + \sum_{k,l=1}^{M} \alpha_{kl} c_k^* c_l^* + \sum_{k,l=1}^{M} \beta_{kl} c_k c_l + \sum_{k,l=1}^{M} \kappa_{kl} c_k^* c_l + \sum_{k,l=1}^{M} \eta_{kl} c_k c_l^*,$$

where $\nu, \alpha_k, \beta_k, \alpha_{kl}, \beta_{kl}, \kappa_{kl}, \eta_{kl} \in \mathbb{C}$, for all $1 \leq k, l \leq M$. Using the CAR, we rewrite $\mathcal{P}_2$ as

$$\mathcal{P}_2 = \mathcal{P}_1 + \mathcal{P}_{2,\alpha} + \mathcal{P}_{2,\beta} + \mathcal{P}_{2,\eta},$$

where

$$\mathcal{P}_1 := \mu + \sum_{k=1}^{M} (\alpha_k c_k^* + \beta_k c_k), \qquad \mathcal{P}_{2,\alpha} := \sum_{k,l=1} \alpha_{kl} c_k^* c_k^*,$$

$$\mathcal{P}_{2,\beta} := \sum_{k=1}^{M} \beta_{kl} c_k c_l, \qquad \mathcal{P}_{2,\theta} := \sum_{k,l=1}^{M} \theta_{kl} (c_k^* c_l - c_l c_k^*),$$

and

$$\mu := \nu + \frac{1}{2} \sum_{k=1}^{M} (\kappa_{kk} + \eta_{kk}), \quad \theta_{kl} := \frac{1}{2} (\kappa_{kl} - \eta_{lk}).$$

Then

$$\begin{aligned}
&\mathrm{tr}_{\mathcal{F}}\left\{\rho\,\mathcal{P}_2^*\mathcal{P}_2\right\}\\
&\quad=\mathrm{tr}_{\mathcal{F}}\left\{\rho\left(\mathcal{P}_1^*+\mathcal{P}_{2,\alpha}^*+\mathcal{P}_{2,\beta}^*+\mathcal{P}_{2,\eta}^*\right)\left(\mathcal{P}_1+\mathcal{P}_{2,\alpha}+\mathcal{P}_{2,\beta}+\mathcal{P}_{2,\theta}\right)\right\}\\
&\quad=\mathrm{tr}_{\mathcal{F}}\left\{\rho\,\mathcal{P}_1^*\mathcal{P}_1\right\}+\mathrm{tr}_{\mathcal{F}}\left\{\rho\,\mathcal{P}_{2,\alpha}^*\mathcal{P}_{2,\alpha}\right\}+\mathrm{tr}_{\mathcal{F}}\left\{\rho\,\mathcal{P}_{2,\beta}^*\mathcal{P}_{2,\beta}\right\}\\
&\qquad\qquad+\mathrm{tr}_{\mathcal{F}}\left\{\rho\,\mathcal{P}_{2,\theta}^*\mathcal{P}_{2,\theta}\right\},
\end{aligned}$$

where we use that $\mathrm{tr}_{\mathcal{F}}\{\rho\,\mathcal{P}_a^*\mathcal{P}_b\}=0$ whenever $a\neq b$, since ρ conserves the particle number. Now, e) implies $\mathrm{tr}_{\mathcal{F}}\{\rho\,\mathcal{P}_1^*\mathcal{P}_1\}\geq 0$, (34) yields $\mathrm{tr}_{\mathcal{F}}\left\{\rho\,\mathcal{P}_{2,\alpha}^*\mathcal{P}_{2,\alpha}\right\}\geq 0$ (see d)), (33) yields $\mathrm{tr}_{\mathcal{F}}\left\{\rho\,\mathcal{P}_{2,\beta}^*\mathcal{P}_{2,\beta}\right\}\geq 0$ (see c)), and $\mathrm{tr}_{\mathcal{F}}\left\{\rho\,\mathcal{P}_{2,\theta}^*\mathcal{P}_{2,\theta}\right\}\geq 0$ follows from (32), see b). Hence, $\mathrm{tr}_{\mathcal{F}}\{\rho\,\mathcal{P}_2^*\mathcal{P}_2\}\geq 0$.

□

Lemma 3.2 is the algebraic part of the proof of Theorem 3.1. To conclude, we have to extend the proof to infinite dimensions.

Proof of Theorem 3.1. Since *(ii)* contains (24)-(27) of Lemma 3.2, the implication *(ii)* ⇒ *(i)* is obvious. For *(i)* ⇒ *(ii)*, let ϕ,ψ and Φ,Ψ be normalized vectors in $\mathfrak{h}$ and $\mathfrak{h}\otimes\mathfrak{h}$, respectively, and set $\alpha_i:=\langle\varphi_i|\phi\rangle$, $\beta_i:=\langle\varphi_i|\psi\rangle$ and $\alpha_{ij}:=\langle\varphi_i\otimes\varphi_j|\Phi\rangle$, $\beta_{ij}:=\langle\varphi_i\otimes\varphi_j|\Psi\rangle$ for all $i,j\in\mathbb{N}$. For $M\in\mathbb{N}$, we define the orthogonal projection $P_M:=\sum_{k=1}^{M}|\varphi_k\rangle\langle\varphi_k|$ and set $\phi_M:=P_M\phi=\sum_{i=1}^{M}\alpha_i\varphi_i$ and $\Psi_M:=(P_M\otimes P_M)\,\Psi=\sum_{i,j=1}^{M}\beta_{ij}\,(\varphi_i\otimes\varphi_j)$. The admissibility and the G-, P-, and Q-Condititions follow from Lemma 3.2 as follows:

a) For the 1-pdm we have $\|\gamma_\rho\|_{\mathrm{op}}<\infty$, since

$$\begin{aligned}
|\langle\phi|\,\gamma_\rho\psi\rangle|&=|\mathrm{tr}_{\mathcal{F}}\{\rho\,c^*(\psi)c(\phi)\}|\\
&\leq\mathrm{tr}_{\mathcal{F}}\{|\rho|\}\,\|\psi\|\|\phi\|=\mathrm{tr}_{\mathcal{F}}\{|\rho|\}<\infty
\end{aligned}$$

by the Cauchy–Schwarz inequality and $c^*(\phi)c(\phi)\leq\mathbb{1}\,\langle\phi|\phi\rangle$. Afterwards, we infer by the triangle inequality

$$\begin{aligned}
|\langle\phi|\,\gamma_\rho\phi\rangle-\langle\phi_M|\,\gamma_\rho\phi_M\rangle|&=|\langle\phi-\phi_M|\,\gamma_\rho\phi\rangle+\langle\phi_M|\,\gamma_\rho(\phi-\phi_M)\rangle|\\
&\leq|\langle\phi-\phi_M|\,\gamma_\rho\phi\rangle|+|\langle\phi_M|\,\gamma_\rho(\phi-\phi_M)\rangle|\\
&\leq\|\phi-\phi_M\|\,(\|\phi\|+\|\phi_M\|)\,\|\gamma_\rho\|_{\mathrm{op}}\\
&\leq 2\,\|\phi-\phi_M\|\|\gamma_\rho\|_{\mathrm{op}}.
\end{aligned}\tag{36}$$

As $M\to\infty$, $\|\phi-\phi_M\|$ vanishes and we conclude with $\langle\phi_M|\,\gamma_\rho\phi_M\rangle\geq 0$ that also $\langle\phi|\,\gamma_\rho\phi\rangle\geq 0$ for all $\phi\in\mathfrak{h}$. The same argument with γ_ρ replaced by $\mathbb{1}-\gamma_\rho$ leads to $\langle\phi|\,(\mathbb{1}-\gamma_\rho)\phi\rangle\geq 0$ for all $\phi\in\mathfrak{h}$.

b) $\gamma_\rho \in \mathcal{L}^1(\mathfrak{h})$ follows by monotone convergence since $\gamma_\rho \geq 0$. For any ONB $\{\psi_i\}_{i=1}^\infty \subseteq \mathfrak{h}$ and $\epsilon > 0$, we have

$$\begin{aligned}\sum_{k=1}^\infty \langle \psi_k | \, \gamma_\rho \psi_k \rangle &\leq \sup_M \left\{ \sum_{k=1}^M \mathrm{tr}_\mathcal{F} \{\rho \, c_k^* c_k\} \right\} \\ &= \sup_M \left\{ \mathrm{tr}_\mathcal{F} \left\{ \rho \sum_{k=1}^M c_k^* c_k \right\} \right\} \\ &= (N+\epsilon) \sup_M \left\{ \mathrm{tr}_\mathcal{F} \left\{ \rho \left(\frac{1}{\widehat{\mathbb{N}}+\epsilon} \right)^{\frac{1}{2}} \left(\sum_{k=1}^M c_k^* c_k \right) \left(\frac{1}{\widehat{\mathbb{N}}+\epsilon} \right)^{\frac{1}{2}} \right\} \right\} \\ &\leq (N+\epsilon) \, \mathrm{tr}_\mathcal{F} \{|\rho|\} < \infty,\end{aligned}$$

since $\widehat{\mathbb{N}} \, \rho = N\rho$ and $\left\| \left(\frac{1}{\widehat{\mathbb{N}}+\epsilon} \right)^{\frac{1}{2}} \left(\sum_{k=1}^M c_k^* c_k \right) \left(\frac{1}{\widehat{\mathbb{N}}+\epsilon} \right)^{\frac{1}{2}} \right\|_{\mathrm{op}} \leq 1$.

