Upper bounds for Grothendieck constants, quantum correlation matrices and CCP functions

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Abstract

Within the framework of the search for the still unknown exact value of the real and complex Grothendieck constant $K_G^{\mathbb{F}}$ in the famous Grothendieck inequality (unsolved since 1953), where $\mathbb{F}$ denotes either the real or the complex field, we concentrate our search on their smallest upper bound. To this end, we establish a basic framework, built on functions which map correlation matrices to correlation matrices entrywise by means of the Hadamard product, such as the Krivine function in the real case or the Haagerup function in the complex case. By making use of multivariate real and complex Gaussian analysis, higher transcendental functions, integration over spheres and combinatorics of the inversion of Maclaurin series, we provide an approach by which we also recover all famous upper bounds of Grothendieck himself ($K_G^{\mathbb{R}} \leq \sinh(\pi/2) \approx 2.301$ - [52]), Krivine ($K_G^{\mathbb{R}} \leq \frac{\pi}{2\ln(1+\sqrt{2})} \approx 1,782$ - [90]) and Haagerup ($K_G^{\mathbb{C}} \leq 1.405$, numerically approximated - [57]); each of them as a special case. In doing so, we aim to unify the real and complex cases as much as possible and apply our results to several concrete examples, including the Walsh-Hadamard transform ("quantum gate") and the multivariate Gaussian copula - with foundations of quantum theory and quantum information theory in mind. Moreover, we propose a shortening and a simplification of the proof of the strongest estimation until now; namely that $K_G^{\mathbb{R}} < \frac{\pi}{2\ln(1+\sqrt{2})}$ ([22]). We summarise our key results in form of an algorithmic scheme and shed light on related open problems for future research works.

Key words and phrases. Grothendieck inequality, Grothendieck real constant, Grothendieck complex constant, Gram matrix, quantum correlation, Bell inequality, Hadamard product, Kronecker product, Pearson correlation coefficient, completely correlation preserving function, Schoenberg's theorem, Hermite polynomial, Ornstein-Uhlenbeck semigroup, Gamma function, Stein's lemma, spherical integration, Gaussian hypergeometric function, real and complex Gaussian random vector, Gaussian copula, noise stability, operator ideal, Taylor series inversion, Bell polynomial

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1. Introduction and motivation

1.1. Problem background

Despite its emergence more than six decades ago, the techniques and results of the actually pathbreaking work of A. Grothendieck in the metric theory of tensor products are still not widely known nor appreciated. Very likely this is due to the fact that Grothendieck included virtually no proofs, and that he used the (duality) theory of the rather abstract (yet very powerful) notion of tensor products of Banach spaces (cf. [2, 33, 37, 52]). Actually, [52] appeared in 1956. The fundamental idea exploited in [33] is a one-to-one correspondence between Grothendieck's finitely generated tensor norms and maximal Banach operator ideals (in the sense of Pietsch - cf. [117]) via trace duality. Theory and applications of operator ideals are widely known (not by functional analysts only), as opposed to the tensor norm theory of Grothendieck. In this respect, [33, 37, 77] are very valuable sources which strongly help to make Grothendieck's approach accessible to a wider community.

In particular, the famous Grothendieck inequality (also known as *the fundamental theorem of the metric theory of tensor products*), published in Grothendieck's seminal paper [52] had a profound influence on the geometry of Banach spaces and operator theory; particularly between 1970 and 1990. We highly recommend those readers who have a solid knowledge of functional analysis to study Chapter 8 of the superb monograph [2]. Here is worked out in great clarity, step-by-step (without the use of tensor products of Banach spaces, and without the use of abstract operator ideal theory), how the Grothendieck inequality can be equivalently characterised, including Grothendieck's key result, that the inequality is equivalent to the deep fact that *any* bounded linear operator $T \in \mathcal{L}(L^1(\mu), l_2)$ (where the measure μ lives on a σ-finite measure space) already is absolutely 1-summing and satisfies the norm inequality $\|T\|_{\mathcal{P}_1} \leq K_G^{\mathbb{F}} \|T\|$ (cf. [2, Remark 8.3.2 (b)], [33, Theorem 23.10], [34], [77, Theorem 10.7] and Remark 4.10). An exceptional proof of the latter result (which is built on a factorisation of $T \in \mathcal{L}(l_1, l_2)$ over the disc algebra $A(\mathbb{D})$) is given in [150, Theorem III.F.7] (cf. also Remark 5.13 below).

Meanwhile, in addition to this impact, the Grothendieck inequality exhibits deep applications in different fields (including theoretical computer science, computational complexity, analysis of Boolean functions, random graphs (including the mathematics of the systemic risk in financial networks, analysis of nearest-neighbour interactions in a crystal structure (Ising model), correlation clustering and image segmentation in the field of computer vision), NP-hard combinatorial optimisation, non-convex optimisation and semidefinite programming (cf. [54]), foundations and philosophy of quantum mechanics, quantum information theory, quantum correlations (cf. Subsection 3.1), quantum cryptography, communication complexity protocols and even high-dimensional private data analysis (cf. [39])! Also in these fields there exist many challenging related open problems.

The interest in Grothendieck's work revived when J. Lindenstrauss and A. Pełczyński recast its main results in the more traditional language of operators and matrices (see [37, Theorem A.3.1] and [97]) which is also the basis of our own research.

Theorem 1.1 (**Grothendieck inequality in matrix form**). *Let* $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$. *There is an absolute constant* $K > 0$ *such that for any* $m, n \in \mathbb{N}$, *for any* $A = (a_{ij}) \in \mathbb{M}_{m,n}(\mathbb{F})$, *any* $\mathbb{F}$*-Hilbert space* H, *and any* $(u_1, \ldots, u_m) \in B_H^m$, $(v_1, \ldots, v_n) \in B_H^n$, *the following inequality is satisfied:*

$$\Big|\sum_{i=1}^{m}\sum_{j=1}^{n} a_{ij}\langle u_i, v_j\rangle_H\Big| \leq K \sup\Big\{\Big|\sum_{i=1}^{m}\sum_{j=1}^{n} a_{ij}p_i q_j\Big| : |p_i| \leq 1, |q_j| \leq 1 \,\forall i, j\Big\}.$$

The smallest possible value of the corresponding absolute constant K is called the *Grothendieck constant* $K_G^{\mathbb{F}}$ (cf. also Theorem 3.7). The superscripts $\mathbb{R}$ and $\mathbb{C}$ are used to indicate the different values in the real and complex cases. Regarding functional analytic key reformulations of the Grothendieck inequality, involving the infinite-dimensional Banach spaces of type $C(K)$, $C(L)'$ and $L^1(\mu)$, we highly recommend the readers to study [119, Section 2], including the detailed and very helpful proof of the equivalence of [119, Theorem 2.3] and the Grothendieck inequality in matrix form (on which our paper is based). Observe that in the case $m = n = 1$, already $K = 1$ satisfies the Grothendieck inequality. However, it is well-known that $K_G^{\mathbb{R}} > K_G^{\mathbb{C}} > 1$ (cf. also Corollary 3.33). In his seminal paper [52], Grothendieck proved that $K_G^{\mathbb{R}} \leq \sinh(\frac{\pi}{2}) \approx 2.301$ (within our framework recovered as special case in Example 6.48). In 1974, Grothendieck's result could be improved by R. E. Rietz, who showed that $K_G^{\mathbb{R}} < 2.261$ (cf. [123]). Until present (rounded to three digits) the following encapsulation of $K_G^{\mathbb{R}}$ holds; rounded to 3 digits (cf. [22], Example 6.48 and Example 6.51):

$$1,676 < K_G^{\mathbb{R}} \overset{(!)}{<} \frac{1}{\frac{2}{\pi}\sinh^{-1}(1)} = \frac{\pi}{2\ln(1+\sqrt{2})} \approx 1,782\,.$$

The complex constant is strictly smaller than the real one. Namely, if we merge the values of the upper bounds of $K_G^{\mathbb{C}}$ achieved to date (cf. [57, 90, 118, 119], Theorem 1.3 and our approximative calculation of the number $\frac{1}{c^*} \approx 1.40449$ at the end of Example 7.15), we obtain (rounded to three digits):

$$1 < \frac{4}{\pi} < 1.338 \leq K_G^{\mathbb{C}} \leq 1.405 < \sqrt{2} < e^{1-\gamma} < \frac{\pi}{2} < K_G^{\mathbb{R}} \leq \sqrt{2}\, K_G^{\mathbb{C}}\,, \tag{1.1}$$

where $\gamma := \sum_{n=2}^{\infty}(-1)^n\frac{\zeta(n)}{n} = -\Gamma'(1) \approx 0.577$ denotes the Euler-Mascheroni constant. Until present, the best-known lowest upper bound of $K_G^{\mathbb{C}}$ is given by $K_G^{\mathbb{C}} \leq 1.40491$, carried out by U. Haagerup in [57] (approximatively achieved again in Example 7.15).

Regarding apparently surprising equivalent formulations of Theorem 1.1 (including their detailed verifications), revealing the depth of the structure beneath the "surface of the inequality", we refer to [77, Equivalent formulations, p. 109 ff].

Computing the exact numerical value of the constants $K_G^{\mathbb{R}}$ and $K_G^{\mathbb{C}}$ is still an open problem (unsolved since 1953). This is where our own research continues. We look for a general framework (primarily build on methods originating from (block) matrix analysis (cf. [68]), multivariate statistics with real and complex Gaussian random vectors, theory of special functions, modelling of statistical dependence with copulas and combinatorics, whose complexity increases rapidly in dimension, though) which allows us either to give the value of $K_G^{\mathbb{R}}$, respectively $K_G^{\mathbb{C}}$ explicitly or to approximate these values from above and from below at least. However, our approach - which in particular allows a short proof of the real and complex Grothendieck inequality, even with J.-L. Krivine's upper bound of $K_G^{\mathbb{R}}$ - confronts us strongly with the question whether the seemingly non-avoidable combinatoric complexity actually allows us to determine the values of $K_G^{\mathbb{R}}$, respectively $K_G^{\mathbb{F}}$ explicitly, or not. A detailed description of this research problem can be studied in Subsection 9.1 of our paper.

If either the size $m \times n$ of the arbitrarily chosen matrix $A \in \mathbb{M}_{m,n}(\mathbb{F})$ or the dimension d of the finite-dimensional Hilbert space $\mathbb{F}_2^d$ is predefined, we obtain the corresponding two weakened forms of Theorem 1.1:

Proposition 1.2. *Let* $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$.

(i) *For any* $d \in \mathbb{N}$ *there is a constant* $K^{\mathbb{F}}(d) > 1$ *such that*

$$\Big|\sum_{i=1}^{m}\sum_{j=1}^{n} a_{ij}\langle u_i, v_j\rangle_{\mathbb{F}_2^d}\Big| \leq K^{\mathbb{F}}(d)\, \sup\Big\{\Big|\sum_{i=1}^{m}\sum_{j=1}^{n} a_{ij}p_i q_j\Big| : |p_i| \leq 1, |q_j| \leq 1\, \forall i,j\Big\} \tag{1.2}$$

for any $m, n \in \mathbb{N}$, *for any* $A \in \mathbb{M}_{m,n}(\mathbb{F})$, *for any* $(u_1, \ldots, u_m) \in B_d^m$, *and for any* $(v_1, \ldots, v_n) \in B_d^n$.

(ii) *For any* $(m,n) \in \mathbb{N}^2$ *there is a constant* $K^{\mathbb{F}}(m,n) > 1$ *such that*

$$\Big|\sum_{i=1}^{m}\sum_{j=1}^{n} a_{ij}\langle u_i, v_j\rangle_{H}\Big| \leq K^{\mathbb{F}}(m,n)\, \sup\Big\{\Big|\sum_{i=1}^{m}\sum_{j=1}^{n} a_{ij}p_i q_j\Big| : |p_i| \leq 1, |q_j| \leq 1\, \forall i,j\Big\} \tag{1.3}$$

for any Hilbert space H, *for any* $A \in \mathbb{M}_{m,n}(\mathbb{F})$, *for any* $(u_1, \ldots, u_m) \in B_H^m$, *and for any* $(v_1, \ldots, v_n) \in B_H^n$.

Let $K_G^{\mathbb{F}}(d)$ denote the smallest possible value of the corresponding constant $K^{\mathbb{F}}(d)$, introduced by Krivine (cf. [33, Proposition 20.17]), and let $K_G^{\mathbb{F}}(m,n)$ be the smallest possible value of the constant $K^{\mathbb{F}}(m,n)$, introduced by B. S. Tsirel'son for $\mathbb{F} = \mathbb{R}$ (cf. [141] and the detailed elaboration in [93, 94]). Consequently, $K_G^{\mathbb{F}}(d) \leq K_G^{\mathbb{F}}$ for all $d \in \mathbb{N}$, whence $\sup\limits_{d\in\mathbb{N}} K_G^{\mathbb{F}}(d) \leq K_G^{\mathbb{F}}$. Similarly, it follows that $\sup\limits_{(m,n)\in\mathbb{N}^2} K_G^{\mathbb{F}}(m,n) \leq K_G^{\mathbb{F}}$. It seems to us that the numbers $K_G^{\mathbb{F}}(m,n)$ and $K_G^{\mathbb{F}}(d)$ in general do not stand in relation to each other. Hence, to avoid any risk of confusion, it is important to understand whether authors refer to $K_G^{\mathbb{F}}(m,n)$ or to $K_G^{\mathbb{F}}(d)$ (or even to $K_G^{\mathbb{F}}$) in their work, when they talk about "the Grothendieck constant" (such as it is the case in [14, 23, 43, 44, 83]). For any $d \in \mathbb{N}_3$, explicit *lower* bounds of $K_G^{\mathbb{R}}(d)$ in closed, analytic form are provided in [23, Theorem 1] and [43, Theorem 2.2]. Very recently, the lower bound of $K_G^{\mathbb{R}}(3)$ (which is precisely the threshold value for the nonlocality of the two-qubit Werner state for projective measurements in quantum information theory (cf. [1], [43, Section 3] and Example 3.25)) could be improved. [14] namely reveals that $1.4367 \leq K_G^{\mathbb{R}}(3) \leq 1.4546$. To achieve this result, however, a high computing power was required. In [83], an application of duality in semidefinite programming (implemented via the so-called "convex hull algorithm" in MATLAB) lead to the following values of $K_G^{\mathbb{R}}(m,n)$: $K_G^{\mathbb{R}}(5,5) = K_G^{\mathbb{R}}(4,n) = \sqrt{2}$, where $n \in \{4,5,6,7\}$.

Note that $K_G^{\mathbb{F}}(1) = 1$. Since the sequence $(K_G^{\mathbb{F}}(d))_{d\in\mathbb{N}}$ is non-decreasing it even follows that $K_G^{\mathbb{F}} = \lim\limits_{d\to\infty} K_G^{\mathbb{F}}(d) = \sup\{K_G^{\mathbb{F}}(d) : d \in \mathbb{N}\}$ (see Proposition 3.18). Moreover, we may add (see Corollary 3.35):

$$K_G^{\mathbb{R}}(2d) \leq K_G^{\mathbb{R}}(2)\, K_G^{\mathbb{C}}(d) = \sqrt{2}\, K_G^{\mathbb{C}}(d) \text{ for all } d \in \mathbb{N}\,.$$

In particular, by taking the limit $d \to \infty$, we reobtain $K_G^{\mathbb{R}} \leq \sqrt{2}\, K_G^{\mathbb{C}}$.

Another important special case of the Grothendieck inequality (known as *the little Grothendieck inequality*) appears if just positive semidefinite matrices A are considered. Let $k_G^{\mathbb{F}}$ denote the Grothendieck constant, derived from the Grothendieck inequality restricted to the set of all positive semidefinite $n \times n$ matrices, with entries in $\mathbb{F}$. Then (cf. [108, 116] and Remark 4.10):

Theorem 1.3 (Grothendieck, 1953; Niemi, 1983). *Let $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$ and H be an arbitrary Hilbert space over $\mathbb{F}$. Let $n \in \mathbb{N}$. Then*

(i)
$$k_G^{\mathbb{R}} = \frac{\pi}{2} \quad \textit{(Grothendieck)}$$

and

(ii)
$$k_G^{\mathbb{C}} = \frac{4}{\pi} \quad \textit{(Niemi)}\,.$$

An approximation of the largest lower bounds of both Grothendieck constants (which is not the subject of our current work) can be found in [32]. The real case is treated in [122] as well.

1.2. Preliminaries, terminology and notation

This subsection serves to provide the foundation upon which our whole work is built. To this end, we list the basic notation and symbolic abbreviations used throughout our paper. More specific terminology, including terms introduced for the first time and related symbolic shortcuts will be introduced on the spot. The few remaining symbolic shortcuts which are not explicitly described, are either self-explanatory or can be found in any well-established and relevant undergraduate textbook in mathematics.

Numbers and sets – As is usual, we denote the set of complex numbers by $\mathbb{C}$ and the set of real numbers by $\mathbb{R}$. $\mathbb{Z}$ represents the set of all integers and $\mathbb{N}$ stands for the subset of positive integers. We will use the symbol $\mathbb{F}$ to denote either the real field $\mathbb{R}$ or the complex field $\mathbb{C}$. If we wish to state a definition or a result that is satisfied for either real or complex numbers (i.e., if $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$), we simply will make use of the letter symbol $\mathbb{F}$. Where there is no risk of confusion, we suppress the symbol $\mathbb{F}$. In order to save unnecessary case distinctions, we constantly view the set $\mathbb{R}$ as a subset of $\mathbb{C}$, so that $\mathbb{R} = \{z \in \mathbb{F} : z = \overline{z}\} = \{z \in \mathbb{F} : \mathrm{Im}(z) = 0\}$. $\mathbb{T} := \{z \in \mathbb{C} : |z| = 1\}$ denotes the unit circle ("one-dimensional torus"), $\mathbb{D} := \{z \in \mathbb{C} : |z| < 1\}$ the open unit disk and $\overline{\mathbb{D}} := \{z \in \mathbb{C} : |z| \leq 1\}$ the closed unit disk. If F is an arbitrary normed space, then $S_F := \{x \in F : \|x\|_F = 1\}$ denotes its unit sphere and $B_F := \{x \in F : \|x\|_F \leq 1\}$ its closed unit ball. Thus, $S_{\mathbb{F}} = \mathbb{F} \cap \mathbb{T}$. In particular, $S_{\mathbb{R}} = \{-1, 1\}$ and $S_{\mathbb{C}} = \mathbb{T}$. $\mathbb{N}_0 := \{0\} \cup \mathbb{N}$ denotes the set of all non-negative integers (often also somewhat unhappily denoted as $\mathbb{Z}_+$). If $m \in \mathbb{N}$, we put $[m] := \mathbb{N} \cap [1, m] = \{1, 2, \ldots, m\}$ and $\mathbb{N}_m := \mathbb{N} \cap [m, \infty) = \{m, m+1, m+2, \ldots\}$. Fix $n \in \mathbb{N}_0$. In addition to the factorial $n! := \prod_{i=1}^{n}(n-i) \in \mathbb{N}$, the double factorial $n!! \in \mathbb{N}$ will play a dominant role. The latter is defined as

$$n!! := \prod_{i=0}^{\lfloor \frac{n-1}{2} \rfloor} (n-2i),$$

where $\mathbb{R} \ni x \mapsto \lfloor x \rfloor := \max\{\nu \in \mathbb{Z} : \nu \leq x\}$ denotes the floor function (and $\mathbb{R} \ni x \mapsto \lceil x \rceil := \min\{\nu \in \mathbb{Z} : x \leq \nu\}$ the ceiling function). We adopt the usual approach to include $(-1)!! := 1$ as well. A straightforward proof by induction on $n \in \mathbb{N}_0$, including the well-known fact that $\Gamma(\frac{1}{2}) = \sqrt{\pi}$ shows that

$$n!! = \begin{cases} 2^{\frac{n}{2}}\, \Gamma(\frac{n}{2}+1) & \text{if } n \text{ is even} \\ \sqrt{\frac{2}{\pi}}\, 2^{\frac{n}{2}}\, \Gamma(\frac{n}{2}+1) & \text{if } n \text{ is odd} \end{cases},$$

where $\{z \in \mathbb{F} : \mathrm{Re}(z) > 0\} \ni z \mapsto \Gamma(z) := \int_0^\infty e^{-t}\, t^{z-1}\, dt$ denotes the Gamma function which will play an important role in our paper (cf. [135, Chapter 6.1] and Lemma 4.3).

Vectors, matrices, norms and linear operators in general – Fix $m, n \in \mathbb{N}$. The set of all $m \times n$-matrices with entries in a given non-empty subset $S \subseteq \mathbb{F}$ is denoted by $\mathbb{M}_{m,n}(S)$. The matrix ring $\mathbb{M}_{n,n}(\mathbb{F})$ is abbreviated as $\mathbb{M}_n(\mathbb{F})$. As usual, $e_i \in \mathbb{F}^n$ denotes the column vector having a 1 in the ith place and zeros elsewhere. If we wish to emphasize the dependence on the dimension n of the vector space $\mathbb{F}^n$, then we speak of the set $\{e_1^{(n)}, e_2^{(n)}, \ldots, e_n^{(n)}\} \subseteq \mathbb{F}^n$ (cf., e.g., (3.71)). $I_n := (e_1 \,\vdots\, e_2 \,\vdots\, \cdots \,\vdots\, e_n) \in \mathbb{M}_n(\mathbb{F})$ describes the identity matrix. Initially, if not indicated otherwise, any vector (deterministic or random) $x \in \mathbb{F}^n$ is set as column vector, so that the allocated row vector is decribed by transposition ($x \mapsto x^\top$). Translated into Dirac's bra-ket language, which is also used in quantum information theory, it holds that $e_i = |i-1\rangle$ and $e_i^\top = \langle i-1|$ ($i \in [n]$). In particular, $|0\rangle = e_1$, $|1\rangle = e_2$ and $|n-1\rangle\langle 1| = e_n e_2^\top \in \mathbb{M}_n(\mathbb{F})$ (cf. [107, 134] and (3.72)). If $A \in \mathbb{M}_{m,n}(S)$ is given, it is sometimes very fruitful to represent the entries of A as $A_{ij} := e_i^\top A e_j = e_j^\top A^\top e_i = (A^\top)_{ji}$, so that $A = (a_{ij})$, where $a_{ij} := A_{ij}$. $\overline{A} \in \mathbb{M}_{m,n}(\mathbb{F})$ is defined as $\overline{A}_{ij} := \overline{A_{ij}}$, implying that $A^* := \overline{A}^\top = \overline{A^\top}$ and $x^* := \overline{x}^\top = \overline{x^\top}$. Recall that the Euclidean norm is given by $\|x\|_2 := \sqrt{x^*\, x} = \sqrt{\sum_{i=1}^n |x_i|^2}$ for any $x = (x_1, \ldots, x_n)^\top \in \mathbb{F}^n$. If we equip the n-dimensional vector space $\mathbb{F}^n$ with the Euclidean inner product, we obtain the n-dimensional Hilbert space $\mathbb{F}_2^n := (\mathbb{F}^n, \langle \cdot, \cdot \rangle_2)$, where the inner product on $\mathbb{F}^n$ is given by $\langle x, y\rangle_2 := \langle x, y\rangle_{\mathbb{F}_2^n} := y^* x = \sum_{i=1}^n x_i \overline{y_i}$. In particular, $\langle z, w\rangle_{\mathbb{F}_2^1} = z \cdot \overline{w}$ for all $z, w \in \mathbb{F}$. As usual in mathematics, we adopt the convention that any inner product $\langle \cdot, \cdot \rangle_H$, defined on an arbitrary Hilbert space H, is linear in the first argument and conjugate linear in the second one, implying that $\langle x, y\rangle_H^{[P]} := \overline{\langle x, y\rangle_H} = \langle y, x\rangle_H$ ($x, y \in H$) is conjugate linear in the first argument and linear in the second one; a rather common approach in (quantum) physics. An orthonormal basis in $\mathbb{F}_2^n$ is given by the set of vectors $\{e_1, e_2, \ldots, e_n\}$; i.e., by the standard basis of $\mathbb{F}^n$. Occasionally, if $1 \leq p \leq \infty$, we put $\mathbb{F}_p^n := (\mathbb{F}^n, \|\cdot\|_p)$, where

$$\|x\|_p := \begin{cases} (\sum_{i=1}^n |x_i|^p)^{1/p} & \text{if } 1 < p < \infty \\ \max\{|x_i| : i \in [n]\} & \text{if } p = \infty \end{cases}$$

denotes the p-norm of $x = (x_1, \ldots, x_m)^\top \in \mathbb{F}^n$. If there is no risk of confusion regarding $\mathbb{F}$, we simply speak of the space l_p^n (as usual). As usual, if $n \in \mathbb{N}_2$, then $\mathbb{S}^{n-1}$ denotes the unit sphere in $\mathbb{R}_2^n$. Throughout the paper, we also identify any linear operator $T : \mathbb{F}^n \longrightarrow \mathbb{F}^m$ with its representing matrix with respect to the respective standard bases: $T \equiv (T_{ij})_{(i,j)\in[m]\times[n]}$. In particular, we have

$$T_{ij} \equiv e_i^\top T e_j = \langle T e_j, e_i\rangle_{\mathbb{F}_2^m} = \langle e_j, T^* e_i\rangle_{\mathbb{F}_2^n} \equiv (T^*)_{ji} \text{ for all } i,j \in [m]\times[n]\,,$$

where $T^* : \mathbb{F}_2^m \longrightarrow \mathbb{F}_2^n$ is the adjoint operator. Furthermore, in the case $n = 1$, $\mathbb{F}$ is considered throughout as the one-dimensional Hilbert space $(\mathbb{F}_2^1, \langle\cdot,\cdot\rangle_2)$, where $\langle z, w\rangle_2 := z\,\overline{w}$ for all $z, w \in \mathbb{F}$. As usual, $O(n)$ denotes the orthogonal group, consisting of all invertible matrices $A \in \mathbb{M}_n(\mathbb{R})$ such that $A^{-1} = A^\top$. $U(n)$ describes the unitary group, consisting of all invertible matrices $A \in \mathbb{M}_n(\mathbb{C})$ such that $A^{-1} = A^*$. $SO(n) := \{A \in O(n) : \det(A) = 1\}$ is the special orthogonal group, and $SU(n) := \{A \in U(n) : \det(A) = 1\}$ describes the special unitary group.

An important inner product on the $\mathbb{F}$-vector space $\mathbb{M}_{m,n}(\mathbb{F})$ of all $m\times n$-matrices with entries in $\mathbb{F}$, which turns $\mathbb{M}_{m,n}(\mathbb{F})$ into an mn-dimensional Hilbert space, is the Frobenius inner product, which is defined as follows: if $A = (a_{ij}) \in \mathbb{M}_{m,n}(\mathbb{F})$ and $B = (b_{ij}) \in \mathbb{M}_{m,n}(\mathbb{F})$, then

$$\langle A, B\rangle_F := \mathrm{tr}(AB^*) = \mathrm{tr}(B^*A) = \sum_{i=1}^m \sum_{j=1}^n a_{ij}\,\overline{b_{ij}} = \overline{\langle B, A\rangle_F}\,,$$

where

$$\mathrm{tr}(C) := \sum_{i=1}^n \langle Ce_i, e_i\rangle_2 = \sum_{i=1}^n c_{ii} = \mathrm{tr}(C^\top) = \overline{\mathrm{tr}(C^*)} = \overline{\mathrm{tr}(\overline{C})}$$

denotes the trace of a given (quadratic) matrix $C = (c_{ij}) \in \mathbb{M}_{n,n}(\mathbb{F})$. One can easily verify the well-known fact that the set of all elementary matrices $\{e_i\, e_j^\top : (i,j) \in [m]\times[n]\}$ is an orthonormal basis in the mn-dimensional $\mathbb{F}$-Hilbert space $(\mathbb{M}_{m,n}(\mathbb{F}), \|\cdot\|_F)$ (since $(e_i\, e_j^\top)_{\alpha\beta} = \delta_{i\alpha}\,\delta_{j\beta}$ for all $(\alpha,\beta) \in [m]\times[n]$ and $\mathrm{tr}(xy^\top) = y^\top x$ for all $x, y \in \mathbb{F}^n$). We adopt the symbolic notation of the "$\mathcal{L}$-community" to represent the set of all bounded linear operators between two normed spaces $(E, \|\cdot\|_E)$ and $(F, \|\cdot\|_F)$ by $\mathcal{L}(E,F)$. As usual, the Banach space $E' := \mathcal{L}(E, \mathbb{F})$ denotes the dual space of E. (The "$\mathcal{B}$-community", often encountered among researchers in the field of C^*-algebras, uses $\mathcal{B}(E,F)$ instead, so that for example, $\mathcal{B}(H) = \mathcal{L}(H,H)$, if H is a given Hilbert space (cf., e.g., [64, Chapter 1.3])). Remember that every linear operator $T : E_0 \longrightarrow F$ from a finite-dimensional normed space E_0 to an arbitrary normed space F already is bounded. It should also be noted that actually $\langle A, B\rangle_F = \langle A, B\rangle_{HS}$ coincides with the Hilbert-Schmidt inner product, defined on the Hilbert space $\mathcal{L}(\mathbb{F}_2^n, \mathbb{F}_2^m)$. To this end, recall that if H and K are arbitrarily given $\mathbb{F}$-Hilbert spaces, $T \in \mathcal{L}(H,K)$ is a Hilbert-Schmidt operator if and only if $(\|Te_\iota\|_K)_{\iota\in J} \in l^2(J)$ for some orthonormal basis $(e_\iota)_{\iota\in J}$ in H. Here, J denotes an arbitrary index set which must be neither finite nor at most countable (cf., e.g., [78, Proposition 20.2.7]). Hence, if $S, T \in \mathcal{S}_2(H,K)$ are two Hilbert-Schmidt operators, the Cauchy-Schwarz inequality implies that

$$\langle S, T\rangle_{HS} := \sum_{\iota\in J} \langle Te_\iota, Se_\iota\rangle_K = \sum_{\iota\in J} \langle e_\iota, T^*Se_\iota\rangle_K = \mathrm{tr}(T^*S)\,,$$

is a well-defined inner product on the $\mathbb{F}$-vector space $\mathcal{S}_2(H,K)$ of all Hilbert-Schmidt operators. In fact, it turns $\mathcal{S}_2(H,K)$ into a Hilbert space itself (cf. [29, Exercises IX.2.19, IX.2.20] and [78, Proposition 20.2.7]). Let us also note the easy-to-prove fact that

$$\Pi : (\mathbb{M}_{m,n}(\mathbb{F}), \|\cdot\|_F) \xrightarrow{\cong} (\mathbb{M}_{m,n}(\mathbb{F}), \|\cdot\|_F)', A \mapsto (B \mapsto \mathrm{tr}(BA^\top))$$

is an isometric isomorphism, whose inverse is given by $\Pi^{-1} = \Psi$, where

$$\mathbb{M}_{m,n}(\mathbb{F}) \ni \Psi(t) := (t(e_i e_j^\top))_{i,j} \text{ for all } t \in (\mathbb{M}_{m,n}(\mathbb{F}), \| \cdot \|_F)'.$$

Obviously, also the canonically defined mapping

$$\Theta : (\mathbb{M}_{m,n}(\mathbb{F}), \| \cdot \|_F)' \xrightarrow{\cong} (\mathbb{M}_{n,m}(\mathbb{F}), \| \cdot \|_F)', t \mapsto (M \mapsto \langle M^\top, t \rangle)$$

is an isometric isomorphism, implying that the composition of these two isometric isomorphisms lead to the finite-dimensional version of *trace duality* with respect to the norm $\| \cdot \|_F = \| \cdot \|_{HS}$ (cf. [79, Theorem 6.4]):

$$\Pi \circ \Theta : (\mathbb{M}_{m,n}(\mathbb{F}), \| \cdot \|_F) \xrightarrow{\cong} (\mathbb{M}_{n,m}(\mathbb{F}), \| \cdot \|_F)', A \mapsto (B \mapsto \operatorname{tr}(BA)).$$

Although it is our intention that the main ideas developed in our paper can be captured without knowledge of advanced functional analysis and related operator theory, we will add a few text passages which should show how also our approach extends into the area of functional analysis and operator ideal theory. Related references will be listed, of course. In particular - despite its elegance and power - we intentionally avoid the explicit use of the language of abstract tensor products of Banach spaces and related tensor norms (originally coined by A. Grothendieck in his seminal paper [52]) as far as possible. Of course, any attentive reader will recognise that tensor products occasionally also are lurking in our framework (primarily in the form of concrete Kronecker products of matrices). Remarks in this regard could be skipped at the first reading. However, for particularly stubborn readers and authors, we strongly refer to [29, 33, 64, 77, 79, 117, 147].

Since (symmetrically) partitioned random vectors and block matrices play a key role in our analysis, it is sometimes very useful to transform matrices into column vectors by making use of a technique known as matrix vectorisation (cf. [98, Chapter 10]). If $A = (a_1 \mid a_2 \mid \cdots \mid a_n) \in \mathbb{M}_{m,n}(\mathbb{F})$, with columns $a_j \in \mathbb{F}^m$ ($j \in [n]$), then

$$\operatorname{vec}(A) := \operatorname{vec}(a_1, \ldots, a_n) := (a_1^\top \mid \ldots \mid a_n^\top)^\top \in \mathbb{F}^{mn}$$

denotes the *column* vector constructed by stacking the columns of A on top of each other. A concise *entrywise* implementable construction (built on Euclidian division with remainder) of $\operatorname{vec}(A)$ will be treated at the beginning of Subsection 3.4 (cf. (3.69)). Obviously,

$$\operatorname{vec} : (\mathbb{M}_{m,n}(\mathbb{F}), \langle \cdot, \cdot \rangle_F) \xrightarrow{\cong} \mathbb{F}_2^{mn}, A \mapsto \operatorname{vec}(A)$$

is an isometric isomorphism (between finite-dimensional Hilbert spaces). In particular,

$$\langle \operatorname{vec}(A), \operatorname{vec}(B) \rangle_2 = \operatorname{tr}(B^* A) \text{ and } \| \operatorname{vec}(A) \|_2 = \sqrt{\operatorname{tr}(A^* A)} \tag{1.4}$$

for all $A, B \in \mathbb{M}_{m,n}(\mathbb{F})$. We also need vec's cousin, the Kronecker product of matrices (cf. [98, Chapter 10]), on which the construction of a matrix is based which delivers $\sqrt{2}$ as a lower bound of the real Grothendieck constant $K_G^{\mathbb{R}}$ *and* plays a key role in the foundations of quantum mechanics, quantum information and even in evolutionary biology: the Walsh-Hadamard transform (cf. Example 3.27, Remark 3.29 and Remark 3.30)! The Kronecker product is constructed as follows: if $A \in \mathbb{M}_{m,n}(\mathbb{F})$ and $B \in \mathbb{M}_{p,q}(\mathbb{F})$, then

$$\mathbb{M}_{mp,nq}(\mathbb{F}) \ni A \otimes B = \begin{pmatrix} M_{11} & M_{12} & \cdots & M_{1n} \\ M_{21} & M_{22} & \cdots & M_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ M_{m1} & M_{m2} & \cdots & M_{mn} \end{pmatrix},$$

where $M_{ij} := a_{ij}B \in \mathbb{M}_{p,q}(\mathbb{F})$. If $C \in \mathbb{M}_{n,r}(\mathbb{F})$ and $D \in \mathbb{M}_{q,s}(\mathbb{F})$ are two further matrices, then elementary block matrix multiplication instantly results into the well-known fact that

$$(A \otimes B)(C \otimes D) = AC \otimes BD\,. \tag{1.5}$$

We will also provide a rigorous *entrywise* implementable construction of the Kronecker product at the beginning of Subsection 3.4 (again built on Euclidian division with remainder). In the context of partitioned random vectors, we will apply the vec operator in the following sense: if $x = (x_1, \ldots, x_n, x_{n+1}, \ldots, x_{2n})^\top \in \mathbb{F}^{2n}$, then $x = \text{vec}(a_1, a_2)$, where $a_1 := (x_1, \ldots, x_n)^\top \in \mathbb{F}^n$ and $a_2 := (x_{n+1}, \ldots, x_{2n})^\top \in \mathbb{F}^n$.

Fix $v = (v_1, \ldots, v_l)^\top \in \mathbb{F}^l$ and $A = (a_{ij}) \in \mathbb{M}_{m,n}(\mathbb{F})$. Let $\Psi : [m] \times [n] \longrightarrow [l]$ and $\Lambda : [l] \longrightarrow [m] \times [n]$ be given. In the context of our analysis, Ψ should be viewed as a mapping which maps an index $(i, j) \in [m] \times [n]$ of the matrix element $a_{ij} \in \mathbb{F}$ to the index $\Psi(i, j) \in [l]$ of an allocated vector element. Conversely, Λ should be regarded as a mapping which maps the index $\alpha \in [l]$ of the vector element $v_\alpha \in \mathbb{F}$ to an index $\Lambda(\alpha) = (\Lambda_1(\alpha), \Lambda_2(\alpha)) \in [m] \times [n]$ of an allocated matrix element. More precisely formulated, if we consider the (linear) composition operator $C_\psi : \mathbb{F}^l \longrightarrow \mathbb{M}_{m,n}(\mathbb{F})$, we map the given vector $v \in \mathbb{F}^l$ to a matrix $C_\Psi(v) := v_\Psi \in \mathbb{M}_{m,n}(\mathbb{F})$ as follows:

$$(v_\Psi)_{i,j} := v_{\Psi(i,j)} \text{ for all } (i, j) \in [m] \times [n].$$

Analogously, we map the matrix $A = (a_{ij}) \in \mathbb{M}_{m,n}(\mathbb{F})$ to a vector $A_\Lambda \in \mathbb{F}^l$, according to the rule

$$(C_\Lambda(A))_\alpha := (A_\Lambda)_\alpha := a_{\Lambda(\alpha)} = a_{(\Lambda_1(\alpha),\Lambda_2(\alpha))} \text{ for all } \alpha \in [l],$$

where $C_\Lambda : \mathbb{M}_{m,n}(\mathbb{F}) \longrightarrow \mathbb{F}^l$ denotes the related linear composition operator. Similarly, the matrix $A \in \mathbb{M}_{m,n}(\mathbb{F})$ can be mapped to the matrix $A_\sigma \in \mathbb{M}_{r,s}(\mathbb{F})$, where σ is now a given mapping of type $\sigma : [r] \times [s] \longrightarrow [m] \times [n]$. Observe that A_σ consists of entries of the originally given matrix A, so that we could view A_σ as a subordinated matrix of A (cf. Remark 5.3). For example, $A^\top = A_\tau = C_\tau(A)$, where the mapping $\tau : [n] \times [m] \longrightarrow [m] \times [n]$ is defined as transposition: $\tau(\nu, \mu) := (\mu, \nu)$ (cf. (3.69)). A very recent application of vectorisation within the framework of single quantum systems (where entangled states do not play a role), including a related application of the Grothendieck inequality can be found in [145, 146].

Partitioning, $\mathbb{C}^{2n}$ versus $\mathbb{R}^{4n}$, matrices with special form and positive semidefiniteness – With regard to the study of a class of crucially important partitioned multivariate complex Gaussian random vectors for our analysis (cf. Section 2), we firstly have to shed some light on the structure of the following two important mappings, which we will encounter many times in this paper. Similar constructions and particular cases are listed in [5, Chapter 1.2] and [68, Problem 1.3.P20 and Problem 1.3.P21]. To this end, fix $m, n \in \mathbb{N}$ and $w \in \mathbb{C}^n$. Put

$$\mathbb{C}^n \ni w = \text{Re}(w) + i\,\text{Im}(w) \mapsto J_2(w) \equiv J_2^{[n]}(w) := \text{vec}(\text{Re}(w), \text{Im}(w)) \in \mathbb{R}^{2n} \tag{1.6}$$

and

$$M_{m,n}(\mathbb{C}) \ni A \mapsto R_2(A) := \begin{pmatrix} \mathrm{Re}(A) & -\mathrm{Im}(A) \\ \mathrm{Im}(A) & \mathrm{Re}(A) \end{pmatrix} \in \mathbb{M}_{2m,2n}(\mathbb{R}) \tag{1.7}$$

Observe, that if $n \geq 2$, $J_2(w) = \mathrm{vec}(\mathrm{Re}(w), \mathrm{Im}(w)) = \mathrm{vec}(\mathrm{Re}(w_1), \ldots, \mathrm{Re}(w_n), \mathrm{Im}(w_1), \ldots, \mathrm{Im}(w_n))$ in general does not coincide with $\mathrm{vec}(J_2(w_1), J_2(w_2), \ldots, J_2(w_n))$. However, given arbitrary $z, w \in \mathbb{C}^n$, we obtain an important equality which will be applied several times in our paper; namely:

$$\begin{aligned} J_2^{[2n]}\mathrm{vec}(z, w) &= \mathrm{vec}(\mathrm{Re}(z), \mathrm{Re}(w), \mathrm{Im}(z), \mathrm{Im}(w)) \\ &= G\,\mathrm{vec}(\mathrm{Re}(z), \mathrm{Im}(z), \mathrm{Re}(w), \mathrm{Im}(w)) = G\,\mathrm{vec}(J_2(z), J_2(w))\,, \end{aligned} \tag{1.8}$$

where

$$G \equiv G_n := \begin{pmatrix} I_n & 0 & 0 & 0 \\ 0 & 0 & I_n & 0 \\ 0 & I_n & 0 & 0 \\ 0 & 0 & 0 & I_n \end{pmatrix} = G^\top = G^{-1} \in O(4n) \text{ is orthogonal}\,. \tag{1.9}$$

Observe that the matrix $G_1 \in O(4)$ precisely coincides with the “swap gate” (also known as “flip operator”), used in quantum information theory (cf. [134, Problem 28] and Example 3.25). In general, if $\mathrm{vec}(x_1, x_2, x_3, x_4) \in \mathbb{R}^{4n}$ is given, then $G \equiv G_n$ swaps the column vectors $x_2 \in \mathbb{R}^n$ and $x_3 \in \mathbb{R}^n$ and maps $\mathrm{vec}(x_1, x_2, x_3, x_4)$ to $\mathrm{vec}(x_1, x_3, x_2, x_4)$. Also the matrix G will be needed repeatedly; for example, in the proofs of Lemma 2.14 and Corollary 2.15.