c) Thanks to b) we can compute $\sum_{k=1}^\infty \langle \varphi_k | \, \gamma_\rho \varphi_k \rangle$ using monotone convergence and $\widehat{\mathbb{N}} \, \rho = N\rho$. This gives the trace of γ_ρ.

$$\begin{aligned}\mathrm{tr}_1 \{\gamma_\rho\} &:= \sum_{k=1}^\infty \langle \varphi_k | \, \gamma_\rho \varphi_k \rangle = \sum_{k=1}^\infty \mathrm{tr}_\mathcal{F} \{\rho \, c_k^* c_k\} \\ &= \mathrm{tr}_\mathcal{F} \left\{ \rho \sum_{k=1}^\infty c_k^* c_k \right\} = \mathrm{tr}_\mathcal{F} \left\{ \rho \, \widehat{\mathbb{N}} \right\} = N.\end{aligned}$$

d) For any basis of $\mathfrak{h}$, the identities $\mathrm{Ex} \, \Gamma_\rho = \Gamma_\rho \, \mathrm{Ex} = -\Gamma_\rho$ are a consequence of the definition of Γ_ρ and the CAR.

e) We conclude from the definition of Γ_ρ by the Cauchy–Schwarz inequality

$$\begin{aligned}|\langle \Psi | \, \Gamma_\rho \Phi \rangle| &= \left| \mathrm{tr}_\mathcal{F} \left\{ \rho \left(\sum_{m,n=1}^\infty \beta_{mn} c_n c_m \right)^* \left(\sum_{k,l=1}^\infty \alpha_{kl} c_l c_k \right) \right\} \right| \\ &\leq \mathrm{tr}_\mathcal{F} \{|\rho|\} \, \|\Psi\| \|\Phi\| = \mathrm{tr}_\mathcal{F} \{|\rho|\} < \infty.\end{aligned}$$

Therefore, we have $\|\Gamma_\rho\|_{\mathrm{op}} < \infty$. Afterwards, we infer analogously to (36)

$$|\langle \Psi | \, \Gamma_\rho \Psi \rangle - \langle \Psi_M | \, \Gamma_\rho \Psi_M \rangle| \leq 2 \, \|\Psi - \Psi_M\| \|\Gamma_\rho\|_{\mathrm{op}},$$

which tends to zero as $M \to \infty$ due to the definition of Ψ_M. With $\langle \Psi_M | \, \Gamma_\rho \Psi_M \rangle \geq 0$ from (33), this means $\langle \Psi | \, \Gamma_\rho \Psi \rangle \geq 0$ for all $\Psi \in \mathfrak{h} \otimes \mathfrak{h}$.

f) To prove that $\Gamma_\rho \in \mathcal{L}^1(\mathfrak{h} \otimes \mathfrak{h})$ we show that there is an ONB $\{\psi_i\}_{i=1}^\infty \subseteq \mathfrak{h}$ such that $\sum_{k,l=1}^\infty \langle \psi_k \otimes \psi_l | \, \Gamma_\rho (\psi_k \otimes \psi_l) \rangle$ is finite, again using $\Gamma_\rho \geq 0$. For

any $\epsilon > 0$ we have, using $\widehat{\mathbb{N}}\,\rho = N\rho$ and monotone convergence,

$$\begin{aligned}
\sum_{k,l=1}^{\infty} \langle \psi_k \otimes \psi_l | \, \Gamma_\rho(\psi_k \otimes \psi_l) \rangle &\leq \sup_M \Big\{ \sum_{k,l=1}^{M} \operatorname{tr}_{\mathcal{F}} \{ \rho \, c_l^* c_k c_k^* c_l \} \Big\} \\
&= \sup_M \Big\{ \operatorname{tr}_{\mathcal{F}} \Big\{ \rho \Big[\Big(\sum_{k=1}^{M} c_k^* c_k \Big)^2 - \Big(\sum_{k=1}^{M} c_k^* c_k \Big) \Big] \Big\} \Big\} \\
&\leq \sup_M \Big\{ \big(N^2 + \epsilon\big) \operatorname{tr}_{\mathcal{F}} \Big\{ |\rho| \Big(\frac{1}{\widehat{\mathbb{N}}^2 + \epsilon} \Big)^{\frac{1}{2}} \Big(\sum_{k=1}^{M} c_k^* c_k \Big)^2 \Big(\frac{1}{\widehat{\mathbb{N}}^2 + \epsilon} \Big)^{\frac{1}{2}} \Big\} \Big\} \\
&\leq \big(N^2 + \epsilon\big) \operatorname{tr}_{\mathcal{F}} \{ |\rho| \} < \infty
\end{aligned}$$

since $\sum\limits_{k=1}^{M} c_k^* c_k \geq 0$ and, due to $\Big(\sum\limits_{k=1}^{M} c_k^* c_k \Big)^2 \leq \widehat{\mathbb{N}}^2$,

$$\Big\| \Big(\frac{1}{\widehat{\mathbb{N}}^2 + \epsilon} \Big)^{\frac{1}{2}} \Big(\sum_{k=1}^{M} c_k^* c_k \Big)^2 \Big(\frac{1}{\widehat{\mathbb{N}}^2 + \epsilon} \Big)^{\frac{1}{2}} \Big\|_{\mathrm{op}} \leq 1.$$

g) To check (32) for any bounded A (not necessarily of finite rank) we abbreviate $\Lambda_{\mathrm{G}} := \Gamma_\rho + \operatorname{Ex}(\gamma_\rho \otimes \mathbb{1}) - \gamma_\rho \otimes \gamma_\rho$ and set $A_M := P_M A P_M$. Clearly, A_M is of finite rank and we observe

$$\begin{aligned}
&\big| \operatorname{tr}_2 \{ (A^* \otimes A) \, \Lambda_{\mathrm{G}} \} - \operatorname{tr}_2 \{ (A_M^* \otimes A_M) \, \Lambda_{\mathrm{G}} \} \big| \\
&\quad = \big| \operatorname{tr}_2 \big\{ \big[(A - A_M)^* \otimes A + A_M^* \otimes (A - A_M) \big] \, \Lambda_{\mathrm{G}} \big\} \big| \\
&\quad = \Big| \operatorname{tr}_2 \Big\{ \Big[\big(P_M A^* P_M^\perp + P_M^\perp A^* P_M + P_M^\perp A^* P_M^\perp \big) \otimes A \\
&\qquad\qquad + A_M^* \otimes \big(P_M^\perp A P_M + P_M A P_M^\perp + P_M^\perp A P_M^\perp \big) \Big] \Lambda_{\mathrm{G}} \Big\} \Big| \qquad (37)
\end{aligned}$$

using $P_M^\perp := \mathbb{1} - P_M$. For $\big| \operatorname{tr}_2 \big\{ \big(P_M^\perp A^* P_M \otimes A \big) \, \Lambda_{\mathrm{G}} \big\} \big|$, for instance, we find

$$\begin{aligned}
&\big| \operatorname{tr}_2 \big\{ \big(P_M^\perp A^* P_M \otimes A \big) \, \Lambda_{\mathrm{G}} \big\} \big| \\
&\quad = \big| \operatorname{tr}_2 \big\{ \big(P_M^\perp A^* P_M \otimes A \big) \, \Gamma_\rho \big\} + \operatorname{tr}_1 \big\{ P_M^\perp A^* P_M \gamma_\rho A \big\} \\
&\qquad\qquad - \operatorname{tr}_1 \big\{ P_M^\perp A^* P_M \gamma_\rho \big\} \operatorname{tr}_1 \{ A \gamma_\rho \} \big| \\
&\quad \leq \big| \operatorname{tr}_2 \big\{ \big(P_M^\perp A^* P_M \otimes A \big) \, \Gamma_\rho \big\} \big| + \big| \operatorname{tr}_1 \big\{ P_M^\perp A^* P_M \gamma_\rho A \big\} \big| \\
&\qquad\qquad + \big| \operatorname{tr}_1 \big\{ P_M^\perp A^* P_M \gamma_\rho \big\} \operatorname{tr}_1 \{ A \gamma_\rho \} \big| \, . \qquad (38)
\end{aligned}$$

Since $\Gamma_\rho \geq 0$ due to the P-Condition (see e)), $P_M^\perp, P_M \geq 0$ and $\widehat{\mathbb{N}}\,\rho = N\rho$ we have on the one hand

$$\begin{aligned}
\big| \operatorname{tr}_2 \big\{ \big(P_M^\perp A^* P_M \otimes A \big) \, \Gamma_\rho \big\} \big| &\leq \|A\|_{\mathrm{op}}^2 \operatorname{tr}_2 \big\{ \big(P_M^\perp \otimes \mathbb{1} \big) \, \Gamma_\rho \big\} \\
&= (N-1) \, \|A\|_{\mathrm{op}}^2 \operatorname{tr}_1 \big\{ P_M^\perp \gamma_\rho \big\} \, ,
\end{aligned}$$

and on the other hand with $0 \leq \gamma_\rho \leq \mathbb{1}$ and $P_M \leq \mathbb{1}$

$$\left|\mathrm{tr}_1\left\{P_M^\perp A^* P_M \gamma_\rho A\right\}\right| \leq \|A\|_{\mathrm{op}}^2 \,\mathrm{tr}_1\left\{P_M^\perp \gamma_\rho\right\},$$

and

$$\left|\mathrm{tr}_1\left\{P_M^\perp A^* P_M \gamma_\rho\right\} \mathrm{tr}_1\left\{A\gamma_\rho\right\}\right| \leq N\,\|A\|_{\mathrm{op}}^2 \,\mathrm{tr}_1\left\{P_M^\perp \gamma_\rho\right\}.$$

Note that $\mathrm{tr}_1\left\{P_M^\perp \gamma_\rho\right\} = \sum_{k=M+1}^{\infty} \langle\varphi_k|\,\gamma_\rho\varphi_k\rangle \to 0$, as $M \to \infty$, since $\sum_{k=1}^{\infty} \langle\varphi_k|\,\gamma_\rho\varphi_k\rangle = \mathrm{tr}_1\{\gamma_\rho\} = N$ is convergent. Analogously, one finds that all terms on the right hand side of (37) tend to zero, as $M \to \infty$. This, in turn, implies $\mathrm{tr}_2\{(A^* \otimes A)\,\Lambda_{\mathrm{G}}\} \geq 0$ for any bounded A since $\mathrm{tr}_2\{(A_M^* \otimes A_M)\,\Lambda_{\mathrm{G}}\} \geq 0$ due to (32).

h) Again by the Cauchy–Schwarz inequality we find

$$\begin{aligned}
&\left|\left\langle\Psi\middle|\Big(\Gamma_\rho + (1-\mathrm{Ex})(\mathbb{1}\otimes\mathbb{1} - \gamma_\rho\otimes\mathbb{1} - \mathbb{1}\otimes\gamma_\rho)\Big)\Phi\right\rangle\right| \\
&\qquad = \left|\mathrm{tr}_{\mathcal{F}}\left\{\rho\left(\sum_{m,n=1}^{\infty} \overline{\beta}_{mn} c_m c_n\right)\left(\sum_{k,l=1}^{\infty} \overline{\alpha}_{kl} c_k c_l\right)^*\right\}\right| \\
&\qquad \leq \mathrm{tr}_{\mathcal{F}}\{|\rho|\}\,\|\Psi\|\|\Phi\|
\end{aligned}$$

and, therefore, $\|\Gamma_\rho + (1-\mathrm{Ex})(\mathbb{1}\otimes\mathbb{1} - \gamma_\rho\otimes\mathbb{1} - \mathbb{1}\otimes\gamma_\rho)\|_{\mathrm{op}} < \infty$. Following (36) with $\Gamma_\rho + (1-\mathrm{Ex})(\mathbb{1}\otimes\mathbb{1} - \gamma_\rho\otimes\mathbb{1} - \mathbb{1}\otimes\gamma_\rho)$ instead of Γ_ρ, we arrive at

$$\left\langle\Psi\middle|\Big(\Gamma_\rho + (1-\mathrm{Ex})(\mathbb{1}\otimes\mathbb{1} - \gamma_\rho\otimes\mathbb{1} - \mathbb{1}\otimes\gamma_\rho)\Big)\Psi\right\rangle \geq 0 \quad \forall\Psi \in \mathfrak{h}\otimes\mathfrak{h}.$$

$(\gamma_\rho, \Gamma_\rho)$ obeys the P-, G-, and Q-Conditions by e), g) and h). The admissibility is ensured in a) to d), and f). □

A simple consequence of Theorem 3.1 is

COROLLARY 3.3. *Let $N \in \mathbb{N}$ and assume that (γ, Γ) is N-representable. Then (γ, Γ) is admissible and fulfills the G-, P- and Q-Conditions.*

Proof. Since (γ, Γ) is N-representable, there exists a density matrix $\rho \in \mathcal{L}_+^1(\mathcal{F})$ with $(\gamma, \Gamma) \equiv (\gamma_\rho, \Gamma_\rho)$. By the last theorem, (γ, Γ) then is admissible and fulfills the G-, P- and Q-Conditions. □

Remark 3.4. The G-Condition (27) seems to be asymmetric in terms of γ_ρ. However, since $\mathrm{tr}_2\{(A\otimes B)\,\Gamma_\rho\} = \mathrm{tr}_2\{(B\otimes A)\,\Gamma_\rho\}$, it is easy to show that also $\mathrm{tr}_2\{(A^*\otimes A)\,(\Gamma_\rho + \mathrm{Ex}\,(\mathbb{1}\otimes\gamma_\rho))\} \geq |\mathrm{tr}_1\{A\gamma_\rho\}|^2$ holds. Thus, we have a symmetrized, but weaker, G-Condition given by

$$\mathrm{tr}_2\left\{(A^*\otimes A)\left(\Gamma_\rho + \frac{1}{2}\mathrm{Ex}\,(\mathbb{1}\otimes\gamma_\rho + \gamma_\rho\otimes\mathbb{1})\right)\right\} \geq |\mathrm{tr}_1\{A\gamma_\rho\}|^2.$$

4 Correlation inequalities from G- and P-Conditions

In [1], a lower bound on the difference of the ground state functional $\mathcal{E}(\gamma, \Gamma)$ and the Hartree–Fock functional $\mathcal{E}(\gamma, (1 - \mathrm{Ex}(\gamma \otimes \gamma)))$, i.e.,

$$\mathrm{tr}_2 \left\{ V\Gamma^{(\mathrm{T})} \right\} = \mathrm{tr}_2 \left\{ V \left(\Gamma - (1 - \mathrm{Ex}) (\gamma \otimes \gamma) \right) \right\}, \tag{39}$$

is derived using the decomposition of the potential V according to Fefferman and de la Llave [7]. It turns out that this decomposition is also useful to derive lower bounds only by means of N-representability. The main result of this section is the following theorem.

THEOREM 4.1. *Let $X = X^* = X^2 \in \mathcal{B}(\mathfrak{h})$ be an orthogonal projection on $\mathfrak{h}$. Assume that (γ, Γ) is admissible and fulfills the G- and P-Conditions. Then*

$$\begin{aligned} \mathrm{tr}_2 \left\{ (X \otimes X) \Gamma^{(\mathrm{T})} \right\} \geq - \mathrm{tr}_1 \{X\gamma\} \min \Big\{ 1;\ 38 \,\mathrm{tr}_1 \left\{ X \left(\gamma - \gamma^2 \right) \right\} \\ + 4 \Big[\mathrm{tr}_1 \left\{ X \left(\gamma - \gamma^2 \right) \right\} \left(2 + 8 \,\mathrm{tr}_1 \left\{ X \left(\gamma - \gamma^2 \right) \right\}^2 \right) \Big]^{\frac{1}{2}} \Big\}. \end{aligned} \tag{40}$$

Proof. The proof is carried out in several parts in the following sections. The first inequality is derived in Theorem 4.4. The second inequality follows from Theorems 4.15, 4.17 and 4.19. □

In order to apply Theorem 4.1 to (39), the potential V on $\mathfrak{h} \otimes \mathfrak{h}$ is decomposed into an integral of a tensor product of two copies of the one-particle operator X. This decomposition is called Fefferman–de la Llave identity.

LEMMA 4.2. *For all $x, y \in \mathbb{R}^3$, $x \neq y$, one has*

$$\frac{1}{|x - y|} = \int_0^\infty \frac{\mathrm{d}r}{\pi r^5} \int_{\mathbb{R}^3} \mathrm{d}^3 z \ \chi_{B(z,r)}(x) \ \chi_{B(z,r)}(y), \tag{41}$$

where $\chi_{B(z,r)}$ is the characteristic function of the ball $B(z, r) := \left\{ x \in \mathbb{R}^3 \mid |x - z| \leq r \right\}$ of radius $r > 0$ centered at $z \in \mathbb{R}^3$.

The proof of the decomposition can be found in the original work of Fefferman and de la Llave in [7]. In [12], Hainzl and Seiringer have derived sufficient conditions on a pair potential $V : \mathbb{R}^n \to \mathbb{R}$ so as to admit a decomposition of the form (41).

Remark 4.3. The multiplication operator corresponding to $\chi_{B(z,r)}$ is denoted by $X_{r,z} \equiv X$. Clearly,

$$\mathcal{B}(\mathfrak{h}) \ni X = X^* = X^2 \tag{42}$$

is an orthogonal projection.

Instead of (39) we consider from now on

$$\mathrm{tr}_2\left\{(X\otimes X)\,\Gamma^{(\mathrm{T})}\right\} = \mathrm{tr}_2\left\{(X\otimes X)\,(\Gamma-(1-\mathrm{Ex})\,(\gamma\otimes\gamma))\right\}. \tag{43}$$

A first estimation of this quantity is immediately obtained by applying the G-Condition directly on $\mathrm{tr}_2\{(X\otimes X)\,\Gamma\}$. This yields the first inequality of (40).