Not only in this context, we occasionally need the following construction. Let $f, g : \mathbb{F}^k \longrightarrow \mathbb{F}$ be two arbitrary functions ($k \in \mathbb{N}$). Then the function $f \otimes g : \mathbb{F}^{2k} \longrightarrow \mathbb{F}$ is (purely symbolic) defined as

$$(f \otimes g)(\mathrm{vec}(x, y)) := f(x)g(y) \text{ for all } x, y \in \mathbb{F}^k\,.$$

Clearly the mapping $J_2 : \mathbb{C}^n \longrightarrow \mathbb{R}^{2n}$ is bijective, and $\|J_2(a)\|_{\mathbb{R}_2^{2n}} = \|a\|_{\mathbb{C}_2^n}$ for any $a \in \mathbb{C}^n$. Moreover,

$$J_2(\overline{a}) = \begin{pmatrix} I_n & 0 \\ 0 & -I_n \end{pmatrix} J_2(a) \text{ for all } a \in \mathbb{C}^n\,. \tag{1.10}$$

Recall that $\mathbb{S}^{\nu-1}$ denotes the unit sphere in $\mathbb{R}_2^\nu$ ($\nu \in \mathbb{N}_2$). Thus, $S_{\mathbb{C}_2^n} = J_2^{-1}(\mathbb{S}^{2n-1})$ describes the unit sphere in $\mathbb{C}_2^n$. Let $z, w \in \mathbb{C}^n$. Then,

$$\mathrm{Re}(\langle w, z\rangle_{\mathbb{C}_2^n}) = \mathrm{Re}(z^*\, w) = J_2(z)^\top J_2(w) = \langle J_2(w), J_2(z)\rangle_{\mathbb{R}_2^{2n}} \tag{1.11}$$

induces an inner product which turns $\mathbb{C}^n$ into a *real* finite-dimensional Hilbert space and J_2 into an isometric isomorphism between the *real* Hilbert spaces $(\mathbb{C}^n, \mathrm{Re}(\langle\cdot,\cdot\rangle_{\mathbb{C}_2^n}))$ and $\mathbb{R}_2^{2n}$. Clearly, J_2 cannot be extended to a linear mapping between $\mathbb{C}^n$ and $\mathbb{C}^{2n} \supseteq \mathbb{R}^{2n}$. However, by construction $J_2^{-1} : \mathbb{R}^{2n} \longrightarrow \mathbb{C}^n$ clearly satisfies

$$x_1 + i\,x_2 = J_2^{-1}x = (I_n \,\vdots\, iI_n)x \text{ for all } x = \mathrm{vec}(x_1, x_2) \in \mathbb{R}^{2n} \cong \mathbb{R}^n \times \mathbb{R}^n\,, \tag{1.12}$$

$$\begin{array}{ccc} \mathbb{C}^n & \xrightarrow{\quad A \quad} & \mathbb{C}^m \\ {\scriptstyle J_2}\downarrow & & \downarrow{\scriptstyle J_2} \\ \mathbb{R}^{2n} & \xrightarrow{\quad R_2(A) \quad} & \mathbb{R}^{2m} \end{array} .$$

Figure 1: $R_2(A) = J_2 \circ A \circ J_2^{-1}$

implying that the linear and non-injective mapping between the complex vector spaces $\mathbb{C}^{2n}$ and $\mathbb{C}^n$, induced by the matrix $(I_n \,\vdots\, iI_n) \in \mathbb{M}_{n,2n}(\mathbb{C})$ actually is a linear extension of J_2^{-1}. Moreover, it follows that

$$\mathrm{Im}(\langle w, z\rangle_{\mathbb{C}_2^n}) = \mathrm{Im}(z^* w) = \mathrm{Re}(z^*(-iw)) = J_2(z)^\top J_2(-iw) = \langle J_2(-iw), J_2(z)\rangle_{\mathbb{R}_2^{2n}} \tag{1.13}$$

and $J_2(Aw) = R_2(A)\, J_2(w)$ and $R_2(rA) = rR_2(A)$ for all $r \in \mathbb{R}$, $z, w \in \mathbb{C}^n$ and $A \in \mathbb{M}_{m,n}(\mathbb{C})$. In particular, the following diagram commutes
Note also that $R_2(I_n) = I_{2n}$ and

$$R_2(GH) = R_2(G)R_2(H) \text{ for all } (G, H) \in \mathbb{M}_{k,m}(\mathbb{C}) \times \mathbb{M}_{m,n}(\mathbb{C})\,.$$

Moreover,

$$R_2(A^*) = R_2(A)^\top \text{ for any } A \in \mathbb{M}_{m,n}(\mathbb{C})\,. \tag{1.14}$$

In particular,

$$R_2(A^\top)^\top = R_2(\overline{A}) = \begin{pmatrix} I_n & 0 \\ 0 & -I_n \end{pmatrix} R_2(A) \begin{pmatrix} I_n & 0 \\ 0 & -I_n \end{pmatrix} \text{ for any } A \in \mathbb{M}_{m,n}(\mathbb{C})\,.$$

Thus, from the algebraic viewpoint, $R_2 : M_n(\mathbb{C}) \longrightarrow \mathbb{M}_{2n}(\mathbb{R})$ is an injective unitary *-ring homomorphism. In particular, $A \in M_n(\mathbb{C})$ is invertible if and only if $R_2(A) \in \mathbb{M}_{2n}(\mathbb{R})$ is invertible (since $R_2(A)R_2(A^{-1}) = I_{2n} = R_2(A^{-1})R_2(A)$ for any $A \in GL(n;\mathbb{C})$). In the case $n = 1$, we reobtain the well-known Abelian group isomorphism $R_2 : \mathbb{T} \overset{\cong}{\longrightarrow} SO(2)$. Consequently, it follows that

$$\begin{aligned} &\mathrm{Re}(\langle A\, w, z\rangle_{\mathbb{C}_2^m}) = \mathrm{Re}(z^* A\, w) = J_2(z)^\top R_2(A) J_2(w) = \langle R_2(A) J_2(w), J_2(z)\rangle_{\mathbb{R}_2^{2m}} \text{ and} \\ &\mathrm{Im}(\langle A\, w, z\rangle_{\mathbb{C}_2^m}) = \mathrm{Im}(z^* A\, w) = -J_2(z)^\top R_2(i\, A) J_2(w) = -\langle R_2(i\, A) J_2(w), J_2(z)\rangle_{\mathbb{R}_2^{2m}} \end{aligned} \tag{1.15}$$

for all $(z, w) \in \mathbb{C}^m \times \mathbb{C}^n$ and $A \in \mathbb{M}_{m,n}(\mathbb{C})$.

Lemma 1.4. *Let $n \in \mathbb{N}$ and $C \in M_n(\mathbb{R})$. Then the following statements are equivalent*

(i) *C is skew symmetric.*

(ii) *$x^\top C y = -y^\top C x$ for all $x, y \in \mathbb{R}^n$.*

(iii) *$z^\top C z = 0$ for all $z \in \mathbb{C}^n$.*

(iv) *$x^\top C x = 0$ for all $x \in \mathbb{R}^n$.*

Proof. Since C is skew symmetric, it follows that $x^\top C y = (x^\top C y)^\top = y^\top(-C)x$ for all $x, y \in \mathbb{R}^n$, wherefrom the implication $(i) \Rightarrow (ii)$ follows. (ii) obviously implies condition (iii): we just have to factor out $(x^\top + iy^\top)C(x + iy)$ for arbitrary $x, y \in \mathbb{R}^n$ and apply (ii) to the four consecutive factors. $(iii) \Rightarrow (iv)$ is trivial. Assume that the hypothesis (iv) holds. Let $x, y \in \mathbb{R}^n$ be given. Then $x^\top C x = 0$, $y^\top C y = 0$ and $(x^\top + y^\top)C(x+y) = 0$. Consequently,

$$0 = (x^\top + y^\top)C(x + y) = x^\top C y + y^\top C x = x^\top(C + C^\top)y\,,$$

and (i) follows. □

Combining Lemma 1.4 with (1.14) and (1.15), we immediately obtain another neat result, including a full characterisation of Hermitian matrices $A = A^* \in M_n(\mathbb{C})$ by their symmetric real representation $R_2(A) = R_2(A)^\top \in \mathbb{M}_{2n}(\mathbb{R})$.

Proposition 1.5. *Let $n \in \mathbb{N}$ and $\Gamma = \mathrm{Re}(\Gamma) + i\,\mathrm{Im}(\Gamma) \in M_n(\mathbb{C})$. Then the following statements are equivalent:*

(i) *Γ is Hermitian.*

(ii) *$i\Gamma$ is skew Hermitian.*

(iii) *$\mathrm{Re}(\Gamma) \in M_n(\mathbb{R})$ is symmetric and $\mathrm{Im}(\Gamma) \in M_n(\mathbb{R})$ is skew symmetric.*

(iv) *$R_2(\Gamma)$ is symmetric.*

(v) *$z^*\Gamma\, z \in \mathbb{R}$ for all $z \in \mathbb{C}^n$.*

(vi) *$R_2(i\,\Gamma)$ is skew symmetric.*

In particular, if $\Sigma = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \in \mathbb{M}_2(M_n(\mathbb{R}))$, then the following applies:

$$\begin{aligned}&\Sigma = R_2(\Gamma) \text{ for some Hermitian matrix } \Gamma \in \mathbb{M}_n(\mathbb{C}) \text{ if and only if } A = D\\ &\text{and } B + C = 0 \text{ and } \Sigma \text{ is symmetric.}\end{aligned} \tag{1.16}$$

Thereby, the uniquely defined Hermitian matrix is given by $\Gamma = A + iC$.

Another important implication refers to the role of the matrix $R_2(A)$ regarding a full clarification of the reason for the difference between the structure of positive semidefinite matrices in $\mathbb{M}_n(\mathbb{C})$ and the structure of positive semidefinite matrices in $\mathbb{M}_n(\mathbb{R})$ (cf. e.g. [68, Theorem 4.1.10] and the field-independent definition in the form of Lemma 1.7 below):

Corollary 1.6. *Let $n \in \mathbb{N}$ and $A = \mathrm{Re}(A) + i\,\mathrm{Im}(A) \in M_n(\mathbb{C})$. Then the following statements are equivalent:*

(i) *$z^* A\, z \geq 0$ for all $z \in \mathbb{C}^n$.*

(ii) *$z^* A\, z \geq 0$ for all $z \in \mathbb{C}^n$ and A is Hermitian.*

(iii) *$x^\top R_2(A)\, x \geq 0$ for all $x \in \mathbb{R}^{2n}$ and $R_2(A)$ is symmetric.*

If in addition $\mathrm{Im}(A) = 0$, then (i) is equivalent to

(i) $x^\top A\, x \geq 0$ *for all* $x \in \mathbb{R}^n$ *and* A *is symmetric.*

Corollary 1.6 reveals the role of symmetry in the established definition of a positive semidefinite real matrix. For example, if we consider the non-symmetric real matrix $A := \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ and $z := (1, i)^\top \in \mathbb{C}^2$, then $x^\top A\, x = 0$ for all $x \in \mathbb{R}^2$, but $z^* A\, z = 2i$. Thus, throughout the paper, we apply the following characterisation of positive semidefinite (respectively positive definite) matrices, which does not depend on the choice of the field $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$:

Lemma 1.7. *Let* $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}, n \in \mathbb{N}$ *and* $A \in M_n(\mathbb{F})$*.* A *is positive semidefinite (respectively positive definite) in* $\mathbb{M}_n(\mathbb{F})$ *if the following two conditions are satisfied:*

(i) $A = A^*$*.*

(ii) $z^* A z \geq 0$ *(respectively* $z^* A z > 0$*) for all* $z \in \mathbb{F}^n \setminus \{0\}$*.*

In particular, $A \in M_n(\mathbb{R})$ *is positive semidefinite in* $M_n(\mathbb{R})$*, if and only if* $A \in M_n(\mathbb{R}) \subseteq M_n(\mathbb{C})$ *is positive semidefinite in* $M_n(\mathbb{C})$*.*

Remark 1.8. If we identify (bounded) linear operators $A \in \mathcal{L}(\mathbb{F}^n, \mathbb{F}^n)$ and matrices $A \in M_n(\mathbb{F})$, then $A \in \mathcal{L}(\mathbb{F}^n, \mathbb{F}^n)$ is positive semidefinite if and only if A is a positive self-adjoint operator. Since any positive operator $A \in \mathcal{L}(\mathbb{C}^n, \mathbb{C}^n)$ is self-adjoint, positivity coincides with positive semidefiniteness on $\mathcal{L}(\mathbb{C}^n, \mathbb{C}^n)$, in contrast to positivity on $\mathcal{L}(\mathbb{R}^n, \mathbb{R}^n)$; i.e., there are positive non-symmetric operators $B \in \mathcal{L}(\mathbb{R}^n, \mathbb{R}^n)$ (such as $B := \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$), implying that these operators cannot be positive semidefinite in $M_n(\mathbb{C})$.

Given $\emptyset \neq S \subseteq \mathbb{F}$, we put (cf. [56])

$$\mathbb{M}_n(S)^+ := \{A : A \in \mathbb{M}_n(S) \text{ and } A \text{ is psd in } \mathbb{M}_n(\mathbb{F})\}\,.$$

Thus, $M_n(\mathbb{C})^+ = \{A \in M_n(\mathbb{C}) : z^* A z \geq 0 \text{ for all } z \in \mathbb{C}^n\}$ and $\mathbb{M}_n(\mathbb{R})^+ = \{A \in M_n(\mathbb{R}) : A = A^\top \text{ and } x^\top A x \geq 0 \text{ for all } x \in \mathbb{R}^n\}$. Moreover, $A \in \mathbb{M}_n(\mathbb{C})^+$ if and only if $R_2(A) \in \mathbb{M}_{2n}(\mathbb{R})^+$. Here, the subclass of all correlation matrices, i.e., of all psd matrices with ones on their diagonal (cf. [82, Definition 2.14.] and Lemma 3.2) plays the main role in our work. Only through their structure, including the deep impact of correlation-preserving mappings (cf. Definition 5.16) our main results could be developed. We actually work with exactly those correlation matrices that are used in statistics. So, our approach could also be interesting for the statistical community; especially for those researchers who are working in spatiotemporal modelling and functional data analysis (FDA).

All basic properties of positive semidefinite (respectively, positive definite) matrices including the "striking if not almost magical" structure of related 2×2 block matrices, used and listed throughout our paper (without proof) can be found in [16, Chapter 1]. A further, very detailed analysis of the convex psd cone and its geometry, considered from the point of view of convex optimisation is listed in [31, Chapter 2.9]. (Note also that in addition to the symbol " $\mathbb{M}_n(\mathbb{R})^+$ ", the terms " $\mathbb{S}_n^+$ " and " $\mathbb{P}_n$ " are often found in the literature.)

Measurability, probability, random vectors – If not specified differently,$(\Omega, \mathcal{F})$ always denotes a measurable space which is not specified in more detail. However, we have to make use of different probability spaces, including $(\mathbb{F}^k, \mathcal{B}(\mathbb{F}^k), \gamma_k^{\mathbb{F}})$, where $\gamma_k^{\mathbb{F}}$ denotes the real or complex

Gaussian measure, described in detail in Subsection 2.1. As usual, if $\mathbb{P}$ is a given probability measure on some $(\Omega, \mathcal{F})$ and $X : \Omega \longrightarrow \mathbb{F}$ a $\mathbb{P}$-integrable $\mathbb{F}$-valued random variable, then (cf., e.g., [11])

$$\mathbb{E}_{\mathbb{P}}[X] := \mathbb{E}_{\mathbb{P}}[\mathrm{Re}(X)] + i\,\mathbb{E}_{\mathbb{P}}[\mathrm{Im}(X)] := \int_{\Omega} \mathrm{Re}(X)\,\mathrm{d}\mathbb{P} + i \int_{\Omega} \mathrm{Im}(X)\,\mathrm{d}\mathbb{P}\,.$$

In order not to unnecessarily complicate readability, we use the symbols $\mathrm{d}^n x$ and λ_n interchangeably to denote the real n-dimensional Lebesgue measure (e.g., $\int_{\mathbb{R}^n} f\,\mathrm{d}\lambda_n = \int_{\mathbb{R}^n} f(x)\lambda_n(\mathrm{d}x) = \int_{\mathbb{R}^n} f(x)\,\mathrm{d}^n x$). Unless otherwise stated, random *variables* will be denoted by capital letters (such as $X : \Omega \longrightarrow \mathbb{R}$, or $Z : \Omega \longrightarrow \mathbb{C}$), whereas random *vectors* will be denoted by bold capital letters (such as $\mathbf{X} : \Omega \longrightarrow \mathbb{R}^n$ or $\mathrm{vec}(\mathbf{Z}, \mathbf{W}) : \Omega \longrightarrow \mathbb{C}^{2n}$). $\mathbf{X} \overset{d}{=} \mathbf{Y}$ stands for the equality $\mathbb{P}_{\mathbf{X}} = \mathbb{P}_{\mathbf{Y}}$ of the respective probability laws.

Within the framework of standard measure theory (including classical L^p-spaces), we will tacitly assume that we always are working with equivalence classes of almost everywhere coinciding $\mathbb{F}$-valued functions, respectively vector valued measurable mappings on some underlying measure space $(\Omega, \mathcal{F}, \mu)$. However, since paths of stochastic processes will not play a role in this paper, we do not have to pay special attention to the structure of null sets. In this regard, a typical example is the real-valued signum function:

$$\mathrm{sign}(x) := \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x = 0 \\ -1 & \text{if } x < 0 \end{cases}.$$

If we namely view sign as an element of $L^\infty(\mathbb{R})$ (with $\|\mathrm{sign}\|_\infty = 1$), it follows that

$$\mathrm{sign} = 2\,\mathbb{1}_{[0,\infty)} - 1 \text{ in } L^\infty(\mathbb{R})$$

(since $\{0\}$ is a Lebesgue null set), where $\mathbb{1}_A$ denotes the indicator function of $A \in \mathcal{F}$. Observe that $H := \mathbb{1}_{[0,\infty)}$ is also well-known as Heaviside step function, which is especially used for applications of Fourier analysis in electricity engineering. This perspective will become an important part of our approach (cf. Example 6.27).

Finally, let us remark, that we also make use of the purely symbolic notation $x \equiv y$ to indicate that x can be canonically identified with the quantity y (such as $\mathbb{M}_{n,1}(\mathbb{F}) \equiv \mathbb{F}^n$) or that it is just a shortcut for the previously rigorously defined quantity y (cf., e.g., (2.18)).

2. Complex Gaussian random vectors and the probability law $\mathbb{C}N_{2n}(0, \Sigma_{2n}(\zeta))$

2.1. General complex Gaussian random vectors in $\mathbb{C}^n$ and their probability distribution

Regarding a deeper analysis of the underlying structure of the Grothendieck inequality in the complex case, including the Haagerup equality, it is very helpful to work with centred random vectors whose probability law follows the multivariate *complex* Gaussian distribution, fully characterised through certain correlation matrices, whose entries are elements of $\overline{\mathbb{D}}$.

This approach allows us to generalise the Haagerup equality by *substituting* the complex sign function, chosen by Haagerup (see [57]), through arbitrary "circularly odd" functions $b : \mathbb{C}^k \longrightarrow \mathbb{T}$, where $k \in \mathbb{N}$ (see Corollary 7.4).

It is far beyond the scope of this paper, to recall the rich structure of the multivariate complex Gaussian distribution in detail. However, for the convenience of the readers we list and describe all those properties of that probability law which are implemented in some of our following proofs in relation to the complex version of the Grothendieck inequality and beyond in a self-contained way. We highly recommend the readers to study related chapters in the references [5, 51], respectively [69, Chapter 2.1] and [72, Appendix E.2], where that class of random vectors and their distribution functions is comprehensively and rigorously introduced including the corresponding symbolic (mostly self-explaining) notation. Significant facts about real Gaussian random vectors are also listed and discussed thoroughly in [95, Chapter 5.II.1] and [129, Chapter 1.10]. In [11, Chapter 30], a real Gaussian random vector is viewed and treated as a special case of a measurable mapping between a probability space and a measurable space. Recall the powerful general characterisation of the Gaussian law of random vectors with values in $\mathbb{R}^n$ (cf. e.g. [11, Theorem 30.2]):

Proposition 2.1. *Let $(\mu, \Sigma) \in \mathbb{R}^n \times \mathbb{M}_n(\mathbb{R})^+$ and $\boldsymbol{X} = vec(X_1, X_2, \ldots, X_n)$ be a random vector in $\mathbb{R}^n$. Then the following statements are equivalent:*

(i)
$$\boldsymbol{X} \sim N_n(\mu, \Sigma);$$

(ii) *For all $a \in \mathbb{R}^n$,*
$$a^\top \boldsymbol{X} = \sum_{i=1}^n a_i\, X_i \sim N_1(a^\top \mu, a^\top \Sigma\, a);$$

(iii) *The characteristic function of $\boldsymbol{X}$ is given by*
$$\mathbb{R}^n \ni a \mapsto \phi_{\boldsymbol{X}}(a) := \mathbb{E}[\exp(ia^\top \boldsymbol{X})] = \exp(ia^\top \mu - \tfrac{1}{2} a^\top \Sigma a).$$

Consequently, the following important fact (which we apply in this paper frequently) follows at once:

$$\text{If } \mathbf{X} \sim N_n(\mu, \Sigma), \text{ then } A\mathbf{X} + b \sim N_n(A\mu + b, A\Sigma A^\top) \text{ for all } m \in \mathbb{N} \text{ and } (b, A) \in \mathbb{R}^m \times \mathbb{M}_{m,n}(\mathbb{R}). \tag{2.17}$$

Furthermore, recall that a random vector $\mathbf{Z} = \text{vec}(Z_1, Z_2, \ldots, Z_n)$ which maps into $\mathbb{C}^n$ is a complex random vector if for all $\nu \in [n]$ $Z_\nu = X_\nu + i\, Y_\nu$, where $X_\nu = \text{Re}(Z_\nu)$ and $Y_\nu = \text{Im}(Z_\nu)$ both are real random variables (each one defined on the same probability space). Along the lines of the notation for (deterministic) vectors in $\mathbb{C}^n$ one puts

$$\mathbf{X} \equiv \text{Re}(\mathbf{Z}) := \text{vec}(\text{Re}(Z_1), \text{Re}(Z_2), \ldots, \text{Re}(Z_n)) = \text{vec}(X_1, X_2, \ldots, X_n)$$

and
$$\mathbf{Y} \equiv \text{Im}(\mathbf{Z}) := \text{vec}(\text{Im}(Z_1), \text{Im}(Z_2), \ldots, \text{Im}(Z_n)) = \text{vec}(Y_1, Y_2, \ldots, Y_n),$$
implying that $\mathbf{Z} = \mathbf{X} + i\, \mathbf{Y} = \text{Re}(\mathbf{Z}) + i\, \text{Im}(\mathbf{Z})$. Let

$$\lambda_n^{\mathbb{C}} := (J_2^{-1})_* \lambda_{2n}$$

be the Lebesgue measure on $\mathbb{C}^n$ (i. e., the image measure of the real Lebesgue measure λ_{2n}). Fix $0 < p < \infty$. If $z = x + iy \in \mathbb{C}$, then

$$|z|^p = (x^2 + y^2)^{p/2} \leq \max\{2^{(p/2)-1}, 1\}(|x|^p + |y|^p) \leq \max\{2^{p/2}, 2\}|z|^p$$

(see [78, 2.10.E]). Consequently, the change-of-variables formula (cf. e.g. [12, Chapter 19]), applied to the image measure $\lambda_n^{\mathbb{C}}$, implies that

$$h \in L^p(\mathbb{C}^n, \lambda_n^{\mathbb{C}}) \text{ if and only if } \mathrm{Re}(h) \circ J_2^{-1} \in L^p(\mathbb{R}^{2n}, \lambda_{2n}) \text{ and } \mathrm{Im}(h) \circ J_2^{-1} \in L^p(\mathbb{R}^{2n}, \lambda_{2n}).$$

The construction of $\lambda_n^{\mathbb{C}}$ namely implies that

$$\int_{\mathbb{C}^n} |h(z)|^p \, \lambda_n^{\mathbb{C}}(\mathrm{d}z) \equiv \int_{\mathbb{C}^n} |h|^p \, \mathrm{d}\lambda_n^{\mathbb{C}} = \int_{\mathbb{R}^{2n}} |h|^p \circ J_2^{-1} \, \mathrm{d}\lambda_{2n} \equiv \int_{\mathbb{R}^{2n}} |h(x + iy)|^p \, \lambda_{2n}(\mathrm{d}(x, y)). \tag{2.18}$$

Equipped with these basic, well-known facts about the Lebesgue measure on $\mathbb{C}^n$, we reintroduce complex Gaussian random vectors in the following, seemingly elementary way:

Definition 2.2 (Complex Gaussian random vector). An n-dimensional complex random vector $\mathbf{Z}$ is a complex Gaussian random vector if the real $2n$-dimensional random vector $J_2(\mathbf{Z}) = \mathrm{vec}(\mathrm{Re}(\mathbf{Z}), \mathrm{Im}(\mathbf{Z}))$ is a real Gaussian random vector.

Although that definition of complex Gaussian random vectors seems to be a quite inconspicuous one, it encapsulates a rich underlying structure which strongly differs from that one of real Gaussian random vectors. Firstly, without having to know any further details about the structure of complex Gaussian random vectors, the change-of-variables formula (cf. e.g. [12, Chapter 19]) implies that

$$\mathbb{E}[g(\mathbf{Z})] \equiv \mathbb{E}[g \circ \mathbf{Z}] = \int_{\Omega} g \circ \mathbf{Z} \, \mathrm{d}\mathbb{P} = \int_{\mathbb{C}^n} g \, \mathrm{d}\mathbb{P}_{\mathbf{Z}} = \int_{\mathbb{C}^n} g \, \mathrm{d}\,(J_2^{-1})_* \mathbb{P}_{J_2(\mathbf{Z})}$$

can be written as

$$\mathbb{E}[g(\mathbf{Z})] = \mathbb{E}_{\mathbb{P}_{\mathbf{X}}}[g \circ J_2^{-1}] = \mathbb{E}[\mathrm{Re}(g(J_2^{-1}(\mathbf{X})))] + i\,\mathbb{E}[\mathrm{Im}(g(J_2^{-1}(\mathbf{X})))]$$

for any $\mathbb{P}_{\mathbf{Z}}$-integrable function $g = \mathrm{Re}(g) + i\ \mathrm{Im}(g)$ and any complex Gaussian random vector $\mathbf{Z}$, where $\mathbf{X} \stackrel{d}{=} J_2(\mathbf{Z})$ is a real $2n$-dimensional Gaussian random vector. Consequently, the expectation vector $\mu \equiv \mathbb{E}[\mathbf{Z}] := \mathrm{vec}(\mathbb{E}[Z_1], \mathbb{E}[Z_2], \ldots, \mathbb{E}[Z_n])$ as well as the variance matrix $\Gamma \equiv \mathrm{var}(\mathbf{Z}) := \mathbb{E}[(\mathbf{Z} - \mu)(\mathbf{Z} - \mu)^*] = (\mathbb{E}[(Z_i - \mu_i)(\overline{Z_j} - \overline{\mu_j})])_{1 \leq i,j \leq n} \in \mathbb{M}_n(\mathbb{C})^+$ and the cross-covariance matrix $C \equiv \mathrm{cov}(\mathbf{Z}, \overline{\mathbf{Z}}) := \mathbb{E}[(\mathbf{Z} - \mu)(\overline{\mathbf{Z} - \mu})^*] = \mathbb{E}[(\mathbf{Z} - \mu)(\mathbf{Z} - \mu)^\top] = (\mathbb{E}[(Z_i - \mu_i)(Z_j - \mu_j)])_{1 \leq i,j \leq n} \in M_n(\mathbb{C})$ are well-defined. Let $S \in \mathbb{M}_{2n}(\mathbb{R})^+$ be the variance matrix of $J_2(\mathbf{Z})$. Then

$$J_2(\mathbf{Z}) \sim N_{2n}(J_2(\mu), S)\,,$$

where $S = \mathbb{E}[J_2(\mathbf{Z} - \mu) J_2(\mathbf{Z} - \mu)^\top]$. A straightforward computation of $C + \Gamma = 2\mathbb{E}[(\mathbf{Z} - \mu)(\mathrm{Re}(\mathbf{Z} - \mu))^\top]$ and $C - \Gamma = 2i\,\mathbb{E}[(\mathbf{Z} - \mu)(\mathrm{Im}(\mathbf{Z} - \mu))^\top]$ implies that

$$\begin{aligned} 2\,S &= \begin{pmatrix} \mathrm{Re}(C + \Gamma) & \mathrm{Im}(C - \Gamma) \\ \mathrm{Im}(C + \Gamma) & -\mathrm{Re}(C - \Gamma) \end{pmatrix} = R_2(\Gamma) + \begin{pmatrix} \mathrm{Re}(C) & \mathrm{Im}(C) \\ \mathrm{Im}(C) & -\mathrm{Re}(C) \end{pmatrix} \\ &= \Lambda_{2n}^* \begin{pmatrix} \Gamma & C \\ \overline{C} & \overline{\Gamma} \end{pmatrix} \Lambda_{2n}\,, \end{aligned} \tag{2.19}$$

where $\Lambda_{2n} := \frac{1}{\sqrt{2}}\begin{pmatrix} I_n & i\,I_n \\ I_n & -i\,I_n \end{pmatrix} \in U(2n)$ is an unitary matrix (with $\det(\Lambda_{2n}) = (-i)^n$). Observe that

$$\begin{pmatrix} \Gamma & C \\ \overline{C} & \overline{\Gamma} \end{pmatrix} = \mathbb{E}[\mathbf{W}\mathbf{W}^*],$$

where the complex random vector $\mathbf{W} := \mathrm{vec}(\mathbf{Z} - \mu, \overline{\mathbf{Z} - \mu}) = \mathrm{vec}(\mathbf{Z}, \overline{\mathbf{Z}}) - \widetilde{\mu}$, with $\widetilde{\mu} := \mathrm{vec}(\mu, \overline{\mu})$, maps into $\mathbb{C}^{2n}$. Consequently, $\begin{pmatrix} \Gamma & C \\ \overline{C} & \overline{\Gamma} \end{pmatrix}$ is the variance matrix of the random vector $\mathrm{vec}(\mathbf{Z}, \overline{\mathbf{Z}})$. Observe that

$$\mathbb{R}^{4n} \ni J_2(\mathrm{vec}(\mathbf{Z}, \overline{\mathbf{Z}})) = AJ_2(\mathbf{Z}) \sim N_{4n}(AJ_2(\mu), ASA^\top), \tag{2.20}$$

where $A := \begin{pmatrix} I_n & 0 \\ I_n & 0 \\ 0 & I_n \\ 0 & -I_n \end{pmatrix} \in \mathbb{M}_{4n,2n}(\mathbb{R})$. Thus, since $a^\top S a = \frac{1}{2}(\Lambda_{2n}\, a)^* \begin{pmatrix} \Gamma & C \\ \overline{C} & \overline{\Gamma} \end{pmatrix} \Lambda_{2n}\, a = \frac{1}{2}\,\mathbb{E}[(\Lambda_{2n}\, a)^* \mathbf{W}\mathbf{W}^*\, \Lambda_{2n}\, a] = \mathbb{E}[(\mathbf{W}^*\, \Lambda_{2n}\, a)^* \mathbf{W}^*\, \Lambda_{2n}\, a]$ for all $a \in \mathbb{R}^{2n}$, it follows that the real matrix S is always positive semidefinite (cf. Corollary 1.6); i.e., $S \in \mathbb{M}_{2n}(\mathbb{R})^+$. *If in addition* $C\Gamma = \Gamma C$, then (see [132, Theorem 3])

$$\det(S) = \frac{1}{4^n}\det\left(R_2(\Gamma) + \begin{pmatrix} \mathrm{Re}(C) & \mathrm{Im}(C) \\ \mathrm{Im}(C) & -\mathrm{Re}(C) \end{pmatrix}\right) = \frac{1}{4^n}\det(\Gamma\overline{\Gamma} - C\overline{C})\,.$$

In particular, if $C = 0$, then $\frac{1}{2}R_2(\Gamma) = S$ is positive semidefinite, implying that

$$\mathrm{Re}(\Gamma) = \mathrm{Re}(\Gamma)^\top \text{ and } -\mathrm{Im}(\Gamma) = \mathrm{Im}(\Gamma)^\top \tag{2.21}$$

(cf. Proposition 1.5-(iii)) and

$$\det(R_2(\Gamma)) = |\det(\Gamma)|^2\,. \tag{2.22}$$

Hence, $\det(\sqrt{R_2(\Gamma)}) = |\det(\Gamma)|$. In particular, $\mathrm{Re}(\mathbf{Z}) \sim N_n(\mathrm{Re}(\mu), \frac{1}{2}\,\mathrm{Re}(\Gamma))$, $\mathrm{Im}(\mathbf{Z}) \sim N_n(\mathrm{Im}(\mu), \frac{1}{2}\,\mathrm{Re}(\Gamma))$ and $\mathbb{E}[\mathrm{Re}(Z_i)\,\mathrm{Im}(Z_i)] = \mathrm{Im}(\Gamma_{ii}) = 0$ for all $i \in [n]$. However, because of Proposition 2.5, the random *vectors* $\mathrm{Re}(\mathbf{Z})$ and $\mathrm{Im}(\mathbf{Z})$ in general are not independent!

Since the distribution of $J_2(\mathbf{Z})$ is fully specified by μ, Γ and C (due to (2.19)), we write $\mathbf{Z} \sim \mathbb{C}N_n(\mu, \Gamma, C)$ if $\mathbf{Z}$ is an n-dimensional complex Gaussian random vector. Thus, if $\mathbf{X}$ and $\mathbf{Y}$ are n-dimensional real random vectors, then

$$\tfrac{1}{\sqrt{2}}\mathbf{X} + i\,\tfrac{1}{\sqrt{2}}\mathbf{Y} \sim \mathbb{C}N_n(\mu, \Gamma, C) \text{ if and only if } \mathrm{vec}(\mathbf{X}, \mathbf{Y}) \sim N_{2n}\Big(J_2(\mu), R_2(\Gamma) + \begin{pmatrix} \mathrm{Re}(C) & \mathrm{Im}(C) \\ \mathrm{Im}(C) & -\mathrm{Re}(C) \end{pmatrix}\Big),$$

or equivalently that

$$\mathbf{Z} \sim \mathbb{C}N_n(\mu, \Gamma, C) \text{ if and only if } J_2(\sqrt{2}\,\mathbf{Z}) \sim N_{2n}\Big(J_2(\mu), R_2(\Gamma) + \begin{pmatrix} \mathrm{Re}(C) & \mathrm{Im}(C) \\ \mathrm{Im}(C) & -\mathrm{Re}(C) \end{pmatrix}\Big).$$

Regarding the main topic of our paper, we only need to work with $C = 0$, what will happen from now on. In this case, we just write $\mathbf{Z} \sim \mathbb{C}N_n(\mu, \Gamma)$. Thus, $\mathbf{Z} = \frac{1}{\sqrt{2}}\mathbf{X} + i\,\frac{1}{\sqrt{2}}\mathbf{Y} \sim \mathbb{C}N_n(\mu, \Gamma)$, if and only if

$$\mathrm{vec}(\mathbf{X}, \mathbf{Y}) = \sqrt{2}J_2(\mathbf{Z}) = \sqrt{2}\mathrm{vec}(\mathrm{Re}(Z_1), \ldots, \mathrm{Re}(Z_n), \mathrm{Im}(Z_1), \ldots, \mathrm{Im}(Z_n)) \sim N_{2n}(J_2(\mu), R_2(\Gamma)),$$

implying that (2.17) carries over to the complex case:

$$\text{if } \mathbf{Z} \sim \mathbb{C}N_n(\mu, \Gamma), \text{ then } A\mathbf{Z} + b \sim \mathbb{C}N_n(A\mu + b, A\Gamma A^*) \text{ for all } m \in \mathbb{N} \text{ and } (b, A) \in \mathbb{C}^m \times \mathbb{M}_{m,n}(\mathbb{C}). \tag{2.23}$$

Remark 2.3. Let $n \in \mathbb{N}$ and $0 \neq \Sigma \in \mathbb{M}_n(\mathbb{R})^+$ be given. Fix some $\mathbf{X} \sim N_n(0, \Sigma)$. A natural question would be, to ask whether $\mathbf{Z} := \frac{1}{\sqrt{2}}\mathbf{X} + i\,\mathbf{0} \sim \mathbb{C}N_n(0, \Sigma)$ in particular is a complex Gaussian random vector? However, if this were the case, it would follow that

$$\operatorname{vec}(\mathbf{X}, \mathbf{0}) = J_2(\sqrt{2}\mathbf{Z}) \sim N_{2n}(0, R_2(\Sigma)) = N_{2n}\Big(0, \begin{pmatrix} \Sigma & 0 \\ 0 & \Sigma \end{pmatrix}\Big),$$

implying that $0 \neq \Sigma = \mathbb{E}[\mathbf{X}\mathbf{X}^\top] = \mathbb{E}[\mathbf{0}\mathbf{0}^\top] = 0$, which is absurd.

Remark 2.4. In general, the random vector $\operatorname{vec}(\mathbf{Z}, \overline{\mathbf{Z}})$ is not a complex Gaussian one, even if $\mathbf{Z}$ is. In order to recognise this, let e.g. $Z \sim \mathbb{C}N_1(0, 1)$ be given. Then $J_2(\sqrt{2}Z) \sim N_2(0, I_2)$. Thus, (2.20) implies that

$$J_2(\sqrt{2}\operatorname{vec}(Z, \overline{Z})) \sim N_4(0, AA^\top).$$

However, since the matrix

$$AA^\top = \left(\begin{array}{cc|cc} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ \hline 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \end{array}\right)$$

does not coincide with a block matrix of type $\left(\begin{array}{c|c} A & -B \\ \hline B & A \end{array}\right) \in M_2(M_2(\mathbb{R}))$, $\operatorname{vec}(Z, \overline{Z})$ is not a complex Gaussian random vector. That observation also holds in the multi-dimensional case (see Lemma 2.7-(iii)).

Occasionally, in view of embedding both, the complex and the real case into a single statement, we also unambiguously say that $\mathbf{Z} \sim \mathbb{F}N_n(\mu, \Gamma)$ if the random vector $\mathbf{Z}$ maps into $\mathbb{F}^n$, where $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$. Note that for both fields, we explicitly include the case of variance matrices $\Gamma \in \mathbb{M}_n(\mathbb{F})^+$ which are not invertible, so that a probability *density* function of $\mathbf{Z} \sim \mathbb{F}N_n(\mu, \Gamma)$ would not have to exist; as opposed to the characteristic function of $\mathbf{Z}$ which completely determines the probability law $\mathbb{P}_{\mathbf{Z}}$. The characteristic function of $\mathbf{Z} \sim \mathbb{C}N_n(\mu, \Gamma)$ can be reduced to the well-known characteristic function of the $2n$-dimensional real Gaussian random vector $J_2(\mathbf{Z}) \sim N_{2n}(J_2(\mu), \frac{1}{2}R_2(\Gamma))$. This follows from

$$\begin{aligned}
\mathbb{C}^n \ni c \mapsto \phi_{\mathbf{Z}}(c) :&= \mathbb{E}[\exp(i\operatorname{Re}(c^*\mathbf{Z}))] = \mathbb{E}[\exp(iJ_2^\top(c)J_2(\mathbf{Z}))] \\
&= \exp(iJ_2(c)^\top J_2(\mu))\exp(-\tfrac{1}{4}J_2(c)^\top R_2(\Gamma)J_2(c)) \\
&= \exp(i\operatorname{Re}(c^*\mu))\exp(-\tfrac{1}{4}\operatorname{Re}(c^*\Gamma c)) \\
&= \exp(i\operatorname{Re}(c^*\mu))\exp(-\tfrac{1}{4}c^*\Gamma c)
\end{aligned}$$

(cf. [5, Theorem 2.7], [11, Theorem 30.2], [72, Definition E.1.13 and Theorem E.1.16] and Lemma 2.7-(ii) below).

Proposition 2.5. *Let $n \in \mathbb{N}$, $\mu \in \mathbb{C}^n$, $\Gamma \in \mathbb{M}_n(\mathbb{C})^+$ and $\boldsymbol{Z} \sim \mathbb{C}N_n(\mu, \Gamma)$. Then* $\operatorname{Re}(\boldsymbol{Z})$ *and* $\operatorname{Im}(\boldsymbol{Z})$ *are independent if and only if* $\operatorname{Im}(\Gamma) = 0$.

Proof. (2.21) and Lemma 1.4 imply that

$$\begin{aligned}\phi_{\mathrm{vec}(\mathrm{Re}(\mathbf{Z}),\mathrm{Im}(\mathbf{Z}))}(\mathrm{vec}(\mathrm{Re}(c),\mathrm{Im}(c))) &= \phi_{\mathbf{Z}}(c)\\ &= \phi_{\mathrm{Re}(\mathbf{Z})}(\mathrm{Re}(c))\,\phi_{\mathrm{Im}(\mathbf{Z})}(\mathrm{Re}(c))\exp(-\tfrac{1}{2}\,\mathrm{Im}(c)^\top\,\mathrm{Im}(\Gamma)\,\mathrm{Re}(c))\end{aligned}$$

for all $c \in \mathbb{C}^n$. Hence, $\mathrm{Re}(\mathbf{Z})$ and $\mathrm{Im}(\mathbf{Z})$ are independent if and only if

$$\phi_{\mathrm{Re}(\mathbf{Z})}(\mathrm{Re}(c))\,\phi_{\mathrm{Im}(\mathbf{Z})}(\mathrm{Re}(c))(1-\exp(-\tfrac{1}{2}\,\mathrm{Im}(c)^\top\,\mathrm{Im}(\Gamma)\,\mathrm{Re}(c))=0$$

for all $c \in \mathbb{C}^n$. Consequently, if we apply the absolute value of the latter equality to any vector $e_l + ie_k \in \mathbb{C}^n$, where $k, l \in [n]$, it follows that

$$|1-\exp(-\tfrac{1}{2}\,\mathrm{Im}(\Gamma_{kl}))| = 0$$

for all $k, l \in [n]$, and the claim follows. □

Similarly, if Γ (respectively $R_2(\Gamma)$) is invertible, the complex density function under the Lebesgue measure $\lambda_n^{\mathbb{C}}$ on $\mathbb{C}^n$ can be constructed as

$$\begin{aligned}\mathbb{C}^n \ni a \mapsto \varphi_{\mu,\Gamma}(a) &:= \varphi_{J_2(\mu),\frac{1}{2}R_2(\Gamma)}(J_2(a))\\ &= \frac{1}{\pi^n\sqrt{\det(R_2(\Gamma))}}\exp(-(J_2(a-\mu))^* R_2(\Gamma^{-1})(J_2(a-\mu)))\\ &\overset{(2.22)}{=} \frac{1}{\pi^n\,|\det(\Gamma)|}\exp(-(a-\mu)^*\,\Gamma^{-1}\,(a-\mu))\,.\end{aligned}$$

These facts, including (2.17), (2.21), (2.23) and Proposition 2.1, immediately imply the following comprehensive characterisation of the probability law $\mathbb{C}N_n(\mu, \Gamma)$.