THEOREM 4.4. *Let X be as in (42). Assume that (γ,Γ) is admissible and fulfills the G-Condition. Then*

$$\mathrm{tr}_2\left\{(X\otimes X)\,\Gamma^{(\mathrm{T})}\right\} \geq -\,\mathrm{tr}_1\{X\gamma\}.$$

Proof. As mentioned, we apply the G-Condition (20) with $A^* = A := X$ directly on $\mathrm{tr}_2\{(X\otimes X)\,\Gamma\}$. The HF-part is carried out:

$$\begin{aligned}&\mathrm{tr}_2\{(X\otimes X)\,(\Gamma-(1-\mathrm{Ex})\,(\gamma\otimes\gamma))\}\\ &\quad\geq (\mathrm{tr}_1\{X\gamma\})^2-\mathrm{tr}_1\{X\gamma\}-(\mathrm{tr}_1\{X\gamma\})^2+\mathrm{tr}_1\{X\gamma X\gamma\}\\ &\quad\geq -\,\mathrm{tr}_1\{X\gamma\}.\end{aligned} \tag{44}$$

The last inequality follows from $\mathrm{tr}_1\{X\gamma X\gamma\} = \mathrm{tr}_1\{X\gamma X\gamma X\}\geq 0$. □

The goal of the next sections is an estimation of (43) in terms of $\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}$.

4.1 PREPARATION

A crucial step in [1] is the decomposition of the spectrum of γ into eigenvalues which are larger than $\frac{1}{2}$, and those which are smaller or equal $\frac{1}{2}$. Following this step, the decomposition is denoted by two orthogonal projections, P and $P^\perp$ (a comparable strategy was also used by Graf and Solovej in [13]). The first one, P, projects on the space which is spanned by the eigenvectors of γ corresponding to eigenvalues larger than $\frac{1}{2}$. The second one treats the eigenvectors with eigenvalues smaller or equal $\frac{1}{2}$. Furthermore, the eigenvectors of γ, $\{\varphi_i \mid \gamma\varphi_i=\lambda_i\varphi_i\}_{i=1}^{\infty}$, are used as an ONB of $\mathfrak{h}$ which we mainly refer to. In this basis the two projections can be defined straightforwardly.

DEFINITION 4.5. On $\mathfrak{h}$, the orthogonal projections P and $P^\perp$ are defined by

$$P := \mathbb{1}\left[\gamma>\frac{1}{2}\right] = \sum_{k>\frac{1}{2}} |\varphi_k\rangle\langle\varphi_k| \quad\text{and}\quad P^\perp := \mathbb{1}\left[\gamma\leq\frac{1}{2}\right] = \sum_{k\leq\frac{1}{2}} |\varphi_k\rangle\langle\varphi_k|. \tag{45}$$

Here, the summation over "$k>\frac{1}{2}$" denotes the summation over $\left\{k \mid \lambda_k>\frac{1}{2}\right\}$ and for "$k\leq\frac{1}{2}$" analogously. Obviously,

$$P+P^\perp=\mathbb{1},\quad PP^\perp=P^\perp P=0,\quad P\gamma=\gamma P\quad\text{and}\quad P^\perp\gamma=\gamma P^\perp.$$

Moreover, the projections are bounded from above.

LEMMA 4.6. *For P and $P^\perp$ defined in (45)*

$$P \leq 2\gamma \quad \textit{and} \quad P^\perp \leq 2\,(\mathbb{1} - \gamma) \tag{46}$$

hold true.

Note that, since $\operatorname{rk}\{P\} \leq 2N$, P is of finite rank and, hence, trace class.

Proof. Using the definition of the projections together with $0 \leq \gamma \leq \mathbb{1}$, one finds for P:

$$P = \sum_{k>\frac{1}{2}} |\varphi_k\rangle\,\langle\varphi_k| \leq \sum_{k>\frac{1}{2}} 2\lambda_k\,|\varphi_k\rangle\,\langle\varphi_k| \leq 2\sum_{k=1}^{\infty} \lambda_k\,|\varphi_k\rangle\,\langle\varphi_k| = 2\gamma,$$

and for $P^\perp$:

$$P^\perp = \sum_{k<\frac{1}{2}} |\varphi_k\rangle\,\langle\varphi_k| \leq \sum_{k<\frac{1}{2}} 2\,(1-\lambda_k)\,|\varphi_k\rangle\,\langle\varphi_k| \leq 2\,(\mathbb{1} - \gamma)\,.$$

□

Thanks to $P^\perp + P = \mathbb{1}$ we can expand $\operatorname{tr}_2\{(X \otimes X)\,\Gamma\}$ into three parts to have expressions on which we can apply the conditions on (γ, Γ). We denote this three parts by Main Part (MP), Remainder (R) and Main Error Term (MET).

LEMMA 4.7. *Let X, and P and $P^\perp$ be as defined in (42) and (45), respectively. Then*

$$\begin{aligned}
&\operatorname{tr}_2\{(X\otimes X)\,\Gamma\} \\
&\quad = \operatorname{tr}_2\{(PXP\otimes PXP)\,\Gamma\} + 4\,\mathfrak{Re}\left\{\operatorname{tr}_2\left\{\left(PXP\otimes P^\perp XP\right)\Gamma\right\}\right\} \\
&\qquad\qquad + 2\operatorname{tr}_2\left\{\left(PXP^\perp\otimes P^\perp XP\right)\Gamma\right\} \\
&\qquad + \operatorname{tr}_2\left\{\left(P^\perp XP^\perp\otimes P^\perp XP^\perp\right)\Gamma\right\} + 4\,\mathfrak{Re}\left\{\operatorname{tr}_2\left\{\left(P^\perp XP\otimes P^\perp XP^\perp\right)\Gamma\right\}\right\} \\
&\qquad\qquad + 2\operatorname{tr}_2\left\{\left(P^\perp XP^\perp\otimes PXP\right)\Gamma\right\} \\
&\qquad + 2\,\mathfrak{Re}\left\{\operatorname{tr}_2\left\{\left(PXP^\perp\otimes PXP^\perp\right)\Gamma\right\}\right\}.
\end{aligned} \tag{47}$$

Proof. After replacing the identity operator on each side of X in each factor of the tensor product $X \otimes X$ by $\left(P + P^\perp\right)$, one can expand the r.h.s. of

$$\begin{aligned}
&\operatorname{tr}_2\{(X\otimes X)\,\Gamma\} \\
&\qquad = \operatorname{tr}_2\left\{\left(\left(P+P^\perp\right)X\left(P+P^\perp\right)\otimes\left(P+P^\perp\right)X\left(P+P^\perp\right)\right)\Gamma\right\}.
\end{aligned}$$

Using $\operatorname{tr}_2\{(A\otimes B)\,\Gamma\} = \operatorname{tr}_2\{(B\otimes A)\,\Gamma\}$, which is a consequence of $\operatorname{Ex}\Gamma\operatorname{Ex} = \Gamma$, one arrives at the assertion after rearranging. □

Afterwards, we collect the terms of (47) in a suitable way. Note that compared to [1] the definitions of the Main Part and the Remainder are slightly changed.

DEFINITION 4.8. The term

$$T_{\mathrm{MP}} := \mathrm{tr}_2\left\{(PXP\otimes PXP)\,\Gamma\right\} + 4\,\mathfrak{Re}\left\{\mathrm{tr}_2\left\{\left(PXP\otimes P^{\perp}XP\right)\Gamma\right\}\right\} + 4\,\mathrm{tr}_2\left\{\left(PXP^{\perp}\otimes P^{\perp}XP\right)\Gamma\right\}$$

is called Main Part,

$$T_{\mathrm{R}} := \mathrm{tr}_2\left\{\left(P^{\perp}XP^{\perp}\otimes P^{\perp}XP^{\perp}\right)\Gamma\right\} + 4\,\mathfrak{Re}\left\{\mathrm{tr}_2\left\{\left(P^{\perp}XP\otimes P^{\perp}XP^{\perp}\right)\Gamma\right\}\right\} + 2\,\mathrm{tr}_2\left\{\left(P^{\perp}XP^{\perp}\otimes PXP\right)\Gamma\right\} - 2\,\mathrm{tr}_2\left\{\left(PXP^{\perp}\otimes P^{\perp}XP\right)\Gamma\right\}$$

is called Remainder, and

$$T_{\mathrm{MET}} := 2\,\mathfrak{Re}\left\{\mathrm{tr}_2\left\{\left(PXP^{\perp}\otimes PXP^{\perp}\right)\Gamma\right\}\right\}$$

is called Main Error Term.

One estimate is used more than once when considering the terms in the Remainder and Main Error Term. This estimate requires the following lemma.