Proposition 2.6. *Let $n \in \mathbb{N}$, $\mu \in \mathbb{C}^n$, $\Gamma \in \mathbb{M}_n(\mathbb{C})^+$ and $\boldsymbol{Z}$ a complex n-dimensional random vector. Then the following statements are equivalent:*

(i) *For all $c \in \mathbb{C}^n$, $\phi_{\boldsymbol{Z}}(c) = \mathbb{E}[\exp(i\ \mathrm{Re}(c^*\boldsymbol{Z})] = \exp(i\,\mathrm{Re}(c^*\mu))\exp(-\frac{1}{4}c^*\Gamma\, c)$.*

(ii) *$\sqrt{2}\,J_2(\boldsymbol{Z}) = vec(\sqrt{2}\,\mathrm{Re}(Z_1), \ldots, \sqrt{2}\,\mathrm{Re}(Z_n), \sqrt{2}\,\mathrm{Im}(Z_1), \ldots, \sqrt{2}\,\mathrm{Im}(Z_n)) \sim N_{2n}(\sqrt{2}\,J_2(\mu), R_2(\Gamma))$.*

(iii) *$\boldsymbol{Z} \sim \mathbb{C}N_n(\mu, \Gamma)$.*

(iv) *For all $\alpha \in \mathbb{T}$, $\alpha\boldsymbol{Z} \sim \mathbb{C}N_n(\alpha\mu, \Gamma)$.*

(v) *For all $c \in \mathbb{C}^n$, $c^*\boldsymbol{Z} \sim \mathbb{C}N_1(c^*\mu, c^*\Gamma\, c)$.*

(vi) *For all $c \in \mathbb{C}^n$, $\sqrt{2}\,J_2(c^*\boldsymbol{Z}) \sim N_2(\sqrt{2}\,J_2(c^*\mu), R_2(c^*\Gamma\, c))$.*

(vii) *For all $c \in \mathbb{C}^n$, $\sqrt{2}\,\mathrm{Re}(c^*\boldsymbol{Z}) \sim N_1(\sqrt{2}\,\mathrm{Re}(c^*\mu), c^*\Gamma\, c)$.*

In particular, if $\boldsymbol{Z} \sim \mathbb{C}N_n(\mu, \Gamma)$, then $\mathrm{Re}(\boldsymbol{Z}) \overset{d}{=} \mathrm{Im}(\boldsymbol{Z}) \sim N_n(0, \mathrm{Re}(\Gamma))$, and $\mathrm{Re}(Z_i)$ and $\mathrm{Im}(Z_i)$ are independent for all $i \in \mathbb{N}$. $\boldsymbol{Z} \sim \mathbb{C}N_n(\mu, \Gamma)$ if and only if $\overline{\boldsymbol{Z}} \sim \mathbb{C}N_n(\overline{\mu}, \overline{\Gamma})$. Moreover, if $\mu = 0$ and $\Gamma = I_n$, then $\{\mathrm{Re}(Z_1), \ldots, \mathrm{Re}(Z_n), \mathrm{Im}(Z_1), \ldots, \mathrm{Im}(Z_n)\}$ are pairwise independent.

In relation to a further investigation of the complex Grothendieck constant (built on complex Hermite polynomials), we need a further analysis of the structure of the random vector $\text{vec}(\mathbf{Z}, \overline{\mathbf{Z}})$ (cf. Theorem 7.11). That analysis, encapsulated in the next lemma, includes a short proof of a generalisation of a result of L. J. Halliwell (see [58, Appendix B]), built on a "change of mean trick", that allows us to pull both, the characteristic function and the moment generating function of a real Gaussian random vector out of a single formula, without having to assume the existence of a density function. In doing so, we will recognise again that in general, the complex random vector $\text{vec}(\mathbf{Z}, \overline{\mathbf{Z}})$ in $\mathbb{C}^{2n}$ is not Gaussian, even if the random vector $\mathbf{Z}$ in $\mathbb{C}^n$ were a complex Gaussian one.

Lemma 2.7. *Let $n \in \mathbb{N}, \Sigma \in \mathbb{M}_n(\mathbb{R})^+$ and $\Gamma \in \mathbb{M}_n(\mathbb{C})^+$. Let $\boldsymbol{X} \sim N_n(0, \Sigma)$ and $\boldsymbol{Z} \sim \mathbb{C}N_n(0, \Gamma)$. Then*

(i) $\mathbb{E}[\exp(c^\top \boldsymbol{X})] = \exp(\frac{1}{2} c^\top \Sigma c)$ *for all* $c \in \mathbb{C}^n$.

(ii) $\mathbb{E}[\exp(a^* \boldsymbol{Z} + b^* \overline{\boldsymbol{Z}})] = \exp(a^* \Gamma \overline{b})$ *for all* $a, b \in \mathbb{C}^n$.

(iii) *For all* $a, b \in \mathbb{C}^n$,

$$\begin{aligned}\phi_{vec(\boldsymbol{Z},\overline{\boldsymbol{Z}})}(vec(a,b)) &= \exp(-\tfrac{1}{4}a^*\Gamma a)\exp(-\tfrac{1}{4}b^*\overline{\Gamma}b)\exp(-\tfrac{1}{2}\operatorname{Re}(a^*\Gamma\overline{b}))\\ &= \exp\Big(-\tfrac{1}{4}vec(a,b)^\top\begin{pmatrix}\Gamma & 0\\ 0 & \overline{\Gamma}\end{pmatrix}vec(a,b)\Big)\exp(-\tfrac{1}{2}\operatorname{Re}(a^*\Gamma\overline{b})).\end{aligned}$$

In particular, $vec(\boldsymbol{Z}, \overline{\boldsymbol{Z}}) \sim \mathbb{C}N_{2n}\Big(0, \begin{pmatrix}\Gamma & 0\\ 0 & \overline{\Gamma}\end{pmatrix}\Big)$ *if and only if* $\Gamma = 0$. *Moreover,* $\mathbb{E}[\exp(a^* \boldsymbol{Z})] = 1$ *for all* $a \in \mathbb{C}^n$.

Proof. (i) Let $c = \alpha + i\beta \in \mathbb{C}^n$ be given, where $\alpha, \beta \in \mathbb{R}^n$. Fix an arbitrary $\mathbf{Y} \sim N_n(0, I_n)$. Since $\Sigma = R^2$, for some (uniquely determined and not necessarily invertible) matrix $R \in \mathbb{M}_n(\mathbb{R})^+$, (2.17) implies that $\mathbf{X} \stackrel{d}{=} R\mathbf{Y}$. Hence,

$$\begin{aligned}\mathbb{E}[\exp(c^\top \mathbf{X})] &= \mathbb{E}[\exp(\alpha^\top R\mathbf{Y})\exp(i(R\beta)^\top \mathbf{Y})]\\ &= (2\pi)^{-\frac{n}{2}}\int_{\mathbb{R}^n}\exp(\alpha^\top Ry - \tfrac{1}{2}\|y\|_2^2)\exp(i(R\beta)^\top y)\,\mathrm{d}^n y.\end{aligned}$$

An easy calculation shows that

$$\exp(\alpha^\top Ry - \tfrac{1}{2}\|y\|_2^2) = \exp(-\tfrac{1}{2}\|y - R\alpha\|_2^2)\exp(\tfrac{1}{2}\alpha^\top R^2\alpha) = (2\pi)^{\frac{n}{2}}\varphi_{R\alpha, I_n}(y)\exp(\tfrac{1}{2}\alpha^\top\Sigma\alpha).$$

Consequently, it follows that

$$\mathbb{E}[\exp(c^\top \mathbf{X})] = \mathbb{E}[\exp(i(R\beta)^\top\widetilde{\mathbf{Y}})]\exp(\tfrac{1}{2}\alpha^\top\Sigma\alpha) = \phi_{\widetilde{\mathbf{Y}}}(R\beta)\exp(\tfrac{1}{2}\alpha^\top\Sigma\alpha)$$

is the product of the value of the characteristic function of the random vector $\widetilde{\mathbf{Y}} \stackrel{d}{=} \mathbf{Y} + R\alpha \sim N_n(R\alpha, I_n)$ at $R\beta$ and the real number $\exp(\frac{1}{2}\alpha^\top\Sigma\alpha)$. Thus, since $\mathbb{E}[\exp(i(R\beta)^\top\widetilde{\mathbf{Y}})] = \exp(i\beta^\top\Sigma\alpha)\exp(-\frac{1}{2}\beta^\top\Sigma\beta)$, we finally obtain

$$\mathbb{E}[\exp(c^\top \mathbf{X})] = \exp(i\beta^\top\Sigma\alpha)\exp(-\tfrac{1}{2}\beta^\top\Sigma\beta)\exp(\tfrac{1}{2}\alpha^\top\Sigma\alpha) = \exp(\tfrac{1}{2}c^\top\Sigma c).$$

(ii) Put $\mathbb{C}^{2n} \ni c := \text{vec}(\overline{a}+\overline{b}, i\,\overline{a}-i\,\overline{b})$. Then $c = \begin{pmatrix} I_n & I_n \\ i\,I_n & -i\,I_n \end{pmatrix} \text{vec}(\overline{a}, \overline{b}) = \sqrt{2}\,\Lambda_{2n}\text{vec}(\overline{a}, \overline{b})$ (cf. (2.19)) and $a^*\mathbf{Z} + b^*\overline{\mathbf{Z}} = c^\top J_2(\mathbf{Z})$. Since $\mathbf{X} := J_2(\mathbf{Z}) \sim N_{2n}(0, \frac{1}{2}\,R_2(\Gamma))$ (due to Proposition 2.6), we may consequently apply (i) to $\mathbf{X}$ and c, and it follows that

$$\mathbb{E}[\exp(a^*\mathbf{Z} + b^*\overline{\mathbf{Z}})] = \exp(\tfrac{1}{4}c^\top R_2(\Gamma)c).$$

A straightforward calculation shows that

$$\Lambda_{2n}^\top\,R_2(\Gamma) = \begin{pmatrix} 0 & \Gamma \\ \overline{\Gamma} & 0 \end{pmatrix} \Lambda_{2n}^*\,.$$

Consequently, since $\Lambda_{2n} = (\Lambda_{2n}^*)^{-1}$ is unitary, the construction of the vector c implies that

$$\begin{aligned} c^\top R_2(\Gamma)c &= 2\text{vec}(\overline{a}, \overline{b})^\top(\Lambda_{2n}^\top\,R_2(\Gamma)\Lambda_{2n})\text{vec}(\overline{a}, \overline{b}) \\ &= 2\text{vec}(\overline{a}, \overline{b})^\top \begin{pmatrix} 0 & \Gamma \\ \overline{\Gamma} & 0 \end{pmatrix} \text{vec}(\overline{a}, \overline{b}) = 2(a^*\Gamma\overline{b} + b^*\overline{\Gamma}\overline{a}) \\ &= 2(a^*\Gamma\overline{b} + a^*\Gamma^*\overline{b}). \end{aligned}$$

Since $\Gamma = \Gamma^*$, the equality (ii) follows.
(iii) If we apply (2.20) and equality (i) to $c := i\,A^\top J_2(\text{vec}(a, b)) = i\,J_2(a + \overline{b}) \in \mathbb{C}^{2n}$ and $\mathbf{X} := J_2(\mathbf{Z}) \sim N_{2n}(0, \frac{1}{2}R_2(\Gamma))$, it follows that

$$\begin{aligned} \phi_{\text{vec}(\mathbf{Z},\overline{\mathbf{Z}})}(\text{vec}(a, b)) &= \mathbb{E}[\exp(i\,J_2(\text{vec}(a, b))^\top A J_2(\mathbf{Z}))] = \mathbb{E}[c^\top J_2(\mathbf{Z})] \\ &= \exp(\tfrac{1}{4}c^\top R_2(\Gamma)c) \\ &= \exp(-\tfrac{1}{4}\,\text{Re}((a^* + b^\top)\Gamma(a + \overline{b}))) \end{aligned}$$

However, since Γ is Hermitian, it follows that $b^\top\Gamma\overline{b} = (b^\top\Gamma\overline{b})^\top = b^*\overline{\Gamma}b$. In the same way, we obtain $b^\top\Gamma a = \overline{a^*\Gamma\overline{b}}$, which completes the proof of (iii). □

Remark 2.8. The main difficulty in the proof of Lemma 2.7-(i) arises from the fact that the normal random variables $\alpha^\top\mathbf{X}$ and $\beta^\top\mathbf{X}$ are correlated, so that we cannot simply represent $\mathbb{E}_{\mathbb{P}_\mathbf{X}}[\exp(\alpha^\top\mathbf{X})\exp(i\beta^\top\mathbf{X})]$ as a product of two expectations. However, it is possible to construct a completely different proof of Lemma 2.7-(i), which is built on (an application of the one-dimensional case of) Theorem 6.5. We strongly encourage the readers to work out the details.

Let $p \in \mathbb{N}$. It is well-known that the image measure $\mathbb{P}_\mathbf{X}$ of a real Gaussian random vector $\mathbf{X} \sim N_p(0, I_p)$ actually coincides with the Gaussian measure γ_p on $\mathbb{R}^p$ (cf. e.g. [20, Proposition 1.2.2.]), constructed via

$$\mathcal{B}(\mathbb{R}^p) \ni B \mapsto \gamma_p(B) := (2\pi)^{-p/2} \int_B \exp(-\frac{1}{2}\|x\|_2^2)\lambda_p(\mathrm{d}x) = \mathbb{P}(\mathbf{X} \in B).$$

Due to Proposition 2.6 this fact can be easily transferred to the complex case. To this end, let $n \in \mathbb{N}$, $\mathbf{Z} \sim \mathbb{C}N_n(0, I_n)$ and $b = \text{Re}(b) + i\,\text{Im}(b) : \mathbb{C}^n \longrightarrow \mathbb{C}$. Consider the two mappings

$$r(b) := \text{Re}(b) \circ \frac{1}{\sqrt{2}}\,J_2^{-1} : \mathbb{R}^{2n} \longrightarrow \mathbb{R} \text{ and } s(b) := \text{Im}(b) \circ \frac{1}{\sqrt{2}}\,J_2^{-1} : \mathbb{R}^{2n} \longrightarrow \mathbb{R}\,.$$

By construction, it follows that for any $x, y \in \mathbb{R}^n$,

$$r(b)(\mathrm{vec}(x,y)) = \mathrm{Re}(b(\tfrac{1}{\sqrt{2}}\,x + i\,\tfrac{1}{\sqrt{2}}\,y)) \text{ and } s(b)(\mathrm{vec}(x,y)) = \mathrm{Im}(b(\tfrac{1}{\sqrt{2}}\,x + i\,\tfrac{1}{\sqrt{2}}\,y)). \tag{2.24}$$

Obviously, $s(b) = r(-i\,b)$, $b \circ \frac{1}{\sqrt{2}}\,J_2^{-1} = r(b) + is(b)$, $\mathrm{Re}(b) = r(b) \circ \sqrt{2}J_2$, $\mathrm{Im}(b) = s(b) \circ \sqrt{2}J_2$ and $r(\alpha b) = \alpha r(b)$ for any $\alpha \in \mathbb{R}$.

Let $p, q \in [1, \infty)$, such that $\frac{1}{p} + \frac{1}{q} = 1$. A direct application of Hölder's inequality (to the vectors $(r(b), s(b))^\top \in \mathbb{R}^2$ and $(1,1)^\top \in \mathbb{R}^2$) implies that

$$\max\{|r(b)|^p, |s(b)|^p\} \leq r(|b|)^p = (|b|^p \circ \frac{1}{\sqrt{2}}\,J_2^{-1}) \leq (|r(b)| \cdot 1 + |s(b)| \cdot 1)^p \leq 2^{p/q}\,(|r(b)|^p + |s(b)|^p).$$

Hence, $\max\{|r(b)|^p, |s(b)|^p\} \in L^p(\mathbb{R}^{2n}, \gamma_{2n})$, if and only if $b \in L^p(\mathbb{C}^n, \mathbb{P}_{\mathbf{Z}})$, and

$$\begin{aligned}\mathbb{E}[b(\mathbf{Z})] &= \int_{\mathbb{C}^n} b\,\mathrm{d}\mathbb{P}_{\mathbf{Z}} = \int_{\mathbb{C}^n} b\,\mathrm{d}\,(\tfrac{1}{\sqrt{2}}J_2^{-1})_*\mathbb{P}_{\sqrt{2}J_2(\mathbf{Z})} = \int_{\mathbb{R}^{2n}} b(\tfrac{1}{\sqrt{2}}(x+iy))\gamma_{2n}(\mathrm{d}(x,y)) \\ &= \int_{\mathbb{R}^{2n}} r(b)\,\mathrm{d}\gamma_{2n} + i\int_{\mathbb{R}^{2n}} s(b)\,\mathrm{d}\gamma_{2n} = \mathbb{E}[r(b)(\mathbf{X})] + i\,\mathbb{E}[s(b)(\mathbf{X})],\end{aligned} \tag{2.25}$$

where $\mathbf{X} \overset{d}{=} \sqrt{2}\,J_2(\mathbf{Z}) \sim N_{2n}(0, I_{2n})$. In particular,

$$\begin{aligned}\mathcal{B}(\mathbb{C}^n) \ni A \mapsto \gamma_n^{\mathbb{C}}(A) :&= \mathbb{P}(\mathbf{Z} \in A) = \mathbb{E}[\mathbb{1}_A(\mathbf{Z})] \overset{(2.25)}{=} \gamma_{2n}(J_2(\sqrt{2}A)) \\ &= \pi^{-n}\int_{J_2(A)} \exp(-\|x\|_2^2)\,\lambda_{2n}(\mathrm{d}x) \overset{(2.18)}{=} \pi^{-n}\int_A \exp(-\|J_2(z)\|_2^2)\,\lambda_n^{\mathbb{C}}(\mathrm{d}z)\end{aligned}$$

emerges as the Gaussian measure on $\mathbb{C}^n$, implying that

$$\gamma_n^{\mathbb{C}} = (\tfrac{1}{\sqrt{2}}J_2^{-1})_*\gamma_{2n} = \mathbb{P}_{\mathbf{Z}}$$

is absolutely continuous with respect to $\lambda_n^{\mathbb{C}}$, with Radon-Nikodým derivative $\frac{\mathrm{d}\gamma_n^{\mathbb{C}}}{\mathrm{d}\lambda_n^{\mathbb{C}}} = \pi^{-n}\exp(-\|J_2(z)\|_2^2)$.

Remark 2.9. In [33, Section 8.7], the complex Gaussian measure on $\mathbb{C}^n$ is defined in such a manner that it coincides with the real Gaussian measure γ_{2n} on $\mathbb{R}^{2n}$. Given that construction, the important factor $\sqrt{2}$ - which actually emerges from the underlying structure of the probability law of a complex Gaussian random vector - is ignored. In our view, that approach creates a bit of dissonance. For example, Corollary 4.8, which shows us that for both fields, $\mathbb{F} = \mathbb{R}$ and $\mathbb{F} = \mathbb{C}$, the little Grothendieck constant $k_G^{\mathbb{F}}$ actually emerges from a common source, can no longer be maintained.

Hence, $b \in L^p(\mathbb{C}^n, \gamma_n^{\mathbb{C}})$ if and only if $\max\{|r(b)|^p, |s(b)|^p\} \in L^p(\mathbb{R}^{2n}, \gamma_{2n}^{\mathbb{R}})$, and

$$\int_{\mathbb{C}^n} \mathrm{Re}(b)\,\mathrm{d}\gamma_n^{\mathbb{C}} + i\int_{\mathbb{C}^n} \mathrm{Im}(b)\,\mathrm{d}\gamma_n^{\mathbb{C}} = \int_{\mathbb{C}^n} b\,\mathrm{d}\gamma_n^{\mathbb{C}} = \mathbb{E}[b(\mathbf{Z})] \overset{(2.25)}{=} \int_{\mathbb{R}^{2n}} r(b)\,\mathrm{d}\gamma_{2n} + i\int_{\mathbb{R}^{2n}} s(b)\,\mathrm{d}\gamma_{2n}\,. \tag{2.26}$$

In particular, $b \in L^2(\mathbb{C}^n, \gamma_n^{\mathbb{C}})$ if and only if $r(b) \in L^2(\mathbb{R}^{2n}, \gamma_{2n})$ and $s(b) \in L^2(\mathbb{R}^{2n}, \gamma_{2n})$, so that (in either case)

$$\mathbb{E}[b(\mathbf{Z})\bar{b}(\mathbf{Z})] = \|b\|_{\gamma_n^{\mathbb{C}}}^2 = \int_{\mathbb{C}^n} |b|^2\mathrm{d}\gamma_n^{\mathbb{C}} \overset{(2.26)}{=} \int_{\mathbb{R}^{2n}} r(|b|^2)\,\mathrm{d}\gamma_{2n} = \|r(b)\|_{\gamma_{2n}}^2 + \|s(b)\|_{\gamma_{2n}}^2 \tag{2.27}$$

(since $r(|b|^2) = r(b)^2 + s(b)^2$). In particular, for any function $f : \mathbb{R}^{2n} \longrightarrow \mathbb{C}$, it follows that $f \circ \sqrt{2} J_2 \in L^2(\mathbb{C}^n, \gamma_n^{\mathbb{C}})$ if and only if $\mathrm{Re}(f) \in L^2(\mathbb{R}^{2n}, \gamma_{2n})$ and $\mathrm{Im}(f) \in L^2(\mathbb{R}^{2n}, \gamma_{2n})$, whence

$$\|f \circ \sqrt{2} J_2\|^2_{\gamma_n^{\mathbb{C}}} = \|\mathrm{Re}(f)\|^2_{\gamma_{2n}} + \|\mathrm{Im}(f)\|^2_{\gamma_{2n}} . \tag{2.28}$$

in either case. Consequently,

$$\|g^{\mathbb{C}}\|_{\gamma_n^{\mathbb{C}}} = \|g\|_{\gamma_n} \tag{2.29}$$

for any real-valued function $g : \mathbb{R}^n \longrightarrow \mathbb{R}$, where $g^{\mathbb{C}} := (g \otimes 1) \circ \sqrt{2}\, J_2$ (since $\gamma_{2n} = \gamma_n \otimes \gamma_n$). Moreover, if $b, c \in L^2(\mathbb{C}^n, \gamma_n^{\mathbb{C}})$, then $r(b\bar{c}) = r(b)r(c) + s(b)s(c)$ and $s(b\bar{c}) = s(b)r(c) - r(b)s(c)$. (2.26) therefore implies that

$$\begin{aligned} \langle b, c\rangle_{\gamma_n^{\mathbb{C}}} &= \langle r(b), r(c)\rangle_{\gamma_{2n}} + \langle s(b), s(c)\rangle_{\gamma_{2n}} \\ &\quad + i\,\langle s(b), r(c)\rangle_{\gamma_{2n}} - i\,\langle r(b), s(c)\rangle_{\gamma_{2n}} . \end{aligned} \tag{2.30}$$

Remark 2.10. If in addition the function $b : \mathbb{C}^n \longrightarrow \mathbb{C}$ is holomorphic, then b actually is an element of the Segal-Bergmann space (cf. [71, Chapter 3.10])

$$\mathcal{H}L^2(\mathbb{C}^n) := \{c : \mathbb{C}^d \longrightarrow \mathbb{C} : c \text{ is holomorphic and } \|c\|_{\gamma_n^{\mathbb{C}}} < \infty\}.$$

In a similar vein, one can now prove easily the more comprehensive

Corollary 2.11. *Let $n \in \mathbb{N}$, $p \in [1, \infty)$, $\mu \in \mathbb{C}^n$, $\Gamma \in M_n(\mathbb{C})^+$ and $\boldsymbol{Z} \sim \mathbb{C}N_n(\mu, \Gamma)$. Let $b = \mathrm{Re}(b) + i\ \mathrm{Im}(b) : \mathbb{C}^n \longrightarrow \mathbb{C}$, such that*

$$\mathbb{R}^{2n} \ni y \mapsto r(b)(y + \sqrt{2}\, J_2(\mu)) \in L^p(\mathbb{R}^{2n}, \gamma_{2n})$$

and

$$\mathbb{R}^{2n} \ni y \mapsto s(b)(y + \sqrt{2}\, J_2(\mu)) \in L^p(\mathbb{R}^{2n}, \gamma_{2n}).$$

Then $b \in L^p(\mathbb{C}^n, \mathbb{P}_{\boldsymbol{Z}})$, and

$$\mathbb{E}[b(\boldsymbol{Z})] = |\det(\Gamma)|\Big(\int_{\mathbb{R}^{2n}} r(b)(y + \sqrt{2}\, J_2(\mu))\gamma_{2n}(\mathrm{d}y) + i \int_{\mathbb{R}^{2n}} s(b)(y + \sqrt{2}\, J_2(\mu))\gamma_{2n}(\mathrm{d}y)\Big).$$

Proof. We just have to observe that

$$\begin{aligned} \mathbb{E}[b(\mathbf{Z})] &= \mathbb{E}[r(b)(\mathbf{Y})] + i\,\mathbb{E}[s(b)(\mathbf{Y})] \\ &= \int_{\mathbb{R}^{2n}} r(b)(\sqrt{R_2(\Gamma)}x + \sqrt{2}\, J_2(\mu))\gamma_{2n}(\mathrm{d}x) + i \int_{\mathbb{R}^{2n}} s(b)(\sqrt{R_2(\Gamma)}x + \sqrt{2}\, J_2(\mu))\gamma_{2n}(\mathrm{d}x) \\ &\overset{(2.22)}{=} |\det(\Gamma)|\Big(\int_{\mathbb{R}^{2n}} r(b)(y + \sqrt{2}\, J_2(\mu))\gamma_{2n}(\mathrm{d}y) + i \int_{\mathbb{R}^{2n}} s(b)(y + \sqrt{2}\, J_2(\mu))\gamma_{2n}(\mathrm{d}y)\Big), \end{aligned}$$

where $\mathbf{Y} \overset{d}{=} \sqrt{2}\, J_2(\mathbf{Z}) \sim N_{2n}(\sqrt{2}\, J_2(\mu), R_2(\Gamma))$. □

2.2. Partitioned complex Gaussian random vectors in $\mathbb{C}^{2n}$ and the probability law $\mathbb{C}N_{2n}(0, \Sigma_{2n}(\zeta))$

For the remainder of the paper we put, without loss of generality, $\mu = 0$, so that we are working with centred Gaussian random vectors (with respect to both fields, $\mathbb{R}$ and $\mathbb{C}$). Moreover, we make use of a specific class of partitioned correlation matrices, which turns out to be of crucial importance regarding the topic of the paper. To this end, let $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$, $n \in \mathbb{N}$ and $\zeta \in \mathbb{F} \cap \overline{\mathbb{D}}$. Put

$$\Sigma_{2n}(\zeta) := \begin{pmatrix} I_n & \zeta\, I_n \\ \overline{\zeta}\, I_n & I_n \end{pmatrix} = \Sigma_2(\zeta) \otimes I_n = \begin{pmatrix} 1 & 0 & \dots & 0 & \zeta & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 & 0 & \zeta & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 & 0 & 0 & \dots & \zeta \\ \overline{\zeta} & 0 & \dots & 0 & 1 & 0 & \dots & 0 \\ 0 & \overline{\zeta} & \dots & 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \overline{\zeta} & 0 & 0 & \dots & 1 \end{pmatrix} \tag{2.31}$$
$$= \Sigma_{2n}(\mathrm{Re}(\zeta)) + R_2(-i\ \mathrm{Im}(\zeta) I_n).$$

Since $|\zeta| \leq 1$, it follows that

$$\Big\langle \begin{pmatrix} I_n & \zeta\, I_n \\ \overline{\zeta}\, I_n & I_n \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}, \begin{pmatrix} a \\ b \end{pmatrix} \Big\rangle_{\mathbb{F}^{2n}} = \|a + \zeta\, b\|^2_{\mathbb{F}^n} + (1 - |\zeta|^2)\, \|b\|^2_{\mathbb{F}^n} \geq 0$$

for all $a, b \in \mathbb{F}^n$, implying that $\Sigma_{2n}(\zeta)$ in fact is positive semidefinite and hence a correlation matrix (due to Lemma 3.2). Lemma 3.2 also clearly implies that

$$C(2; \mathbb{F}) = \Big\{ \Sigma_2(\zeta) = \begin{pmatrix} 1 & \zeta \\ \overline{\zeta} & 1 \end{pmatrix} : \zeta \in \mathbb{F} \cap \overline{\mathbb{D}} \Big\}. \tag{2.32}$$

Moreover, the determinant of the Kronecker product $\Sigma_{2n}(\zeta) = \Sigma_2(\zeta) \otimes I_n$ is calculated as (cf. [67, Problem 4.2.1]):

$$\det(\Sigma_{2n}(\zeta)) = \det(I_n)^2\ \det(\Sigma_2(\zeta))^n = (1 - |\zeta|^2)^n\,.$$

If in addition $|\zeta| < 1$, then $\|a + \zeta\, b\|^2_{\mathbb{F}^n} + (1 - |\zeta|^2)\|b\|^2_{\mathbb{F}^n} > 0$ for all $(a, b) \in (\mathbb{F}^n \times \mathbb{F}^n) \setminus \{(0, 0)\}$, implying that in this case $\Sigma_{2n}(\zeta)$ even is positive definite and hence invertible, with inverse $\Sigma_{2n}(\zeta)^{-1} = \frac{1}{1-|\zeta|^2} \Sigma_{2n}(-\zeta) = \frac{1}{1-|\zeta|^2} \begin{pmatrix} I_n & -\zeta\, I_n \\ -\overline{\zeta}\, I_n & I_n \end{pmatrix}$, implying that also $(1 - |\zeta|^2)\, \Sigma_{2n}(\zeta)^{-1} = \Sigma_{2n}(-\zeta)$ is a correlation matrix of rank $2n$.

In particular, for any $\rho \in (-1, 1)$, the density function of the $2n$-dimensional random vector $\mathrm{vec}(\mathbf{X}_1, \mathbf{X}_2) \sim N_{2n}(0, \Sigma_{2n}(\rho))$, where both, $\mathbf{X}_1$ and $\mathbf{X}_2$ are n-dimensional random vectors, exists. It is given by

$$\begin{aligned} \varphi_{0,\Sigma_{2n}(\rho)}(x_1, x_2) &= \frac{1}{(2\pi)^n\, (1 - \rho^2)^{n/2}} \exp\Big(- \frac{1}{2(1 - \rho^2)} \langle \Sigma_{2n}(-\rho)x, x \rangle_{\mathbb{R}^{2n}_2} \Big) \\ &= \frac{1}{(2\pi)^n\, (1 - \rho^2)^{n/2}} \exp\Big(- \frac{\|x_1\|^2 + \|x_2\|^2 - 2\rho\langle x_1, x_2\rangle}{2(1 - \rho^2)} \Big) \\ &= M_\rho(x_1, x_2; n)\, \varphi_{0,I_{2n}}(x_1, x_2) \\ &= M_\rho(x_1, x_2; n)\, \varphi_{0,I_n}(x_1)\, \varphi_{0,I_n}(x_2) \\ &= \varphi_{0,\Sigma_{2n}(\rho)}(x_2, x_1)\,, \end{aligned} \tag{2.33}$$

where $x_1, x_2 \in \mathbb{R}^n$, $x := \text{vec}(x_1, x_2)$ and

$$M_\rho(x_1, x_2; n) := \frac{1}{(1-\rho^2)^{n/2}} \exp\Big(\frac{2\rho\langle x_1, x_2\rangle - \rho^2(\|x_1\|^2 + \|x_2\|^2)}{2(1-\rho^2)}\Big) = M_{-\rho}(x_1, -x_2; n) \tag{2.34}$$

denotes the n-dimensional Mehler kernel (cf. [60]). Moreover, since $\det(\Sigma_{2n}(\zeta)) = 0$ if and only if $\zeta \in \mathbb{D}$, we achieve the following result:

Proposition 2.12. *Let $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$, $n \in \mathbb{N}$ and $\zeta \in \overline{\mathbb{D}} \cap \mathbb{F}$. Then*

$$\Sigma_{2n}(\zeta) := \begin{pmatrix} I_n & \zeta\, I_n \\ \overline{\zeta}\, I_n & I_n \end{pmatrix} \in C(2n; \mathbb{F}).$$

Moreover, the following statements are equivalent

(i) *$\Sigma_{2n}(\zeta)$ is a correlation matrix of rank $2n$.*

(ii) *$\Sigma_{2n}(\zeta)$ is invertible.*

(iii) *$\zeta \in \mathbb{D}$.*

If one of these equivalent statements is given, then $\Sigma_{2n}(\zeta)^{-1} = \frac{1}{1-|\zeta|^2}\,\Sigma_{2n}(-\zeta)$. In particular, also the $2n \times 2n$-matrix $(1-|\zeta|^2)\Sigma_{2n}(\zeta)^{-1}$ is a correlation matrix of rank $2n$.

It is not obvious that the probablity law $N_{2n}(0, \Sigma_{2n}(\rho))$ can also be described as follows (cf. [110, Definition 11.6 and Definition 11.10]):

Proposition 2.13. *Let $n \in \mathbb{N}$ and $\rho \in [-1, 1]$. Let $\boldsymbol{X} = (X_1, \ldots, X_n)^\top$ and $\boldsymbol{Y} = (Y_1, \ldots, Y_n)^\top$ be two $\mathbb{R}^n$-valued random vectors. Then the following statements are equivalent:*

(i) *$vec(\boldsymbol{X}, \boldsymbol{Y}) \sim N_{2n}(0, \Sigma_{2n}(\rho))$.*

(ii) *$vec(X_i, Y_i, X_j, Y_j) \sim N_{2n}\Big(0, \begin{pmatrix} \Sigma_2(\rho) & 0 \\ 0 & \Sigma_2(\rho) \end{pmatrix}\Big)$ for all $i \neq j \in [n]$.*

(iii) *The random component vector pairs $vec(X_i, Y_i), \ldots, vec(X_n, Y_n)$ are mutually independent, and $vec(X_i, Y_i) \sim N_2(0, \Sigma_2(\rho))$ for all $i \in [n]$.*

Proof. We just sketch the main ideas and leave the elaboration of the proof to the readers. Suppose that (i) holds. Since

$$\text{vec}(X_i, Y_i, X_j, Y_j) = A(i,j)\text{vec}(\mathbf{X}, \mathbf{Y}),$$

where $\mathbb{M}_{4,2n}(\mathbb{R}) \ni A(i,j) := \begin{pmatrix} e_i^\top & 0^\top \\ 0^\top & e_i^\top \\ e_j^\top & 0^\top \\ 0^\top & e_j^\top \end{pmatrix}$, it follows that

$$A(i,j)\Sigma_{2n}(\rho)A(i,j)^\top = \begin{pmatrix} \Sigma_2(\rho) & 0 \\ 0 & \Sigma_2(\rho) \end{pmatrix}$$

is the correlation matrix of the Gaussian random vector $\text{vec}(X_i, Y_i, X_j, Y_j)$ (cf. (2.17)), which proves (ii). If (ii) is given, the structure of the correlation matrix $\begin{pmatrix} \Sigma_2(\rho) & 0 \\ 0 & \Sigma_2(\rho) \end{pmatrix}$ implies that for $i \neq j$ the characteristic function of $\text{vec}(X_i, Y_i, X_j, Y_j)$ can be written as the product of the two characteristic functions of the pairs $\text{vec}(X_i, Y_i)$ and $\text{vec}(X_j, Y_j)$, respectively. Finally, if (iii) is given, it follows that for all $a, b \in \mathbb{R}^n$

$$(\text{vec}(a,b))^\top \text{vec}(\mathbf{X}, \mathbf{Y}) = \sum_{i=1}^n V_i\,,$$

where $V_i := a_i\, X_i + b_i\, Y_i \sim N_1(0, a_i^2 + 2\rho a_i b_i + b_i^2)$ for all $i \in [n]$ and $V_1, \ldots, V_n$ are mutually independent. Consequently, it follows that $(\text{vec}(a,b))^\top \text{vec}(\mathbf{X}, \mathbf{Y}) \sim N_1(0, \|a\|^2 + 2\rho a^\top b + \|b\|^2)$, and (i) is achieved. □

Regarding the underlying structure of the Haagerup equality (and its generalisation - see Theorem 7.2) an analysis of the structure of partitioned complex $2n$-dimensional Gaussian random vectors whose probability law is induced by the correlation matrix $\Sigma_{2n}(\zeta)$ leads to another important

Lemma 2.14. *Let $n \in \mathbb{N}$, $\zeta = x + iy \in \overline{\mathbb{D}}$ and $vec(\boldsymbol{Z}, \boldsymbol{W}) \sim \mathbb{C}N_{2n}(0, \Sigma_{2n}(\zeta))$, where the complex random vectors $\boldsymbol{Z}$ and $\boldsymbol{W}$ both map into $\mathbb{C}^n$. Then the following statements hold:*

(i) *For any $\alpha, \beta \in \mathbb{T}$, $vec(\alpha \boldsymbol{Z}, \beta\, \boldsymbol{W}) \sim \mathbb{C}N_{2n}(0, \Sigma_{2n}(\alpha\, \overline{\beta}\, \zeta))$.*

(ii) *$vec(\boldsymbol{W}, \boldsymbol{Z}) \sim \mathbb{C}N_{2n}(0, \Sigma_{2n}(\overline{\zeta}))$.*

(iii) *$\sqrt{2}\, vec(\text{Re}(\boldsymbol{Z}), \text{Re}(\boldsymbol{W})) \sim N_{2n}(0, \Sigma_{2n}(\text{Re}(\zeta)))$ and $\sqrt{2}\, vec(\text{Im}(\boldsymbol{Z}), \text{Im}(\boldsymbol{W})) \sim N_{2n}(0, \Sigma_{2n}(\text{Re}(\zeta)))$.*

(iv) *If $\zeta \in [-1, 1]$, then $\sqrt{2}\, vec(\text{Re}(\boldsymbol{Z}), \text{Im}(\boldsymbol{Z}), \text{Re}(\boldsymbol{W}), \text{Im}(\boldsymbol{W})) = \sqrt{2}\, vec(J_2(\boldsymbol{Z}), J_2(\boldsymbol{W})) \sim N_{4n}(0, \Sigma_{4n}(\zeta))$, and $vec(\text{Re}(\boldsymbol{Z}), \text{Re}(\boldsymbol{W}))$ and $vec(\text{Im}(\boldsymbol{Z}), \text{Im}(\boldsymbol{W}))$ are independent.*

(v) *If $\zeta \in \overline{\mathbb{D}} \setminus \{0\}$, then $vec(sign(\overline{\zeta})\boldsymbol{Z}, \boldsymbol{W}) \stackrel{d}{=} vec(sign(\zeta)\boldsymbol{Z}, \boldsymbol{W}) \sim \mathbb{C}N_{2n}(0, \Sigma_{2n}(|\zeta|))$. Moreover, $\sqrt{2}\, vec(J_2(sign(\overline{\zeta})\boldsymbol{Z}), J_2(\boldsymbol{W})) \stackrel{d}{=} \sqrt{2}\, vec(J_2(sign(\zeta)\boldsymbol{Z}), J_2(\boldsymbol{W})) \sim N_{4n}(0, \Sigma_{4n}(|\zeta|))$.*

Proof. (i) Let $\alpha, \beta \in \mathbb{T}$. Then

$$\begin{pmatrix} \alpha\, \mathbf{Z} \\ \beta\, \mathbf{W} \end{pmatrix} = \begin{pmatrix} \alpha\, I_n & 0 \\ 0 & \beta\, I_n \end{pmatrix} \begin{pmatrix} \mathbf{Z} \\ \mathbf{W} \end{pmatrix}$$

and

$$\begin{pmatrix} \alpha\, I_n & 0 \\ 0 & \beta\, I_n \end{pmatrix} \begin{pmatrix} I_n & z\, I_n \\ \overline{z}\, I_n & I_n \end{pmatrix} \begin{pmatrix} \overline{\alpha}\, I_n & 0 \\ 0 & \overline{\beta}\, I_n \end{pmatrix} = \begin{pmatrix} I_n & \alpha\, \overline{\beta}\, z\, I_n \\ \overline{\alpha\, \overline{\beta}\, z}\, I_n & I_n \end{pmatrix}.$$

The claim now follows from [5, Theorem 2.8].
(ii) Again, by analogy with the above approach, the claim from from [5, Theorem 2.8].
(iii) Since $\sqrt{2}\, J_2(\text{vec}(\mathbf{Z}, \mathbf{W})) = \sqrt{2}\, \text{vec}(\text{Re}(\mathbf{Z}), \text{Re}(\mathbf{W}), \text{Im}(\mathbf{Z}), \text{Im}(\mathbf{W})) \sim N_{4n}(0, R_2(\Sigma_{2n}(\zeta)))$ and

$$R_2(\Sigma_{2n}(\zeta)) = \begin{pmatrix} \text{Re}(\Sigma_{2n}(\zeta)) & -\text{Im}(\Sigma_{2n}(\zeta)) \\ \text{Im}(\Sigma_{2n}(\zeta)) & \text{Re}(\Sigma_{2n}(\zeta)) \end{pmatrix} = \begin{pmatrix} \Sigma_{2n}(\text{Re}(\zeta)) & -\Sigma_{2n}(\text{Im}(\zeta)) \\ \Sigma_{2n}(\text{Im}(\zeta)) & \Sigma_{2n}(\text{Re}(\zeta)) \end{pmatrix},$$

claim (iii) follows.
(iv) Firstly, we fix an arbitrary $\zeta = x + iy \in \overline{\mathbb{D}}$. (1.8) implies that

$$\operatorname{vec}(\operatorname{Re}(\mathbf{Z}), \operatorname{Im}(\mathbf{Z}), \operatorname{Re}(\mathbf{W}), \operatorname{Im}(\mathbf{W})) = G \operatorname{vec}(\operatorname{Re}(\mathbf{Z}), \operatorname{Re}(\mathbf{W}), \operatorname{Im}(\mathbf{Z}), \operatorname{Im}(\mathbf{W})),$$

where $G \in O(4n)$ is the matrix, introduced in (1.9). Since $\sqrt{2} \operatorname{vec}(\operatorname{Re}(\mathbf{Z}), \operatorname{Re}(\mathbf{W}), \operatorname{Im}(\mathbf{Z}), \operatorname{Im}(\mathbf{W})) = \sqrt{2}\, J_2(\operatorname{vec}(\mathbf{Z}, \mathbf{W})) \sim N_{4n}(0, R_2(\Sigma_{2n}(\zeta)))$, an application of (2.17) therefore implies that

$$\sqrt{2} \operatorname{vec}(\operatorname{Re}(\mathbf{Z}), \operatorname{Im}(\mathbf{Z}), \operatorname{Re}(\mathbf{W}), \operatorname{Im}(\mathbf{W})) \sim N_{4n}(0, G R_2(\Sigma_{2n}(\zeta)) G).$$

A straightforward block matrix multiplication shows that

$$G R_2(\Sigma_{2n}(\zeta)) G = \begin{pmatrix} I_n & 0 & x\, I_n & -y\, I_n \\ 0 & I_n & y\, I_n & x\, I_n \\ x\, I_n & y\, I_n & I_n & 0 \\ -y\, I_n & x\, I_n & 0 & I_n \end{pmatrix} = \Sigma_{4n}(x) + \begin{pmatrix} 0 & 0 & 0 & -y\, I_n \\ 0 & 0 & y\, I_n & 0 \\ 0 & y\, I_n & 0 & 0 \\ -y\, I_n & 0 & 0 & 0 \end{pmatrix}.$$

Since by assumption $\zeta \in [-1, 1] = \overline{\mathbb{D}} \cap \mathbb{R}$, $y = \operatorname{Im}(\zeta) = 0$, and the first part of claim (iv) follows. To verify the independence assertion, put $\mathbf{X} := \sqrt{2} \operatorname{vec}(\operatorname{Re}(\mathbf{Z}), \operatorname{Re}(\mathbf{W})) = \sqrt{2}\, \operatorname{Re}(\operatorname{vec}(\mathbf{Z}_1, \mathbf{Z}_2))$ and $\mathbf{Y} := \sqrt{2} \operatorname{vec}(\operatorname{Im}(\mathbf{Z}), \operatorname{Im}(\mathbf{W})) = \sqrt{2}\, \operatorname{Im}(\operatorname{vec}(\mathbf{Z}_1, \mathbf{Z}_2))$. Since

$$\operatorname{vec}(\mathbf{X}, \mathbf{Y}) = \sqrt{2} J_2(\operatorname{vec}(\mathbf{Z}, \mathbf{W})) \sim N_{4n}(0, R_2(\Sigma_{2n}(\zeta))),$$

it follows that for all $(a, b) \in \mathbb{R}^{2n} \times \mathbb{R}^{2n}$

$$\phi_{\operatorname{vec}(\mathbf{X},\mathbf{Y})}(\operatorname{vec}(a, b)) = \exp(-\frac{1}{2}(a^\top \Sigma_{2n}(\zeta) a + b^\top \Sigma_{2n}(\zeta) b)) = \phi_{\mathbf{X}}(a) \phi_{\mathbf{Y}}(b).$$

Thus, $\mathbf{X}$ and $\mathbf{Y}$ are independent, and (iv) follows.
(v) follows from (i) and (iv). □

Next, we will recognise that for any $\rho \in [-1, 1]$, the real probability law $N_{4n}(0, \Sigma_{4n}(\rho))$ actually originates from the complex probability law $\mathbb{C}N_{2n}(0, \Sigma_{2n}(\rho))$! Since:

Corollary 2.15. *Let $\rho \in [-1, 1]$. Let $\boldsymbol{X}_1$, $\boldsymbol{Y}_1$, $\boldsymbol{X}_2$ and $\boldsymbol{Y}_2$ be four $\mathbb{R}^n$-valued random vectors. Then the following statements are equivalent:*

(i) *$\operatorname{vec}(\boldsymbol{X}_1, \boldsymbol{X}_2) \sim N_{2n}(0, \Sigma_{2n}(\rho))$, $\operatorname{vec}(\boldsymbol{Y}_1, \boldsymbol{Y}_2) \sim N_{2n}(0, \Sigma_{2n}(\rho))$, and $\operatorname{vec}(\boldsymbol{X}_1, \boldsymbol{X}_2)$ and $\operatorname{vec}(\boldsymbol{Y}_1, \boldsymbol{Y}_2)$ are independent.*

(ii) *$\operatorname{vec}(\boldsymbol{X}_1, \boldsymbol{X}_2, \boldsymbol{Y}_1, \boldsymbol{Y}_2) \sim N_{4n}(0, R_2(\Sigma_{2n}(\rho)))$.*

(iii) *$\operatorname{vec}(\boldsymbol{X}_1, \boldsymbol{Y}_1, \boldsymbol{X}_2, \boldsymbol{Y}_2) \sim N_{4n}(0, \Sigma_{4n}(\rho))$.*

(iv) *$\operatorname{vec}(\boldsymbol{X}_1, \boldsymbol{Y}_1, \boldsymbol{X}_2, \boldsymbol{Y}_2) = \sqrt{2} \operatorname{vec}(\operatorname{Re}(\boldsymbol{Z}_1), \operatorname{Im}(\boldsymbol{Z}_1), \operatorname{Re}(\boldsymbol{Z}_2), \operatorname{Im}(\boldsymbol{Z}_2)) = \operatorname{vec}(J_2(\boldsymbol{Z}_1), J_2(\boldsymbol{Z}_2))$, where $\operatorname{vec}(\boldsymbol{Z}_1, \boldsymbol{Z}_2) \sim \mathbb{C}N_{2n}(0, \Sigma_{2n}(\rho))$.*

Proof. Let (i) be given. Since $\operatorname{vec}(\mathbf{X}_1, \mathbf{X}_2, \mathbf{Y}_1, \mathbf{Y}_2) = \operatorname{vec}(\mathbf{X}, \mathbf{Y})$, where $\mathbf{X} := \operatorname{vec}(\mathbf{X}_1, \mathbf{X}_2)$ and $\mathbf{Y} := \operatorname{vec}(\mathbf{Y}_1, \mathbf{Y}_2)$, the assumed independence of the random vectors $\mathbf{X}$ and $\mathbf{Y}$ implies that for all $a, b \in \mathbb{R}^{2n}$

$$\begin{aligned}\phi_{\operatorname{vec}(\mathbf{X},\mathbf{Y})}(\operatorname{vec}(a,b)) &= \phi_{\mathbf{X}}(a)\phi_{\mathbf{Y}}(b)\\ &= \exp(-\frac{1}{2}(a^\top \Sigma_{2n}(\rho)a + b^\top \Sigma_{2n}(\rho)b))\\ &= \exp(-\frac{1}{2}\operatorname{vec}(a,b)^\top R_2(\Sigma_{2n}(\rho))\operatorname{vec}(a,b)).\end{aligned}$$

Proposition 2.1 therefore concludes the proof of (ii).
Now, assume that (ii) holds. Then (2.17) implies that

$$\operatorname{vec}(\mathbf{X}_1, \mathbf{Y}_1, \mathbf{X}_2, \mathbf{Y}_2) = G\operatorname{vec}(\mathbf{X}_1, \mathbf{X}_2, \mathbf{Y}_1, \mathbf{Y}_2) \sim N_{4n}(0, GR_2(\Sigma_{2n}(\rho))G^\top),$$

where $G \in O(4n)$ is the matrix, introduced in (1.9). Since $GR_2(\Sigma_{2n}(\rho))G^\top = \Sigma_{4n}(\rho)$, (iii) follows.
Suppose that (iii) is given. Put $\mathbf{Z}_1 := \frac{1}{\sqrt{2}}(\mathbf{X}_1 + i\mathbf{Y}_1)$ and $\mathbf{Z}_2 := \frac{1}{\sqrt{2}}(\mathbf{X}_2 + i\mathbf{Y}_2)$. Then $\operatorname{vec}(\mathbf{Z}_1, \mathbf{Z}_2) = \operatorname{vec}(\frac{\mathbf{X}_1}{\sqrt{2}}, \frac{\mathbf{X}_2}{\sqrt{2}}) + i\operatorname{vec}(\frac{\mathbf{Y}_1}{\sqrt{2}}, \frac{\mathbf{Y}_2}{\sqrt{2}})$. Hence,

$$\sqrt{2}J_2(\operatorname{vec}(\mathbf{Z}_1, \mathbf{Z}_2)) = \operatorname{vec}(\mathbf{X}_1, \mathbf{X}_2, \mathbf{Y}_1, \mathbf{Y}_2).$$

This, since $\operatorname{vec}(\mathbf{X}_1, \mathbf{X}_2, \mathbf{Y}_1, \mathbf{Y}_2) = G\operatorname{vec}(\mathbf{X}_1, \mathbf{Y}_1, \mathbf{X}_2, \mathbf{Y}_2)$ and $G\Sigma_{4n}(\rho)G^\top = R_2(\Sigma_{2n}(\rho))$, (iv) follows from Proposition 2.6 .
Finally, if (iv) holds, then we may apply Lemma 2.14 and assertion (i) follows. □

Similarly, under the inclusion of Corollary 4.5, respectively [33, Proposition 8.7] (including a minor adjustment of the factor c_1 of the complex Gaussian probability measure in their proof, required due to the shape of the complex density function induced by the law $\mathbb{C}N_1(0,1) = \mathbb{R}N_2(0, \frac{1}{2}I_2)$), we obtain

Lemma 2.16. *Let $n \in \mathbb{N}$, $z \in \overline{\mathbb{D}} \cap \mathbb{F}$, $\boldsymbol{X} = vec(X_1, \ldots, X_n) \sim \mathbb{F}N_n(0, I_n)$, $vec(\boldsymbol{Y}, \boldsymbol{Z}) \sim \mathbb{F}N_{2n}(0, \Sigma_{2n}(z))$ and $u, v \in S_{\mathbb{F}^n}$. Then*

$$u^\top \boldsymbol{X} \overset{d}{=} u^* \boldsymbol{X} \sim \mathbb{F}N_1(0,1) \ \ \textit{and} \ \ \begin{pmatrix} u^* \boldsymbol{Y} \\ v^* \boldsymbol{Z}\end{pmatrix} \sim \mathbb{F}N_2(0, \Sigma_2((u^*v)z))\,.$$

In particular, $\begin{pmatrix} u^* \boldsymbol{X} \\ v^* \boldsymbol{X}\end{pmatrix} \sim \mathbb{F}N_2(0, \Sigma_2(u^*v))$ *and*

$$\mathbb{E}\Big[\Big|\sum_{k=1}^n a_k X_k\Big|^p\Big] = \mathbb{E}\Big[|a^\top \boldsymbol{X}|^p\Big] = \|a\|^p_{\mathbb{F}_2^n}\,\mathbb{E}[|X_1|^p] = \|a\|^p_{\mathbb{F}_2^n}\,C_p^{\mathbb{F}}$$

for all $a \equiv (a_1, \ldots, a_n)^\top \in \mathbb{F}^n$ and $p \in (-1, \infty)$, where $C_p^{\mathbb{R}} := \frac{(\sqrt{2})^p}{\sqrt{\pi}}\,\Gamma(\frac{p+1}{2})$ and $C_p^{\mathbb{C}} := \Gamma(1+\frac{p}{2})$.

3. A quantum correlation matrix version of the Grothendieck inequality

3.1. Gram matrices, quantum correlation, and beyond

In this section, we aim at another equivalent reformulation of the Grothendieck inequality (occasionally abbreviated by "GT") for both fields, built on the inclusion of correlation matrices; i.e., positive semidefinite matrices with entries in $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$ whose diagonal is occupied with 1's only. Since we need equivalent descriptions of a correlation matrix including its fundamental representation as a Gram matrix (cf. [68, Theorem 2.7.10]), we proceed with a fundamental acronym, to indicate a comprehensive class of matrices with entries in $\mathbb{F}$ which properly contains the class of all Gram matrices (cf. [68, page 441]) and reveals a deep connection to the foundations and philosophy of quantum mechanics.

Definition 3.1. Let $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$, $m, n \in \mathbb{N}$ and H be an $\mathbb{F}$-inner product space with inner product $\langle \cdot, \cdot \rangle \equiv \langle \cdot, \cdot \rangle_H$. Let $u \equiv (u_1, u_2, \ldots, u_m) \in H^m$ and $v \equiv (v_1, v_2, \ldots, v_n) \in H^n$. We put

$$\Gamma_H(u, v) := (\langle v_j, u_i \rangle)_{(i,j) \in [m] \times [n]} = \begin{pmatrix} \langle v_1, u_1 \rangle & \langle v_2, u_1 \rangle & \ldots & \langle v_n, u_1 \rangle \\ \langle v_1, u_2 \rangle & \langle v_2, u_2 \rangle & \ldots & \langle v_n, u_2 \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle v_1, u_m \rangle & \langle v_2, u_m \rangle & \ldots & \langle v_n, u_m \rangle \end{pmatrix} \in \mathbb{M}_{m,n}(\mathbb{F}).$$

Observe that $\Gamma_H(u, v)^* = \Gamma_H(v, u)$ for all $(u, v) \in H^m \times H^n$. $\Gamma_H(u, v)$ should be viewed as an element of the image of the matrix-valued sesquilinear mapping

$$\Gamma_H : H^m \times H^n \longrightarrow \mathbb{M}_{m,n}(\mathbb{F}).$$

In particular, if Γ_H were restricted to the product $S_H^m \times S_H^n$, we would obtain a matrix-valued sesquilinear mapping, which is defined on the infinite-dimensional C^∞-manifold $S_H^m \times S_H^n$; an interesting fact, which actually underlies our chosen notation (cf. [130, Example 1.34 and Definition 1.36]. If $m = n$ and $u = v \in H^m$, we get again the Gram matrix of the vectors $u_1, \ldots, u_m \in H$:

$$\Gamma_H(u, u) = \begin{pmatrix} \|u_1\|^2 & \langle u_2, u_1 \rangle & \ldots & \langle u_m, u_1 \rangle \\ \langle u_1, u_2 \rangle & \|u_2\|^2 & \ldots & \langle u_m, u_2 \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle u_1, u_m \rangle & \langle u_2, u_m \rangle & \ldots & \|u_m\|^2 \end{pmatrix} \in M_m(\mathbb{F})^+ .$$

If $(r, s) \in \mathbb{F}^m \times \mathbb{F}^n$, then

$$\Gamma_{\mathbb{F}}(r, s) \equiv \Gamma_{\mathbb{F}_2^1}(r, s) = \overline{r} s^\top = \overline{r} \otimes s^\top = \begin{pmatrix} \overline{r_1}\, s_1 & \overline{r_1}\, s_2 & \ldots & \overline{r_1}\, s_n \\ \overline{r_2}\, s_1 & \overline{r_2}\, s_2 & \ldots & \overline{r_2}\, s_n \\ \vdots & \vdots & \vdots & \vdots \\ \overline{r_m}\, s_1 & \overline{r_1}\, s_2 & \ldots & \overline{r_m}\, s_n \end{pmatrix} .$$

More generally, if $H = \mathbb{F}_2^d$ for some $d \in \mathbb{N}$, it follows that $\langle x, y \rangle_H = y^* x$ for all $x, y \in H$. Consequently, we obtain an important factorisation:

$$\Gamma_{\mathbb{F}_2^d}(u, v) = U^* V \text{ for all } (u, v) \in (\mathbb{F}_2^d)^m \times (\mathbb{F}_2^d)^n, \tag{3.35}$$

where $U := (u_1 \mid u_2 \mid \cdots \mid u_m) \in \mathbb{M}_{d,m}(\mathbb{F})$ and $V := (v_1 \mid v_2 \mid \cdots \mid v_n) \in \mathbb{M}_{d,n}(\mathbb{F})$. Thus,

$$\operatorname{tr}(A^* \Gamma_{\mathbb{F}_2^d}(u,v)) = \overline{\operatorname{tr}(\Gamma_{\mathbb{F}_2^d}(u,v)^* A)} = \overline{\operatorname{tr}(V^*(UA))} = \overline{\langle UA, V\rangle_F} \tag{3.36}$$

for all $A \in \mathbb{M}_{m,n}(\mathbb{F})$ (cf. also Proposition 3.13). A straightforward proof shows that any Gram matrix is positive semidefinite (cf. [68, Theorem 2.7.10]). Moreover, if $(a_{ij}) \equiv A = (A^{1/2})^2 = A^{1/2}(A^{1/2})^\top \in M_n(\mathbb{F})^+$ is positive semidefinite and $\mathbf{X} \sim \mathbb{F}N_n(0, I_n)$, then $\mathbf{Z} := A^{1/2}\mathbf{X} \sim \mathbb{F}N_n(0, A)$, implying that $A = A^{1/2}\mathbb{E}[\mathbf{X}\mathbf{X}^*]A^{1/2} = \mathbb{E}[\mathbf{Z}\mathbf{Z}^*]$ (cf., e.g., [115, Lemma 12.10.]) and $a_{ij} = \langle A^{1/2}e_j, A^{1/2}e_i\rangle_{\mathbb{F}_2^n}$ for all $i, j \in [n]$. Let us also recall the following characterisation of the set $C(n;\mathbb{F})$ of all $n \times n$ correlation matrices (with entries in $\mathbb{F}$):

Lemma 3.2. *Let $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$, $n \in \mathbb{N}$ and $\Sigma = (\sigma_{ij}) \in \mathbb{M}_n(\mathbb{F})$. Then the following statements are equivalent:*

(i) $\Sigma \in C(n;\mathbb{F})$.

(ii) $\Sigma \in \mathbb{M}_n(\mathbb{F})^+$ *and* $\sigma_{ii} = 1$ *for all* $i \in [n]$.

(iii) *There exist vectors* $x_1, \ldots, x_n \in S_{\mathbb{F}_2^n}$ *such that*

$$\sigma_{ij} = \langle x_j, x_i\rangle_{\mathbb{F}_2^n} = x_i^* x_j \text{ for all } i, j \in [n].$$

(iv) *There exist an $\mathbb{F}$-Hilbert space L and $x = (x_1, x_2, \ldots, x_n) \in L^n$ such that $\|x_i\|_L = 1$ for all $i \in [n]$ and*

$$\Sigma = \Gamma_L(x, x).$$

(v) $\Sigma = \mathbb{E}[\boldsymbol{Z}\boldsymbol{Z}^*]$ *for some n-dimensional Gaussian random vector $\boldsymbol{Z} \sim \mathbb{F}N_n(0, \Sigma)$, and $\sigma_{ii} = 1$ for all $i \in [n]$.*

In particular, the set $C(n;\mathbb{F})$ is convex, and $|\sigma_{ij}| \leq 1$ for all $i, j \in [n]$.

Remark 3.3 (The elliptope $\mathcal{E}_n \equiv C(n;\mathbb{R})$). In the real case, the set of all $n \times n$-correlation matrices, which is very rich in geometrical and combinatorial structure, is also known as the so-called *elliptope* (standing for *ellip*soid and poly*tope*) $\mathcal{E}_n$, studied in detail by M. Laurent and S. Poljak (cf. [19, Example 5.44.], [31, Chapter 5.9.1] and [35, Chapter 31.5]). From these sources, we learn, among many other deep facts, that for any $n \in \mathbb{N}$ the set $\mathcal{E}_n \equiv C(n;\mathbb{R})$ is a convex polytope, which in general is not a polyhedron, so that it cannot be described as a finite intersection of weak half spaces (cf. [3, Chapter 5.10]). Since both sets, $C(n;\mathbb{R})$ and $C(n;\mathbb{C})$ are compact (with respect to the topology of pointwise convergence), and since norms on finite-dimensional $\mathbb{F}$-vector spaces are equivalent, it follows that any linear functional on the finite-dimensional Hilbert space $(\mathbb{M}_n(\mathbb{F}), \|\cdot\|_F) \cong \mathbb{F}_2^{n^2}$ attains its maximum (and minimum) on the compact set $C(n;\mathbb{F}) \subseteq \mathbb{M}_n(\mathbb{F})$, including the linear functional $\operatorname{tr}(A^* \cdot) : \mathbb{M}_n(\mathbb{F}) \longrightarrow \mathbb{F}$, where $A \in \mathbb{M}_n(\mathbb{F})$ is given. From the point of view of real (convex) semidefinite optimisation, both, the primal SDP

$$\sup_{\Sigma \in C(m+n;\mathbb{R})} \operatorname{tr}(A^\top \Sigma) = \sup\left\{\operatorname{tr}(A^\top \Sigma) : \operatorname{tr}(e_\nu e_\nu^\top \Sigma) = 1 \text{ for all } \nu \in [m+n], \Sigma \in \mathbb{M}_\nu(\mathbb{R})^+\right\}$$

and its dual SDP have non-empty, compact sets of optimal solutions and hence attain their respective optima (cf. [19, Theorem 2.15, Theorem 2.29 and Exercise 2.41] and [21, Chapter 5]). We do not know whether this "strong duality" is also valid in the complex case (cf. Lemma 3.10).

Of particular relevance is the set

$$C_1(n;\mathbb{F}) := \{\Theta : \Theta \in C(k;\mathbb{F}) \text{ and } \mathrm{rk}(\Theta) = 1\}$$

of all $n \times n$ correlation matrices of rank 1. The Gram matrix structure implies a neat characterisation of $C_1(n;\mathbb{F})$. At the same time, we recognise again the structure of all pure states on the Hilbert space $\mathbb{F}_2^n$. To this end, recall that $S_{\mathbb{R}} = \{-1, 1\}$ and $S_{\mathbb{C}} = \mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$.

Proposition 3.4. *Let $m, n \in \mathbb{N}$. Then the following statements hold:*

(i)

$$\begin{aligned}\{A : A \in \mathbb{M}_{m,n}(\mathbb{F}) \textit{ and } rk(A) = 1\} &= \{\overline{p}q^\top : (p,q) \in \mathbb{F}^m \setminus \{0\} \times \mathbb{F}^n \setminus \{0\}\} \\ &= \{\Gamma_{\mathbb{F}}(p,q) : (p,q) \in \mathbb{F}^m \setminus \{0\} \times \mathbb{F}^n \setminus \{0\}\}.\end{aligned}$$

(ii)

$$\{A : A \in \mathbb{M}_n(\mathbb{F})^+ \textit{ and } rk(A) = 1\} = \{xx^* : x \in \mathbb{F}^m \setminus \{0\}\} = \{\Gamma_{\mathbb{F}}(z,z) : z \in \mathbb{F}^m \setminus \{0\}\}.$$

In particular,

$$\{A : A \in \mathbb{M}_n(\mathbb{F})^+ \textit{ and } rk(A) = 1 \textit{ and } tr(A) = 1\} = \{xx^* : x \in S_{\mathbb{F}}^m\} = \{\Gamma_{\mathbb{F}}(z,z) : z \in S_{\mathbb{F}}^m\}.$$

Moreover,

$$\mathbb{M}_n(S_{\mathbb{F}})^+ = \{xx^* : x \in S_{\mathbb{F}}^k\} = \{\Gamma_{\mathbb{F}}(z,z) : z \in S_{\mathbb{F}}^n\} = C_1(n;\mathbb{F}).$$

Proof. (i): Let $\mathrm{rank}(A) = 1$. Then $\{Ax : x \in \mathbb{F}^n\}$ is contained in the linear hull $[v]$ of some $v \in \mathbb{F}^m \setminus \{0\}$. Thus, for any $j \in [n]$, $Ae_j = \lambda_j v$ for some $\lambda_j \in \mathbb{F}$. Put $q := (\lambda_1, \ldots, \lambda_n)^\top \in \mathbb{F}^n$ and $p := \overline{v} \in \mathbb{F}^m \setminus \{0\}$. Then $a_{ij} = e_i^\top A e_j = \overline{p_i}\, q_j$ for all $(i,j) \in [m] \times [n]$. Hence, $A = \overline{p}\, q^\top$. Since $A \neq 0$, it also follows that $q \neq 0$. The remaining part of (i) is trivial.
(ii): Let $A \equiv (a_{ij}) \in \mathbb{M}_n(\mathbb{F})^+$. Then $A = B^2$ for some $B \in \mathbb{M}_n(\mathbb{F})^+$, where $\mathrm{rk}(B) = 1$ (cf. [67, Theorem 7.2.6]). Let $b \in \mathbb{F}^n \setminus \{0\}$ such that $\{Bx : x \in \mathbb{F}^n\} \subseteq [b]$. For any $i \in [n]$, $Be_i = \lambda_i\, b$ for some $\lambda_i \in \mathbb{F}$. Put $y := (y_1, \ldots, y_n)^\top$, where $y_i := \|b\|_2\, \lambda_i$. Then

$$(y\, y^*)_{ij} = y_i\, \overline{y_j} = \|b\|_2^2\, \lambda_i\, \overline{\lambda_j} = \langle Be_i, Be_j \rangle_{\mathbb{F}_2^n} = e_j^\top B^2 e_i = a_{ji} = \overline{a_{ij}}$$

for all $i, j \in [n]$. Thus, $A = xx^*$, where $x := \overline{y} \neq 0$. In particular, if $|a_{ij}| = 1$ for all $i, j \in [n]$, then $|x_i|^2 = 1$ for all $i \in [n]$.
To conclude (ii), fix $\Theta \in \mathbb{M}_n(S_{\mathbb{F}})^+ = \mathbb{M}_n(\mathbb{F})^+ \cap \mathbb{M}_n(S_{\mathbb{F}})$. Nothing is to show for $n = 1$, of course. So, let $n \geq 2$. Since $\Theta^* = \Theta \equiv (\vartheta_{ij}) \in \mathbb{M}_n(\mathbb{F})^+$ is positive semidefinite and satisfies $|\vartheta_{ij}| = 1$ for all $i, j \in [n]$, it follows that $\vartheta_{ii} = e_i^\top \Theta e_i = e_i^* \Theta e_i \geq 0$, implying that $\vartheta_{ii} = |\vartheta_{ii}| = 1$ for all $i \in \mathbb{N}$ and hence $\Theta \in C(n;\mathbb{F})$. Thus,

$$\Theta = \begin{pmatrix} \Sigma & b \\ b^* & 1 \end{pmatrix}$$

for some correlation matrix $\Sigma \equiv (\sigma_{ij}) \in C(n-1;\mathbb{F})$ and $b \in S_{\mathbb{F}}^{n-1}$. Let $x \in \mathbb{F}^{n-1}$ be arbitrary and put $\mathbb{F}^n \ni \widetilde{y} := \mathrm{vec}(x, -b^* x)$. Since

$$x^*(\Sigma - bb^*)x = \widetilde{y}^* \, \Theta \widetilde{y} \geq 0$$

(by construction), the matrix $(c_{ij}) \equiv C := \Sigma - bb^* \in \mathbb{M}_{n-1}(\mathbb{F})^+$ is positive semidefinite as well. Consequently, C can be represented as a Gram matrix: $C = \Gamma_H(w, w)$, $w = (w_1, \ldots, w_{n-1}) \in H^{n-1}$. The Cauchy-Schwarz inequality therefore implies that $|c_{ij}| = |\langle w_j, w_i \rangle_H| \leq \sqrt{|c_{ii}|}\sqrt{|c_{jj}|}$ for all $i, j \in [n-1]$. However, since $\sigma_{ii} = \vartheta_{ii} = 1 = |b_i|^2$ for all $i \in [n-1]$, it follows that $c_{ij} = 0$ for all $i, j \in [n-1]$. Thus, $\Sigma = b\, b^*$ and

$$\Theta = \begin{pmatrix} \Sigma & b \\ b^* & 1 \end{pmatrix} = \widetilde{b}\, \widetilde{b}^* \,,$$

where $\widetilde{b} := \mathrm{vec}(b, 1) \in S_{\mathbb{F}}^n$. □

Note that for all $m, n, \mu, \nu \in \mathbb{N}$, for all Hilbert spaces H, for all $(u, v) \in H^{m+n} \equiv H^m \times H^n$ and for all $(w, z) \in H^{\mu+\nu} \equiv H^\mu \times H^\nu$, the following block matrix representation in $\mathbb{M}_{m+n,\mu+\nu}(\mathbb{F})$ always is satisfied:

$$\begin{pmatrix} \Gamma_H(u, w) & \Gamma_H(u, z) \\ \Gamma_H(v, w) & \Gamma_H(v, z) \end{pmatrix} = \Gamma_H((u, v), (w, z)).$$

In particular,

$$\Gamma_{l_2^d}((u, v), (u, v)) = \begin{pmatrix} U^*U & U^*V \\ V^*U & V^*V \end{pmatrix} = \begin{pmatrix} U^* & 0 \\ V^* & 0 \end{pmatrix} \begin{pmatrix} U & V \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} U & V \\ 0 & 0 \end{pmatrix}^* \begin{pmatrix} U & V \\ 0 & 0 \end{pmatrix} \tag{3.37}$$

for any $d \in \mathbb{N}$, where $U := (u_1 \,\vdots\, u_2 \,\vdots\, \cdots \,\vdots\, u_m) \in \mathbb{M}_{d,m}(\mathbb{F})$ and $V := (v_1 \,\vdots\, v_2 \,\vdots\, \cdots \,\vdots\, v_n) \in \mathbb{M}_{d,n}(\mathbb{F})$. (due to (3.35)). Regarding the topic of our paper, the block structure of the elements of $C(m+n;\mathbb{F})$ is of particular interest. To this end, put

$$\mathcal{Q}_{m,n}(\mathbb{F}) := \{S : S = \Gamma_H(u, v) \text{ for some } \mathbb{F}\text{-Hilbert space } H \text{ and } (u, v) \in S_H^m \times S_H^n\}.$$

Any Hilbert space $(H, \langle \cdot, \cdot \rangle_H)$ can be isometrically embedded into the Hilbert space

$$(\widetilde{H}, \langle \cdot, \cdot \rangle_{\widetilde{H}}) := (H \oplus \mathbb{F}_2^2, \langle \cdot, \cdot \rangle_H + \langle \cdot, \cdot \rangle_{\mathbb{F}_2^2})$$

(external direct sum of H and $\mathbb{F}_2^2$). Thus, for any $(h, k) \in B_H \times B_H$, it follows by construction that

$$\widetilde{h} := (h, 0, \sqrt{1 - \|h\|_H}) \in S_{\widetilde{H}},\ \widetilde{k} := (k, \sqrt{1 - \|k\|_H}, 0) \in S_{\widetilde{H}} \text{ and } \langle \widetilde{k}, \widetilde{h} \rangle_{\widetilde{H}} = \langle k, l \rangle_H \,. \tag{3.38}$$

Note that $\dim(\widetilde{H}) \geq 3$. Consequently,

$$\mathcal{Q}_{m,n}(\mathbb{F}) = \{S : S = \Gamma_H(x, y) \text{ for some } \mathbb{F}\text{-Hilbert space } H \text{ and } (x, y) \in B_H^m \times B_H^n\}. \tag{3.39}$$

Observe also that for $C(\nu;\mathbb{F}) \subseteq \mathcal{Q}_{\nu,\nu}(\mathbb{F})$ for all $\nu \in \mathbb{N}$. By "inflating" the set $\mathcal{Q}_{m,n}(\mathbb{F})$ to a $(m+n) \times (m+n)$ - correlation matrix, we obtain the non-trivial fact that $\mathcal{Q}_{m,n}(\mathbb{F})$ is absolutely convex:

Corollary 3.5. *Let $m, n \in \mathbb{N}$ and $\Sigma \in \mathbb{M}_{m+n}(\mathbb{F})$. Then the following statements are equivalent:*

(i) $\Sigma \in C(m+n;\mathbb{F})$.

(ii) $\Sigma = \begin{pmatrix} \Gamma_H(u,u) & \Gamma_H(u,v) \\ \Gamma_H(u,v)^* & \Gamma_H(v,v) \end{pmatrix}$, *for some Hilbert space H over $\mathbb{F}$ and some $(u,v) \in S_H^m \times S_H^n$.*

(iii) $\Sigma = \begin{pmatrix} \Gamma_H(u,u) & \Gamma_H(u,v) \\ \Gamma_H(u,v)^* & \Gamma_H(v,v) \end{pmatrix}$, *for some Hilbert space H over $\mathbb{F}$ and some $(u,v) \in B_H^m \times B_H^n$.*

(iv) *There exist $d \in \mathbb{N}$, $U \in \mathbb{M}_{d,m}(\mathbb{F})$ and $V \in \mathbb{M}_{d,n}(\mathbb{F})$, such that $u_i := Ue_i \in S_{\mathbb{F}_2^d}$ for all $i \in [m]$, $v_j := Ve_j \in S_{\mathbb{F}_2^d}$ for all $j \in [n]$ and*

$$\Sigma = \begin{pmatrix} U^*U & U^*V \\ V^*U & V^*V \end{pmatrix} = \begin{pmatrix} U^* & 0 \\ V^* & 0 \end{pmatrix}\begin{pmatrix} U & V \\ 0 & 0 \end{pmatrix}.$$

In particular, $S \in \mathcal{Q}_{m,n}(\mathbb{F})$ if and only if there exist correlation matrices $A \in C(m;\mathbb{F})$ and $B \in C(n;\mathbb{F})$, such that $\begin{pmatrix} A & S \\ S^* & B \end{pmatrix} \in C(m+n;\mathbb{F})$ is a correlation matrix. The set $\mathcal{Q}_{m,n}(\mathbb{F})$ is absolutely convex.

Proof. (i) $\Rightarrow$ (ii): If (i) holds, then $\Sigma = \Gamma_H(w,w)$ for some $\mathbb{F}$-Hilbert space H and some $w = (w_1, \ldots, w_m, w_{m+1}, \ldots, w_{m+n}) \in S_H^{m+n}$ (due to Lemma 3.2). Thus, if we put $u_i := w_i$ for $i \in [m]$ and $v_j := w_{m+j}$ for $j \in [n]$, then (ii) follows.
(iii) $\Rightarrow$ (iv): Since $H = [u_1, \ldots u_m, v_1, \ldots, v_n] \oplus [u_1, \ldots u_m, v_1, \ldots, v_n]^\perp$, the orthogonal projection from H onto the finite-dimensional Hilbert space $[u_1, \ldots u_m, v_1, \ldots, v_n]$ does not alter any of the inner product entries of $\Gamma_H(u,v)$, so that we may assume without loss of generality that the Hilbert space $H \equiv \mathbb{F}_2^k$ is finite-dimensional (for some $k \in [m+n]$). (iv) now follows from (a potential application of) (3.38) and (3.37), where $d \in \{k, k+2\}$.
(iv) $\Rightarrow$ (i): (iv), respectively (3.37) implies that $\Sigma \in \mathbb{M}_{m+n}(\mathbb{F})^+$. Since $(U^*U)_{ii} = (e_i^\top U^*)(Ue_i) = (\overline{Ue_i})^\top (Ue_i) = \|u_i\|^2 = 1$ for all $i \in [m]$ and $(V^*V)_{jj} = 1$ for all $j \in [n]$, it also follows that $\Sigma_{\nu\nu} = 1$ for all $\nu \in [m+n]$.
To verify the absolute convexity statement, we have to show that $\mathcal{Q}_{m,n}(\mathbb{F})$ is convex and satisfies $(\mathbb{F} \cap \overline{\mathbb{D}}) \cdot \mathcal{Q}_{m,n}(\mathbb{F}) = \mathcal{Q}_{m,n}(\mathbb{F})$ (cf., e.g., [78, Proposition 6.1.1]). So, let $S_1, S_2 \in \mathcal{Q}_{m,n}(\mathbb{F})$. Choose $A_1, A_2 \in C(m;\mathbb{F})$ and $B_1, B_2 \in C(n;\mathbb{F})$, such that

$$\begin{pmatrix} A_1 & S_1 \\ S_1^* & B_1 \end{pmatrix} \in C(m+n;\mathbb{F}) \text{ and } \begin{pmatrix} A_2 & S_2 \\ S_2^* & B_2 \end{pmatrix} \in C(m+n;\mathbb{F}).$$

Let $\lambda \in [0,1]$. Since $C(\nu;\mathbb{F})$ is convex for all $\nu \in \mathbb{N}$, it follows that $\lambda A_1 + (1-\lambda)A_2 \in C(m;\mathbb{F})$, $\lambda B_1 + (1-\lambda)B_2 \in C(n;\mathbb{F})$ and

$$\begin{pmatrix} \lambda A_1 + (1-\lambda)A_2 & \lambda S_1 + (1-\lambda)S_2 \\ (\lambda S_1 + (1-\lambda)S_2)^* & \lambda B_1 + (1-\lambda)B_2 \end{pmatrix} = \lambda \begin{pmatrix} A_1 & S_1 \\ S_1^* & B_1 \end{pmatrix} + (1-\lambda)\begin{pmatrix} A_2 & S_2 \\ S_2^* & B_2 \end{pmatrix} \in C(m+n;\mathbb{F}).$$

Consequently, $\lambda S_1 + (1-\lambda)S_2 \in \mathcal{Q}_{m,n}(\mathbb{F})$. $(\mathbb{F} \cap \overline{\mathbb{D}}) \cdot \mathcal{Q}_{m,n}(\mathbb{F}) = \mathcal{Q}_{m,n}(\mathbb{F})$ follows from (3.39). $\square$

Remark 3.6 (Tsirel'son's characterisation of quantum correlation matrices). In the real case, i.e., if $\mathbb{F} = \mathbb{R}$, $\mathcal{Q}_{m,n} \equiv \mathcal{Q}_{m,n}(\mathbb{R})$ *coincides* with the class of so-called *quantum correlation matrices*. These matrices are particularly essential in the foundations and philosophy of quantum mechanics (cf. [9, Chapter 11], [93, 94], [140, Theorem 1] and [141, Section 4]). To this end, recall that in quantum mechanics a *matrix* $\rho \in \mathbb{M}_{n,n}(\mathbb{C})$ is called a *(quantum) state* if $\rho \in \mathbb{M}_{n,n}(\mathbb{C})^+$ and $\mathrm{tr}(\rho) = 1$ (cf., e.g., [9, Chapter 0.10]). In fact, we have (cf. [9, Chapter 11]):

Theorem (Tsirel'son, 1980). *Let $m, n \in \mathbb{N}$ and $S \equiv (s_{ij}) \in \mathbb{M}_{m,n}(\mathbb{R})$. Then the following statements are equivalent:*

(i) $S \in \mathcal{Q}_{m,n}(\mathbb{R})$.

(ii) *There exists a unital C^*-algebra $\mathcal{A}$, self-adjoint elements $A_1, \ldots, A_m$, $B_1, \ldots, B_n$ and a state τ on $\mathcal{A}$, such that $A_i\, B_j = B_j\, A_i$, $\max\{\|A_i\|, \|B_j\|\} \leq 1$ and $S_{ij} = \tau(A_i B_j)$ for all $(i,j) \in [m] \times [n]$.*

(iii) *There is a state $\rho \in \mathbb{M}_{d_1 \cdot d_2}(\mathbb{C})$ (for some $d_1, d_2 \in \mathbb{N}$), Hermitian matrix families $(W_1, \ldots, W_m) \in \mathbb{M}_{d_1}(\overline{\mathbb{D}})^m$ and $(Z_1, \ldots, Z_n) \in \mathbb{M}_{d_2}(\overline{\mathbb{D}})^n$, such that*

$$s_{ij} = tr((W_i \otimes Z_j)\rho) \;\; for\ all \;\; (i,j) \in [m] \times [n]\,.$$

Here, according to the construction, the Hermitian matrix $W_i \otimes Z_j \in \mathbb{M}_{d_1 \cdot d_2}(\overline{\mathbb{D}})$ is given by the Kronecker product of $W_i \in \mathbb{M}_{d_1}(\overline{\mathbb{D}})$ and $Z_j \in \mathbb{M}_{d_2}(\overline{\mathbb{D}})$.

In particular, if $k \in \mathbb{N}_3$, then *every* real standard $(k \times k)$-correlation matrix – used in everyday statistical calculations – actually contains a *quantum* correlation matrix block part $\in \mathcal{Q}_{m,k-m}$ $(m \in [k-1])$ and its transpose! Although, the Grothendieck inequality actually "compares" the set $\mathcal{Q}_{m,n}(\mathbb{F})$ of all real (respectively complex!) quantum correlation matrices with their extreme counterparts of rank 1 (cf. Proposition 3.4-(i), (3.40), (3.41), Theorem 3.7, Corollary 3.15 and Theorem 3.20), Tsirel'son's groundbreaking result, per se, won't be discussed in technical depth in this paper, though. Regarding a detailed introduction to this fascinating subject including full and detailed proofs of Tsirel'son's results, we particularly refer to [9, Ch. 11.2] and [50, 93, 94], and the cited sources there.

3.2. The Grothendieck inequality, correlation matrices and the matrix norm $\|\cdot\|_{\infty,1}^{\mathbb{F}}$

Fix $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$ and $m, n \in \mathbb{N}$. Let $A \in \mathbb{M}_{m,n}(\mathbb{F})$ and H be an arbitrary Hilbert space. If $(x, y) \in H^m \times H^n$, then

$$\overline{\sum_{i=1}^{m}\sum_{j=1}^{n} a_{ij}\langle x_i, y_j\rangle_H} = \sum_{i=1}^{m}\sum_{j=1}^{n} \overline{a_{ij}}\, \langle y_j, x_i\rangle_H = \mathrm{tr}(A^*\Gamma_H(x,y)) = \overline{\mathrm{tr}(A\,\Gamma_H(y,x))}.$$

Moreover, observe that (cf. [46, Lemma 2.2.], [77, Remark 10.1] and Remark 3.16 regarding the existence of the respective maxima)

$$\begin{aligned}\|A\|_H^{\mathrm{G}} &:= \max_{\|u_i\|=1, \|v_j\|=1} \Big|\sum_{i=1}^{m}\sum_{j=1}^{n} a_{ij}\, \langle u_i, v_j\rangle_H\Big| = \max_{(u,v)\in S_H^m \times S_H^n} |\mathrm{tr}(A^*\Gamma_H(u,v))| \\ &= \max_{\|u_i\|\leq 1, \|v_j\|\leq 1} \Big|\sum_{i=1}^{m}\sum_{j=1}^{n} a_{ij}\langle u_i, v_j\rangle_H\Big|\,. \end{aligned} \tag{3.40}$$

In particular (if $H = \mathbb{F}$, where $\langle z, w\rangle_H = \overline{w}z$ for all $z, w \in \mathbb{F}$), we have:

$$\|A\|_{\mathbb{F}}^{\mathrm{G}} = \max_{(p,q)\in S_{\mathbb{F}}^m\times S_{\mathbb{F}}^n} |\mathrm{tr}(A^*\Gamma_{\mathbb{F}}(p,q))| = \max_{|p_i|\le 1, |q_j|\le 1} \Big|\sum_{i=1}^{m}\sum_{j=1}^{n} a_{ij}p_i\overline{q_j}\Big|, \tag{3.41}$$

Consequently, if the matrix $A \in \mathbb{M}_{m,n}(\mathbb{F})$ is viewed as a bounded linear operator from l_∞^n into l_1^m, then (3.41) and the fact that l_∞^m is isometrically isomorphic to the dual space of l_1^m (via the linear map $\chi : l_\infty^m \longrightarrow (l_1^m)'$, defined as $l_1^m \ni z \mapsto \langle z, \chi(q)\rangle := q^\top z = \sum_{i=1}^m q_i z_i$), implies that

$$\begin{aligned}\|A\|_{\mathbb{F}}^{\mathrm{G}} &= \max_{(p,q)\in S_{\mathbb{F}}^m\times S_{\mathbb{F}}^n} |\mathrm{tr}(A^*\Gamma_{\mathbb{F}}(p,q))| \overset{(3.41)}{=} \max_{(p,q)\in B_\infty^m\times B_\infty^n} |\mathrm{tr}(A^*\Gamma_{\mathbb{F}}(p,q))| \\ &= \max_{(p,q)\in B_\infty^m\times B_\infty^n} |\mathrm{tr}(A\,\overline{q}p^\top)| = \max_{(p,q)\in B_\infty^m\times B_\infty^n} |\mathrm{tr}(A\,qp^\top)| = \max_{(p,q)\in B_\infty^m\times B_\infty^n} |\langle Aq, \chi(p)\rangle| \\ &= \|A\|_{\mathcal{L}(l_\infty^n, l_1^m)} =: \|A\|_{\infty,1}^{\mathbb{F}},\end{aligned} \tag{3.42}$$

where $B_\infty^\nu := B_{l_\infty^\nu}$, $\nu \in \mathbb{N}$. Consequently, Theorem 1.1 is equivalent to

Theorem 3.7. *Let $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$. There is an absolute constant $K > 0$ such that for any $m, n \in \mathbb{N}$, for any $A \in \mathbb{M}_{m,n}(\mathbb{F})$ and any $\mathbb{F}$-Hilbert space H, the following inequality is satisfied:*

$$\max_{(u,v)\in S_H^m\times S_H^n} |tr(A^*\,\Gamma_H(u,v))| = \|A\|_H^G \le K\,\|A\|_{\infty,1}^{\mathbb{F}}.$$

$K_G^{\mathbb{F}} > 1$ is the smallest possible value of the corresponding absolute constant K.