LEMMA 4.9. *Let $\{\psi_i\}_{i=1}^{\infty}\subseteq\mathfrak{h}$ be an ONB, $Q=Q^*=Q^2$, $Q^{\perp}:=\mathbb{1}-Q$, and $Y=Y^*=Y^2\in\mathcal{B}(\mathfrak{h})$ orthogonal projections. For $r,s\in\mathbb{N}$ define*

$$B(r,s) := |QY\psi_r\rangle\left\langle Q^{\perp}Y\psi_s\right| \in \mathcal{B}(\mathfrak{h}). \tag{48}$$

Then one has

$$\sum_{r,s=1}^{\infty}\mathrm{tr}_2\left\{\left(B^*(r,s)\otimes B(r,s)\right)\left(\Gamma+\mathrm{Ex}\left(\gamma\otimes\mathbb{1}\right)\right)\right\} = \mathrm{tr}_2\left\{\left(QYQ\otimes Q^{\perp}YQ^{\perp}\right)\left(-\Gamma+\mathbb{1}\otimes\gamma\right)\right\}. \tag{49}$$

Proof. Denoting $K := \sum_{r,s=1}^{\infty}\mathrm{tr}_2\left\{\left(B^*(r,s)\otimes B(r,s)\right)\left(\Gamma+\mathrm{Ex}\left(\gamma\otimes\mathbb{1}\right)\right)\right\}$, we calculate the trace using the ONB $\{\psi_i\}_{i=1}^{\infty}\subseteq\mathfrak{h}$.

$$K = \sum_{r,s=1}^{\infty}\sum_{k,l,m,n=1}^{\infty}\left\langle\psi_k\otimes\psi_l\right|\left(B^*(r,s)\otimes B(r,s)\right)\left(\psi_m\otimes\psi_n\right)\rangle \times\left\langle\psi_m\otimes\psi_n\right|\left(\Gamma+\mathrm{Ex}\left(\gamma\otimes\mathbb{1}\right)\right)\left(\psi_k\otimes\psi_l\right)\rangle.$$

In the next step, the definition of $B(r,s)$ together with $(A)_{ij}:=\langle\psi_i|\,A\psi_j\rangle$, for any $A\in\mathcal{B}(\mathfrak{h})$, can be used to write

$$K = \sum_{r,s=1}^{\infty}\sum_{k,l,m,n=1}^{\infty}(YQ)_{rm}\left(Q^{\perp}Y\right)_{ks}(QY)_{lr}\left(YQ^{\perp}\right)_{sn} \times\left\langle\psi_m\otimes\psi_n\right|\left(\Gamma+\mathrm{Ex}\left(\gamma\otimes\mathbb{1}\right)\right)\left(\psi_k\otimes\psi_l\right)\rangle.$$

Performing the summation over r and s leads to

$$\begin{aligned} K &= \sum_{k,l,m,n=1}^{\infty} (QYQ)_{lm} \left(Q^{\perp}YQ^{\perp}\right)_{kn} \\ &\qquad \times \left\langle \psi_m \otimes \psi_n \right| \left(\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1})\right) \left(\psi_k \otimes \psi_l\right) \rangle \\ &= \sum_{k,l,m,n=1}^{\infty} \left\langle \psi_l \otimes \psi_k \right| \left(QYQ \otimes Q^{\perp}YQ^{\perp}\right) \left(\psi_m \otimes \psi_n\right) \rangle \\ &\qquad \times \left\langle \psi_m \otimes \psi_n \right| \left(\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1})\right) \left(\psi_k \otimes \psi_l\right) \rangle . \end{aligned}$$

The summation over m and n can also be carried out. Finally, the summation over k and l gives

$$\begin{aligned} K &= \sum_{k,l=1}^{\infty} \left\langle \psi_k \otimes \psi_l \right| \left(\mathrm{Ex}\left(QYQ \otimes Q^{\perp}YQ^{\perp}\right) \left(\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1})\right)\right) \left(\psi_k \otimes \psi_l\right) \rangle \\ &= \mathrm{tr}_2 \left\{ \left(QYQ \otimes Q^{\perp}YQ^{\perp}\right) \left(-\Gamma + \mathbb{1} \otimes \gamma\right) \right\} , \end{aligned}$$

using the cyclicity of the trace, $\Gamma\,\mathrm{Ex} = -\Gamma$, and $\mathrm{Ex}\,(\mathbb{1} \otimes \gamma)\,\mathrm{Ex} = \gamma \otimes \mathbb{1}$. □

Remark 4.10. By changing the definition of $B\,(r,s)$ it is also possible to treat, for example, $QYQ \otimes QYQ$ similarly. However, it is important to notice that $\sum_{r,s} B^*\,(r,s) \otimes B\,(r,s)$ is, in general, indefinite. In fact, the trace of $B\,(r,s)$ is vanishing in our case and so is the trace of $B^*\,(r,s) \otimes B\,(r,s)$. Hence, $B^*\,(r,s) \otimes B\,(r,s)$ is either indefinite or zero. Furthermore, since $P^{\perp}$ and P commute with γ, we also have $\mathrm{tr}_1\,\{B\,(r,s)\,\gamma\} = 0$.

A consequence of Lemma 4.9 is a key inequality for proving the estimate on the Remainder and the Main Error Term. This inequality is given in (50).

LEMMA 4.11. *Let X, and P and $P^{\perp}$ be as defined in (42) and (45), respectively. Assume that (γ, Γ) is admissible and fulfills the G-Condition. Then*

$$\mathrm{tr}_2 \left\{ \left(PXP \otimes P^{\perp}XP^{\perp}\right) \Gamma \right\} \leq 4\,\mathrm{tr}_1\,\{X\gamma\}\,\mathrm{tr}_1 \left\{ X\left(\gamma - \gamma^2\right) \right\} . \tag{50}$$

Proof. First, we observe that (49) with $Y = X$ and $Q = P$ and the G-Condition immediately lead to

$$\begin{aligned} 0 &\leq \sum_{p,q} \mathrm{tr}_2 \left\{ \left(B^*\,(r,s) \otimes B\,(r,s)\right) \left(\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1})\right) \right\} \\ &= \mathrm{tr}_2 \left\{ \left(PXP \otimes P^{\perp}XP^{\perp}\right) \left(-\Gamma + (\mathbb{1} \otimes \gamma)\right) \right\} . \end{aligned}$$

Consequently,

$$\begin{aligned} \mathrm{tr}_2 \left\{ \left(PXP \otimes P^{\perp}XP^{\perp}\right) \Gamma \right\} &\leq \mathrm{tr}_2 \left\{ \left(PXP \otimes P^{\perp}XP^{\perp}\right) (\mathbb{1} \otimes \gamma) \right\} \\ &= \mathrm{tr}_1\,\{PX\}\,\mathrm{tr}_1 \left\{ P^{\perp}X\gamma \right\} . \end{aligned}$$

Secondly, we permute the arguments in the trace cyclically and use that γ is trace class and PX and $P^\perp X$ are bounded. Then we use (46) to estimate the projections:

$$\begin{aligned}\operatorname{tr}_1\{PX\}\operatorname{tr}_1\left\{P^\perp X\gamma\right\} &= \operatorname{tr}_1\{XPX\}\operatorname{tr}_1\left\{X\sqrt{\gamma}P^\perp\sqrt{\gamma}X\right\}\\ &\leq 4\operatorname{tr}_1\{X\gamma\}\operatorname{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}\end{aligned}$$

since $\gamma P^\perp = \sqrt{\gamma}P^\perp\sqrt{\gamma}$. □

Remark 4.12. ¿From $\operatorname{tr}_2\{(A\otimes B)\,\Gamma\} = \operatorname{tr}_2\{(B\otimes A)\,\Gamma\}$, for $A, B \in \mathcal{B}(\mathfrak{h})$, one directly can conclude

$$\operatorname{tr}_2\left\{\left(P^\perp XP^\perp\otimes PXP\right)\Gamma\right\} \leq 4\operatorname{tr}_1\{X\gamma\}\operatorname{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}. \tag{51}$$

4.2 Estimation of the Remainder

Now we consider the Remainder of (47):

$$\begin{aligned}T_{\mathrm{R}} := \operatorname{tr}_2\left\{\left(P^\perp XP^\perp\otimes P^\perp XP^\perp\right)\Gamma\right\} + 4\,\mathfrak{Re}\left\{\operatorname{tr}_2\left\{\left(P^\perp XP\otimes P^\perp XP^\perp\right)\Gamma\right\}\right\}\\ + 2\operatorname{tr}_2\left\{\left(P^\perp XP^\perp\otimes PXP\right)\Gamma\right\} - 2\operatorname{tr}_2\left\{\left(PXP^\perp\otimes P^\perp XP\right)\Gamma\right\}.\end{aligned}$$

The first three terms, summed up in T_{R_1} and the last term, called T_{R_2}, are treated separately to derive a lower bound.

Lemma 4.13. *Let X, and P and $P^\perp$ be as defined in (42) and (45), respectively. Assume that (γ,Γ) is admissible and fulfills the G- and P-Conditions. Then*

$$\begin{aligned}T_{\mathrm{R}_1} &:= \operatorname{tr}_2\left\{\left(P^\perp XP^\perp\otimes P^\perp XP^\perp\right)\Gamma\right\} + 2\operatorname{tr}_2\left\{\left(P^\perp XP^\perp\otimes PXP\right)\Gamma\right\}\\ &\qquad + 4\,\mathfrak{Re}\left\{\operatorname{tr}_2\left\{\left(P^\perp XP^\perp\otimes PXP^\perp\right)\Gamma\right\}\right\}\\ &\geq -8\operatorname{tr}_1\{X\gamma\}\operatorname{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}.\end{aligned}$$

Proof. First, we use $\mathfrak{Re}(\zeta) \geq -|\zeta|$, for any complex number ζ, and $P^\perp XP\otimes P^\perp XP^\perp = \left(P^\perp X\otimes P^\perp X\right)\left(XP\otimes XP^\perp\right)$ to infer

$$\begin{aligned}T_{\mathrm{R}_1} &= \operatorname{tr}_2\left\{\left(P^\perp XP^\perp\otimes P^\perp XP^\perp\right)\Gamma\right\} + 2\operatorname{tr}_2\left\{\left(PXP\otimes P^\perp XP^\perp\right)\Gamma\right\}\\ &\qquad + 4\,\mathfrak{Re}\left\{\operatorname{tr}_2\left\{\left(P^\perp XP\otimes P^\perp XP^\perp\right)\Gamma\right\}\right\}\\ &\geq \operatorname{tr}_2\left\{\left(P^\perp XP^\perp\otimes P^\perp XP^\perp\right)\Gamma\right\} + 2\operatorname{tr}_2\left\{\left(PXP\otimes P^\perp XP^\perp\right)\Gamma\right\}\\ &\qquad - 4\left|\operatorname{tr}_2\left\{\left(P^\perp X\otimes P^\perp X\right)\left(XP\otimes XP^\perp\right)\Gamma\right\}\right|.\end{aligned}$$