The operator norm $\|\cdot\|_{\infty,1}^{\mathbb{F}}$ on the right side of the Grothendieck inequality is a particular example of a *mixed subordinate matrix norm* (cf., e.g., [21, A.1.5] and [124, 136]). Here, we have to recall two key results, particularly regarding the computational complexity of $\|A\|_{\infty,1}^{\mathbb{R}}$ (cf. [66, 121, 124, 136]):

Theorem 3.8 (Rohn, 2000). *Computing $\|A\|_{\infty,1}^{\mathbb{R}}$ is NP-hard in the class of Maximum Cut Matrices.*

Even an approximation of $\|A\|_{\infty,1}^{\mathbb{R}}$ is NP-hard (see also [124, Theorem 6]):

Theorem 3.9 (Hendrickx and Olshevsky, 2010). *Unless $P = NP$, there is no polynomial time algorithm which, given a real matrix A with entries in $\{-1, 0, 1\}$, approximates $\|A\|_{\infty,1}^{\mathbb{R}}$ to some fixed error with polynomial running time in the dimensions of the matrix.*

These observations immediately result in another important well-known fact which will be used later in this paper to show that *for both fields* the calculation of $K_G^{\mathbb{F}}$ can also be elaborated by means of semidefinite programming, which is a *convex* optimisation problem (cf. Corollary 3.15, Proposition 3.11 and [21, Chapter 4.6.2]). Namely,

Lemma 3.10. *Let $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$, $m, n \in \mathbb{N}$ and $A \in \mathbb{M}_{m,n}(\mathbb{F})$. Let $\mathtt{HIL}^{\mathbb{F}}$ denote the class of all $\mathbb{F}$-Hilbert spaces. Put*

$$\Delta(A) \equiv \Delta^{\mathbb{F}}(A) := \tfrac{1}{2}\begin{pmatrix} 0 & A \\ A^* & 0 \end{pmatrix}. \tag{3.43}$$

Then $\Delta(A)$ *is Hermitian and*

$$vec(x,y)^*\Delta(A)vec(x,y) = \mathrm{Re}(x^*Ay) \text{ for all } (x,y) \in \mathbb{F}^m \times \mathbb{F}^n\,. \tag{3.44}$$

In particular, $\Delta(A) \in \mathbb{M}_{m+n}(\mathbb{F})^+$ *if and only if* $A = 0$. *Moreover,*

$$tr\Big(\Delta(A)\begin{pmatrix} C & S \\ R^* & D \end{pmatrix}\Big) = \tfrac{1}{2}\big(\overline{tr(A^*R)} + tr(A^*S)\big) \tag{3.45}$$

for all $(C,D) \in \mathbb{M}_m(\mathbb{F}) \times \mathbb{M}_n(\mathbb{F})$ *and* $S, R \in \mathbb{M}_{m,n}(\mathbb{F})$. $0 \leq \max\limits_{\Sigma \in C(m+n;\mathbb{F})} tr(\Delta(A)\Sigma) < \infty$, *and*

$$\begin{aligned} \sup_{H \in HIL^{\mathbb{F}}} \|A\|_H^G &= \max_{S \in \mathcal{Q}_{m,n}(\mathbb{F})} |tr(A^*S)| = \max_{S \in \mathcal{Q}_{m,n}(\mathbb{F})} \mathrm{Re}(tr(A^*S)) \\ &= \max_{\Sigma \in C(m+n;\mathbb{F})} tr(\Delta(A)\Sigma) \leq K_G^{\mathbb{F}}(m,n)\|A\|_{\infty,1} \end{aligned} \tag{3.46}$$

Proof. (3.44) and its impact on the positive semidefiniteness of $\Delta(A)$ follows immediately. Since

$$\Delta(A)\begin{pmatrix} C & S \\ R^* & D \end{pmatrix} = \tfrac{1}{2}\begin{pmatrix} AR^* & AD \\ A^*C & A^*S \end{pmatrix},$$

it follows that

$$\mathrm{tr}\Big(\Delta(A)\begin{pmatrix} C & S \\ R^* & D \end{pmatrix}\Big) = \tfrac{1}{2}(\mathrm{tr}(AR^*) + \mathrm{tr}(A^*S)) = \tfrac{1}{2}(\overline{\mathrm{tr}(A^*R)} + \mathrm{tr}(A^*S)).$$

Observe, that (3.45) does not at all depend on the choice of the matrices C and D! Regarding the proof of (3.46), we firstly verify the second equality. To this end, fix $S \in \mathcal{Q}_{m,n}(\mathbb{F})$. Since any $z \in \mathbb{F}$ satisfies $|z| = \mathrm{Re}(\zeta z)$, where $\zeta := 1$ if $z = 0$ and $\zeta := \frac{\overline{z}}{|z|}$ if $z \neq 0$, it follows in particular that $|\mathrm{tr}(A^*S)| = \mathrm{Re}(\alpha\,\mathrm{tr}(A^*S)) = \mathrm{Re}(\mathrm{tr}(A^*\alpha S)) \geq 0$ for some $\alpha \in S_{\mathbb{F}}$. Since $\alpha S \in \mathcal{Q}_{m,n}(\mathbb{F})$, the completion of the proof of (3.46) now follows by applying (3.45) twice, including the fact that $|\mathrm{tr}(\Delta(A)\Sigma)| \leq \max\limits_{V \in \mathcal{Q}_{m+n,m+n}(\mathbb{F})} |\mathrm{tr}(\Delta(A)V)|$ for any $\Sigma \in C(m+n;\mathbb{F}) \subseteq \mathcal{Q}_{m+n,m+n}(\mathbb{F})$. □

Let $A \in \mathbb{M}_n(\mathbb{F})$. Put $d_1(A) \equiv d_1^{\mathbb{F}}(A) := \sup\limits_{\Theta \in C_1(n;\mathbb{F})} |\mathrm{tr}(A^*\Theta)|$. Because of Proposition 3.4-(ii) it follows that

$$d_1(A) = \max_{x \in S_{\mathbb{F}}^n} |x^*Ax| = \max_{x \in S_{\mathbb{F}}^n} |\mathrm{tr}(A^*xx^*)| \leq \|A\|_{\infty,1}^{\mathbb{F}}\,.$$

Observe that $d_1 \neq \|\cdot\|_{\infty,1}^{\mathbb{F}}$ (due to [45, Corollary 2.11]). If B is symmetric, respectively Hermitian, then $d_1(B)$ coincides with the seminorm $\|B\|_{\gamma,1}$ of S. Friedland and L.-H. Lim (cf. [45, Proposition 2.5]). Moreover, in the positive semidefinite case [45, Proposition 2.8] implies that

$$d_1(M) = \max_{x \in S_{\mathbb{F}}^n} |x^*Mx| = \max_{x \in [-1,1]^n} |x^*Mx| \text{ for all } M \in \mathbb{M}_n(\mathbb{F})^+\,. \tag{3.47}$$

Recall from Lemma 3.10 the Hermitian matrix $\Delta(A) \equiv \Delta^{\mathbb{F}}(A) := \frac{1}{2}\begin{pmatrix} 0 & A \\ A^* & 0 \end{pmatrix}$, where $m, n \in \mathbb{N}$ and $A \in M(m \times n;\mathbb{F})$. Observe that in the following inequalities, which are an immediate application of [45, Corollary 2.6., (29) and Proposition 2.8., (31)], seemingly no Hilbert space presence is required (cf. also (3.46) and Corollary 6.41).

Proposition 3.11. *Let* $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$ *and* $m, n \in \mathbb{N}$*. Then* $K_G^{\mathbb{F}}(m, n)$ *is the smallest constant* $c > 0$*, satisfying*

$$|tr(\Delta(A)\,\Sigma)| \leq c\,\|A\|_{\infty,1} \text{ for all } \Sigma \in C(m+n;\mathbb{F}) \text{ and } A \in \mathbb{M}_{m,n}(\mathbb{F}). \tag{3.48}$$

The little Grothendieck constant $k_G^{\mathbb{F}}$ *is the smallest constant* $\gamma > 0$*, such that*

$$|tr(B\,\Sigma)| \leq \gamma\,\|B\|_{\infty,1} \text{ for all } \Sigma \in C(n;\mathbb{F}) \text{ and } B \in \mathbb{M}_n(\mathbb{F})^+. \tag{3.49}$$

In fact, if we allow the implementation of a possibly strictly larger absolute constant than $K_G^{\mathbb{F}}$, our approach leads to a further, more general inequality, which encompasses the real and the complex Grothendieck inequality as a special case (cf. Theorem 6.40 (real case), respectively Theorem 7.14 (complex case)). Moreover, it extends the symmetric Grothendieck equality of Friedberg and Lim in [45] from symmetric $\mathbb{F}$-matrices to arbitrary $\mathbb{F}$-matrices (cf. (3.62) and Remark 3.22):

Theorem 3.12. *Let* $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$*. Then there exists an absolute constant* $K_*^{\mathbb{F}} > 1$ *such that*

$$|tr(B^*\,\Sigma)| \leq K_*^{\mathbb{F}} d_1(B)\,.$$

for any $k \in \mathbb{N}$*, any* $\Sigma \in C(k;\mathbb{F})$ *and any* $B \in \mathbb{M}_k(\mathbb{F})$*. Moreover,*

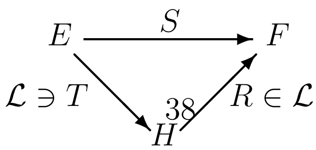
$$C(k;\mathbb{F}) \subseteq K_*^{\mathbb{F}}\, acx(C_1(k;\mathbb{F})) \text{ for all } k \in \mathbb{N}\,,$$

$K_*^{\mathbb{R}} \in [K_G^{\mathbb{R}}, \sinh(\frac{\pi}{2})]$ *and* $K_*^{\mathbb{C}} \in [K_G^{\mathbb{C}}, \frac{8}{\pi} - 1]$*.*

3.3. Characterisation of $K_G^{\mathbb{F}}$ through operator ideals and violation of Bell inequalities (a brief digression)

Readers who are familiar with operator ideals in the sense of A. Pietsch (cf. [33, 79, 117]) should take notice of Remark 3.17 below regarding the Grothendieck norm (3.40) on the left side of the Grothendieck inequality. To round out the picture, we list a rather elementary result (Proposition 3.13), which however unveals the link between matrices in $\mathcal{Q}_{m,n}(\mathbb{F})$ and a well-known functional analytic formulation of the Grothendieck inequality; namely as an inequality between Banach ideal matrix norms, when matrices are viewed as bounded linear operators from l_∞^n into l_1^m (respectively from l_1^n into l_∞^m), being elements of certain 1-Banach ideals (in the sense of A. Pietsch), or equivalently as an inequality between certain tensor product norms on tensor products of Banach spaces. The latter approach was developed by Grothendieck. Regarding the underlying functional analytic details, we refer the readers to [33, 117]. Primarily, we need an intuitive understanding of bounded linear operators between (finite-dimensional) Banach spaces, *factoring* through a Hilbert space and the basics of nuclear operators (cf. [117, Chapter 6.3]).

So, let E and F be $\mathbb{F}$-Banach spaces and $S \in \mathcal{L}(E, F)$. By definition, $S \in \mathcal{L}_2(E, F)$ if and only if there exist an $\mathbb{F}$-Hilbert space H and bounded linear operators $R \in \mathcal{L}(H, F)$, $T \in \mathcal{L}(E, H)$, such that $S = RT$. $S \in \mathcal{L}_2(E, F)$ is said to be *2-factorable* (cf., e.g., [33, Corollary 18.6.2]).



It can be shown that $(\mathcal{L}_2(E,F), \|\cdot\|_{\mathcal{L}_2(E,F)})$ is an $\mathbb{F}$-Banach space. The norm is defined as

$$\|S : E \longrightarrow F\|_{\mathcal{L}_2} \equiv \|S\|_{\mathcal{L}_2(E,F)} := \inf \|R\|\,\|T\|,$$

where the infimum is taken over all factorisations $S = RT$ through any Hilbert space.

The unit ball of the Banach space $\mathcal{L}_2(l_1^n, l_\infty^m)$ completely characterises the convex set $\mathcal{Q}_{m,n}(\mathbb{F})$, since:

Proposition 3.13. *Let $m, n \in \mathbb{N}$ and $S \in \mathbb{M}_{m,n}(\mathbb{F})$. Then the following statements are equivalent:*

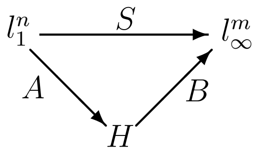
(i) $S \in B_{\mathcal{L}_2(l_1^n, l_\infty^m)}$.

(ii) *There exist $d \in \mathbb{N}$ and $(u,v) \in (S_{\mathbb{F}_2^d})^m \times (S_{\mathbb{F}_2^d})^n$ such that $S = \Gamma_{\mathbb{F}_2^d}(u,v)$.*

(iii) *There exist an $\mathbb{F}$-Hilbert space H and $(u,v) \in B_H^m \times B_H^n$ such that $S = \Gamma_H(u,v)$.*

(iv) *There exist $d \in \mathbb{N}$, $U \in \mathbb{M}_{d,m}(\mathbb{F})$ and $V \in \mathbb{M}_{d,n}(\mathbb{F})$ such that $\|U : l_1^m \longrightarrow l_2^d\| = 1$, $\|V : l_1^n \longrightarrow l_2^d\| = 1$ and $S = U^* V$.*

Proof. (i) $\Rightarrow$ (ii): Let



for some Hilbert space H and $\|B\|\|A\| = \|S\|_{\mathcal{L}_2} \leq 1$ (cf. [33, Corollary 18.6.2]). Obviously, we may assume without loss of generality that $H = l_2^k$, for some $k \in \mathbb{N}$, $\|B\| \leq 1$ and $\|A\| \leq 1$. As usual, we identify H' and H (by the Riesz representation theorem). Let $\Lambda \in \mathcal{L}(l_1^m, (l_\infty^m)')$ be the well-known linear mapping (which even is an isometric isomorphism, since $\dim(l_\infty^m) = m < \infty$), whose duality bracket is given by

$$\langle z, \Lambda x \rangle := x^\top z = \sum_{i=1}^m z_i x_i \quad ((z,x) \in l_\infty^m \times l_1^m)\,.$$

Obviously, $\|\Lambda\| \leq 1$. Let $B' \in \mathcal{L}((l_\infty^m)', (l_2^k)')$ the dual operator of B. Then $\|B'\| = \|B\| \leq 1$. By construction, it follows that the matrix of S (with respect to the standard bases) is given entrywise as

$$S_{ij} = (BA)_{ij} = e_i^\top BAe_j = \langle BAe_j, \Lambda e_i \rangle = \langle Ae_j, (B'\Lambda)e_i \rangle = \langle y_j, x_i \rangle_H \text{ for all } (i,j) \in [m] \times [n]\,,$$

where $y_j := Ae_j \in B_H$ and $x_i := (B'\Lambda)e_i \in B_{H'} \equiv B_H$. Consequently, $S = \Gamma_{\mathbb{F}_2^d}(u,v)$ for some $(u,v) \in (S_{\mathbb{F}_2^d})^m \times (S_{\mathbb{F}_2^d})^n$, where $d \in \{k, k+2\}$ (due to (3.38)).

(iii) $\Rightarrow$ (iv): Since $H = [u_1, \ldots u_m, v_1, \ldots, v_n] \oplus [u_1, \ldots u_m, v_1, \ldots, v_n]^\perp$, the orthogonal projection from H onto the finite-dimensional Hilbert space $[u_1, \ldots u_m, v_1, \ldots, v_n]$ does not alter any of the inner product entries of $\Gamma_H(u,v)$, so that we may assume without loss of generality that the Hilbert space $H \equiv l_2^d$ is finite-dimensional. Due to (3.38), we can assume (after a possible transition from l_2^d to l_2^{d+2}) that $(u,v) \in S_H^m \times S_H^n$. Hence, we may apply the factorisation (3.35), implying that $S = \Gamma_H(u,v) = U^* V$, where $U := (u_1 \mid u_2 \mid \cdots \mid u_m) \in \mathbb{M}_{d,m}(\mathbb{F})$

and $V := (v_1 \,|\, v_2 \,|\, \cdots \,|\, v_n) \in \mathbb{M}_{d,n}(\mathbb{F})$. If we view U as $U \in \mathcal{L}(l_1^m, l_2^d)$ and V as $V \in \mathcal{L}(l_1^n, l_2^d)$, then a straightforward calculation shows that for any $y = (y_1, \ldots, y_n)^\top = \sum_{j=1}^n y_j e_j \in l_1^n$,

$$\|Vy\|_2 = \Big\| \sum_{j=1}^n y_j (V e_j) \Big\|_2 = \Big\| \sum_{j=1}^n y_j v_j \Big\|_2 \leq \|y\|_{l_1^n} \, (\max_{j \in [n]} \|v_j\|_2) = \|y\|_{l_1^n} \,,$$

whence $\|V\| \leq 1 = \|v_1\|_2 = \|Ve_1\|_2 \leq \|V\|$. Thus, $\|V\| = 1$. Similarly, we obtain that $\|U\| = 1$, and (iv) follows.

(iv) $\Rightarrow$ (i): Again, we identify l_2^d with its dual. It is also well-known that $\Psi : (l_1^m)' \stackrel{\cong}{\longrightarrow} l_\infty^m$ is an isometric isomorphism, defined as

$$\Psi a := \sum_{i=1}^m \langle e_i, a \rangle e_i \quad (a \in (l_1^m)').$$

Put $W := \Psi \overline{U}' : l_2^d \equiv (l_2^d)' \longrightarrow l_\infty^m$. ($l_2^d \ni \overline{U}x := \overline{Ux}$ for all $x \in l_1^m$, of course.) The mapping rule of Ψ implies that for any $j \in [n]$,

$$\begin{aligned}(WV)e_j &= \sum_{i=1}^m \langle e_i, \overline{U}' V e_j \rangle e_i = \sum_{i=1}^m \langle \overline{U} e_i, V e_j \rangle_{l_2^d} \, e_i \\ &= \sum_{i=1}^m \langle e_i, (U^* V) e_j \rangle_{l_2^d} \, e_i = \sum_{i=1}^m (e_i^\top (U^* V) e_j) e_i = S e_j \,.\end{aligned}$$

Consequently, $S = WV \in \mathcal{L}_2(l_1^n, l_\infty^m)$, and $\|S\|_{\mathcal{L}_2} \leq \|W\| \, \|V\| \leq \|\overline{U}'\| \, \|V\| = \|U\| \, \|V\| \leq 1$. □

In other words, if $m, n \in \mathbb{N}$ and $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$, then

$$B_{\mathcal{L}_2(l_1^n, l_\infty^m)} = \mathcal{Q}_{m,n}(\mathbb{F}) = \bigcup_{d=1}^\infty \{\Gamma_{\mathbb{F}_2^d}(u, v) : (u, v) \in (S_{\mathbb{F}_2^d})^m \times (S_{\mathbb{F}_2^d})^n\}. \tag{3.50}$$

Corollary 3.14. *Let $d, m, n \in \mathbb{N}$, $(z, w) \in (\mathbb{C}_2^d)^m \times (\mathbb{C}_2^d)^n$ and $(a, b) \in (\mathbb{R}_2^{2d})^m \times (\mathbb{R}_2^{2d})^n$. Then*

$$\Gamma_{\mathbb{C}_2^d}(z, w) = \Gamma_{\mathbb{R}_2^{2d}}(x, y) + i \, \Gamma_{\mathbb{R}_2^{2d}}(x, y') \,,$$

and

$$\Gamma_{\mathbb{R}_2^{2d}}(a, b) = \mathrm{Re}(\Gamma_{\mathbb{C}_2^d}(\zeta, \xi)),$$

where $(\zeta, \xi) \in (\mathbb{C}_2^d)^m \times (\mathbb{C}_2^d)^n$, $(x, y) \in (\mathbb{R}_2^{2d})^m \times (\mathbb{R}_2^{2d})^n$ and $y' \in (\mathbb{R}_2^{2d})^n$ are given as $x_i := J_2(z_i), y_j := J_2(w_j)$, $y'_j := J_2(-i \, w_j) = R_2(-i \, I_d) y_j$, $\zeta_i := J_2^{-1}(a)$ and $\xi_j := J_2^{-1}(b)$ ($(i, j) \in [m] \times [n]$). In particular, $\{\mathrm{Re}(S) : S \in \mathcal{Q}_{m,n}(\mathbb{C})\} \subseteq \mathcal{Q}_{m,n}(\mathbb{R})$, $\{\mathrm{Im}(S) : S \in \mathcal{Q}_{m,n}(\mathbb{C})\} \subseteq \mathcal{Q}_{m,n}(\mathbb{R})$ and $\mathcal{Q}_{m,n}(\mathbb{C}) \subseteq \mathcal{Q}_{m,n}(\mathbb{R}) + i \, \mathcal{Q}_{m,n}(\mathbb{R})$. Moreover, $\{\mathrm{Re}(\Sigma) : \Sigma \in C(n; \mathbb{C})\} \subseteq C(n; \mathbb{R})$.

Proof. We just have to apply (3.50), (1.11) and (1.13), taking into account the algebraic properties of the mappings J_2 and R_2. □

Let $(u, v) \in S_H^m \times S_H^n$. Since $\Gamma_H(u, v)^* = \Gamma_H(v, u)$, it follows that also $\Gamma_H(u, v)^* \in \mathcal{Q}_{n,m}(\mathbb{F})$. Consequently, if we recall Theorem 3.7 and Lemma 3.10, we arrive at the following crucial implication of Proposition 3.13 (cf. [50]):

Corollary 3.15. *Let* $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$ *and* $m, n \in \mathbb{N}$. *Let* $A \in \mathbb{M}_{m,n}(\mathbb{F})$ *such that* $\|A\|_{\infty,1}^{\mathbb{F}} \leq 1$. *Then the following statements are equivalent to each other and to* (1.3)*:*

(i)

$$|tr(A^* \, \Gamma_H(u, v))| \leq K_G^{\mathbb{F}}(m, n) \text{ for all Hilbert spaces } H \text{ and for all } (u, v) \in S_H^m \times S_H^n .$$

(ii)

$$\max_{S \in \mathcal{Q}_{m,n}(\mathbb{F})} |tr(A^* \, S)| = \max_{R \in B_{\mathcal{L}_2(l_1^m, l_\infty^n)}} |tr(A \, R)| \leq K_G^{\mathbb{F}}(m, n) .$$

(iii)

$$\max_{\Sigma \in C(m+n; \mathbb{F})} tr(\Delta(A)\Sigma) \leq K_G^{\mathbb{F}}(m, n).$$

Recall that for any $\nu \in \mathbb{N}$, the canonical isometric isomorphisms $(l_1^\nu)' \cong l_\infty^\nu$, and $(l_\infty^\nu)' \cong l_1^\nu$ (since l_∞^ν is finite-dimensional) explicitly characterise the respective dual spaces. Put

$$X := \mathcal{L}_2(l_1^n, l_\infty^m), Y := \mathcal{L}(l_\infty^m, l_1^n), Z := \mathcal{N}(l_1^n, l_\infty^m) \text{ and } W := \mathcal{L}(l_\infty^n, l_1^m), \tag{3.51}$$

where $(\mathcal{N}, \|\cdot\|_{\mathcal{N}})$ denotes the 1-Banach ideal of all nuclear operators, which is the smallest 1-Banach ideal (originally created by A. Grothendieck in his famous thesis [53]). Let us quickly recall that a linear operator $T : E \longrightarrow F$ between two $\mathbb{F}$-Banach spaces E and F is said to be *nuclear* if there exist sequences $(a_n)_{n \in \mathbb{N}} \subseteq B_{E'}$, $(y_n)_{n \in \mathbb{N}} \subseteq B_F$ and $(\lambda_n)_{n \in \mathbb{N}} \in l_1$ such that

$$T = \sum_{n=1}^{\infty} \lambda_n \langle \cdot, a_n \rangle y_n \,,$$

and the series converges in $\mathcal{L}(E, F)$ (cf. Remark 3.19, [53] and [117, Chapter 6.3 and Theorem 9.2.1.]). It is a well-known fact that the Banach space Z is isometrically isomorphic to the dual Banach space Y'. The isometric isomorphism $\tau : Z \longrightarrow Y'$ is given by canonical trace duality

$$Z \ni S \mapsto \tau_S \equiv \tau(S), \text{ where } \langle B, \tau_S \rangle := \text{tr}(BS) \text{ for all } B \in Y \tag{3.52}$$

(see [117, Theorem 9.2.1]). Readers, who are familiar with tensor norms and Banach ideals could verify the above trace duality very quickly, (since $Y' \cong (l_1^m \otimes_\varepsilon l_1^n)' \cong (l_1^n \otimes_\varepsilon l_1^m)' \cong \mathcal{I}(l_1^n, l_\infty^m) = Z$ (cf. [33, Corollary 5.7.1 and Proposition 16.7])). Observe that Proposition 3.13 implies that $B_Z \subseteq B_X = \mathcal{Q}_{m,n}(\mathbb{F})$. However, since X consists of elementary operators only (i.e., linear operators between finite-dimensional $\mathbb{F}$-vector spaces), it follows that we may identify the equivalently normed finite-dimensional Banach spaces $(Z, \|\cdot\|_Z)$ and $(X, \|\cdot\|_X)$ topologically (yet not isometrically!), implying that $\mathcal{Q}_{m,n}(\mathbb{F}) = B_X \subseteq X \subseteq Z$. Fix $B \in Y$. Then $A := B^* \in W$, and $\|B\|_Y = \|A^*\|_Y = \|A\|_W = \|A\|_{\infty,1}$. (3.46) implies that

$$|\text{tr}(BS)| = |\text{tr}(A^* S)| \leq K_G^{\mathbb{F}}(m, n) \, \|A\|_{\infty,1} = K_G^{\mathbb{F}}(m, n) \, \|B\|_Y \text{ for all } (B, S) \in Y \times \mathcal{Q}_{m,n}(\mathbb{F}) .$$

By making use of polarisation with respect to the dual pairing (Y, Z) (cf., e.g., [78, Chapter 8.2]), the latter inquality is equivalent to

$$\mathcal{Q}_{m,n}(\mathbb{F}) \subseteq K_G^{\mathbb{F}}(m, n) \, B_Y^\circ = K_G^{\mathbb{F}}(m, n) \, B_Z .$$

So, we get again a well-known norm inequality variant of the Grothendieck inequality (cf. also [33, Corollary 14.3] and [50, Section 1.2]); namely:

$$\mathcal{Q}_{m,n}(\mathbb{F}) \subseteq K_G^{\mathbb{F}}(m,n)\, B_Z \subseteq K_G^{\mathbb{F}}\, B_Z \tag{3.53}$$

and $\|S\|_Z \leq K_G^{\mathbb{F}}(m,n) \leq K_G^{\mathbb{F}}$ for all $m, n \in \mathbb{N}$ and $S \in \mathcal{Q}_{m,n}(\mathbb{F})$.

Thus, we recognise that the isometric isomorphism $\tau : Z \longrightarrow Y'$ can be *extended* to the well-defined bounded linear operator $\widetilde{\tau} : X \longrightarrow Y'$, where the latter is given as $\widetilde{\tau}(R) := K_G^{\mathbb{F}}(m,n)\, \tau\big(\frac{1}{K_G^{\mathbb{F}}(m,n)}\, R\big)$ for all $R \in X$; i.e.,

$$Y \times X \ni (B, R) \mapsto \langle B, \widetilde{\tau}(R)\rangle := K_G^{\mathbb{F}}(m,n) \Big\langle B, \tau\Big(\frac{1}{K_G^{\mathbb{F}}(m,n)}\, R\Big)\Big\rangle = \mathrm{tr}(BR)\,. \tag{3.54}$$

Note that $\|\widetilde{\tau}(R)\| = K_G^{\mathbb{F}}(m,n)\, \|\frac{1}{K_G^{\mathbb{F}}(m,n)}\, R\|_Z \leq K_G^{\mathbb{F}}(m,n)\, \|R\|_X \leq K_G^{\mathbb{F}}\, \|R\|_X$ for all $R \in X$ (due to (3.53)), whence $\|\widetilde{\tau}\| \leq K_G^{\mathbb{F}}(m,n) \leq K_G^{\mathbb{F}}$.

Consequently, since $K_G^{\mathbb{F}}(m,n)$ is the smallest constant which satisfies inequality (1.3) (or equivalently (3.46)), it even follows that

$$K_G^{\mathbb{F}}(m,n) = \sup_{S \in \mathcal{Q}_{m,n}(\mathbb{F})} \|S\|_Z \tag{3.55}$$

(since $|\mathrm{tr}(A^* S)| \overset{(3.54)}{=} |\langle A^*, \widetilde{\tau}(S)\rangle| \leq K_G^{\mathbb{F}}(m,n)\, \|\tau(\frac{1}{K_G^{\mathbb{F}}(m,n)}\, S)\|\, \|A^*\|_Y \overset{(3.52)}{\leq} K_G^{\mathbb{F}}(m,n)\, \|\frac{1}{K_G^{\mathbb{F}}(m,n)}\, S\|_Z$ for all $S \in \mathcal{Q}_{m,n}(\mathbb{F})$ and $A \in B_W$).

Remark 3.16. (**Attainability of maximum in GT**) For any $A \in W$ the linear functional $f_A : X \longrightarrow \mathbb{R}, R \mapsto \langle A^*, \widetilde{\tau}(R)\rangle = \mathrm{tr}(A^* R)$ satisfies $|f_A(R)| \leq \|\widetilde{\tau}(R)\|\, \|A\|_W \leq K_G^{\mathbb{F}} \|R\|_X\, \|A\|_{\infty,1}$ for all $R \in X$. Hence, $f_A : X \longrightarrow \mathbb{R}$ is continuous and attains it maximum on the *compact* unit ball $B_X = \mathcal{Q}_{m,n}(\mathbb{F})$ (since X is finite-dimensional). Thus, we may indeed replace the supremum by the maximum in Theorem 3.7. Similarly, the maximum is attained in (3.55), whence

$$K_G^{\mathbb{F}}(m,n) = \|S_0\|_Z > 1$$

for some $S_0 \in B_X \setminus B_Z = \mathcal{Q}_{m,n}(\mathbb{F})$. Recall that $\tau : Z \xrightarrow{\cong} Y'$ is an isometric isomorphism (cf. (3.52)) and observe that

$$\langle S, (\tau' j_Y)(B)\rangle = \langle B, \tau(S)\rangle = \mathrm{tr}(BS) \text{ for all } (S, B) \in Z \times Y\,.$$

Thus, $\tau' j_Y : Y \xrightarrow{\cong} Z'$ again is an isometric isomorphism (since Y is finite-dimensional). It therefore follows the existence of some $B_0 \in S_Y$, such that

$$K_G^{\mathbb{F}}(m,n) = \|S_0\|_Z = |\mathrm{tr}(A_0^* S_0)|\,,$$

where $A_0 := B_0^* \in S_W$. Moreover, the polar of B_Z satisfies

$$B_Z^\circ = B_{Z'} = \tau' j_Y(B_Y). \tag{3.56}$$

Consequently, for *any* matrix $A \in \mathbb{M}_{m,n}(\mathbb{F})$, the following equivalence holds: $|\mathrm{tr}(A^* R)| \leq 1$ for all $R \in B_Z$ *if and only if* $\|A\|_W = \|A\|_{\infty,1} \leq 1$. In summary, we have:

$$K_G^{\mathbb{F}}(m,n) = |\mathrm{tr}(A_0^* S_0)| > 1 \;\text{ and }\; |\mathrm{tr}(A_0^* R)| \leq 1 \;\text{ for all }\; R \in B_Z\,; \tag{3.57}$$

a fact which plays a key role in quantum mechanics (cf. Remark 3.21). Moreover, due to (3.50), $S_0 = \Gamma_{\mathbb{F}_2^{d_0}}(u_0, v_0)$, for some $d_0 \equiv d_0(m,n) \in \mathbb{N}$ and $(u_0, v_0) \in (S_{\mathbb{F}_2^{d_0}})^m \times (S_{\mathbb{F}_2^{d_0}})^n$. Hence, $K_G^{\mathbb{F}}(m,n) \leq \sup_{(u,v)\in(S_{\mathbb{F}_2^{d_0}})^m \times (S_{\mathbb{F}_2^{d_0}})^n} |\mathrm{tr}(A_0^* \Gamma_{\mathbb{F}_2^{d_0}}(u,v))| \leq K_G^{\mathbb{F}}(d_0)$.

Remark 3.17 (**Adjoining GT**)**.** Readers who are familiar with adjoint normed operator ideals and trace duality in general (cf. [117, Chapter 9.1]) immediately recognise that Corollary 3.15-(ii) implies that the Grothendieck inequality actually is equivalent to an inequality between two matrix norms, induced by two (adjoint) Banach ideals; namely:

$$\sup_{H \in \mathtt{HIL}^{\mathbb{F}}} \|A\|_H^{\mathrm{G}} \overset{(3.46)}{=} \|A\|_{\mathcal{D}_2} \leq K_G^{\mathbb{F}}(m,n)\, \|A\|_{\infty,1} \leq K_G^{\mathbb{F}}\, \|A\|_{\infty,1}$$

for all matrices $A \in \mathbb{M}_{m,n}(\mathbb{F}), m, n \in \mathbb{N}$, or, equivalently,

$$B_{\mathcal{L}(l_\infty^n, l_1^m)} \subseteq K_G^{\mathbb{F}}(m,n)\, B_{\mathcal{D}_2(l_\infty^n, l_1^m)} \subseteq K_G^{\mathbb{F}}\, B_{\mathcal{D}_2(l_\infty^n, l_1^m)} \tag{3.58}$$

for all $m, n \in \mathbb{N}$, where $(\mathcal{D}_2, \|\cdot\|_{\mathcal{D}_2}) = (\mathcal{L}_2^*, \|\cdot\|_{\mathcal{L}_2^*}) = (\mathcal{P}_2^d \circ \mathcal{P}_2, \|\cdot\|_{\mathcal{P}_2^d \circ \mathcal{P}_2})$ characterises the Banach ideal of 2-dominated operators (cf. [33, Table 17.12, Theorem 17.14 and Chapter 19] and Remark 4.10). The latter inclusion also follows directly from "adjoining" (3.53) above. In fact, if K and L are arbitrary compact sets, the following deep result of Grothendieck holds:

$$\mathcal{L}(C(K), C(L)') \subseteq \mathcal{D}_2(C(K), C(L)') \subseteq \mathcal{P}_2(C(K), C(L)') \subseteq \mathcal{L}_2(C(K), C(L)')\,,$$

and

$$\|T\|_{\mathcal{L}_2} \leq \|T\|_{\mathcal{P}_2} \leq \|T\|_{\mathcal{D}_2} \leq K_G^{\mathbb{F}}\, \|T\|$$

for all $T \in \mathcal{L}(C(K), C(L)')$. To recognise this highly noteworthy statement, we just have to note that [119, Theorem 2.1] implies that any $T \in \mathcal{L}(C(K), C(L)')$ can be represented as $T = (J_{\mathbb{P}_L})' U J_{\mathbb{P}_K}$, where for $\Delta \in \{K, L\}$, $\mathbb{P}_\Delta$ is a well-defined *probability* measure on Δ, $J_{\mathbb{P}_\Delta} : C(\Delta) \hookrightarrow L^2(\mathbb{P}_\Delta)$ denotes the canonical (norm 1) inclusion and $\|U\| \leq K_G^{\mathbb{F}} \|T\|$. Each of the two operators $J_{\mathbb{P}_\Delta}$ is absolutely 2-summing (such as their biduals - cf. [33, Corollary 17.8.4]) and satisfies $\|J_{\mathbb{P}_\Delta}\|_{\mathcal{P}_2} = \mathbb{P}_\Delta(\Delta)^{1/2} = 1$ (cf. [33, Subsection 11.2])). In particular, we reobtain [119, Corollary 2.2]. It is quite instructive to compare this result with [33, Corollary 14.5.2 and Theorem 17.14], [70, Section 5] and [80, Theorem G].

Given that trace duality view, the role of the "free parameters" $m, n, d \in \mathbb{N}$, where the pair $(m, n) \in \mathbb{N}^2$ describes the size of the matrices and d is the dimension of the underlying finite-dimensional Hibert space $\mathbb{F}_2^d$ is explicitly described in

Proposition 3.18. *Let* $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$ *and* $m, n, d \in \mathbb{N}$. *Put*

$$K_G^{\mathbb{F}}(m,n;d) := \sup\Big\{\|\Gamma_{\mathbb{F}_2^d}(u,v) : l_1^n \longrightarrow l_\infty^m\|_{\mathcal{N}} : (u,v) \in (S_{\mathbb{F}_2^d})^m \times (S_{\mathbb{F}_2^d})^n\Big\}.$$

Then

$$K_G^{\mathbb{F}}(d) = \sup_{(m,n)\in\mathbb{N}^2} K_G^{\mathbb{F}}(m,n;d). \tag{3.59}$$

and

$$K_G^{\mathbb{F}}(m,n) = \sup_{S \in \mathcal{Q}_{m,n}(\mathbb{F})} \|S\|_{\mathcal{N}} = \sup_{d \in \mathbb{N}} K_G^{\mathbb{F}}(m,n;d). \tag{3.60}$$

The sequence $(K_G^{\mathbb{F}}(d))_{d\in\mathbb{N}}$ *is non-decreasing, and*

$$K_G^{\mathbb{F}} = \sup\Big\{\|S\|_{\mathcal{N}} : m,n \in \mathbb{N}, S \in \mathcal{Q}_{m,n}(\mathbb{F})\Big\} = \sup_{(m,n)\in\mathbb{N}^2} K_G^{\mathbb{F}}(m,n) = \sup_{d\in\mathbb{N}} K_G^{\mathbb{F}}(d) = \lim_{d\to\infty} K_G^{\mathbb{F}}(d). \tag{3.61}$$

In particular, $K_G^{\mathbb{F}}(1,1) = 1$ *and* $K_G^{\mathbb{F}}(m,n;1) = K_G^{\mathbb{F}}(1) = 1$ *for all* $m,n \in \mathbb{N}$.

Proof. First of all, it follows from (3.50) and (3.55) that

$$K_G^{\mathbb{F}}(m,n) = \sup_{S \in \mathcal{Q}_{m,n}(\mathbb{F})} \|S\|_{\mathcal{N}} = \sup_{d\in\mathbb{N}} K_G^{\mathbb{F}}(m,n;d) \leq \sup\Big\{\|S\|_{\mathcal{N}} : m,n \in \mathbb{N}, S \in \mathcal{Q}_{m,n}(\mathbb{F})\Big\}.$$

Since

$$\sup_{A\in B_W} |\mathrm{tr}(A^*S)| \overset{(3.52)}{=} \sup_{A\in B_W} |\langle A^*, \tau_S\rangle| = \|\tau_S\| = \|S\|_{\mathcal{N}}$$

for any $S \in \mathcal{Q}_{m,n}(\mathbb{F})$, Theorem 3.7 and (1.3) imply that

$$\sup\Big\{\|S\|_{\mathcal{N}} : m,n \in \mathbb{N}, S \in \mathcal{Q}_{m,n}(\mathbb{F})\Big\} = K_G^{\mathbb{F}} \leq \sup_{(m,n)\in\mathbb{N}^2} K_G^{\mathbb{F}}(m,n).$$

Hence,

$$\begin{aligned}\sup_{d\in\mathbb{N}}\Big(\sup_{(m,n)\in\mathbb{N}^2} K_G^{\mathbb{F}}(m,n;d)\Big) &= \sup_{(m,n)\in\mathbb{N}^2}\Big(\sup_{d\in\mathbb{N}} K_G^{\mathbb{F}}(m,n;d)\Big)\\ &= \sup_{(m,n)\in\mathbb{N}^2} K_G^{\mathbb{F}}(m,n) = \sup\Big\{\|S\|_{\mathcal{N}} : m,n \in \mathbb{N}, S \in \mathcal{Q}_{m,n}(\mathbb{F})\Big\} = K_G^{\mathbb{F}}.\end{aligned}$$

Moreover, if $m,n,d \in \mathbb{N}$ are given, recall that

$$\begin{aligned}K_G^{\mathbb{F}}(m,n;d) &= \sup\Big\{\|\Gamma_{\mathbb{F}_2^d}(u,v) : l_1^n \longrightarrow l_\infty^m\|_{\mathcal{N}} : (u,v) \in (S_{\mathbb{F}_2^d})^m \times (S_{\mathbb{F}_2^d})^n\Big\}\\ &= \sup\Big\{|\mathrm{tr}(A^*\,\Gamma_{\mathbb{F}_2^d}(u,v))| : A \in B_W, (u,v) \in (S_{\mathbb{F}_2^d})^m \times (S_{\mathbb{F}_2^d})^n\Big\},\end{aligned}$$

whence $\sup_{(m,n)\in\mathbb{N}^2} K_G^{\mathbb{F}}(m,n;d) \leq K_G^{\mathbb{F}}(d)$ (due to (1.2) and (3.40)). By definition, $K_G^{\mathbb{F}}(d)$ is the smallest constant $K(d)$ which satisfies inequality (1.2). Thus, $\sup_{(m,n)\in\mathbb{N}^2} K_G^{\mathbb{F}}(m,n;d) = K_G^{\mathbb{F}}(d)$. Finally, since $\langle v,u\rangle_{\mathbb{F}_2^d} = \langle Jv, Ju\rangle_{\mathbb{F}_2^{d+1}}$ for all $d \in \mathbb{N}$ and $u,v \in \mathbb{F}_2^d$, where $J : \mathbb{F}_2^d \longrightarrow \mathbb{F}_2^{d+1}, (x_1,\ldots,x_d) \mapsto (x_1,\ldots,x_d,0)$ denotes the canonical isometric injection from $\mathbb{F}_2^d$ into $\mathbb{F}_2^{d+1}$, it follows that $K_G^{\mathbb{F}}(d) \leq K_G^{\mathbb{F}}(d+1)$ for all $d \in \mathbb{N}$. □

Remark 3.19. Even in the matrix case, the Banach space $(\mathcal{N}(l_1^n, l_\infty^m), \|\cdot\|_{\mathcal{N}})$ should not be confused with the Banach space $(\mathcal{N}(\mathbb{F}_2^n, \mathbb{F}_2^m), \|\cdot\|_{\mathcal{N}}) = (\mathcal{S}_1(\mathbb{F}_2^n, \mathbb{F}_2^m), \sigma_1)$! The latter space namely consists of matrices - viewed as operators - between (finite-dimensional) *Hilbert spaces*, contained in the so-called *Schatten-von Neumann class of index 1*, also known as *trace-class operators* (cf., e.g., [67] and [78, Chapter 20.2]). In particular, if we view a given matrix

$M \in \mathbb{M}_{m,n}(\mathbb{F})$ as linear operator *from* l_1^n *to* l_∞^m, the norm $\|M\|_{\mathcal{N}}$ in general does *not* coincide with the so-called *trace norm* of M (also known as *nuclear norm*). The latter is given by $\|M\|_* := \operatorname{tr}(|M|)$, where $|M| := (M^* M)^{1/2}$. Since the trace norm of M coincides with the Schatten 1-norm $\sigma_1(M)$, it equals the sum of the singular values of the matrix M (cf., e.g., [15, Chapter IV.2], [29, Exercises IX.2.19, IX.2.20 and IX.2.21] and [68, Chapter 5.6 and Chapter 7.4.7]).

Let us recall the isometric isomorphism $\tau : Z \overset{\cong}{\longrightarrow} Y'$, induced by the Banach spaces $Y := \mathcal{L}(l_\infty^m, l_1^n)$ and $Z := \mathcal{N}(l_1^n, l_\infty^m) \cong Y'$ (cf. (3.52)). Put $\delta := \tau' j_Y : Y \overset{\cong}{\longrightarrow} Z'$. As we have seen, also δ is an isometric isomorphism (cf. Remark 3.16). Its inverse is given by $\delta^{-1} = j_Y^{-1}(\tau^{-1})'$ (since Y is finite-dimensional). An application of the bipolar theorem to the dual pairing $\langle Z, Z' \rangle = \langle Z, \delta(Y) \rangle$, induced by the bilinear form $Z \times Z' \longrightarrow \mathbb{F}, (R, z') \mapsto \langle R, z' \rangle := \operatorname{tr}(R\,\delta^{-1}(z'))$ (cf. [29, V.1.8] and [78, Chapter 8.2]) implies the following explicit representation result for the so-called “local correlation polytope”. To the best of our knowledge, the outcome for the complex case (i.e., if $\mathbb{F} = \mathbb{C}$) is new. A (different) part of our proof for the real case can be found in the proof of [9, Proposition 11.7]. In particular, we are going to shed some light on the geometry of the unit ball of $\mathcal{N}(l_1^n, l_\infty^m)$. To this end, recall that for any subset S of an $\mathbb{F}$-vector space

$$\operatorname{cx}(S) := \bigcup_{n \in \mathbb{N}} \Big\{ \sum_{i=1}^n \alpha_i x_i : x_1, \ldots, x_n \in S, \alpha_1, \ldots, \alpha_n \geq 0 \text{ and } \sum_{i=1}^n \alpha_i = 1 \Big\}$$

denotes the convex hull of S and that

$$\operatorname{acx}(S) := \bigcup_{n \in \mathbb{N}} \Big\{ \sum_{i=1}^n \alpha_i x_i : x_1, \ldots, x_n \in S, \alpha_1, \ldots, \alpha_n \in \mathbb{F} \text{ and } \sum_{i=1}^n |\alpha_i| \leq 1 \Big\} \tag{3.62}$$

marks the absolute convex hull of S. Here we adopt the notation, introduced right below [78, Proposition 6.1.3]. Recall also that $\operatorname{acx}(S) = \operatorname{cx}(\breve{S})$, where $\breve{S} := (\mathbb{F} \cap \overline{\mathbb{D}})S$ denotes the circled hull of S (cf. [78, Proposition 6.1.4]).

Theorem 3.20. *Let* $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$ *and* $m, n \in \mathbb{N}$. *Put*

$$\mathcal{G}_{m,n}(\mathbb{F}) := \{\overline{p} q^\top : (p, q) \in S_{\mathbb{F}}^m \times S_{\mathbb{F}}^n\} = \Big\{\Gamma_{\mathbb{F}}(p, q) : (p, q) \in S_{\mathbb{F}}^m \times S_{\mathbb{F}}^n\Big\}$$

and

$$\mathcal{H}_{m,n}(\mathbb{F}) := \{\overline{x} y^\top : (x, y) \in (\mathbb{F} \cap \overline{\mathbb{D}})^m \times (\mathbb{F} \cap \overline{\mathbb{D}})^n\} = \Big\{\Gamma_{\mathbb{F}}(x, y) : (x, y) \in (\mathbb{F} \cap \overline{\mathbb{D}})^m \times (\mathbb{F} \cap \overline{\mathbb{D}})^n\Big\}.$$

Then

$$B_{\mathcal{N}(l_1^n, l_\infty^m)} = acx(\mathcal{G}_{m,n}(\mathbb{F})) = cx(\widetilde{\mathcal{G}_{m,n}(\mathbb{F})}) = cx(\mathcal{H}_{m,n}(\mathbb{F})). \tag{3.63}$$

(i) *If* $\mathbb{F} = \mathbb{R}$, *then the set* $\mathcal{G}_{m,n}(\mathbb{R})$ *even coincides with the set of all extreme points of* $B_{\mathcal{N}(l_1^n, l_\infty^m)}$ *and*

$$\begin{aligned} B_{\mathcal{N}(l_1^n, l_\infty^m)} &= cx(\mathcal{G}_{m,n}(\mathbb{F})) = \Big\{ \sum_{i=1}^{mn+1} \lambda_i\, x_i : x_i \in \mathcal{G}_{m,n}(\mathbb{R}), 0 \leq \lambda_i \leq 1, \sum_{i=1}^{mn+1} \lambda_i = 1 \Big\} \\ &= \Big\{ \mathbb{E}[\boldsymbol{X}\boldsymbol{Y}^\top] : \max\{|X_i|, |Y_j|\} \leq 1 \textit{ a.s., for all } (i, j) \in [m] \times [n] \Big\}. \end{aligned}$$

(ii) *If $\mathbb{F} = \mathbb{C}$, then*

$$B_{\mathcal{N}(l_1^n, l_\infty^m)} = \Big\{ \sum_{i=1}^{2mn+1} \lambda_i\, x_i : x_i \in \widetilde{\mathcal{G}_{m,n}(\mathbb{C})}, 0 \leq \lambda_i \leq 1, \sum_{i=1}^{2mn+1} \lambda_i = 1 \Big\}.$$

Proof. Put $Y := \mathcal{L}(l_\infty^m, l_1^n)$ and $Z := \mathcal{N}(l_1^n, l_\infty^m)$. Fix $(p, q) \in S_{\mathbb{F}}^m \times S_{\mathbb{F}}^n$. Recall the well-known isometric isomorphism $\chi : l_\infty^n \overset{\cong}{\longrightarrow} (l_1^n)'$, defined as

$$\langle z, \chi(q) \rangle := z^\top q = \sum_{j=1}^{n} q_j\, z_j \quad ((z, q) \in l_1^n \times l_\infty^n).$$

Since $\overline{p}_i\, q_j = e_i^\top \Big(\langle \cdot, \chi(q) \rangle\, \overline{p} \Big) e_j$ for all $(i, j) \in [m] \times [n]$, it follows that $\overline{p} q^\top$ is the matrix representation of the linear operator $\langle \cdot, \chi(q) \rangle\, \overline{p} : \mathbb{F}^n \longrightarrow \mathbb{F}^m$ with respect to the standard bases. By definition of the nuclear norm it therefore follows that $\|\overline{p} q^\top\|_{\mathcal{N}} \equiv \|\langle \cdot, \chi(q) \rangle\, \overline{p}\|_{\mathcal{N}} = \|q\|_\infty\, \|p\|_\infty = 1$ (cf. [117, Chapter 6.3]). Hence,

$$\text{acx}(\mathcal{G}_{m,n}(\mathbb{F})) \subseteq B_Z.$$

Moreover, $\mathcal{G}_{m,n}(\mathbb{F}) = f(S_{\mathbb{F}}^m \times S_{\mathbb{F}}^n)$, where $f : l_\infty^m \times l_\infty^n \longrightarrow Z$ is defined as $f(p, q) := \overline{p} q^\top$. A standard application of the triangle inequality implies that f is continuous. Hence, $\mathcal{G}_{m,n}(\mathbb{F})$ is a compact subset of the Banach space Z. Similarly it follows that $\mathcal{H}_{m,n}(\mathbb{F}) \subseteq Z$ is compact. Let $z' \in (\mathcal{G}_{m,n}(\mathbb{F}))^\circ \subseteq Z'$. Consider the isometric isomorphism $\delta : Y \longrightarrow Z'$. Then in particular $|\text{tr}(\overline{p} q^\top B_0)| = |\langle \overline{p} q^\top, z' \rangle| \leq 1$ for all $(p, q) \in S_{\mathbb{F}}^m \times S_{\mathbb{F}}^n$, where $B_0 := \delta^{-1}(z') \in Y$. Consequently, $B_0 \in B_Y$ (due to (3.42)), whence

$$(\text{acx}(\mathcal{G}_{m,n}(\mathbb{F})))^\circ \subseteq (\mathcal{G}_{m,n}(\mathbb{F}))^\circ \subseteq \delta(B_Y) = B_{Z'} = B_Z^\circ\,.$$

Consequently, polarisation again (now applied to subsets of Z' - cf., e.g., [29, Definition V.1.6]) implies that

$$B_Z \subseteq B_Z^{\circ\circ} \subseteq (\text{acx}(\mathcal{G}_{m,n}(\mathbb{F})))^{\circ\circ} = \overline{\text{acx}(\mathcal{G}_{m,n}(\mathbb{F}))}^{\|\cdot\|_Z}. \tag{3.64}$$

The last equality follows from the bipolar theorem (cf., e.g., [29, Theorem V.1.8] or [78, Theorem 8.2.2]). However, since actually Z is a finite-dimensional space, it follows that also $\text{acx}(\mathcal{G}_{m,n}(\mathbb{F}))$ is a compact subset of Z (see [78, Proposition 6.7.4]). In particular, it is closed, whence $B_Z = \text{acx}(\mathcal{G}_{m,n}(\mathbb{F}))$.

The inclusion $\text{acx}(\mathcal{G}_{m,n}(\mathbb{F})) \subseteq \text{cx}(\mathcal{H}_{m,n}(\mathbb{F}))$ is trivial. Let $(\lambda_1, \ldots, \lambda_k) \in [0, 1]^k$, such that $\sum_{\nu=1}^k \lambda_\nu = 1$. Since

$$\| \sum_{\nu=1}^{k} \lambda_\nu\, \overline{x} y^\top \|_{\mathcal{N}} \leq \sum_{\nu=1}^{k} \lambda_\nu \|x\|_\infty\, \|y\|_\infty \leq \sum_{\nu=1}^{k} \lambda_\nu = 1,$$

for all $(x, y) \in (\mathbb{F} \cap \mathbb{D})^m \times (\mathbb{F} \cap \mathbb{D})^n$, $l \in \mathbb{N}$, it follows that $\text{cx}(\mathcal{H}_{m,n}(\mathbb{F})) \subseteq B_Z$. Finally, [78, Proposition 6.2.4] implies that $\text{acx}(\mathcal{G}_{m,n}(\mathbb{F})) = \text{cx}(\widetilde{\mathcal{G}_{m,n}(\mathbb{F})})$, which concludes the proof of (3.63).

(i) The non-trivial statement that - in the real case - $\mathcal{G}_{m,n}(\mathbb{R})$ precisely describes the set of all extreme points of the convex compact unit ball B_Z (whose proof requires tensor product

methods and trace duality) follows from [33, Proposition 16.7], together with [128, Theorem 1.3]. Equipped with this deep fact, we may apply the finite-dimensional version of the Krein-Milman Theorem to the non-empty convex compact set B_Z (cf. [3, Theorem 7.68]), whence $B_Z = \text{cx}(\mathcal{G}_{m,n}(\mathbb{F}))$. Now, we may apply Carathéodory's Convexity Theorem (cf. [3, Theorem 5.32]), which gives us the second equality. The last equality follows from [9, Definition 11.5 and Proposition 11.7].
(ii) To proceed in a similar way as in the real case (i), we view $Z \cong \mathbb{M}_{m,n}(\mathbb{C}) \cong \mathbb{C}^{mn}$ as a real finite-dimensional vector space, implying that $\dim_{\mathbb{R}}(Z) = 2mn$. Consequently, we may apply Carathéodory's Convexity Theorem again (cf. [3, Theorem 5.32] and the proof of [78, Proposition 6.7.4]); namely to $\text{cx}(\mathcal{G}_{m,n}(\mathbb{F})) = B_Z \subseteq Z$, from which (ii) follows (due to (3.63)). □

Based on [9, Definition 11.5 and remark right below], we have shown that at least in the real case (i.e., if $\mathbb{F} = \mathbb{R}$), B_Z precisely coincides with the set of all *classical (or local) "correlation" matrices.*

Consequently, (3.53) implies that for all $m, n \in \mathbb{N}$, for all $\mathbb{F}$-Hilbert spaces $H^{\mathbb{F}}$ and $(u, v) \in S^m_{H^{\mathbb{F}}} \times S^n_{H^{\mathbb{F}}}$ there are $x^{\mathbb{F}}_1, \ldots, x^{\mathbb{F}}_{k^{\mathbb{F}}} \in (\mathbb{F} \cap \mathbb{D})^m$, $y^{\mathbb{F}}_1, \ldots, y^{\mathbb{F}}_{k^{\mathbb{F}}} \in (\mathbb{F} \cap \mathbb{D})^n$ and $(\lambda^{\mathbb{F}}_1, \ldots, \lambda^{\mathbb{F}}_{k^{\mathbb{F}}}) \in [0, 1]^{k^{\mathbb{F}}}$, such that $\sum_{\nu=1}^{k^{\mathbb{F}}} \lambda^{\mathbb{F}}_\nu = 1$ and

$$\Gamma_{H^{\mathbb{F}}}(u, v) = K^{\mathbb{F}}_G \sum_{\nu=1}^{k^{\mathbb{F}}} \lambda^{\mathbb{F}}_\nu \, \overline{x^{\mathbb{F}}_\nu} \, (y^{\mathbb{F}}_\nu)^\top, \tag{3.65}$$

where $k_{\mathbb{R}} := mn + 1$ and $k_{\mathbb{C}} := 2mn + 1$. If $\mathbb{F} = \mathbb{R}$, we may assume that $|x^{\mathbb{R}}_\nu| = 1$ and $|y^{\mathbb{R}}_\nu| = 1$ for all $\nu \in [k^{\mathbb{R}}]$. In particular (if $m = n = 1$),

$$\langle u, v \rangle_{H^{\mathbb{R}}} = K^{\mathbb{R}}_G \, (\lambda^{\mathbb{R}}_1 \, x^{\mathbb{R}}_1 \, y^{\mathbb{R}}_1 + (1 - \lambda^{\mathbb{R}}_1) \, x^{\mathbb{R}}_2 \, y^{\mathbb{R}}_2)$$

and

$$\langle b, a \rangle_{H^{\mathbb{C}}} = K^{\mathbb{C}}_G \sum_{\nu=1}^{3} \lambda^{\mathbb{C}}_\nu \, \overline{x^{\mathbb{C}}_\nu} \, y^{\mathbb{C}}_\nu$$

for all $u, v \in S_{H^{\mathbb{R}}}$ and $a, b \in S_{H^{\mathbb{C}}}$. Since $K^{\mathbb{R}}_G > 1$, it follows that $\text{sign}(x^{\mathbb{R}}_1 \, y^{\mathbb{R}}_1) \neq \text{sign}(x^{\mathbb{R}}_2 \, y^{\mathbb{R}}_2)$. Thus, if $\lambda_1 \neq \frac{1}{2}$, then

$$\frac{\pi}{2} < K^{\mathbb{R}}_G \leq \frac{1}{|2\,\lambda_1 - 1|}, \text{ respectively } |\lambda_1| \leq \frac{1 + K^{\mathbb{R}}_G}{2K^{\mathbb{R}}_G} < \frac{\pi + 2}{2\pi} \approx 0.818\,.$$

Remark 3.21 (**Quantum violation of a Bell inequality**). Fix an *arbitrarily given* $S \in \mathcal{Q}_{m,n}(\mathbb{F}) \setminus B_Z$. Recall again the construction of the isometric isomorphism $\tau : Z \xrightarrow{\cong} Y'$ via trace duality (cf. (3.51) and (3.52)). Since B_Z is a non-empty closed and absolutely convex subset of the Banach space Z, we may apply [78, Corollary 7.3.6]. The latter is an implication of hyperplane separation (which is a geometric version of the Hahn-Banach theorem and thus an implication of Zorn's lemma). Hence, due to (3.56), it follows the existence of a matrix $B_0 \in B_Y$, such that

$$\text{tr}(A^*_0 S) = \text{tr}(B_0 S) > 1 \text{ and } |\text{tr}(A^*_0 R)| \leq 1 \text{ for all } R \in B_Z\,,$$

where $A_0 := B_0^* \in B_W$ (compare also with (3.57)). In particular, we have been provided with a matrix $A_0 \in \mathbb{M}_{m,n}(\mathbb{F})$, such that $\|A_0\|_{\infty,1} \leq 1$ and

$$1 < \sup_{H \in \mathtt{HIL}^{\mathbb{F}}} \|A_0\|_H^{\mathrm{G}} = \max_{S \in \mathcal{Q}_{m,n}(\mathbb{F})} |\mathrm{tr}(A_0^* S)| = \max_{S \in \mathcal{Q}_{m,n}(\mathbb{F})} \mathrm{Re}(\mathrm{tr}(A_0^* S)) = \max_{\Sigma \in C(m+n;\mathbb{F})} \mathrm{tr}(\Delta(A_0)\Sigma)$$

(due to (3.46)). In quantum mechanics (if $\mathbb{F} = \mathbb{R}$), the latter inequality is somewhat vaguely referred to as the "maximal quantum violation of a Bell (correlation) inequality". The "maximal violation of the related Bell inequality" coincides precisely with the inequality

$$\|f_{A_0}\| = \max_{S \in \mathcal{Q}_{m,n}(\mathbb{F})} |f_{A_0}(S)| = \max_{S \in \mathcal{Q}_{m,n}(\mathbb{F})} |\mathrm{tr}(A_0^* S)| > 1\,,$$

where f_{A_0} is defined as in Remark 3.16 (for both fields). The term "Bell inequality" (now with respect to any given $A \in B_W$, of course) is therefore to be understood as the inequality

$$\max_{R \in B_Z} |f_A(R)| = \max_{R \in B_Z} |\mathrm{tr}(A^* R)| \leq 1\,,$$

which holds for all $A \in B_W$ (due to (3.56)). That Bell inequality is "violated", if and only if $|f_A(S_0)| > 1$ for some quantum correlation matrix $S_0 \in \mathcal{Q}_{m,n}(\mathbb{F}) \setminus B_Z$. (cf. also Remark 3.16, respectively Theorem 3.20-(i), together with [94, Lemma 2] if $\mathbb{F} = \mathbb{R}$). In this respect, the maximum value $\|f_A\|$ is then referred to as "maximal violation of the Bell inequality". Consequently, due to (3.50) and Remark 3.16, there are $S_* \in \mathcal{Q}_{m,n}(\mathbb{F}) \setminus B_Z$ and - hence - $d_* \in \mathbb{N}$, such that "the maximal violation of the Bell inequality" (i.e., $\|f_A\|$) is uniformly bounded above by $K_G^{\mathbb{F}}(d_*) \leq K_G^{\mathbb{F}}$. More precisely, if $S_* = \Gamma_{\mathbb{F}_2^{d_*}}(u_*, v_*)$, for some $d_* \in \mathbb{N}$ and $(u_*, v_*) \in (S_{\mathbb{F}_2^{d_*}})^m \times (S_{\mathbb{F}_2^{d_*}})^n$, then

$$1 < \|f_A\| = |\mathrm{tr}(A^* S_*)| = \sup_{(u,v) \in (S_{\mathbb{F}_2^{d_*}})^m \times (S_{\mathbb{F}_2^{d_*}})^n} |\mathrm{tr}(A^* \Gamma_{\mathbb{F}_2^{d_*}}(u, v))| \leq K_G^{\mathbb{F}}(d_*) \leq K_G^{\mathbb{F}}\,.$$

Remark 3.22. We don't know whether in (3.48) we may substitute the block matrix $\Delta(A) \in \mathbb{M}_{m+n}(\mathbb{F})$ through an *arbitrary* matrix $B \in \mathbb{M}_{m+n}(\mathbb{F})$. If this were the case, a further application of the bipolar theorem (cf. [78, Theorem 8.2.2]) shows that the latter would be equivalent to

$$C(k;\mathbb{F}) \subseteq K_G^{\mathbb{F}}\,\mathrm{acx}(C_1(k;\mathbb{F})) \text{ for all } k \in \mathbb{N}_2\,.$$

Theorem 3.20 therefore would imply that

$$C(k;\mathbb{F}) \subseteq K_G^{\mathbb{F}}\,\mathrm{acx}(\{\overline{p}q^\top : (p,q) \in S_{\mathbb{F}}^k \times S_{\mathbb{F}}^k\}) \overset{(3.63)}{=} K_G^{\mathbb{F}}\, B_{\mathcal{N}(l_1^k, l_\infty^k)} \text{ for all } k \in \mathbb{N}_2\,,$$

where $B_{\mathcal{N}(l_1^k, l_\infty^k)}$ again denotes the unit ball of the Banach space of nuclear operators between l_1^k and l_∞^k, equipped with the nuclear norm.

3.4. $K_G^{\mathbb{R}}(2)$ and the Walsh-Hadamard transform: Krivine's approach revisited

Regarding explicit constructions of elements of $\mathcal{Q}_{m,n}(\mathbb{F})$, a rigorous description of the *entries* of the Kronecker product of matrices proves to be a very useful tool (cf. Example 3.27). To this end, we consider the mapping:

$$\mathbb{Z} \times \mathbb{N} \ni (\nu, n) \mapsto r_n(\nu) := \begin{cases} n & \text{if } n \text{ is a divisor of } \nu \\ \mathrm{rem}_n(\nu) & \text{if } n \text{ is not a divisor of } \nu\,, \end{cases}$$

where $\operatorname{rem}_n(\nu) \in \{0, 1, \ldots, n-1\}$ denotes the uniquely determined remainder in Euclidian division of ν by n, implying that $r_n(\nu) \in [n]$ (by construction). Thus, if $p \in \mathbb{Z}$ and $\nu = pn + \operatorname{rem}_n(\nu)$, then $p + 1 \geq \frac{\nu+1}{n}$ and

$$f_n(\nu) := \frac{\nu - r_n(\nu)}{n} + 1 = \begin{cases} p + 1 < \frac{\nu}{n} + 1 & \text{if } n \text{ is not a divisor of } \nu \\ \frac{\nu}{n} & \text{if } n \text{ is a divisor of } \nu\,. \end{cases}$$

Consequently, if $l \in \mathbb{N}$ and $\nu \in [ln]$, then $f_n(\nu) \in [l]$. In particular, $r_n(\nu) = \nu$ if $\nu \in [n]$.

Especially with regard to Example 3.27 the "Boolean" case n=2 is of particular importance to us. Here, we obviously obtain:

$$f_2(\nu) = \left\lceil \frac{\nu}{2} \right\rceil = \begin{cases} \frac{\nu}{2} & \text{if } \nu \text{ is even} \\ \frac{\nu+1}{2} & \text{if } \nu \text{ is odd} \end{cases} \text{ and } b_1(\nu) := r_2(\nu) - 1 = \mathbb{1}_{2\mathbb{N}}(\nu) = \begin{cases} 1 & \text{if } \nu \text{ is even} \\ 0 & \text{if } \nu \text{ is odd}\,. \end{cases} \tag{3.66}$$

Note that the structure of f_2 implies that $f_2([2^i]) = [2^{i-1}]$ for all $i \in \mathbb{N}$. In particular, for any $m \in \mathbb{N}_2$ and $i \in \{2, 3, \ldots, m\}$, the well-defined function $b_i := b_1 \circ \underbrace{f_2 \circ \cdots \circ f_2}_{(i-1)-\text{times}}$ is the ith component of the $\{0,1\}^m$-valued function $\pi_m : \mathbb{Z} \longrightarrow \{0,1\}^m$, defined as

$$\pi_m(\nu) := (b_1(\nu), b_2(\nu), \ldots, b_m(\nu))^\top \text{ for all } \nu \in \mathbb{Z}\,. \tag{3.67}$$

The actual role of the sequence of functions $(r_n)_{n \in \mathbb{N}}$ is encoded in

Lemma 3.23. *Let $n \in \mathbb{N}$. Then the mapping*

$$\Psi_n : \mathbb{Z} \times [n] \xrightarrow{\cong} \mathbb{Z}\,, (i,j) \mapsto (i-1)n + j$$

is bijective. Its inverse is given by $\Psi_n^{-1} = \Lambda_n$, where

$$\Lambda_n : \mathbb{Z} \longrightarrow \mathbb{Z} \times [n], \nu \mapsto (f_n(\nu), r_n(\nu)).$$

Moreover, $\Psi_n([l] \times [n]) = [ln]$ for all $l \in \mathbb{N}$.

Proof. Fix $(i,j) \in \mathbb{Z} \times [n]$. If $\Psi(i,j) = (i-1)n + j = ln$ for some $l \in \mathbb{Z}$, it follows that $0 < j = (l - (i-1))n \leq n$, whence $0 < l - (i-1) \leq 1$. Thus, $l = i$, and hence $j = n$. Thus, n is a divisor of $(i-1)n + j$ if and only if $j = n$, implying that $r_n((i-1)n + j) = n$ (by construction of the mapping r). Hence, if n is not a divisor of $(i-1)n + j$, then $j < n$, and it follows that $r_n((i-1)n + j) = j$ is the uniquely determined remainder of $(i-1)n + j$. Now, we only have to use a bit of elementary algebra, to show that $\Lambda_n \circ \Psi_n = \operatorname{id}_{\mathbb{Z} \times [n]}$ and $\Psi_n \circ \Lambda_n = \operatorname{id}_{\mathbb{Z}}$, where $\Lambda(\nu) := \left(\frac{\nu - r_n(\nu)}{n} + 1, r_n(\nu)\right)$ for all $\nu \in \mathbb{Z}$. Consequently, $\Lambda_n = \Psi_n^{-1}$. Finally, if $\Psi_n(i,j) = (i-1)n + j \leq ln$, it follows that $n(l - (i-1)) \geq j > 0$, whence $i - 1 < l$. Thus, $i \in [l]$, and it follows that $[ln] = [ln] \cap \Psi_n(\mathbb{Z} \times [n]) \subseteq \Psi_n([l] \times [n])$ (since Ψ_n is onto). Conversely, if $i \in [l]$ and $j \in [n]$, then $\Psi_n(i,j) = (i-1)n + j \leq in \leq ln$. ☐

Equipped with the remainder mapping r and the both bijections $\Psi_n : \mathbb{Z} \times [n] \longrightarrow \mathbb{Z}$ and $\Psi_m : \mathbb{Z} \times [m] \longrightarrow \mathbb{Z}$, we are now able to describe both, the bijective linear operator vec :

$\mathbb{M}_{m,n}(\mathbb{F}) \longrightarrow \mathbb{F}^{mn}$ and the Kronecker product explicitly *entrywise*. So, fix $m, n, p, q \in \mathbb{N}$. If $A = (a_{ij}) \in \mathbb{M}_{m,n}(\mathbb{F})$, $B = (b_{kl}) \in \mathbb{M}_{p,q}(\mathbb{F})$, $\alpha \in [mp]$, $\beta \in [nq]$ and $\gamma \in [mn]$, put

$$(A \otimes B)_{\alpha,\beta} := a_{f_p(\alpha),f_q(\beta)} \cdot b_{r_p(\alpha),r_q(\beta)} = ((A^\top \otimes B^\top)^\top)_{\alpha,\beta} \tag{3.68}$$

and

$$\mathrm{vec}(A)_\gamma \equiv \mathrm{vec}_m(A)_\gamma := a_{r_m(\gamma),f_m(\gamma)} = (A^\top)_{\Psi_m^{-1}(\gamma)} = \left(A_{\tau\circ\Psi_m^{-1}}\right)_\gamma , \tag{3.69}$$

where $(i, j) \mapsto \tau(i, j) := (j, i)$ denotes transposition. In other words, $\mathrm{vec} \equiv \mathrm{vec}_m = C_{\tau\circ\Psi_m^{-1}}$. In particular,

$$\mathrm{vec}\Big(e_i^{(m)}(e_j^{(n)})^\top\Big) = e^{(nm)}_{(j-1)m+i} \text{ for all } (i, j) \in [m] \times [n].$$

Consequently, Lemma 3.23 implies that

$$e_\nu^{(nm)} = \mathrm{vec}\Big(e^{(m)}_{r_m(\nu)} e^{(n)\top}_{f_m(\nu)}\Big) \text{ for all } \nu \in [nm]\,. \tag{3.70}$$

Moreover, if $n = 1$, it follows that $\mathrm{vec}(A)_i = a_{i,1}$ for all $i \in [m]$. Observe that the vectorisation of the matrix A involves its transpose $A^\top = A_\tau \in \mathbb{M}_{n,m}(\mathbb{F})$. Not too surprisingly, it follows that

$$\mathrm{vec}_n \circ C_\tau(A) = \mathrm{vec}_n(A^\top) = \mathrm{vec}_n(A_\tau) = A_{\Psi_n^{-1}} = C_{\Psi_n^{-1}}(A)$$

(since $\tau \circ \tau = \mathrm{id}$). The construction implies at once the non-trivial fact that $\mathrm{vec}_n(A^\top) = C_{\Psi_m\circ\tau\circ\Psi_n^{-1}}(\mathrm{vec}_m(A))$, where $C_{\Psi_m\circ\tau\circ\Psi_n^{-1}} : \mathbb{F}^{mn} \longrightarrow \mathbb{F}^{nm} = \mathbb{F}^{mn}$ is the related linear composition operator. Consequently,

$$\mathrm{vec}_n(A^\top) = K_{m,n}\,\mathrm{vec}_m(A)\,,$$

where the matrix $K^\top_{n,m} = K_{m,n} \in O(mn)$ satisfies

$$\begin{aligned}
(K_{m,n})_{\nu\mu} &= \delta_{(\Psi_m\circ\tau\circ\Psi_n^{-1})(\nu),\,\mu} = \delta_{(r_n(\nu)-1)m+f_n(\nu),\,\mu} \\
&\overset{(!)}{=} \delta_{f_m(\mu),r_n(\nu)} \cdot \delta_{f_n(\nu),r_m(\mu)} \\
&\overset{(3.68)}{=} \Big(\sum_{i=1}^m \sum_{j=1}^n e_i\, e_j^\top \otimes e_j\, e_i^\top\Big)_{\nu\mu}
\end{aligned}$$

for all $\nu, \mu \in [mn]$. The second equality follows from Lemma 3.23: $(r_n(\nu) - 1)m + f_n(\nu) = \mu$ if and only if $\Psi_m(r_n(\nu), f_n(\nu)) = \mu = \Psi_m(f_m(\mu), r_m(\mu))$. Since $f_n(\nu) \in [m]$, it follows that $r_n(\nu) = f_m(\mu)$ and $f_n(\nu) = r_m(\mu)$. Therefore, Lemma 3.23 (respectively Euclidian division with remainder) allows to extend the results in [98, Chapter 11, including Exercise 11.8] by an explicit entrywise (and hence implementable) description of the commutation matrix $K_{m,n} = \sum_{i=1}^m \sum_{j=1}^n e_i\, e_j^\top \otimes e_j\, e_i^\top$; namely in form of a product of two Kronecker delta symbols.

Moreover, $\mathrm{vec}^{-1} = \mathrm{mat}$, where the "matrixation operator" $\mathrm{mat} : \mathbb{F}^{mn} \longrightarrow \mathbb{M}_{m,n}(\mathbb{F})$ is given by $\mathrm{mat} \equiv \mathrm{mat}_m := C_{\Psi_m\circ\tau}$; i.e.,

$$\mathrm{mat}(x) := x_{\Psi_m\circ\tau} = \left(x_{\Psi_m(\tau(i,j))}\right)_{(i,j)} = \left(x_{(j-1)m+i}\right)_{(i,j)} = \begin{pmatrix} x_1 & x_{m+1} & \dots & x_{(n-1)m+1} \\ x_2 & x_{m+2} & \dots & x_{(n-1)m+2} \\ \vdots & \vdots & \dots & \vdots \\ x_m & x_{2m} & \dots & x_{mn} \end{pmatrix}$$

for all $x \in \mathbb{F}^{mn}$. Again, if $n = 1$, we recognise that $\mathrm{mat}(x)_{i1} = x_i$ for all $i \in [m]$. Consequently, we may identify $\mathrm{mat}(\mathbb{F}^m) \equiv \mathrm{vec}(\mathbb{M}_{m,1}(\mathbb{F})) \equiv \mathbb{F}^m$ for all $m \in \mathbb{N}$, so that we may assume without loss of generality that $(m,n) \in \mathbb{N}_2 \times \mathbb{N}_2$. That assumption also avoids necessarily the review, whether vec maps $\mathbb{F}^{mn}$ into $\mathbb{M}_{m,n}(\mathbb{F})$, or into $\mathbb{M}_{mn,1}(\mathbb{F}) \equiv \mathbb{F}^{mn}$, or into $\mathbb{M}_{1,mn}(\mathbb{F}) \equiv \{x^\top : x \in \mathbb{F}^{mn}\}$!

Example 3.24. Consider $A := \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{pmatrix} \in \mathbb{M}_{2,3}(\mathbb{F})$. Then $4 \in [2 \cdot 3] = [6]$ and $\Psi_3^{-1}(4) = (\frac{4 - r_3(4)}{3} + 1, r_3(4)) = (2,1)$. Thus, $\mathrm{vec}(A^\top)_4 = a_{21}$.

Therefore, we reobtain the well-known (and easy computable) facts that

$$xy^\top \equiv x \otimes y^\top \text{ for all } (x,y) \in \mathbb{F}^m \times \mathbb{F}^n .$$

and

$$\mathrm{vec}(xy^\top) \equiv y \otimes x \text{ for all } (x,y) \in \mathbb{F}^m \times \mathbb{F}^n .$$

In particular,

$$\begin{array}{ccc} e_\nu^{(nm)} & \overset{(3.70)}{=} & e_{f_m(\nu)}^{(n)} \otimes e_{r_m(\nu)}^{(m)} \\ \| & & \| \\ e_{(j-1)m+i}^{(nm)} & & e_j^{(n)} \otimes e_i^{(m)} \end{array} \tag{3.71}$$

for all $\nu \in [nm] = \Psi_m([n] \times [m]) = \{(j-1)m + i : (j,i) \in [n] \times [m]\}$. Equivalently (now translated into Dirac's bra-ket language):

$$|\alpha\, \beta\rangle \equiv |\alpha\rangle\, |\beta\rangle = |\alpha m + \beta\rangle \text{ for all } (\alpha, \beta) \in \{0,1,\ldots,n-1\} \times \{0,1,\ldots,m-1\}. \tag{3.72}$$

Consequently, if $C = \sum\limits_{j=1}^{n} \sum\limits_{k=1}^{p} c_{jk}\, e_j e_k^\top \in \mathbb{M}_{n,p}(\mathbb{F})$ is a third given matrix, then $ACB = \sum\limits_{j=1}^{n} \sum\limits_{k=1}^{p} c_{jk} (A e_j)(B^\top e_k)^\top$ and $\mathrm{vec}(C) = \sum\limits_{j=1}^{n} \sum\limits_{k=1}^{p} c_{jk}\, e_k \otimes e_j$, leading to another important, well-known matrix equality:

$$\mathrm{vec}(ACB) = (B^\top \otimes A)\mathrm{vec}(C).$$

Example 3.25 (Werner state). Let $p \in [0,1]$. Put

$$\mathbb{R}^4 \ni \psi^- := \frac{1}{\sqrt{2}}(0,1,-1,0)^\top \overset{(3.72)}{=} \frac{1}{\sqrt{2}}(|0\,1\rangle - |1\,0\rangle).$$

Consider the matrix

$$\mathbb{M}_4(\mathbb{R}) \ni \rho_p^{\mathrm{W}} := p\, \psi^-(\psi^-)^\top + \frac{1-p}{4} I_4 = \frac{1}{4} \begin{pmatrix} 1-p & 0 & 0 & 0 \\ 0 & 1+p & -2p & 0 \\ 0 & -2p & 1+p & 0 \\ 0 & 0 & 0 & 1-p \end{pmatrix}.$$

Since the rank one matrix $p\, \psi^-(\psi^-)^\top$ is positive semidefinite and $\frac{1-p}{4} I_4$ is positive definite if $p < 1$, it immediately follows that ρ_p^{W} is positive definite if $p < 1$ and $\rho_1^{\mathrm{W}} = \psi^-(\psi^-)^\top$ is positive semidefinite (yet not invertible). Moreover, by construction, it trivially follows that in general $\mathrm{tr}(\rho_p^{\mathrm{W}}) = 1$. Note that ρ_p^{W} can also be written as

$$\rho_p^{\mathrm{W}} = \frac{3-2\lambda(p)}{6} I_4 - \frac{3-4\lambda(p)}{6} G_1 = \frac{3-2\lambda(p)}{6}\Big(I_4 - \frac{3-4\lambda(p)}{3-2\lambda(p)} G_1\Big)\,,$$

where $\lambda(p) := \frac{3}{4}(1-p) \in [0,1]$ and $G_1 \in O(4)$ is the "flip operator" (cf. (1.9)). In quantum physics, the matrix $\rho_p^{\mathrm{W}} \in \mathbb{M}_4(\mathbb{R})^+$ is known as the so-called "two-qubit Werner state". A very detailed discussion of the origin and the meaning of Werner states in the foundations and philosophy of quantum mechanics, particularly in relation to the topic of entanglement and "local hidden-variable theories" can be found, for example, in [9, 25, 43] and in the relevant references, cited there.

Proposition 3.26. *Let $m, n, p, q \in \mathbb{N}$, $S \in \mathbb{M}_{m,n}(\mathbb{F})$ and $R \in \mathbb{M}_{p,q}(\mathbb{F})$. If $S \in \mathcal{Q}_{m,n}(\mathbb{F})$ and $R \in \mathcal{Q}_{p,q}(\mathbb{F})$, then $S \otimes R \in \mathcal{Q}_{mp,nq}(\mathbb{F})$.*

Proof. We only have to apply Proposition 3.13 and the entrywise description (3.68) of the Kronecker product $S \otimes R$. So, choose $\mathbb{F}$-Hilbert spaces $H_1, H_2, (u^{(1)}, v^{(1)}) \in S_{H_1}^m \times S_{H_1}^n$ and $(u^{(2)}, v^{(2)}) \in S_{H_2}^p \times S_{H_2}^q$, such that $S = \Gamma_{H_1}(u^{(1)}, v^{(1)})$ and $R = \Gamma_{H_2}(u^{(2)}, v^{(2)})$. Fix $(\alpha, \beta) \in [mp] \times [nq]$. (3.68) consequently implies that

$$(S \otimes R)_{\alpha,\beta} = \Big\langle v^{(1)}_{\frac{\beta - r_q(\beta)}{q}+1}, u^{(1)}_{\frac{\alpha - r_p(\alpha)}{p}+1}\Big\rangle_{H_1} \cdot \Big\langle v^{(2)}_{r_q(\beta)}, u^{(2)}_{r_p(\alpha)}\Big\rangle_{H_2} = \langle v_\beta, u_\alpha\rangle_H\,,$$

where the Hilbert space $H := H_1 \otimes H_2$ denotes the standard tensor product of the Hilbert spaces H_1 and H_2, $v_\beta := v^{(1)}_{\frac{\beta - r_q(\beta)}{q}+1} \otimes v^{(2)}_{r_q(\beta)}$ and $u_\alpha := u^{(1)}_{\frac{\alpha - r_p(\alpha)}{p}+1} \otimes u^{(2)}_{r_p(\alpha)}$. Since $u_\alpha \in S_H$ and $v_\beta \in S_H$ (by construction), it follows that $S \otimes R = \Gamma_H(u, v)$, where $(u, v) \in S_H^{mp} \times S_H^{nq}$. Thus, $S \otimes R \in \mathcal{Q}_{mp,nq}(\mathbb{F})$ (again, a consequence of Proposition 3.13). □

An important example of a matrix $A \in \mathbb{M}_{2^m}(\{-1, 1\})$, which satisfies $\|A\|_{\infty,1}^{\mathbb{R}} \leq 1$ and delivers $\sqrt{2}$ as a lower bound of $K_G^{\mathbb{R}}$ (cf. Proposition 3.34), and also plays a key role in the foundations of quantum mechanics and quantum information is the so-called *Walsh-Hadamard transform* (also known as *quantum gate* - cf. [25]). In the following enlightening example, we extend the Walsh-Hadamard transform $H_m \in \mathbb{M}_{2^m}(\{-1, 1\})$ to a complex Walsh-Hadamard transform $H_m^{\mathbb{C}} \in \mathbb{M}_{2^m}(\mathbb{T})$ and disclose some surprising properties of that matrix. In particular, we will show that the (value of the) sign of any of the 4^m entries of the real Walsh-Hadamard transform can be specified precisely, in exactly m calculation steps - for any $m \in \mathbb{N}$! To this end, recall the construction of the function $\pi_m : \mathbb{Z} \longrightarrow \{0, 1\}^m$ (cf. (3.67)) and put

$$N_m(\nu, \mu) := \langle \pi_m(\nu), \pi_m(\mu)\rangle_{\mathbb{F}_2^m} = \sum_{i=1}^m b_i(\nu) b_i(\mu) = b_1(\nu) b_1(\mu) + N_{m-1}(f_2(\nu), f_2(\mu)),$$

where $(\nu, \mu) \in [2^m] \times [2^m]$ and $N_0 := 0$. $N_m(\nu, \mu)$ counts the number of all $i \in [m]$, such that $b_i(\nu) b_i(\mu) = 1$. In particular, $N_m(1, \mu) = 0$ for all $\mu \in [2^m]$ (since $b_1(1) = 0$).