Then we use that $(A,B) := \operatorname{tr}_2\{A^*B\,\Gamma\}$ defines a positive semidefinite Hermitian form on $\mathcal{B}(\mathfrak{h}\otimes\mathfrak{h})$, due to $\Gamma \geq 0$, which is the P-Condition. Hence, the Cauchy–Schwarz inequality

$$|(A,B)| \geq (A,A)^{\frac{1}{2}}\,(B,B)^{\frac{1}{2}} \tag{52}$$

holds, and we arrive at

$$\begin{aligned} T_{\mathrm{R}_1} \geq\, & \operatorname{tr}_2\left\{\left(P^\perp X P^\perp \otimes P^\perp X P^\perp\right)\Gamma\right\} + 2\operatorname{tr}_2\left\{\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right\} \\ & - 4\left(\operatorname{tr}_2\left\{\left(P^\perp X P^\perp \otimes P^\perp X P^\perp\right)\Gamma\right\}\right)^{\frac{1}{2}}\left(\operatorname{tr}_2\left\{\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right\}\right)^{\frac{1}{2}}. \end{aligned}$$

As $x^2 - 4bx \geq -4b^2$, for $x := \left(\operatorname{tr}_2\left\{\left(P^\perp X P^\perp \otimes P^\perp X P^\perp\right)\Gamma\right\}\right)^{\frac{1}{2}}$ and $b := \left(\operatorname{tr}_2\left\{\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right\}\right)^{\frac{1}{2}}$, one then easily concludes

$$\begin{aligned} T_{\mathrm{R}_1} &\geq -4\operatorname{tr}_2\left\{\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right\} + 2\operatorname{tr}_2\left\{\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right\} \\ &= -2\operatorname{tr}_2\left\{\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right\}. \end{aligned}$$

The proof is completed by using (50):

$$T_{\mathrm{R}_1} \geq -2\operatorname{tr}_2\left\{\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right\} \geq -8\operatorname{tr}_1\{X\gamma\}\operatorname{tr}_1\left\{X\left(\gamma - \gamma^2\right)\right\}.$$

□

The estimate on $T_{\mathrm{R}_2} := -2\operatorname{tr}_2\left\{\left(P^\perp X P \otimes P X P^\perp\right)\Gamma\right\}$ is addressed in the next lemma.

LEMMA 4.14. *Let X, and P and $P^\perp$ be as defined in (42) and (45), respectively. Assume that (γ, Γ) is admissible and fulfills the G- and P-Conditions. Then*

$$T_{\mathrm{R}_2} = -2\operatorname{tr}_2\left\{\left(P^\perp X P \otimes P X P^\perp\right)\Gamma\right\} \geq -8\operatorname{tr}_1\{X\gamma\}\operatorname{tr}_1\left\{X\left(\gamma - \gamma^2\right)\right\}. \tag{53}$$

Proof. First, the left side is estimated by its absolute value. Then the Cauchy–Schwarz inequality (52) is used:

$$\begin{aligned} & -2\operatorname{tr}_2\left\{\left(P^\perp X P \otimes P X P^\perp\right)\Gamma\right\} \\ & \quad \geq -2\left|\operatorname{tr}_2\left\{\left(P^\perp X P \otimes P X P^\perp\right)\Gamma\right\}\right| \\ & \quad \geq -2\left(\operatorname{tr}_2\left\{\left(P^\perp X P^\perp \otimes PXP\right)\Gamma\right\}\right)^{\frac{1}{2}}\left(\operatorname{tr}_2\left\{\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right\}\right)^{\frac{1}{2}} \\ & \quad = -2\operatorname{tr}_1\left\{\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right\}. \end{aligned} \tag{54}$$

The assertion (53) follows again from (50). □

Summing up the results, we obtain the following estimate of the Remainder directly from Lemmata 4.13 and 4.14.

THEOREM 4.15. *Let X, and P and $P^\perp$ be as defined in (42) and (45), respectively. Assume that (γ, Γ) is admissible and fulfills the G- and P-Conditions. Then*

$$T_{\mathrm{R}} \geq -16\operatorname{tr}_1\{X\gamma\}\operatorname{tr}_1\left\{X\left(\gamma - \gamma^2\right)\right\}.$$

4.3 ESTIMATION OF THE MAIN ERROR TERM

The main error in Theorem 4.1 results from estimating T_{MET} in (47),

$$T_{\mathrm{MET}} = 2\,\mathfrak{Re}\left\{\mathrm{tr}_2\left\{\left(P^\perp XP \otimes P^\perp XP\right)\Gamma\right\}\right\}. \tag{55}$$

A key observation is that terms of the form $A \otimes B \in \mathcal{B}(\mathfrak{h} \otimes \mathfrak{h})$ or $\mathrm{Ex}\,(A \otimes B) \in \mathcal{B}(\mathfrak{h} \otimes \mathfrak{h})$ can be added to Γ in (55) without changing the value of T_{MET}, provided A and B commute with $P^\perp$ and P. Therefore, one can also consider

$$T_{\mathrm{MET}} = 2\,\mathfrak{Re}\left\{\mathrm{tr}_2\left\{\left(P^\perp XP \otimes P^\perp XP\right)(\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}))\right\}\right\}.$$

This expression can now be estimated using a variant of the Cauchy–Schwarz inequality given in the next lemma.

LEMMA 4.16. *Let X, and P and $P^\perp$ be as defined in (42) and (45), respectively. Assume that (γ, Γ) is admissible and fulfills the G-Condition. Then*

$$\begin{aligned}\mathfrak{Re}\left\{\mathrm{tr}_2\left\{\left(P^\perp XP \otimes P^\perp XP\right)(\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}))\right\}\right\}&\\ \geq -\left(\mathrm{tr}_2\left\{\left(PXP^\perp \otimes P^\perp XP\right)(\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}))\right\}\right)^{\frac{1}{2}}&\\ \times\left(\mathrm{tr}_2\left\{\left(P^\perp XP \otimes PXP^\perp\right)(\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}))\right\}\right)^{\frac{1}{2}}.&\end{aligned} \tag{56}$$

Proof. We define

$$(A, B) := \mathrm{tr}_2\left\{(A^* \otimes B)(\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}))\right\}$$

on $\mathcal{B}(\mathfrak{h}) \times \mathcal{B}(\mathfrak{h})$ and observe that, because

$$\mathrm{tr}_2\left\{(B^* \otimes A)\,\Gamma\right\} = \mathrm{tr}_2\left\{(A \otimes B^*)\,\Gamma\right\} = \overline{\mathrm{tr}_2\left\{(A^* \otimes B)\,\Gamma\right\}}$$

and

$$\begin{aligned}\mathrm{tr}_2\left\{(B^* \otimes A)\,\mathrm{Ex}\,(\gamma \otimes \mathbb{1})\right\} &= \mathrm{tr}_1\left\{B^* A\,\gamma\right\} = \overline{\mathrm{tr}_1\left\{A^* B\,\gamma\right\}}\\ &= \overline{\mathrm{tr}_2\left\{(A^* \otimes B)\,\mathrm{Ex}\,(\gamma \otimes \mathbb{1})\right\}},\end{aligned}$$

$(\cdot\,,\cdot)$ defines a Hermitian form on $\mathcal{B}(\mathfrak{h}) \times \mathcal{B}(\mathfrak{h})$. Furthermore, $(\cdot\,,\cdot)$ is positive semidefinite, since

$$\begin{aligned}(A, A) &= \mathrm{tr}_2\left\{(A^* \otimes A)\,(\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}))\right\}\\ &\geq \left|\mathrm{tr}_1\left\{A\gamma\right\}\right|^2 \geq 0\end{aligned}$$

thanks to the G-Condition. Hence, the Cauchy–Schwarz inequality $|(A, B)| \leq (A, A)^{\frac{1}{2}}\,(B, B)^{\frac{1}{2}}$ holds true. Applying this with $A^* := B := P^\perp XP$, we arrive at the asserted estimate (56):

$$\begin{aligned}&\mathfrak{Re}\left\{\mathrm{tr}_2\left\{\left(P^\perp XP \otimes P^\perp XP\right)(\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}))\right\}\right\}\\ &\quad= \mathfrak{Re}\left\{(A^*, A)\right\} \geq -\left|(A^*, A)\right| \geq -\,(A^*, A^*)^{\frac{1}{2}}\,(A, A)^{\frac{1}{2}}\\ &\quad= -\left(\mathrm{tr}_2\left\{\left(PXP^\perp \otimes P^\perp XP\right)(\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}))\right\}\right)^{\frac{1}{2}}\\ &\qquad\qquad\times\left(\mathrm{tr}_2\left\{\left(P^\perp XP \otimes PXP^\perp\right)(\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}))\right\}\right)^{\frac{1}{2}}.\end{aligned}$$

□

Now the Main Error Term can be estimated.

THEOREM 4.17. *Let X, and P and $P^\perp$ be as defined in (42) and (45), respectively. Assume that (γ, Γ) is admissible and fulfills the G- and P-Conditions. Then*

$$T_{\mathrm{MET}} \geq -2\,\mathrm{tr}_1\left\{X\gamma\right\}\left[8\,\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}\left(1+4\,\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}\right)\right]^{\frac{1}{2}}.$$

Proof. We rewrite T_{MET} adding the necessary exchange term to allow for an application of (56):

$$\begin{aligned}
T_{\mathrm{MET}} &= 2\,\mathfrak{Re}\left\{\mathrm{tr}_2\left\{\left(P^\perp XP\otimes P^\perp XP\right)\Gamma\right\}\right\}\\
&= 2\,\mathfrak{Re}\left\{\mathrm{tr}_2\left\{\left(P^\perp XP\otimes P^\perp XP\right)\left(\Gamma+\mathrm{Ex}\left(\gamma\otimes\mathbb{1}\right)\right)\right\}\right\}\\
&\geq -2\left(\mathrm{tr}_2\left\{\left(PXP^\perp\otimes P^\perp XP\right)\left(\Gamma+\mathrm{Ex}\left(\gamma\otimes\mathbb{1}\right)\right)\right\}\right)^{\frac{1}{2}}\\
&\qquad\times\left(\mathrm{tr}_2\left\{\left(P^\perp XP\otimes PXP^\perp\right)\left(\Gamma+\mathrm{Ex}\left(\gamma\otimes\mathbb{1}\right)\right)\right\}\right)^{\frac{1}{2}}.
\end{aligned}$$

Note that $\mathrm{tr}_2\left\{\left(PXP^\perp\otimes P^\perp XP\right)\Gamma\right\} = \mathrm{tr}_2\left\{\left(P^\perp XP\otimes PXP^\perp\right)\Gamma\right\}$, which was already estimated in (54). Together with (50) we obtain

$$\begin{aligned}
\mathrm{tr}_2\left\{\left(PXP^\perp\otimes P^\perp XP\right)\Gamma\right\} &\leq \mathrm{tr}_1\left\{\left(PXP\otimes P^\perp XP^\perp\right)\Gamma\right\}\\
&\leq 4\mathrm{tr}_1\left\{X\gamma\right\}\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}.
\end{aligned}$$

The two exchange terms have to be treated separately. Using $P^\perp, P \leq \mathbb{1}$, we find

$$\begin{aligned}
\mathrm{tr}_2\left\{\left(PXP^\perp\otimes P^\perp XP\right)\mathrm{Ex}\left(\gamma\otimes\mathbb{1}\right)\right\} &= \mathrm{tr}_1\left\{P^\perp XP\gamma PXP^\perp\right\}\\
&= \mathrm{tr}_1\left\{P^\perp X\sqrt{\gamma}P\sqrt{\gamma}XP^\perp\right\}\\
&\leq \mathrm{tr}_1\left\{X\gamma\right\},
\end{aligned}$$

and

$$\begin{aligned}
\mathrm{tr}_2\left\{\left(P^\perp XP\otimes PXP^\perp\right)\mathrm{Ex}\left(\gamma\otimes\mathbb{1}\right)\right\} &= \mathrm{tr}_1\left\{PXP^\perp\gamma P^\perp XP\right\}\\
&= \mathrm{tr}_1\left\{XPXXP^\perp\gamma P^\perp X\right\}\\
&\leq \mathrm{tr}_1\left\{XPX\right\}\mathrm{tr}_1\left\{XP^\perp\gamma P^\perp X\right\}\\
&\leq 4\,\mathrm{tr}_1\left\{X\gamma\right\}\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\},
\end{aligned}$$

where cyclic permutation in the argument of the trace is used together with $X = X^2$, $\left(P^\perp\right)^2 = P^\perp$ and $P^2 = P$ to expand the argument of the trace. Then one can use $XPX \geq 0$ and $XP^\perp\gamma P^\perp X \geq 0$ to estimate by $XPX \leq \mathbb{1}\,\mathrm{tr}_1\left\{XPX\right\}$. Afterwards, (46) can be used. Merging the results, we arrive at the assertion. □

4.4 Estimation of the Main Part

In this section it is shown that the remaining terms of (47),

$$T_{\mathrm{MP}} = \mathrm{tr}_2\left\{(PXP \otimes PXP)\,\Gamma\right\} + 4\,\mathfrak{Re}\left\{\mathrm{tr}_2\left\{\left(PXP^{\perp} \otimes PXP\right)\Gamma\right\}\right\} + 4\,\mathrm{tr}_2\left\{\left(PXP^{\perp} \otimes P^{\perp}XP\right)\Gamma\right\},$$

are large enough to cover the HF-part $\mathrm{tr}_2\left\{(X \otimes X)\,(\mathbb{1} - \mathrm{Ex})\,(\gamma \otimes \gamma)\right\}$ in (43). Due to this, we call this terms the Main Part. As mentioned, the Main Part was extended by an additional term. This extension allows for the following observation.

Lemma 4.18. *Let X, and P and $P^{\perp}$ be as defined in (42) and (45), respectively. Then*

$$T_{\mathrm{MP}} = \mathrm{tr}_2\left\{\left(PX\left(P + 2P^{\perp}\right) \otimes \left(P + 2P^{\perp}\right)XP\right)\Gamma\right\}. \tag{57}$$

Proof. Expanding the parentheses on the right side leads to the assertion by using $\mathrm{tr}_2\left\{(A \otimes B)\,\Gamma\right\} = \mathrm{tr}_2\left\{(B \otimes A)\,\Gamma\right\}$. □

For $A := \left(P + 2P^{\perp}\right)XP$ we have $T_{\mathrm{MP}} = \mathrm{tr}_2\left\{(A^* \otimes A)\,\Gamma\right\}$. This provides the use of the G-Condition.

Theorem 4.19. *Let X, and P and $P^{\perp}$ be as defined in (42) and (45), respectively. Assume that (γ, Γ) is admissible and fulfills the G-Condition. Then*

$$T_{\mathrm{MP}} - \mathrm{tr}_2\left\{(X \otimes X)\,(\mathbb{1} - \mathrm{Ex})\,(\gamma \otimes \gamma)\right\} \geq -\,22\,\mathrm{tr}_1\left\{X\gamma\right\}\mathrm{tr}_1\left\{X\left(\gamma - \gamma^2\right)\right\}. \tag{58}$$

Proof. The proof is split into two parts. In the first part, the trace of the HF-part is calculated. In the second part, the Main Part is estimated by applying the G-Condition with $A := \left(P + 2P^{\perp}\right)XP$.

a) As in (44), the trace of the HF part can be written as

$$\mathrm{tr}_2\left\{(X \otimes X)\,(\mathbb{1} - \mathrm{Ex})\,(\gamma \otimes \gamma)\right\} = \left(\mathrm{tr}_1\left\{X\gamma\right\}\right)^2 - \mathrm{tr}_1\left\{X\gamma X\gamma\right\}.$$

b) Owing to (57), the G-Condition can be applied directly on the Main Part:

$$\begin{aligned} T_{\mathrm{MP}} &= \mathrm{tr}_2\left\{\left(PX\left(P + 2P^{\perp}\right) \otimes \left(P + 2P^{\perp}\right)XP\right)\Gamma\right\} \\ &\geq \left|\mathrm{tr}_1\left\{PX\left(P + 2P^{\perp}\right)\gamma\right\}\right|^2 \\ &\qquad - \mathrm{tr}_1\left\{PX\left(P + 2P^{\perp}\right)\gamma\left(P + 2P^{\perp}\right)XP\right\}. \end{aligned}$$

Due to cyclical permutation, $[\gamma, P] = \left[\gamma, P^{\perp}\right] = 0$ and $P^{\perp}P = PP^{\perp} = 0$, some traces vanish. The result is

$$\begin{aligned} T_{\mathrm{MP}} &\geq \left|\mathrm{tr}_1\left\{PX\gamma\right\}\right|^2 - \mathrm{tr}_1\left\{XPXP\gamma\right\} - 4\,\mathrm{tr}_1\left\{XPXP^{\perp}\gamma\right\} \\ &\geq \left(\mathrm{tr}_1\left\{PX\gamma\right\}\right)^2 - \mathrm{tr}_1\left\{PX\gamma X\right\} - 4\,\mathrm{tr}_1\left\{XP\right\}\mathrm{tr}_1\left\{XP^{\perp}\gamma\right\}. \end{aligned}$$

In $\mathrm{tr}_1\{XPXP\gamma\}$, $[P,\gamma] = 0$ and $P \leq \mathbb{1}$ is used to write $\mathrm{tr}_1\{XPXP\gamma\} = \mathrm{tr}_1\{PX\sqrt{\gamma}P\sqrt{\gamma}XP\} \leq \mathrm{tr}_1\{PX\gamma X\}$. In the last trace, $XP \leq \mathbb{1}\,\mathrm{tr}_1\{XP\}$ is used. This is possible since $\mathrm{tr}_1\{XPXP^\perp\gamma\} = \mathrm{tr}_1\{XPXXP^\perp\gamma X\}$ and $XP^\perp\gamma X = \left|XP^\perp\sqrt{\gamma}\right|^2 \geq 0$ together with $XPX \geq 0$.