Example 3.27 (Real and complex Walsh-Hadamard transform). Let

$$H_1 := \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \text{ and } H_1^{\mathrm{op}} := R_2(i) H_1 = \tfrac{1}{\sqrt{2}}\begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix}.$$

For $m \in \mathbb{N}$, put

$$H_{m+1} := H_m \otimes H_1 = H_1 \otimes H_m = \tfrac{1}{\sqrt{2}} \begin{pmatrix} H_m & H_m \\ H_m & -H_m \end{pmatrix}$$

and

$$H^{\mathrm{op}}_{m+1} := H_m \otimes H^{\mathrm{op}}_1 = H_1 \otimes H^{\mathrm{op}}_m = \tfrac{1}{\sqrt{2}} \begin{pmatrix} H^{\mathrm{op}}_m & H^{\mathrm{op}}_m \\ H^{\mathrm{op}}_m & -H^{\mathrm{op}}_m \end{pmatrix}.$$

Then the following properties are satisfied:

(i) $(H_1)_{\alpha\beta} = \tfrac{1}{\sqrt{2}}\,(-1)^{(\alpha-1)(\beta-1)}$ for all $(\alpha,\beta) \in [2] \times [2]$. $H_1^\top = H_1 \in O(2)$ and $(H_1^{\mathrm{op}})^\top = H_1^{\mathrm{op}} \in O(2)$. If $m \in \mathbb{N}_2$, then $(H_m)^\top = H_m \in SO(2^m)$ and $(H_m^{\mathrm{op}})^\top = H_m^{\mathrm{op}} \in SO(2^m)$.

(ii) Let $m \in \mathbb{N}_2$ and $(\nu,\mu) \in [2^m] \times [2^m]$. Then

$$(H_m)_{\nu\mu} = \frac{1}{\sqrt{2}}\,(H_{m-1})_{f_2(\nu)\,f_2(\mu)} \cdot (-1)^{b_1(\nu)\,b_1(\mu)} = \frac{1}{\sqrt{2^m}}\,(-1)^{N_m(\nu,\mu)}\,, \tag{3.73}$$

In particular,

$$(H_m)_{1\mu} = (H_m)_{\mu 1} = \frac{1}{\sqrt{2^m}}\,.$$

(iii) Let $m \in \mathbb{N}$. Then $H_m = \mathrm{Re}(H_m^{\mathbb{C}}) \in \mathcal{Q}_{2^m,2^m}(\mathbb{R})$ and $H_m^{\mathrm{op}} = \mathrm{Im}(H_m^{\mathbb{C}}) \in \mathcal{Q}_{2^m,2^m}(\mathbb{R})$, where

$$H_m^{\mathbb{C}} := H_m + i\,H_m^{\mathrm{op}} \in \mathcal{Q}_{2^m,2^m}(\mathbb{C})\,.$$

In particular the matrix,

$$H_1^{\mathbb{C}} = \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} H_1 = \tfrac{1}{\sqrt{2}} \begin{pmatrix} 1-i & 1+i \\ 1+i & -1+i \end{pmatrix} = \overline{p}\,q^\top = \Gamma_{\mathbb{C}}(p,q)$$

is of rank 1 and satisfies $\|H_1^{\mathbb{C}}\|_{\infty,1} = \|p\|_1\,\|q\|_1 = 4$, where $p := (i,1)^\top \in \mathbb{T}^2$ and $q := (\tfrac{1+i}{\sqrt{2}}, \tfrac{-1+i}{\sqrt{2}})^\top \in \mathbb{T}^2$ and $H_{m+1}^{\mathbb{C}} = H_1 \otimes H_m^{\mathbb{C}}$ for all $m \in \mathbb{N}$.

(iv) For any $m \in \mathbb{N}$, $\|H_m\|_{\infty,1} = \|H_m^{\mathrm{op}}\|_{\infty,1}$. The sequence $(\|H_m\|_{\infty,1})_{m\in\mathbb{N}}$ is non-decreasing. Moreover,

$$\sqrt{2}\,\|H_m\|_{\infty,1} \leq \|H_{m+1}\|_{\infty,1} \leq 2\sqrt{2}\,\|H_m\|_{\infty,1} \tag{3.74}$$

and

$$(\sqrt{2})^m \leq \|H_m\|_{\infty,1} \leq (\sqrt{2})^{3m-2} \tag{3.75}$$

for all $m \in \mathbb{N}$. In particular, $\|A_m^{\mathrm{Had}}\|_{\infty,1} \leq 1$ for all $m \in \mathbb{N}$, where

$$A_m^{\mathrm{Had}} := \frac{1}{(\sqrt{2})^{3m-2}}\,H_m = \frac{1}{2^{2m-1}}((\sqrt{2})^m\,H_m)$$

and

$$\frac{1}{\sqrt{2}}\,\|H_1\|_{\infty,1} = \|A_1^{\mathrm{Had}}\|_{\infty,1} = 1. \tag{3.76}$$

Proof. First of all, it should be noted that our entire proof (also) involves induction on $m \in \mathbb{N}$.
(i) It is sufficient to verify (i) for H_m only. The case $m = 1$ is trivial. Given the recursive construction of H_m, we only have to apply the rule for the transpose of a Kronecker product of two matrices to recognise that $H_m = H_m^\top$ (cf. (3.68) and [67, 4.2.4]). The recursive construction of H_m also directly implies that $H_m^2 = H_m H_m = I_{2^m}$, whence $H_m \in O(2^m)$. However, since

$$\det(H_{m+1}) = \det(H_1 \otimes H_m) = (\det(H_1))^{2^m} (\det(H_m))^2 = (\det(H_m))^2,$$

(cf. [67, Problem 4.2.1]), the induction hypothesis implies that $\det(H_{m+1}) = 1$, whence $H_{m+1} \in SO(2^{m+1})$.
(ii) The first equality in (3.73) instantly follows from the construction of b_1 and f_2 (cf. (3.66)) and (3.68), where the latter is applied to $p = q = 2$. Because of the obvious fact that $\pi_m \circ f_2 = (b_2, \ldots, b_{m+1})^\top$, a remaining and very elementary proof of induction on m immediately leads to the explicit entrywise determination of the sign of H_m in (3.73).
(iii) Due to Proposition 3.26, it is sufficient to verify the base case $m = 1$ only. Since by construction, $H_{m+1}^{\mathbb{C}} = H_1 \otimes H_m + i(H_1 \otimes H_m^{\text{op}}) = H_1 \otimes (H_m + iH_m^{\text{op}})$ for all $m \in \mathbb{N}$, we just have to prove the claims for H_1 and H_1^{op}. The complex case follows then immediately. To this end, consider the (real) Hilbert space $\mathbb{R}_2^2$. Put $u := (u_1, u_2)$ and $v := (v_1, v_2)$, where

$$u_1 := \begin{pmatrix} 0 \\ 1 \end{pmatrix}, u_2 := \begin{pmatrix} 1 \\ 0 \end{pmatrix}, v_1 := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \text{ and } v_2 := \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix}.$$

Then $(u, v) \in (\mathbb{S}^1)^2 \times (\mathbb{S}^1)^2$, and

$$H_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \Gamma_{\mathbb{R}_2^2}(u, v).$$

Thus, $H_1 \in \mathcal{Q}_{2,2}(\mathbb{R})$ (due to (3.50)). Since obviously, $R_2(i) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ is an isometry from l_∞^2 to l_∞^2, it follows that $\|H_1^{\text{op}}\|_{\mathcal{L}_2} = \|R_2(i) H_1\|_{\mathcal{L}_2} \leq \|H_1\|_{\mathcal{L}_2} \leq 1$ (due to (3.50)). Consequently, a further application of (3.50) implies that $H_1^{\text{op}} \in \mathcal{Q}_{2,2}(\mathbb{R})$. Finally, since for any $\xi \in \mathbb{C}^2$, $\|(\overline{p}\, q^\top)\xi\|_1 = |\overline{q}^* \xi| \, \|p\|_1 = 2|\overline{q}^* \xi|$, and since $(l_\infty^2)' \cong l_1^2$, it follows that $\|H_1^{\mathbb{C}}\|_{\infty,1} = \|p\|_1 \, \|q\|_1 = 4$.
(iv) Firstly, let $m = 1$ (the base case). Let $p = (x_1, x_2)^\top \in \{-1, 1\}^2$ and $q = (y_1, y_2)^\top \in \{-1, 1\}^2$ be arbitrarily given. Then

$$\left|\text{tr}((A_1^{\text{Had}})^\top pq^\top)\right| = \left|\text{tr}(A_1^{\text{Had}} pq^\top)\right| = \left|q^\top A_1^{\text{Had}} p\right| = \tfrac{1}{2} \left|(x_2 y_1 - x_2 y_2) + (x_1 y_1 + x_1 y_2)\right|.$$

Since $\max\{|x_1|, |x_2|, |y_1|, |y_2|\} \leq 1$, the triangle inequality clearly implies that

$$\left|(x_2 y_1 - x_2 y_2) + (x_1 y_1 + x_1 y_2)\right| \leq |y_1 - y_2| + |y_1 - (-y_2)|.$$

However, since $-1 \leq y_2$, it further follows that $y_1(1 + y_2) \leq |y_1(1 + y_2)| \leq 1 + y_2$, whence $y_1 - y_2 \leq 1 - y_1 y_2 = 1 - y_2 y_1$. Consequently, we obtain that $|y_1 - y_2| \leq 1 - y_1 y_2$. Similarly, since also $-1 \leq -y_2$, it follows that $|y_1 - (-y_2)| \leq 1 - y_1(-y_2) = 1 + y_1 y_2$. Hence,

$$\left|\text{tr}((A_1^{\text{Had}})^\top pq^\top)\right| \leq \tfrac{1}{2}(1 - y_1 y_2 + 1 + y_1 y_2) = 1.$$

On the other hand, an easy calculation shows that

$$\operatorname{tr}((A_1^{\text{Had}})^\top \widetilde{p}\widetilde{q}^\top) = \widetilde{q}^\top A_1^{\text{Had}} \widetilde{p} = 1 \leq \|A_1^{\text{Had}}\|_{\infty,1},$$

where $\widetilde{p} := (1,-1)^\top$ and $\widetilde{q} := (1,1)^\top$, which finishes the proof of the base case $m = 1$ as well as of (3.76). So let us now assume that (3.75) is satisfied for a fixed $m \in \mathbb{N}$ (induction hypothesis). Firstly, we consider the upper bound. Let $p = \operatorname{vec}(p_1, p_2) \in \{-1,1\}^{2^{m+1}} \equiv \{-1,1\}^{2^m} \times \{-1,1\}^{2^m}$ and $q = \operatorname{vec}(q_1, q_2) \in \{-1,1\}^{2^{m+1}} \equiv \{-1,1\}^{2^m} \times \{-1,1\}^{2^m}$. Since

$$A_{m+1}^{\text{Had}} = \tfrac{1}{2}(A_1^{\text{Had}} \otimes A_m^{\text{Had}}) = \tfrac{1}{4}\begin{pmatrix} A_m^{\text{Had}} & A_m^{\text{Had}} \\ A_m^{\text{Had}} & -A_m^{\text{Had}} \end{pmatrix},$$

it follows that

$$|\operatorname{tr}(A_{m+1}^{\text{Had}} pq^\top)| = \tfrac{1}{4}\Big|\operatorname{tr}\Big(A_m^{\text{Had}} p_1 q_1^\top + A_m^{\text{Had}} p_2 q_1^\top + A_m^{\text{Had}} p_1 q_2^\top - A_m^{\text{Had}} p_2 q_2^\top\Big)\Big| \leq \|A_m^{\text{Had}}\|_{\infty,1}.$$

The induction hypothesis therefore implies that $\|A_{m+1}^{\text{Had}}\|_{\infty,1} \leq \|A_m^{\text{Had}}\|_{\infty,1} \leq 1$, and hence $\|H_{m+1}\|_{\infty,1} \leq 2\sqrt{2}\,\|H_m\|_{\infty,1} \leq (\sqrt{2})^{3(m+1)-2}$. Now, let us turn to the lower bound. To this end, let $s, r \in \{-1,1\}^{2^m}$ be arbitrarily chosen. Consider $\widetilde{s} := \operatorname{vec}(s,s) \in \{-1,1\}^{2^{m+1}}$ and $\widetilde{r} := \operatorname{vec}(r,r) \in \{-1,1\}^{2^{m+1}}$. Then

$$\Big|\operatorname{tr}(A_{m+1}^{\text{Had}} \widetilde{s}\,\widetilde{r}^\top)\Big| = \frac{1}{4}\Big|\operatorname{tr}(A_m^{\text{Had}} sr^\top + 2\,A_m^{\text{Had}} sr^\top - A_m^{\text{Had}} sr^\top)\Big| = \frac{1}{2}\Big|\operatorname{tr}(A_m^{\text{Had}} sr^\top)\Big|\,.$$

Consequently, it follows that

$$\tfrac{1}{2}\|A_m^{\text{Had}}\|_{\infty,1} \leq \|A_{m+1}^{\text{Had}}\|_{\infty,1},$$

whence $\|H_m\|_{\infty,1} \leq \sqrt{2}\,\|H_m\|_{\infty,1} \leq \|H_{m+1}\|_{\infty,1}$. The induction hypothesis therefore implies that $(\sqrt{2})^{m+1} \leq \|H_{m+1}\|_{\infty,1}$, and it follows that the estimates (3.74) and (3.75) are valid. ☐

Remark 3.28. After some "skillful searching", a then simple calculation shows that also

$$\|A_2^{\text{Had}}\|_{\infty,1} = 1\,.$$

If we namely consider the vectors $\widetilde{p} := (1,1,-1,1)^\top \in \{-1,1\}^4$ and $\widetilde{q} := (1,-1,1,1)^\top \in \{-1,1\}^4$, it follows that

$$\operatorname{tr}(A_2^{\text{Had}} \widetilde{p}\widetilde{q}^\top) = \langle A_2^{\text{Had}} \widetilde{p}, \widetilde{q}\rangle_{\mathbb{R}_2^4} = \frac{1}{8}\left\langle \begin{pmatrix} 2 \\ -2 \\ 2 \\ 2 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \\ 1 \\ 1 \end{pmatrix} \right\rangle = 1\,.$$

In particular,

$$\Big|(A_m^{\text{Had}}\,\widetilde{p})_i\Big| = \frac{1}{2^m} \text{ for all } i \in [2^m] \tag{3.77}$$

(since $m = 2$). This naturally leads to the (open) question, whether $\|A_m^{\text{Had}}\|_{\infty,1} = 1$ for all $m \in \mathbb{N}$ and whether (3.77) holds for all $m \in \mathbb{N}$. It seems that we cannot make use of induction on $m \in \mathbb{N}$ here. In fact, if $\nu \neq 2$ and $\|p\|_{l_\infty^{2^\nu}} \leq 1$, then $\Big|(A_\nu^{\text{Had}}\,p)_{i_0}\Big| \neq \frac{1}{2^\nu}$ for some

$i_0 \in [2^\nu]$! The case $\nu = 1$ follows from the fact that for any $a, b \in [-1,1]$, $|a+b| = 1 = |a-b|$ if and only if $\begin{pmatrix} a \\ b \end{pmatrix} \in \left\{ \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} -1 \\ 0 \end{pmatrix} \right\}$. In order to verify the claim for $\nu > 2$, assume by contradiction that there exist $m \in \mathbb{N}_3$ and $\widetilde{p} \in B_{l_\infty^{2^m}}$, such that $\frac{1}{2^m} = \left|(A_m^{\text{Had}}\,\widetilde{p})_i\right| = \frac{1}{(\sqrt{2})^{3m-2}}\,|(H_m\,\widetilde{p})_i| = \frac{1}{2^{2m-1}}\left|\sum_{j=1}^{2^m}(-1)^{N_m(i,j)}\widetilde{p}_j\right|$ for all $i \in [2^m]$. Put $\widetilde{q} := 2^m A_m^{\text{Had}}\widetilde{p}$. Then $\widetilde{q} \in \{-1,1\}^{2^m}$ (due to the assumption) and

$$\begin{aligned} 1 &= 2^m\,\|A_m^{\text{Had}}\widetilde{p}\|^2_{l_2^{2^m}} = \langle A_m^{\text{Had}}\widetilde{p}, \widetilde{q}\rangle_{\mathbb{R}_2^{2^m}} = 2^m\,\langle \widetilde{p}, (A_m^{\text{Had}})^2\,\widetilde{p}\rangle_{\mathbb{R}_2^{2^m}} \\ &= \frac{2^m}{2^{3m-2}}\,\|\widetilde{p}\|^2_{l_2^{2^m}} \leq \frac{1}{2^{3m-2}}\,2^{2m} = \frac{1}{2^{m-2}}\,. \end{aligned}$$

On the other hand, $\frac{1}{2^{m-2}} \leq \frac{1}{2} < 1$ (since $m \geq 3$ by assumption), which is absurd. Observe that in any case $\left|(A_m^{\text{Had}}\,x)_i\right| \leq \frac{2^m}{2^{2m-1}} = \frac{2}{2^m}$ for all $i \in [2^m]$ and $x \in B_{l_\infty^{2^m}}$. Consequently,

$$\left\|A_m^{\text{Had}}\,\frac{p}{2}\right\|_{l_\infty^{2^m}} < \frac{1}{2^m}$$

for all $m \in \mathbb{N}_3$ and $p \in B_{l_\infty^{2^m}}$. Our conjecture is that there exists $\widetilde{m} \in \mathbb{N}_3$ such that $\|A_{\widetilde{m}}^{\text{Had}}\|_{\infty,1} < 1$.

To be more explicit, note e.g. that

$$H_2 = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}, \quad H_2^{\text{op}} = \frac{1}{2}\begin{pmatrix} -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & -1 \\ 1 & 1 & -1 & -1 \end{pmatrix}$$

and

$$H_3 = \frac{1}{(\sqrt{2})^3}\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{pmatrix}.$$

To see how smoothly and quickly (3.73) can be applied to H_3, let us perform a calculation for the two matrix entries $(H_3)_{6,4}$ and $(H_3)_{7,3}$ as an example. There are two ways to perform the calculation process. Either we go through each step of the recursion relation, or we count, step by step, how often the products $b_i(\nu)b_i(\mu)$ are equal to 1. So, either we proceed with

$$(H_3)_{6,4} = -\frac{1}{\sqrt{2}}\,(H_2)_{3,2} = -\frac{1}{\sqrt{2^2}}\,(H_1)_{2,1} = \frac{1}{\sqrt{2^3}}(-1)$$

and

$$(H_3)_{7,3} = \frac{1}{\sqrt{2}}\,(H_2)_{4,2} = -\frac{1}{\sqrt{2^2}}\,(H_1)_{2,1} = \frac{1}{\sqrt{2^3}}(-1)\,,$$

or we count: $N_3(6,4) = 1$ (since $b_1(6)b_1(4) = 1, b_2(6)b_2(4) = b_1(3)b_1(2) = 0$ and $b_3(6)b_3(4) = b_2(3)b_2(2) = b_1(2)b_1(1) = 0$). Similarly, we obtain that $N_3(7,3) = 1$. However, since $\frac{1}{\sqrt{2^3}}(-1) = (H_3)_{7,3} \neq \frac{1}{\sqrt{2^3}} = \frac{1}{\sqrt{2^3}}(-1)^{(7-1)(3-1)}$, [107, Exercise 2.33, (2.55)] seems to be wrong.

Remark 3.29 (CHSH inequalities). As we have seen (just by making use of elementary calculus on the real line), the following inequality holds

$$|x_1y_1 + x_1y_2 + x_2y_1 - x_2y_2| \leq 2 \text{ for all } (x_1, x_2, y_1, y_2) \in [-1, 1]^4, \tag{3.78}$$

which is equivalent to $A_1^{\mathrm{Had}} = \frac{1}{\sqrt{2}} H_1 \in B_{\mathcal{L}(l_\infty^2, l_1^2)}$. Even $A_1^{\mathrm{Had}} \in S_{\mathcal{L}(l_\infty^2, l_1^2)}$ holds (cf. (3.76)). We also know that $\|A_1^{\mathrm{Had}}\|_{\infty,1} \leq 1$ is equivalent to

$$|\mathrm{tr}(A_1^{\mathrm{Had}} B)| \leq 1 \textit{ for all } B \in B_{\mathcal{N}(l_1^2, l_\infty^2)}$$

(cf. (3.52)). On the other hand,

$$\sqrt{2} = \frac{1}{\sqrt{2}} |\mathrm{tr}(I_2)| = \frac{1}{\sqrt{2}} |\mathrm{tr}(H_1^2)| = |\mathrm{tr}(A_1^{\mathrm{Had}} \widetilde{S})| > 1 \text{ for some } \widetilde{S} \in \mathcal{Q}_{2,2} = B_{\mathcal{L}_2(l_1^2, l_\infty^2)}$$

(namely, $\widetilde{S} := H_1$), implying again that $B_{\mathcal{N}(l_1^2, l_\infty^2)}$ is strictly contained in $B_{\mathcal{L}_2(l_1^2, l_\infty^2)}$. Particularly, physicists, who are working in the foundations and philosophy of quantum mechanics recognise that (3.78) – which are just inequalities between certain real numbers – *instantly imply* the famous CHSH inequalities. CHSH stands for John Clauser, Michael Horne, Abner Shimony, and Richard Holt, who introduced the inequalities (between expectation values) in [27] (cf. `https://www.nobelprize.org/prizes/physics/2022/clauser/facts/`) and used them as a means of proving Bell's theorem. In the 2-dimensional case (i.e., if $m = n = 2$) the CHSH inequalities coincide with the so-called "Bell inequalities", assigned to the matrix A_1^{Had}. Somewhat vaguely, it is said that the matrix $\widetilde{S} = H_1 \in \mathcal{Q}_{2,2}(\mathbb{R})$ "violates the Bell inequalities". That "violation" implies that certain consequences of spatial entanglement in quantum mechanics can not be reproduced by classical probability theory in the sense of A. Kolmogorov (i.e., it cannot be reduced to "local hidden-variable theories").

Remark 3.30 (An application of H_m in evolutionary biology). The Walsh-Hadamard transform can even be found in evolutionary biology, specifically in relation to the challenge of reconstructing evolutionary trees from events several million years in the past. (cf. [65])! In order to recognise this, we consider the orthogonal matrix $I_1^{(-)} := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \in O(2)$. A straightforward proof by induction shows that the matrix family $\{H^{(m)} : m \in \mathbb{N}\} = \{(1)\} \cup \{H^{(m)} : m \in \mathbb{N}_2\}$, consisting of invertible matrices $H^{(m)} \in \mathbb{M}_{2^{m-1}}(\mathbb{R})$, introduced in [65], in fact can be represented as

$$H^{(1)} := (1)$$

and

$$H^{(m)} := \begin{pmatrix} H^{(m-1)} & -H^{(m-1)} \\ H^{(m-1)} & H^{(m-1)} \end{pmatrix} = H^{(2)} \otimes H^{(m-1)} = \bigotimes_{i=1}^{m-1} H^{(2)} = \sqrt{2^{m-1}}\, H_{m-1}\, I_{m-1}^{(-)}$$

if $m \in \mathbb{N}_2$, where $I_l^{(-)} := I_1^{(-)} \otimes I_{l-1}^{(-)} = \bigotimes_{i=1}^{l} I_1^{(-)} \in O(2^l)$ for all $l \in \mathbb{N}_2$.

It is quite instructive to compare (3.65) to (6.182) (real case), (7.228) (complex case) and the following

Proposition 3.31. *Suppose there exist $c \in (1, \infty)$, a sequence $(r_\nu)_{\nu\in\mathbb{N}} \in B_{l_1(\mathbb{F})}$, a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and sequences $(P_{1,\nu})_{\nu\in\mathbb{N}}, \ldots, (P_{m,\nu})_{\nu\in\mathbb{N}}$, $(Q_{1,\nu})_{\nu\in\mathbb{N}}, \ldots, (Q_{n,\nu})_{\nu\in\mathbb{N}}$ of random variables which map into $S_\mathbb{F}$ $\mathbb{P}$-a.s., such that for all $m, n \in \mathbb{N}$, for all $\mathbb{F}$-Hilbert spaces H, for all $(u, v) \in S_H^m \times S_H^n$, and for all $(i, j) \in [m] \times [n]$ the following equality holds:*

$$\langle v_j, u_i \rangle_H = \Gamma_H(u, v)_{ij} = c \sum_{\nu=1}^{\infty} r_\nu \, \mathbb{E}_\mathbb{P}[\overline{P_{i,\nu}} Q_{j,\nu}].$$

Then

$$K_G^\mathbb{F} \leq c\,.$$

Proof.

$$\begin{aligned}|\mathrm{tr}(A^*\Gamma_H(u,v))| &= c\Big|\sum_{\nu=1}^{\infty} r_\nu \Big(\sum_{i=1}^{m}\sum_{j=1}^{n} \overline{a_{ij}}\, \mathbb{E}_\mathbb{P}[\overline{P_{i,\nu}} Q_{j,\nu}]\Big)\Big| \leq c \sum_{\nu=1}^{\infty} |r_\nu| \,\Big|\sum_{i=1}^{m}\sum_{j=1}^{n} \overline{a_{ij}}\, \mathbb{E}_\mathbb{P}[\overline{P_{i,\nu}} Q_{j,\nu}]\Big| \\ &\leq c \sum_{\nu=1}^{\infty} |r_\nu|\, \mathbb{E}_\mathbb{P}\Big[\Big|\sum_{i=1}^{m}\sum_{j=1}^{n} \overline{a_{ij}}\, \overline{P_{i,\nu}} Q_{j,\nu}\Big|\Big] = c \sum_{\nu=1}^{\infty} |r_\nu|\, \mathbb{E}_\mathbb{P}|\mathrm{tr}(A^*\Gamma_\mathbb{F}(\mathbf{P}_\nu, \mathbf{Q}_\nu))|\,,\end{aligned}$$

where the components of the random vectors $\mathbf{P}_\nu : \Omega \longrightarrow \mathbb{F} \cap \overline{\mathbb{D}}^m$ and $\mathbf{Q}_\nu : \Omega \longrightarrow \mathbb{F} \cap \overline{\mathbb{D}}^n$ are defined as $(\mathbf{P}_\nu)_i := P_{i,\nu}$ and $(\mathbf{Q}_\nu)_j := Q_{j,\nu}$. Since $|\mathrm{tr}(A^*\Gamma_\mathbb{F}(\mathbf{P}_\nu(\omega), \mathbf{Q}_\nu(\omega)))| \leq \|A\|_{\infty,1}$ for almost all $\omega \in \Omega$, it therefore follows that

$$|\mathrm{tr}(A^*\Gamma_H(u,v))| \leq c \sum_{\nu=1}^{\infty} |r_\nu| \|A\|_{\infty,1} \leq c\|A\|_{\infty,1}$$

(since $\sum_{\nu=1}^{\infty} |r_\nu| \leq 1$, by assumption). □

Of particular interest is the value of $K_G^\mathbb{R}(2)$. A *lower* bound is rather easy to detect: $\sqrt{2} \leq K_G^\mathbb{R}(2)$, implying the important fact that $K_G^\mathbb{R} > 1$. We just have to work with the Walsh-Hadamard transform $H_1 = \Gamma_{\mathbb{R}_2^2}(u_1, u_2, v_1, v_2) \in \mathcal{Q}_{2,2}(\mathbb{R}) \cap O(2)$ (cf. Example 3.27). To this end, consider again the symmetric matrix $A_1^{\mathrm{Had}} = \frac{1}{\sqrt{2}} H_1$. Recall that $\|A_1^{\mathrm{Had}}\|_{\infty,1} = 1$ (due to (3.76)), and note that $\mathrm{tr}(A_1^{\mathrm{Had}} H_1) = \frac{1}{\sqrt{2}}\mathrm{tr}(H_1^2) = \frac{1}{\sqrt{2}}\mathrm{tr}(I_2) = \sqrt{2}$. Consequently, it follows that

$$\sqrt{2} = |\mathrm{tr}((A_1^{\mathrm{Had}})^\top H_1)| \leq K_G^\mathbb{R}(2,2;2) \leq \min\{K_G^\mathbb{R}(2,2), K_G^\mathbb{R}(2)\} \leq K_G^\mathbb{R}.$$

Much less trivial is the proof of the reverse direction, performed by Krivine in [90, 91]. Within the scope of Proposition 3.18 he namely represented - in the real 2-dimensional case - any $\Gamma_{\mathbb{R}_2^2}(u, v) \in \mathcal{Q}_{2,2}(\mathbb{R})$ as matrix $\sum_{\nu=1}^{\infty} b_\nu T_\nu : l_1^n \longrightarrow l_\infty^m$ such that $\|\Gamma_{\mathbb{R}_2^2}(u, v)\|_\mathcal{N} = \|\sum_{\nu=1}^{\infty} b_\nu T_\nu\|_\mathcal{N} \leq \sqrt{2}$ (which he called "norme de la fonction $\cos(x - y)$ dans le produit tensoriel projectif $C[-\pi, \pi] \widehat{\otimes} C[-\pi, \pi]$" in [90]). Actually, the main building block in his proof is an intricate sophisticated representation of the function $\mathbb{R} \times \mathbb{R} \ni (x, y) \mapsto \cos(x - y)$ by convolution (cf. Theorem 3.32). However, that representation allows us to provide a short, straightforward proof of Corollary 3.33 - without the use of any tensor product structure.

Theorem 3.32 (**Krivine, 1977**). *Consider the probability space $([-\pi, \pi], \mathcal{B}([-\pi, \pi]), \mu)$, where $\mu := \frac{1}{2\pi}\lambda_1\big|_{\mathcal{B}([-\pi,\pi])}$. Then there exist two functions $p, q : \mathbb{R} \longrightarrow [-1, 1]$ and a sequence*

$(r_n)_{n\in\mathbb{N}}$ *of real numbers such that* $\sum_{n=1}^\infty |r_n| = 1$ *and*

$$\cos(x-y) = \sqrt{2}\sum_{n=1}^\infty r_n \mathbb{E}_\mu[p(nx-S)q(ny-S)]$$
$$= \frac{\sqrt{2}}{2\pi}\sum_{n=1}^\infty r_n \int_{[-\pi,\pi]} p(nx-\omega)q(ny-\omega)\lambda_1(\mathrm{d}\omega)$$

for all $x, y \in \mathbb{R}$, *where* $\mathbb{R} \ni t \mapsto q(t) := \mathit{sign}(\cos(t))$ *and* $[-\pi,\pi] \ni \omega \mapsto S(\omega) := \omega$.

Corollary 3.33 (**Krivine, 1977**).

$$K_G^{\mathbb{R}}(2) = \sqrt{2}\,.$$

Proof. Consider the 2-dimensional standard Euclidean vector space $H := \mathbb{R}_2^2$. Let $u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \in S_H = \mathbb{S}^1$ and $v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \in S_H = \mathbb{S}^1$. Since

$$\langle u, v\rangle_H = \Big\langle \begin{pmatrix} \cos(x) \\ \sin(x) \end{pmatrix}, \begin{pmatrix} \cos(y) \\ \sin(y) \end{pmatrix} \Big\rangle_H = \cos(x-y)\,,$$

for some $x, y \in \mathbb{R}$, Theorem 3.32 unveils as a special case of Proposition 3.31, and the claim follows. ☐

Proposition 3.18, together with Corollary 3.33 help us to find a "fitting" relation between $K_G^{\mathbb{R}}(2d)$ and $K_G^{\mathbb{C}}(d)$. To this end, we firstly supplement and prove once again (for the sake of completeness) [45, Corollary 2.14., (38)].

Proposition 3.34. *Let* $d, m, n \in \mathbb{N}$, $A \in \mathbb{M}_{m,n}(\mathbb{R})$ *and* $B \in \mathbb{M}_{m,n}(\mathbb{C})$. *Then*

$$\|A\|^G_{\mathbb{R}_2^d} \le \|A\|^G_{\mathbb{C}_2^d} = \|A\|^G_{\mathbb{R}_2^{2d}} \le K_G^{\mathbb{R}}(m,n;2d)\,\|A\|^{\mathbb{R}}_{\infty,1}\,. \tag{3.79}$$

In particular,

$$\|A\|^{\mathbb{R}}_{\infty,1} \le \|A\|^{\mathbb{C}}_{\infty,1} = \|A\|^G_{\mathbb{R}_2^2} \le \sqrt{2}\,\|A\|^{\mathbb{R}}_{\infty,1} \tag{3.80}$$

and

$$\|\operatorname{Re}(B)\|^G_{\mathbb{C}_2^d} \le \|B\|^G_{\mathbb{C}_2^d} \text{ and } \|\operatorname{Im}(B)\|^G_{\mathbb{C}_2^d} \le \|B\|^G_{\mathbb{C}_2^d}\,. \tag{3.81}$$

Moreover,

$$\|A_1^{Had}\|^{\mathbb{R}}_{\infty,1} = 1 < \sqrt{2} = \|A_1^{Had}\|^{\mathbb{C}}_{\infty,1}\,.$$

Proof. Since

$$xy = \Big(\frac{1-i}{\sqrt{2}}\Big)x\Big(\frac{1+i}{\sqrt{2}}\Big)y \text{ for all } x, y \in \mathbb{R}\,,$$

it follows that for any $(u,v) \in S^m_{\mathbb{R}_2^d} \times S^n_{\mathbb{R}_2^d}$, $\Gamma_{\mathbb{R}_2^d}(u,v) = \Gamma_{\mathbb{C}_2^d}(z,w)$ for some $(z,w) \in S^m_{\mathbb{C}_2^d} \times S^n_{\mathbb{C}_2^d}$. Thus, $\|A\|^{\mathrm{G}}_{\mathbb{R}_2^d} \le \|A\|^{\mathrm{G}}_{\mathbb{C}_2^d}$. In particular, if $d = 1$, it follows that $\|A\|^{\mathbb{R}}_{\infty,1} \le \|A\|^{\mathbb{C}}_{\infty,1}$. Since any $z \in \mathbb{C}$ satisfies $|z| = \operatorname{Re}(\alpha\, z)$, for some $\alpha \in \mathbb{T}$, we may assume that $\|A\|^{\mathrm{G}}_{\mathbb{C}_2^d} = \operatorname{Re}(\operatorname{tr}(A^\top \Gamma_{\mathbb{C}_2^d}(z,w)))$, for some $(z,w) \in S^m_{\mathbb{C}^d_2} \times S^n_{\mathbb{C}^d_2}$. Since A has real entries by assumption, it follows that $\|A\|^{\mathrm{G}}_{\mathbb{C}^d_2} = \mathrm{tr}(A^\top \mathrm{Re}(\Gamma_{\mathbb{C}^d_2}(z,w)))$. Corollary 3.14 therefore implies that

$$\|A\|^{\mathrm{G}}_{\mathbb{C}^d_2} = \mathrm{tr}(A^\top \Gamma_{\mathbb{R}^{2d}_2}(u,v)) \leq \|A\|^{\mathrm{G}}_{\mathbb{R}^{2d}_2} \leq K^{\mathbb{R}}_G(m,n;2d)\, \|A\|^{\mathbb{R}}_{\infty,1}$$

for some $(u,v) \in (\mathbb{S}^{2d-1})^m \times (\mathbb{S}^{2d-1})^n$. In particular,

$$\|A\|^{\mathbb{C}}_{\infty,1} \leq \|A\|^{\mathrm{G}}_{\mathbb{R}^2_2} \leq K^{\mathbb{R}}_G(2)\, \|A\|^{\mathbb{R}}_{\infty,1}\,.$$

Thus, we may apply Krivine's remarkable result (cf. Corollary 3.33), and it follows that

$$\|A\|^{\mathbb{C}}_{\infty,1} \leq \|A\|^{\mathrm{G}}_{\mathbb{R}^2_2} \leq \sqrt{2}\|A\|^{\mathbb{R}}_{\infty,1}\,.$$

On the other hand, Corollary 3.14 clearly implies also that $\|A\|^{\mathrm{G}}_{\mathbb{R}^{2d}_2} = \mathrm{Re}(\mathrm{tr}(A^\top \widetilde{S}))$ for some $\widetilde{S} = \Gamma_{\mathbb{C}^d_2}(z,w) \in \mathcal{Q}_{m,n}(\mathbb{C})$, whence $\|A\|^{\mathrm{G}}_{\mathbb{R}^{2d}_2} \leq \|A\|^{\mathrm{G}}_{\mathbb{C}^d_2}$. In order to verify the complex case (3.81), we must only note that $\|B\|^{\mathrm{G}}_{\mathbb{C}^d_2} = \|\overline{B}\|^{\mathrm{G}}_{\mathbb{C}^d_2}$, implying that

$$\|\mathrm{Re}(B)\|^{\mathrm{G}}_{\mathbb{C}^d_2} \leq \frac{1}{2}(\|B\|^{\mathrm{G}}_{\mathbb{C}^d_2} + \|\overline{B}\|^{\mathrm{G}}_{\mathbb{C}^d_2}) = \|B\|^{\mathrm{G}}_{\mathbb{C}^d_2}$$

(since $|\mathrm{tr}(B^*\Gamma_{\mathbb{C}^d_2}(z,w))| = |\mathrm{tr}((B^*)^\top \Gamma_{\mathbb{C}^d_2}(\overline{w},\overline{z}))|$ for all $(z,w) \in (\mathbb{C}^d)^m \times (\mathbb{C}^d)^n$ - cf. also with (3.35)).
Finally, put $\zeta_0 := (z_0,w_0)^\top := (\frac{1}{\sqrt{2}}(1+i), \frac{1}{\sqrt{2}}(1-i))^\top$. Then $\zeta_0 \in \mathbb{T}^2 \subseteq S_{\mathbb{C}^2_\infty}$, and a further application of the Walsh-Hadamard transform A^{Had}_1 therefore leads to

$$\|A^{\mathrm{Had}}_1\|^{\mathbb{R}}_{\infty,1} \overset{(3.76)}{=} 1 < \sqrt{2} = \frac{1}{2}(|z_0+w_0|+|z_0-w_0|) = \|A^{\mathrm{Had}}_1\,\zeta_0\|_{\mathbb{C}^2_1} \leq \|A^{\mathrm{Had}}_1\|^{\mathbb{C}}_{\infty,1} \leq \sqrt{2}\,\|A^{\mathrm{Had}}_1\|^{\mathbb{R}}_{\infty,1} = \sqrt{2}\,.$$

□

Since

$$\|A\|^{\mathrm{G}}_{\mathbb{R}^{2d}_2} \overset{(3.79)}{=} \|A\|^{\mathrm{G}}_{\mathbb{C}^d_2} \leq K^{\mathbb{C}}_G(d)\, \|A\|^{\mathbb{C}}_{\infty,1} \overset{(3.80)}{\leq} \sqrt{2}\, K^{\mathbb{C}}_G(d)\, \|A\|^{\mathbb{R}}_{\infty,1}$$

for all $m,n \in \mathbb{N}$ and $A \in \mathbb{M}_{m,n}(\mathbb{R})$ and

$$\begin{aligned}\|B\|^{\mathrm{G}}_{\mathbb{C}^d_2} &= \|\mathrm{Re}(B) + i\,\mathrm{Im}(B)\|^{\mathrm{G}}_{\mathbb{C}^d_2} \leq \|\mathrm{Re}(B)\|^{\mathrm{G}}_{\mathbb{C}^d_2} + \|\mathrm{Im}(B)\|^{\mathrm{G}}_{\mathbb{C}^d_2} \\ &\overset{(3.79)}{\leq} K^{\mathbb{R}}_G(2d)(\|\mathrm{Re}(B)\|^{\mathbb{R}}_{\infty,1} + \|\mathrm{Im}(B)\|^{\mathbb{R}}_{\infty,1}) \overset{(3.81)}{\leq} 2\, K^{\mathbb{R}}_G(2d)\, \|B\|^{\mathbb{C}}_{\infty,1}\end{aligned}$$

for all $m,n \in \mathbb{N}$ and $B \in \mathbb{M}_{m,n}(\mathbb{C})$, we obtain

Corollary 3.35.

$$\tfrac{1}{\sqrt{2}}\, K^{\mathbb{R}}_G(2d) \leq K^{\mathbb{C}}_G(d) \leq 2\, K^{\mathbb{R}}_G(2d) \text{ for all } d \in \mathbb{N}.$$

In particular,

$$\tfrac{1}{\sqrt{2}} K^{\mathbb{R}}_G \leq K^{\mathbb{C}}_G \leq 2\, K^{\mathbb{R}}_G\,. \tag{3.82}$$

Note that the implication (3.82) contains [77, Theorem 10.6]. We do not know whether the second estimation could be improved to $K^{\mathbb{C}}_G(d) \overset{?}{\leq} \sqrt{2}\, K^{\mathbb{R}}_G(2d)$ for all $d \in \mathbb{N}$. In particular, since $\mathrm{Re}(B)$ and $\mathrm{Im}(B)$ do not commute, we do not know whether $(\|\mathrm{Re}(B)+i\,\mathrm{Im}(B)\|^{\mathrm{G}}_{\mathbb{C}^d_2})^2 \overset{?}{\leq} (\|\mathrm{Re}(B)\|^{\mathrm{G}}_{\mathbb{C}^d_2})^2 + (\|\mathrm{Im}(B)\|^{\mathrm{G}}_{\mathbb{C}^d_2})^2$ holds for all $m,n \in \mathbb{N}$ and $B \in \mathbb{M}_{m,n}(\mathbb{C})$ (in analogy to $|x+iy|^2 = x^2 + y^2$ for all $x,y \in \mathbb{R}$).

3.5. The Gaussian inner product splitting property

Next, we are going to disclose a crucial *joint* multivariate Gaussian "splitting property" of inner products of vectors on the unit sphere of an arbitrary *separable* $\mathbb{F}$-Hilbert space. That result (which should be compared to the construction of Gaussian Hilbert spaces or Moore's theorem on the characterisation of kernel functions (cf. [115, Theorem 2.14])) runs like a thread through the entire paper, including its implementation in Theorem 6.5 and Theorem 7.12. It holds for both fields, $\mathbb{F} = \mathbb{R}$ and $\mathbb{F} = \mathbb{C}$, and plays a significant role, when we are looking for a specific Gaussian random structure in quantum correlation matrices. So, let $k, m, n \in \mathbb{N}$. Fix $S = \Gamma_H(u, v) = (u_i^* v_j)_{ij} \in Q_{m,n}(\mathbb{F})$, where $(u, v) \in S_H^m \times S_H^n$ and $(i, j) \in [m] \times [n]$. Based on our analysis so far, if $\zeta_{ij} := u_i^* v_j = \langle v_j, u_i \rangle_H$ is given, then we only know about the existence of a joint Gaussian random vector $\text{vec}(\mathbf{Z}_{ij}, \mathbf{W}_{ij}) \sim \mathbb{F}N_{2k}(0, \Sigma_{2k}(\zeta_{ij}))$. A priori, we cannot say whether it is even possible to allocate to $\zeta_{ij} = u_i^* v_j$ a joint Gaussian random vector of type $\text{vec}(\mathbf{Z}_i, \mathbf{W}_j) \sim \mathbb{F}N_{2k}(0, \Sigma_{2k}(\zeta_{ij}))$. In fact, our next cornerstone result reveals that such a "joint Gaussian splitting of an inner product" is guaranteed if we assume that H is separable, $u_i \in S_H$ and $v_j \in S_H$. For this, we fix an arbitrary complete probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and construct a suitable random field.