Before adding up the estimates, we note that

$$\mathrm{tr}_1\left\{P^\perp X\gamma X\gamma\right\} = \mathrm{tr}_1\left\{\sqrt{\gamma}X\sqrt{\gamma}P^\perp\sqrt{\gamma}X\sqrt{\gamma}\right\} \geq 0$$

and

$$\begin{aligned}
&\left(\mathrm{tr}_1\{X\gamma\}\right)^2 - \left(\mathrm{tr}_1\{PX\gamma\}\right)^2 \\
&\qquad = \Big(\mathrm{tr}_1\{X\gamma\} + \mathrm{tr}_1\{PX\gamma\}\Big)\Big(\mathrm{tr}_1\{X\gamma\} - \mathrm{tr}_1\{PX\gamma\}\Big) \\
&\qquad = \Big(\mathrm{tr}_1\{X\gamma\} + \mathrm{tr}_1\{PX\gamma\}\Big)\mathrm{tr}_1\left\{P^\perp X\gamma\right\}. \qquad (59)
\end{aligned}$$

Furthermore, one has $\mathrm{tr}_1\{XP\}\,\mathrm{tr}_1\left\{XP^\perp\gamma\right\} \leq 4\,\mathrm{tr}_1\{X\gamma\}\,\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}$. These results can now be applied together with a) and b) to the left side of (58):

$$\begin{aligned}
&T_{\mathrm{MP}} - \mathrm{tr}_2\{(X\otimes X)(\mathbb{1}-\mathrm{Ex})(\gamma\otimes\gamma)\} \\
&\quad \geq -\Big(\left(\mathrm{tr}_1\{X\gamma\}\right)^2 - \left(\mathrm{tr}_1\{PX\gamma\}\right)^2\Big) + \mathrm{tr}_1\{X\gamma X\gamma\} - \mathrm{tr}_1\{PX\gamma X\} \\
&\qquad\qquad - 16\,\mathrm{tr}_1\{X\gamma\}\,\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}.
\end{aligned}$$

At this point we use (59), split $\mathrm{tr}_1\{X\gamma X\gamma\}$ into $\mathrm{tr}_1\{PX\gamma X\gamma\} + \mathrm{tr}_1\left\{P^\perp X\gamma X\gamma\right\}$, and rearrange:

$$\begin{aligned}
&T_{\mathrm{MP}} - \mathrm{tr}_2\{(X\otimes X)(\mathbb{1}-\mathrm{Ex})(\gamma\otimes\gamma)\} \\
&\quad \geq -\left(\mathrm{tr}_1\{X\gamma\} + \mathrm{tr}_1\{PX\gamma\}\right)\mathrm{tr}_1\left\{P^\perp X\gamma\right\} \\
&\qquad\qquad - \mathrm{tr}_1\{PX\gamma X(\mathbb{1}-\gamma)\} + \mathrm{tr}_1\left\{P^\perp X\gamma X\gamma\right\} \\
&\qquad\qquad - 16\,\mathrm{tr}_1\{X\gamma\}\,\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}.
\end{aligned}$$

Then, with $P \leq \mathbb{1}$, $P^\perp \leq 2(1-\gamma)$, and $\mathrm{tr}_1\left\{P^\perp X\gamma X\gamma\right\} \geq 0$, one obtains

$$\begin{aligned}
&T_{\mathrm{MP}} - \mathrm{tr}_2\{(X\otimes X)(\mathbb{1}-\mathrm{Ex})(\gamma\otimes\gamma)\} \\
&\quad \geq -4\,\mathrm{tr}_1\{X\gamma\}\,\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\} - \mathrm{tr}_1\{PX\gamma X(\mathbb{1}-\gamma)\} \\
&\qquad\qquad - 16\,\mathrm{tr}_1\{X\gamma\}\,\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}.
\end{aligned}$$

We continue with the inequality $X\gamma X \leq \mathbb{1}\mathrm{tr}_1\{X\gamma X\}$. This is allowed because $\mathrm{tr}_1\{PX\gamma X(\mathbb{1}-\gamma)\} = \mathrm{tr}_1\{X\gamma XX(\mathbb{1}-\gamma)PX\}$ and $X(\mathbb{1}-\gamma)PX =$

$X\sqrt{\mathbb{1}-\gamma}P\sqrt{\mathbb{1}-\gamma}X = \left|X\sqrt{\mathbb{1}-\gamma}P\right|^2 \geq 0$ together with $X\gamma X \geq 0$:

$$\begin{aligned} T_{\mathrm{MP}} &- \mathrm{tr}_2\left\{(X\otimes X)\left(\mathbb{1}-\mathrm{Ex}\right)(\gamma\otimes\gamma)\right\} \\ &\geq -20\,\mathrm{tr}_1\left\{X\gamma\right\}\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\} - \mathrm{tr}_1\left\{X\gamma X\right\}\mathrm{tr}_1\left\{X\left(\mathbb{1}-\gamma\right)PX\right\} \\ &\geq -20\,\mathrm{tr}_1\left\{X\gamma\right\}\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\} - 2\,\mathrm{tr}_1\left\{X\gamma\right\}\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\} \\ &= -22\,\mathrm{tr}_1\left\{X\gamma\right\}\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}. \end{aligned}$$

The last inequality follows from $P \leq 2\gamma$. □

Finally, the proof of Theorem 4.1 is completed by the estimation of T_{R} in Theorem 4.15, T_{MET} in Theorem 4.17 and $T_{\mathrm{MP}} - \mathrm{tr}_2\left\{(X\otimes X)\left(\mathbb{1}-\mathrm{Ex}\right)(\gamma\otimes\gamma)\right\}$ in Theorem 4.19. In each of this theorems, the G-Condition was used to generate bounds. The P-Condition was only applied to provide the use of the Cauchy–Schwarz inequality. In the end, it is remarkable that the Q-Condition is not needed for the proof of the correlation estimate.

5 Summary

We have obtained several results in the last section, which were merged in the main theorem, Theorem 4.1:

$$\mathrm{tr}_2\left\{(X\otimes X)\left(\Gamma-(1-\mathrm{Ex})\left(\gamma\otimes\gamma\right)\right)\right\} \geq -\,\mathrm{tr}_1\left\{X\gamma\right\},$$

$$T_{\mathrm{R}} \geq -\,16\,\mathrm{tr}_1\left\{X\gamma\right\}\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\},$$

$$T_{\mathrm{MET}} \geq -\,2\,\mathrm{tr}_1\left\{X\gamma\right\}\left[8\,\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}\left(1+4\,\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}\right)\right]^{\frac{1}{2}},$$

$$T_{\mathrm{MP}} - \mathrm{tr}_2\left\{(X\otimes X)\left(\mathbb{1}-\mathrm{Ex}\right)(\gamma\otimes\gamma)\right\} \geq -\,22\,\mathrm{tr}_1\left\{X\gamma\right\}\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}.$$

Denoting $b := \mathrm{tr}_1\left\{X\gamma\right\}$ and $a := \sqrt{\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}}$, one can rewrite the estimates for $\mathrm{tr}_2\left\{(X\otimes X)\,\Gamma^{(\mathrm{T})}\right\} = \mathrm{tr}_2\left\{(X\otimes X)\left(\Gamma-(1-\mathrm{Ex})\left(\gamma\otimes\gamma\right)\right)\right\}$ as follows:

$$\mathrm{tr}_2\left\{(X\otimes X)\,\Gamma^{(\mathrm{T})}\right\} \geq -\,b\,\min\left\{1;\ a\left(38a+2\sqrt{8+32a^2}\right)\right\}. \tag{60}$$

A suitable choice of $a \leq b$ in (60) leads to the following correlation estimation.

Theorem 5.1. *Let X, and P and $P^{\perp}$ be as defined in (42) and (45), respectively. Assume that (γ,Γ) is admissible and fulfills the G- and P-Conditions. Then*

$$\mathrm{tr}_2\left\{(X\otimes X)\,\Gamma^{(\mathrm{T})}\right\} \geq -\,\mathrm{tr}_1\left\{X\gamma\right\}\,\min\left\{1;\ 10\sqrt{\mathrm{tr}_1\left\{X\left(\gamma-\gamma^2\right)\right\}}\right\}.$$

Proof. The minimum in (60) is $a\left(38a + 2\sqrt{8+32a^2}\right)$ for $0 < a \leq \frac{1}{\sqrt{94}}$ and, thus, $\frac{1}{a} \geq \left(38a + 2\sqrt{8+32a^2}\right)$. Since $\left(38a + 2\sqrt{8+32a^2}\right)$ is monotonously increasing in a, we find

$$\left(38a + 2\sqrt{8+32a^2}\right) \leq \sqrt{94} < 10, \tag{61}$$

which implies the assertion. □

Remark 5.2. In section 4.1, we have split the eigenvalues of γ in eigenvalues which are larger than $\frac{1}{2}$ and lower or equal $\frac{1}{2}$. In fact, this split turns out to be almost optimal and (61) cannot be sharpened by another choice of P and $P^{\perp}$.

Up to the constant (61), Theorem 5.1 is exactly the result which was already obtained in [1]. The difference of the constants comes, on the one hand, from a different arrangement of the terms of $\mathrm{tr}_2\left\{(X \otimes X)\,\Gamma^{(\mathrm{T})}\right\}$ and, on the other hand, from the fact that in [1] also the Q-Condition was used, which can be seen implicitly in estimate (68) in [1]. With the result of Theorem 5.1 we can immediately perform the integration in the Feffermann–de la Llave identity according to [1] which leads to an estimate of $\mathrm{tr}_2\{V\,(\Gamma - (1 - \mathrm{Ex})(\gamma \otimes \gamma))\}$.

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