Proposition 3.36 (**Inner product splitting**). *Let $k \in \mathbb{N}$, $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$ and H be a separable $\mathbb{F}$-Hilbert space. There exists a family $\{\boldsymbol{Z}_x : x \in H\}$ of random vectors $\boldsymbol{Z}_x \equiv (Z_x^{(1)}, Z_x^{(2)}, \ldots, Z_x^{(k)})^\top$ in $\mathbb{F}^k$, such that*

$$vec(\boldsymbol{Z}_x, \boldsymbol{Z}_y) \sim \mathbb{F}N_{2k}(0, C_{2k}(x, y)) \text{ for all } x, y \in H, \tag{3.83}$$

where

$$C_{2k}(x, y) := \begin{pmatrix} \|x\|_H^2 \, I_k & \langle x, y \rangle_H \, I_k \\ \langle y, x \rangle_H \, I_k & \|y\|_H^2 \, I_k \end{pmatrix}.$$

In particular,

$$\mathbb{E}[|Z_x^{(\nu)}|^2] = \|x\|_H^2 \text{ and } \langle x, y \rangle_H = \mathbb{E}[Z_x^{(\nu)} \, \overline{Z_y^{(\nu)}}] \text{ for all } \nu \in [k] \text{ and } x, y \in H\,.$$

If $w \in S_H$, then $\boldsymbol{Z}_w \sim \mathbb{F}N_k(0, I_k)$ and

$$vec(\boldsymbol{Z}_u, \boldsymbol{Z}_v) \sim \mathbb{F}N_{2k}(0, \Sigma_{2k}(\langle u, v \rangle_H)) \text{ for all } u, v \in S_H. \tag{3.84}$$

If $e_1, e_2 \in S_H$ are orthogonal, then

$$vec(\boldsymbol{Z}_\zeta, \boldsymbol{Z}_1) \sim \mathbb{F}N_{2k}(0, \Sigma_{2k}(\zeta)) \text{ for all } \zeta \in \overline{\mathbb{D}}, \tag{3.85}$$

where $\boldsymbol{Z}_\zeta := \boldsymbol{Z}_{\zeta e_1 + \sqrt{1-|\zeta|^2} e_2}$ and $\boldsymbol{Z}_1 := \boldsymbol{Z}_{e_1}$. In particular, $vec(\boldsymbol{Z}_{\langle u,v \rangle_H}, \boldsymbol{Z}_1) \overset{d}{=} vec(\boldsymbol{Z}_u, \boldsymbol{Z}_v)$ for all $u, v \in S_H$. $\boldsymbol{Z}_x \in L^2(\Omega)^k$ for all $x \in H$, and $Tx := \boldsymbol{Z}_x$ defines a bounded linear operator $T \in \mathcal{L}(H, L^2(\Omega)^k)$, such that $\frac{1}{\sqrt{k}} T$ is an isometry. For any $\nu \in [k]$, the family $\{Z_x^{(\nu)} : x \in H\}$ is an H-isonormal process.

Proof. Fix $k \in \mathbb{N}$, and let $n \in \mathbb{N}$. Consider the $n \times k$ random matrix

$$\Xi := (\xi_1 \,\vdots\, \xi_2 \,\vdots\, \ldots \,\vdots\, \xi_k) = \begin{pmatrix} \xi_{11} & \xi_{12} & \ldots & \xi_{1k} \\ \xi_{21} & \xi_{22} & \ldots & \xi_{2k} \\ \vdots & \vdots & \vdots & \vdots \\ \xi_{n1} & \xi_{n2} & \ldots & \xi_{nk} \end{pmatrix},$$

where $\xi_\nu = \mathrm{vec}(\xi_{1\nu}, \ldots, \xi_{n\nu}) \sim \mathbb{F}N_n(0, I_n)$ for all $\nu \in [k]$ and the random vectors $\xi_1, \ldots, \xi_k$ are mutually independent, implying that $\xi_{11}, \ldots, \xi_{n1}, \ldots, \xi_{1k}, \ldots, \xi_{nk}$ are i.i.d. and standard normally distributed $\mathbb{F}$-valued random variables (i.e., with probability law $\mathbb{F}N_1(0,1)$). Thus, the family

$$\{\xi_{i\nu} : (i, \nu) \in \mathbb{N} \times [k]\} \tag{3.86}$$

consists of i.i.d. and standard normally distributed $\mathbb{F}$-valued random variables. Since by assumption the Hilbert space H is separable, then H is either isometrically isomorphic to $\mathbb{F}_2^n$ for some $n \in \mathbb{N}$ or isometrically isomorphic to l_2. Firstly, we treat the finite-dimensional case: $H := \mathbb{F}_2^n$. Given an arbitrary vector $x \in H$, put

$$\mathbf{Z}_x := \Xi^* x = (x^\top \overline{\Xi})^\top = (x^\top \overline{\xi_1}, x^\top \overline{\xi_2}, \ldots, x^\top \overline{\xi_k})^\top, \tag{3.87}$$

respectively

$$Z_x^{(\nu)} := x^\top \overline{\xi_\nu} \quad (\nu \in [k]).$$

To prove (3.83) in the finite-dimensional case, fix $x, y \in H$. Let $a \in \mathbb{F}^{2k}$. Then $a = \mathrm{vec}(s,t)$, for some $s, t \in \mathbb{F}^k$, and

$$a^* \mathrm{vec}(\mathbf{Z}_x, \mathbf{Z}_y) = x^\top \overline{\Xi}\, \overline{s} + y^\top \overline{\Xi}\, \overline{t} = \sum_{\nu=1}^{k} \sum_{i=1}^{n} c_{\nu i}\, \overline{\xi_{i\nu}} = \overline{\sum_{\nu=1}^{k} \sum_{i=1}^{n} \overline{c_{\nu i}}\, \xi_{i\nu}} \sim \mathbb{F}N_1\Big(0, \sum_{\nu=1}^{k} \sum_{i=1}^{n} |c_{\nu i}|^2\Big),$$

where $c_{\nu i} := x_i \overline{s_\nu} + y_i \overline{t_\nu}$ (since all random variables $\xi_{i\nu} \sim \mathbb{F}N_1(0,1)$ are mutually independent). A straightforward calculation shows that

$$0 \leq \sum_{\nu=1}^{k} \sum_{i=1}^{n} |c_{\nu i}|^2 = \|x\|^2 \|s\|^2 + 2\,\mathrm{Re}(\langle x, y\rangle \langle t, s\rangle) + \|y\|^2 \|t\|^2 = a^* C_{2k}(x,y) a\,.$$

Consequently, since $a \in \mathbb{F}^{2k}$ was chosen arbitrarily, $C_{2k}(x,y) \in \mathbb{P}_{2k}(\mathbb{F})$ is positive semidefinite, and [5, Theorem 2.8] implies that

$$\mathrm{vec}(\mathbf{Z}_x, \mathbf{Z}_y) \sim \mathbb{F}N_{2k}(0, C_{2k}(x,y))\,.$$

In particular, if $(u,v) \in S_H \times S_H$, then $C_{2k}(u,v) = \Sigma_{2k}(\langle u, v\rangle_H)$, and (3.84) follows at once. Next, we consider the infinite-dimensional case ($H := l_2$). Fix $x, y \in H$, and let $w \in \{x, y\}$. Put $\pi_n(w) := (w_1, w_2, \ldots, w_n)^\top \in \mathbb{F}_2^n =: H_n$. Since $Z_{\pi_n(w)}^{(\nu)} = \sum_{i=1}^n w_i\, \overline{\xi_{i\,\nu}}$ for all $\nu \in [k]$ (see (3.87)) and $\|w\|_H^2 = \sum_{i=1}^\infty |w_i|^2 < \infty$, the assumed independence structure of the Gaussians $\xi_{i\,\nu}$ (cf. (3.86)) implies that for any $\nu \in [k]$ the sequence $(Z_{\pi_n(w)}^{(\nu)})_{n \in \mathbb{N}}$ is a Cauchy sequence in $L^2(\Omega)$. Thus, for any $\nu \in [k]$, the ν'th component of the k-dimensional random vector $\mathbf{Z}_{\pi_n(w)}$ converges in $L^2(\Omega)$ to $\mathbf{Z}_w^{(\nu)} := \sum_{i=1}^\infty w_i\, \overline{\xi_{i\,\nu}} \in L^2(\Omega)$ (cf. also [20, Theorem 1.1.4.] for the real case). It follows that $s^* \mathbf{Z}_x + t^* \mathbf{Z}_y$ is the L^2-limit of the sequence $(s^* \mathbf{Z}_{\pi_n(x)} + t^* \mathbf{Z}_{\pi_n(y)})_{n \in \mathbb{N}}$ for all $s, t \in \mathbb{F}^k$. From the proof of the finite-dimensional case, we know that in $H_n = \mathbb{F}_2^n$

$$s^* \mathbf{Z}_{\pi_n(x)} + t^* \mathbf{Z}_{\pi_n(y)} \sim N_1\Big(0, a^* C_{2k}(\pi_n(x), \pi_n(y)) a\Big),$$

where $a := \mathrm{vec}(s,t)$. Since $\lim_{n \to \infty} \langle \pi_n(x'), \pi_n(y')\rangle_{H_n} = \langle x', y'\rangle_H$ for all $x', y' \in H$, we obtain

$$\lim_{n \to \infty} a^* C_{2k}(\pi_n(x), \pi_n(y)) a = a^* C_{2k}(x,y) a\,.$$

Consequently, since L^2-convergence implies convergence in probability, and hence convergence in distribution (cf. e.g. [72, Proposition E.1.5.]), we conclude that

$$\mathrm{vec}(\mathbf{Z}_x, \mathbf{Z}_y) \sim \mathbb{F}N_{2k}(0, C_{2k}(x, y)).$$

Finally, (3.85) is a particular case of (3.84), where $u := \zeta\, e_1 + \sqrt{1 - |\zeta|^2}\, e_2 \in S_H$ and $v := e_1 \in S_H$. $\square$

Let $\Sigma = (\sigma_{ij})_{(i,j)\in[n]\times[n]} \in C(n;\mathbb{F})$ be an arbitrary correlation matrix. Then $\Sigma = \Gamma_{H_n}(w, w)$ for some $w \equiv (w_1, w_2, \ldots, w_n) \in S^n_{H_n}$, where $H_n := \mathbb{F}^n_2$ (due to Lemma 3.2), implying that $\sigma_{ij} = w_i^* w_j = \langle w_j, w_i\rangle_{H_n}$ for all $i, j \in [n]$. Consequently, (3.84), applied to all pairs $w_i, w_j \in S_H$, immediately results in

Corollary 3.37 (Correlation matrix splitting). *Let $n \in \mathbb{N}$ and $\Sigma = (\sigma_{ij})_{(i,j)\in[n]\times[n]} \in C(n;\mathbb{F})$. Let $k \in \mathbb{N}$. Then there exist n $\mathbb{F}^k$-valued random vectors $\boldsymbol{Z}_1, \boldsymbol{Z}_2, \ldots, \boldsymbol{Z}_n$ such that*

$$vec(\boldsymbol{Z}_i, \boldsymbol{Z}_j) \sim \mathbb{F}N_{2k}(0, \Sigma_{2k}(\sigma_{ij})) \text{ and } \frac{1}{\sqrt{k}}\boldsymbol{Z}_i \in S_{H_k}$$

for all $(i, j) \in [n] \times [n]$, where $H_k := L^2(\Omega)^k$. In particular,

$$\sigma_{ij} = \mathbb{E}[Z_i^{(\nu)}\, \overline{Z_j^{(\nu)}}] = \Big\langle \frac{1}{\sqrt{k}}\boldsymbol{Z}_i, \frac{1}{\sqrt{k}}\boldsymbol{Z}_j \Big\rangle_{H_k} \text{ for all } (i, j) \in [n] \times [n] \text{ and } \nu \in [k].$$

Moreover, for any $\mathbb{F}$-Hilbert space H, for any $u, v \in S_H$, there exist two joint Gaussian random vectors $\boldsymbol{W}_u$ and $\boldsymbol{W}_v$ in $\mathbb{F}^k$, such that $\frac{1}{\sqrt{k}}\boldsymbol{W}_u \in S_{H_k}$, $\frac{1}{\sqrt{k}}\boldsymbol{W}_v \in S_{H_k}$, $W_u^{(\nu)} \in S_{L^2(\Omega)}$, $W_v^{(\nu)} \in S_{L^2(\Omega)}$ and

$$\langle v, u\rangle_H = \mathbb{E}[W_v^{(\nu)}\, \overline{W_u^{(\nu)}}\,] = \Big\langle \frac{1}{\sqrt{k}}\boldsymbol{W}_v, \frac{1}{\sqrt{k}}\boldsymbol{W}_u \Big\rangle_{H_k} \text{ for all } \nu \in [k].$$

4. Powers of inner products of random vectors, uniformly distributed on the sphere

4.1. Gaussian sign-correlation

It seems to be the case that any rigorous proof of the Grothendieck inequality is built on two *equalities*, namely the Grothendieck equality (if $\mathbb{F} = \mathbb{R}$ - cf. e.g. [46, 85], or the proof of [37, Prop. 4.4.2]) and the Haagerup equality (if $\mathbb{F} = \mathbb{C}$ - see [46, 57, 85]). In fact, if we reveal the inherent *bivariate* Gaussian random structure, these equalities emerge as two special cases of the representation of a single Pearson correlation coefficient which applies likewise for the real case and the complex case (Corollary 4.2). Rewritten in terms of real Gaussian random vectors (if $\mathbb{F} = \mathbb{R}$) and complex Gaussian random vectors (if $\mathbb{F} = \mathbb{C}$) namely, we firstly obtain a representation of the two equalities, indicating an already lurking common underlying probabilistic structure for both fields, $\mathbb{R}$ and $\mathbb{C}$ (cf. also (4.100) and (4.101)). To this end, recall (cf., e.g., [6] and [10, Chapter II]) that for any $a, b \in \mathbb{C}$, any $c \in \mathbb{C} \setminus \{-n : n \in \mathbb{N}_0\}$ and any $z \in \mathbb{D}$ the well-defined power series

$${}_2F_1(a, b, c; z) := \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(b+n)}{\Gamma(c+n)} \frac{z^n}{n!} = 1 + \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{n=1}^{\infty} \frac{\Gamma(a+n)\Gamma(b+n)}{\Gamma(c+n)} \frac{z^n}{n!}$$

denotes the *Gaussian hypergeometric function.* If in addition $\mathrm{Re}(c) > \mathrm{Re}(a+b)$ then the series converges absolutely on $\mathbb{T}$ and satisfies ${}_2F_1(a,b,c;1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}$ (Gauss Summation Theorem). Recall that $S_{\mathbb{C}^n} := \{w \in \mathbb{C}^n : \|w\|_{\mathbb{C}_2^n} = 1\} = J_2^{-1}(\mathbb{S}^{2n-1})$ denotes the the unit sphere in $\mathbb{C}^n$ (where $n \in \mathbb{N}$, of course).

The Grothendieck equality. *Let $n \in \mathbb{N}$ and $u, v \in \mathbb{S}^{n-1}$. Let $\boldsymbol{X} \equiv (X_1, \ldots, X_n)^\top \sim N_n(0, I_n)$ be a standard-normally distributed real Gaussian random vector. Then*

$$
\begin{aligned}
\mathbb{E}[sign(u^\top \boldsymbol{X}) sign(v^\top \boldsymbol{X})] &= \frac{2}{\pi} \arcsin(u^\top v) \\
&= \frac{2}{\pi} u^\top v \; {}_2F_1(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{3}{2}; (u^\top v)^2) \\
&= \mathbb{E}[|X_1|]^2 \, u^\top v \; {}_2F_1(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{3}{2}; (u^\top v)^2).
\end{aligned}
\tag{4.88}
$$

The Haagerup equality. *Let $n \in \mathbb{N}$ and $\boldsymbol{Z} \equiv (Z_1, \ldots, Z_n)^\top \sim \mathbb{C}N_n(0, I_n)$ be a standard-normally distributed complex Gaussian random vector. Then*

$$
\begin{aligned}
\mathbb{E}[sign(u^* \boldsymbol{Z}) sign(\overline{v^* \boldsymbol{Z}})] &= \frac{\pi}{4} sign(u^* v) \Big(\frac{1}{\pi} \int_0^{2\pi} \arcsin(|u^* v| \cos(t)) \cos(t) \, \mathrm{d}t \Big) \\
&= \frac{\pi}{4} sign(u^* v) \, |u^* v| \; {}_2F_1(\tfrac{1}{2}, \tfrac{1}{2}, 2; |u^* v|^2) \\
&= \mathbb{E}[|Z_1|]^2 \, u^* v \; {}_2F_1(\tfrac{1}{2}, \tfrac{1}{2}, 2; |u^* v|^2).
\end{aligned}
\tag{4.89}
$$

Remark 4.1. The second equality in (4.89) is a particular case of the equality

$$
\frac{1}{\pi} \int_0^{2\pi} \arcsin(x \cos(t)) \cos(t) \, \mathrm{d}t = x \, {}_2F_1(\tfrac{1}{2}, \tfrac{1}{2}, 2; x^2) \text{ for all } x \in [-1, 1],
\tag{4.90}
$$

implied by the Maclaurin series representation of the function arcsin and the well-known fact that $\int_0^{2\pi} \cos^{2(n+1)}(t) \, \mathrm{d}t = \frac{2\sqrt{\pi}}{(n+1)!} \Gamma(n + \frac{3}{2}) = \frac{2\sqrt{\pi}}{\Gamma(n+2)} (n + \frac{1}{2}) \Gamma(n + \frac{1}{2})$ for all $n \in \mathbb{N}_0$.

We can see clearly that both, (4.88) and (4.89) do not depend on the choice of the dimension n. The reason for this is Lemma 2.16, but not the use of the sign functions. If we namely fix an arbitrary random vector $\mathbf{W} \sim \mathbb{F}N_n(0, I_n)$ and consider the matrix $A_{u,v} := \begin{pmatrix} u_1 & u_2 & \ldots & u_n \\ v_1 & v_2 & \ldots & v_n \end{pmatrix} \in \mathbb{M}_{2,n}(\mathbb{F})$, then $(u^* \mathbf{W}, v^* \mathbf{W})^\top = A_{u,v} \mathbf{W} \sim N_2(0, \Sigma_2(u^* v))$ (due to Lemma 2.16). Hence, if $(S_1, S_2)^\top \sim N_2(0, \Sigma_2(u^* v))$ is given, then $\mathbb{P}_{(S_1, S_2)^\top} = \mathbb{P}_{(u^* \mathbf{W}, v^* \mathbf{W})^\top} = (A_{u,v})_* \mathbb{P}_{\mathbf{W}}$. The change of variables formula therefore implies that (in particular) *for any* choice of a. e. bounded functions $f, g \in L^\infty(\mathbb{F})$, the following equality holds:

$$
\mathbb{E}[f(u^* \mathbf{W}) g(\overline{v^* \mathbf{W}})] = \mathbb{E}[(f \otimes \overline{g}) \circ A_{u,v}(\mathbf{W})] = \int_{\mathbb{F}^2} f \otimes \overline{g} \, \mathrm{d}((A_{u,v})_* \mathbb{P}_{\mathbf{W}}) = \mathbb{E}[f(S_1) g(\overline{S_2})].
\tag{4.91}
$$

Consequently, if we also include Lemma 3.2 (or the obvious fact that the mapping $S_{\mathbb{F}^n} \times S_{\mathbb{F}^n} \ni (u, v) \mapsto u^* v \in \overline{\mathbb{D}} \cap \mathbb{F}$ is onto for any $n \in \mathbb{N}_2$) and Corollary 4.8, then (4.91), applied to $f := g := \mathrm{sign}$ implies that (4.88) and (4.89) are special cases of an equality which "just" involves the function $\mathrm{sign} : \mathbb{R} \longrightarrow \{-1, 1\}$ and a 2-dimensional Gaussian random vector, where the latter consists of two arbitrarily correlated random variables, though. Remembering the fact (2.32), we obtain:

Corollary 4.2 (**Gaussian sign-correlation coefficient**). *Fix* $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$. *Let* $\Sigma \in C(2;\mathbb{F})$ *and* $(S_1, S_2) \sim \mathbb{F}N_2(0, \Sigma)$. *Then* $\Sigma = \Sigma_2(\zeta)$ *for some* $\zeta \in \mathbb{F} \cap \overline{\mathbb{D}}$, *and the Pearson correlation coefficient between* $sign(S_1)$ *and* $sign(S_2)$ *is given by*

$$\mathbb{E}[sign(S_1)sign(\overline{S_2})] = \mathbb{E}[|S_1|]^2\, \zeta\, {}_2F_1(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{d_{\mathbb{F}}+2}{2}; |\zeta|^2) = \frac{1}{k_G^{\mathbb{F}}}\, \zeta\, {}_2F_1(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{d_{\mathbb{F}}+2}{2}; |\zeta|^2), \tag{4.92}$$

where $d_{\mathbb{R}} := 1$ *and* $d_{\mathbb{C}} := 2$.

4.2. Integration over $\mathbb{S}^{n-1}$ and the Gamma function

In fact, the Grothendieck equality as well as the Haagerup equality instantly unfold as a *special case* of a (much more general) result, where we explicitly describe all non-negative integer powers of an expectation of inner products of suitably correlated - real - random vectors, uniformly distributed on the unit sphere (cf. Theorem 4.12 and Proposition 6.16). In this regard, we possibly should point to the so-called "kernel trick", used also for the computation of inner products in high-dimensional feature spaces using simple functions defined on pairs of input patterns which is a crucial ingredient of support vector machines in statistical learning theory; i.e., learning machines that construct decision functions of sign type. This trick allows the formulation of nonlinear variants of any algorithm that can be cast in terms of inner products (cf. [144, Chapter 5.6]).

Firstly, it is quite helpful to understand the actual source of the values $\frac{2}{\pi}$ and $\frac{\pi}{4}$ (cf. (4.102), Corollary 4.8, Proposition 6.16 and [33, Chapter 8.7]).

Lemma 4.3. *Let* $(b_n)_{n\in\mathbb{N}}$ *be the sequence of real numbers, defined as*

$$b_n := \begin{cases} 1 & \text{if } n \text{ is even} \\ \sqrt{\pi/2} & \text{if } n \text{ is odd} \end{cases}. \tag{4.93}$$

Then

$$\Gamma\Big(\frac{n}{2}\Big) = \frac{(n-2)!!}{\sqrt{2^{n-2}}}\, b_n \quad \text{for all } n \in \mathbb{N}. \tag{4.94}$$

In particular, $b_n = b_{2m+n}$ *for all* $m, n \in \mathbb{N}$, *and*

$${}_2F_1\Big(\frac{k}{2}, \frac{l}{2}, \frac{m}{2}; z\Big) = \frac{(m-2)!!}{(k-2)!!\,(l-2)!!} \sum_{n=0}^{\infty} \frac{(2(n-1)+k)!!\,(2(n-1)+l)!!}{(2n)!!\,(2(n-1)+m)!!}\, z^n \tag{4.95}$$

for all $k, l, m \in \mathbb{N}$ *and* $z \in \mathbb{D}$. *If in addition* $m > k + l$, *then* (4.95) *holds for any* $z \in \mathbb{T}$.

Proof. Regarding the proof of (4.94), we have to distinguish two cases; namely the even case (i.e., $n = 2l$ for some $l \in \mathbb{N}$) and the odd case (i.e., $n = 2k + 1$ for some $k \in \mathbb{N}_0$). However, since $(2l-2)!! = (2(l-1))!! = 2^{l-1}(l-1)!$ and $\Gamma(k + \frac{1}{2}) = \frac{(2k-1)!!}{2^k}\sqrt{\pi}$, (4.94) follows at once. Equipped with (4.94), the proof of the representation (4.95) just involves a few remaining basic algebraic transformations (including a multiple shortening of fractions), implied by the definition of Gaussian hypergeometric functions. □

We also need results about the real and complex Gaussian randomness structure, embedded in the Gamma function, which are of their own interest; built on an important link between the Gamma function and powers of absolute moments of standard normally distributed real random variables. To this end, we consider both, the real and the complex unit sphere as a probability space. Put

$$\sigma_{n-1}(A) := \frac{\omega_n(A)}{\omega_n} = \frac{\Gamma(n/2)}{2\pi^{n/2}}\,\omega_n(A) = \frac{\Gamma(n/2)}{2\pi^{n/2}}\,n\,\lambda_n(\{r\xi : 0 < r \leq 1 \text{ and } \xi \in A\}) \\ = \frac{\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}\,\lambda_n(\{r\xi : 0 < r \leq 1 \text{ and } \xi \in A\}),$$

where $A \in \mathcal{B}(\mathbb{S}^{n-1})$ and $\omega_n \equiv \omega_n(\mathbb{S}^{n-1}) = \frac{2\pi^{n/2}}{\Gamma(n/2)}$ denotes the surface area of the unit sphere $\mathbb{S}^{n-1} \subseteq \mathbb{R}^n$. σ_{n-1} denotes the rotation-invariant probability measure (Haar measure) on $\mathbb{S}^{n-1}$. Moreover, $\sigma_n^{\mathbb{C}} := (J_2^{-1})_* \,\sigma_{2n-1}$ denotes the surface area probability measure on the complex unit sphere $S_{\mathbb{C}^n}$.

Proposition 4.4. *Let $n \in \mathbb{N}$, $X \sim N_1(0,1)$, $\boldsymbol{X} \sim N_n(0, I_n)$, $Z \sim \mathbb{C}N_1(0,1)$, $\boldsymbol{Z} \sim \mathbb{C}N_n(0, I_n)$ and $\boldsymbol{Y} = vec(\boldsymbol{Y}_1, \boldsymbol{Y}_2) \sim N_{2n}(0, I_{2n})$. Let $p, q \in \mathbb{R}$ such that $p > -1$ and $q > 0$. Then*

(i)

$$2\int_0^\infty s^p\,\gamma_1(\mathrm{d}s) = \mathbb{E}[|X|^p] = \frac{2^{p/2}}{\sqrt{\pi}}\,\Gamma(\tfrac{p+1}{2}) \tag{4.96}$$

and

$$\Gamma(q) = \frac{\sqrt{2\pi}}{2^q}\,\mathbb{E}[|X|^{2q-1}].$$

In particular,

$$\mathbb{E}[|X|^k] = \frac{(k-1)!!}{b_k} = \begin{cases} (k-1)!! & \text{if } k \text{ is even} \\ \sqrt{\frac{2}{\pi}}\,(k-1)!! & \text{if } k \text{ is odd} \end{cases} \quad \text{for all } k \in \mathbb{N}_0\,, \tag{4.97}$$

where b_k satisfies (4.93).

(ii) *Let $n \geq 2$ and $f : \mathbb{R}^n \longrightarrow \mathbb{R}$, such that*

$$f(rx) = r^p\,f(x) \text{ for all } (r, x) \in (0,\infty) \times \mathbb{R}^n\,.$$

Then $f \in L^1(\mathbb{R}^n, \gamma_n)$ if and only if $f\big|_{\mathbb{S}^{n-1}} \in L^1(\mathbb{S}^{n-1}, \sigma_{n-1})$, and

$$\mathbb{E}[f(\boldsymbol{X})] = \int_{\mathbb{R}^n} f(x)\gamma_n(\mathrm{d}x) \;=\; 2^{p/2}\,\frac{\Gamma\left(\frac{n+p}{2}\right)}{\Gamma\left(\frac{n}{2}\right)} \int_{\mathbb{S}^{n-1}} f(\xi)\,\mathrm{d}\sigma_{n-1}(\xi)\,. \tag{4.98}$$

(iii) *Let $b : \mathbb{C}^n \longrightarrow \mathbb{C}$, such that*

$$b(rz) = r^p\,b(z) \text{ for all } (r, z) \in (0,\infty) \times \mathbb{C}^n\,.$$

Then $b \in L^1(\mathbb{C}^n, \gamma_n^{\mathbb{C}})$ *if and only if* $\mathrm{Re}(b) \circ J_2^{-1}\big|_{\mathbb{S}^{2n-1}} \in L^1(\mathbb{S}^{2n-1}, \sigma_{2n-1})$ *and* $\mathrm{Im}(b) \circ J_2^{-1}\big|_{\mathbb{S}^{2n-1}} \in L^1(\mathbb{S}^{2n-1}, \sigma_{2n-1})$, *and*

$$\begin{aligned}
\mathbb{E}[b(\boldsymbol{Z})] &= \int_{\mathbb{C}^n} b(z)\gamma_n^{\mathbb{C}}(\mathrm{d}z) = \frac{\Gamma(n+\frac{p}{2})}{(n-1)!} \int\limits_{S_{\mathbb{C}^n}} b(\zeta)\,\mathrm{d}\sigma_n^{\mathbb{C}}(\zeta) \\
&= \frac{\Gamma(n+\frac{p}{2})}{(n-1)!}\Big(\int\limits_{\mathbb{S}^{2n-1}} \mathrm{Re}(b(y_1 + i\,y_2))\,\mathrm{d}\sigma_{2n-1}((y_1,y_2)) + i \int\limits_{\mathbb{S}^{2n-1}} \mathrm{Im}(b(y_1 + i\,y_2))\,\mathrm{d}\sigma_{2n-1}((y_1,y_2))\Big) \\
&= 2^{-p/2}\Big(\mathbb{E}[\mathrm{Re}(b(\boldsymbol{Y}_1 + i\,\boldsymbol{Y}_2))] + i\,\mathbb{E}[\mathrm{Im}(b(\boldsymbol{Y}_1 + i\,\boldsymbol{Y}_2))]\Big).
\end{aligned} \tag{4.99}$$

Proof. (i) Recall that $\Gamma(z) = \int_0^\infty t^{z-1}\,e^{-t}\,\mathrm{d}t$, where $\mathrm{Re}(z) > 0$. Consequently (if we substitute t through $\frac{s^2}{2}$), we obtain

$$\Gamma\Big(\frac{p+1}{2}\Big) = \frac{\sqrt{2\pi}}{(\sqrt{2})^{p-1}} \int_0^\infty s^p\,\gamma_1(\mathrm{d}s)\,,$$

and it follows that

$$\mathbb{E}[|X|^p] = \int_{-\infty}^0 (-s)^p\,\gamma_1(\mathrm{d}s) + \int_0^\infty s^p\,\gamma_1(\mathrm{d}s) = 2\int_0^\infty s^p\,\gamma_1(\mathrm{d}s) = \frac{2^{p/2}}{\sqrt{\pi}}\,\Gamma\Big(\frac{p+1}{2}\Big).$$

(4.94) implies the particular case (4.97).
(ii) Since $\mathbf{X} \equiv (X_1,\ldots,X_n)^\top \sim N_n(0, I_n)$ is a (centered) standard Gaussian random vector, we have

$$\mathbb{E}[f(\mathbf{X})] = \mathbb{E}[f(X_1,\ldots,X_n)] = (2\pi)^{-n/2}\int_{\mathbb{R}^n} f(x)\exp\Big(-\frac{1}{2}\|x\|^2\Big)\lambda_n(\mathrm{d}x)\,.$$

It follows that for λ_n-almost all $r \in (0,\infty)$ we have

$$\begin{aligned}
\int\limits_{\mathbb{R}^n} f(x)\exp(-\tfrac{1}{2}\|x\|^2)\lambda_n(\mathrm{d}x) &= \int\limits_0^\infty \Big(\int\limits_{\mathbb{S}^{n-1}} f(r\xi)\exp(-\tfrac{1}{2}\|r\xi\|^2)\,\mathrm{d}\omega_n(\xi)\Big) r^{n-1}\,\mathrm{d}r \\
&= \int\limits_0^\infty \exp(-\tfrac{1}{2}r^2) r^{n+p-1}\,\mathrm{d}r \cdot \int\limits_{\mathbb{S}^{n-1}} f(\xi)\,\mathrm{d}\omega_n(\xi)\,.
\end{aligned}$$

Hence,

$$\mathbb{E}[f(\mathbf{X})] = (2\pi)^{-n/2}\,\kappa_{n+p} \int\limits_{\mathbb{S}^{n-1}} f(\xi)\,\mathrm{d}\omega_n(\xi)\,,$$

where $\kappa_\nu := \int\limits_0^\infty r^{\nu-1}\,\exp(-\frac{1}{2}r^2)\,\mathrm{d}r = \sqrt{\frac{\pi}{2}}\,\mathbb{E}[|X_1|^{\nu-1}] = 2^{\frac{\nu-2}{2}}\,\Gamma(\frac{\nu}{2})$, $\nu \in \mathbb{N}$. Consequently, since $\frac{2\pi^{n/2}}{\Gamma(\frac{n}{2})} = \omega_n(\mathbb{S}^{n-1})$ is the surface area of $\mathbb{S}^{n-1}$, it follows that

$$\mathbb{E}[f(\mathbf{X})] = (2\,\pi)^{-n/2}\,\frac{2\pi^{n/2}}{\Gamma(\frac{n}{2})}\,\kappa_{n+p} \int\limits_{\mathbb{S}^{n-1}} f(\xi)\,\mathrm{d}\sigma_{n-1}(\xi) = 2^{p/2}\,\frac{\Gamma(\frac{n+p}{2})}{\Gamma(\frac{n}{2})} \int\limits_{\mathbb{S}^{n-1}} f(\xi)\,\mathrm{d}\sigma_{n-1}(\xi)\,.$$

(iii) That equality follows instantly from (ii) and the definition of the measure $\sigma_n^{\mathbb{C}}$. We only have to recall (2.25) and the representation $S_{\mathbb{C}^n} = \{\zeta \in \mathbb{C}^n : \|\zeta\|_{\mathbb{C}_2^n} = 1\} = J_2^{-1}(\mathbb{S}^{2n-1})$ of the unit sphere in $\mathbb{C}^n$. □

Corollary 4.5. *Let $p \in (-1, \infty)$, $m, n \in \mathbb{N}$, $X \sim N_1(0,1)$, $\boldsymbol{X} \sim N_n(0, I_n)$, $\boldsymbol{Y} \sim N_{2n}(0, I_{2n})$, $Z \sim \mathbb{C}N_1(0,1)$ and $\boldsymbol{Z} \sim \mathbb{C}N_n(0, I_n)$. Then*

$$\mathbb{E}[\|\boldsymbol{X}\|_{\mathbb{R}_2^n}^p] = 2^{p/2}\,\frac{\Gamma(\frac{n+p}{2})}{\Gamma(\frac{n}{2})} = \frac{\mathbb{E}[|X|^{n-1+p}]}{\mathbb{E}[|X|^{n-1}]} \tag{4.100}$$

and

$$\mathbb{E}[\|\boldsymbol{Z}\|_{\mathbb{C}_2^n}^p] = \frac{\Gamma(n+\frac{p}{2})}{(n-1)\,!} = 2^{-p/2}\,\mathbb{E}[\|\boldsymbol{X}\|_{\mathbb{R}_2^{2n}}^p] = 2^{-p/2}\,\frac{\mathbb{E}[|X|^{2n-1+p}]}{\mathbb{E}[|X|^{2n-1}]}\,. \tag{4.101}$$

In particular,

$$\mathbb{E}[\|\boldsymbol{X}\|_{\mathbb{R}_2^n}^m] = a_n(m)\,\frac{(n-2+m)!!}{(n-2)!!} \quad \textit{and} \quad \mathbb{E}[\|\boldsymbol{Z}\|_{\mathbb{C}_2^n}^m] = a_{2n}(m)\,2^{-m/2}\,\frac{(2n-2+m)!!}{(2n-2)!!}$$

and

$$\mathbb{E}[|X|] = \sqrt{\frac{2}{\pi}} \quad \textit{and} \quad \mathbb{E}[|Z|] = \sqrt{\frac{\pi}{4}} = \frac{\sqrt{\pi}}{2}\,, \tag{4.102}$$

where

$$a_n(m) := \frac{b_{n+m}}{b_n} = \begin{cases} \sqrt{\pi/2} & \text{if } n \text{ is even and } m \text{ is odd} \\ \sqrt{2/\pi} & \text{if } n \text{ is odd and } m \text{ is odd} \\ 1 & \text{if } m \text{ is even} \end{cases} \tag{4.103}$$

and b_n is defined as in Lemma 4.3.

Proof. We just have to apply Proposition 4.4 to the function $\mathbb{F}^n \ni z \mapsto f_p(z) := \|z\|^p$ (and to recall that by definition $\|\cdot\|_{\mathbb{R}_2^1} := |\cdot|$). □

A further, very important special case (which allows an easy proof of Theorem 4.12) arises if we consider the function $\mathbb{R}^n \ni x \mapsto \langle u, x\rangle_{l_n^2}^m = (u^\top x)^m$, where $m \in \mathbb{N}_0$ and $u \in \mathbb{S}^{n-1}$ are given.

Corollary 4.6. *Let $p \in (-1, \infty), n \in \mathbb{N}_2, x \in \mathbb{S}^{n-1}$ and $Y \sim N_1(0,1)$. Let $f : \mathbb{R} \longrightarrow \mathbb{R}$ be a function such that $f \in L^1(\mathbb{R}, \gamma_1)$ and $f(ry) = r^p f(y)$ for all $(r, y) \in (0, \infty) \times \mathbb{R}$. Then $f(x^\top \cdot) \in L^1(\mathbb{S}^{n-1}, \sigma_{n-1})$, and*

$$\int_{\mathbb{S}^{n-1}} f(x^\top u)\,\sigma_{n-1}(\mathrm{d}u) = 2^{-p/2}\frac{\Gamma(\frac{n}{2})}{\Gamma(\frac{n+p}{2})}\,\mathbb{E}[f(Y)]\,.$$

In particular,

$$\int_{\mathbb{S}^{n-1}} (x^\top u)^m\,\sigma_{n-1}(\mathrm{d}u) = \frac{1+(-1)^m}{2}\,\frac{\Gamma(\frac{m+1}{2})\Gamma(\frac{n}{2})}{\sqrt{\pi}\,\Gamma(\frac{m+n}{2})} = \frac{1+(-1)^m}{2}\Big(\frac{\Gamma(\frac{n}{2})}{\sqrt{\pi}\,\Gamma(\frac{n-1}{2})}\,B(\tfrac{m+1}{2}, \tfrac{n-1}{2})\Big) \tag{4.104}$$

for all $m \in \mathbb{N}_0$. Here, $(0,\infty) \times (0,\infty) \ni (x_1, x_2) \mapsto B(x_1, x_2) := \int_0^1 t^{x_1-1}(1-t)^{x_2-1}\,\mathrm{d}t = \frac{\Gamma(x_1)\Gamma(x_2)}{\Gamma(x_1+x_2)}$ denotes the real beta function.

Proof. Since $\|x\|_{l_n^2} = 1$, it follows that $x^\top \mathbf{Y} \overset{d}{=} Y \sim N_1(0,1)$ for any $\mathbf{Y} \sim N_n(0, I_n)$. Thus, $\mathbb{E}[f(Y)] = \mathbb{E}[f(x^\top \mathbf{Y})]$, so that we may apply (4.98) to the function $\mathbb{R}^n \ni x \mapsto f(x^\top \cdot)$. Regarding the particular case $\mathbb{R} \ni y \mapsto y^m$ (respectively, $\mathbb{R}^n \ni x \mapsto (x^\top \cdot)^m$), we only have to include Lemma 4.3 and the well-known fact that the m-th moment of $Y \sim N_1(0,1)$ satisfies $\mathbb{E}[Y^m] = \frac{1+(-1)^m}{2}\,(m-1)!!\,$. □

Lemma 4.7. *Consider the sequence $(c_k)_{k\in\mathbb{N}}$, defined as*

$$c_k := \frac{1}{\sqrt{{}_2F_1(\frac{1}{2}, \frac{1}{2}, \frac{k+2}{2}; 1)}}\,.$$

Let $\boldsymbol{X} \sim N_k(0, I_k)$ and $\boldsymbol{Z} \sim \mathbb{C}N_k(0, I_k)$. Then

$$c_k = \sqrt{\frac{2}{k}}\,\frac{\Gamma(\frac{k+1}{2})}{\Gamma(\frac{k}{2})} = a_k\,\frac{1}{\sqrt{k}}\,\frac{(k-1)!!}{(k-2)\,!!} = \frac{1}{\sqrt{k}}\,\mathbb{E}[\|\boldsymbol{X}\|_{\mathbb{R}_2^k}] = \sqrt{\frac{2\pi}{k}}\,\frac{\omega_k}{\omega_{k+1}}\,, \tag{4.105}$$

where $a_k := a_k(1)$ satisfies (4.103), $\omega_1 := 2$ and ω_m denotes the surface area of the unit sphere $\mathbb{S}^{m-1}$ $(m \in \mathbb{N}_2)$. In particular, $c_1^2 = \frac{2}{\pi}$, $c_2^2 = \frac{\pi}{4}$ and

$$c_{2k} = \frac{1}{\sqrt{k}}\,\frac{\Gamma(k+\frac{1}{2})}{(k-1)!} = \frac{1}{\sqrt{k}}\,\sqrt{\frac{\pi}{4}}\,\frac{(2k-1)!!}{(2k-2)\,!!} = \frac{1}{\sqrt{k}}\,\mathbb{E}[\|\boldsymbol{Z}\|_{\mathbb{C}_2^k}]\,. \tag{4.106}$$

Moreover, $0 < c_k < 1$ for all $k \in \mathbb{N}$, $\lim\limits_{k\to\infty} c_k = 1$, and

$$\frac{1}{\sqrt{k}}\,\mathbb{E}[\|\boldsymbol{W}\|_{\mathbb{F}_2^k}] = c_{\nu_k^{\mathbb{F}}} = \frac{1}{\sqrt{{}_2F_1(\frac{1}{2}, \frac{1}{2}, \frac{\nu_k^{\mathbb{F}}+2}{2}; 1)}} \overset{k\to\infty}{\longrightarrow} 1 \quad \textit{for all } \boldsymbol{W} \sim \mathbb{F}N_k(0, I_k)\,,$$

where $\nu_k^{\mathbb{R}} := k$ and $\nu_k^{\mathbb{C}} := 2k$.

Proof. Fix $k \in \mathbb{N}$. Firstly, the Gauss Summation Theorem implies that

$${}_2F_1(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{k}{2}+1; 1) = \frac{\Gamma(\frac{k}{2}+1)\,\Gamma(\frac{k}{2})}{\Gamma(\frac{k+1}{2})\Gamma(\frac{k+1}{2})} = \frac{k}{2}\cdot\frac{\Gamma^2(\frac{k}{2})}{\Gamma^2(\frac{k+1}{2})}\,,$$

whence $c_k = \sqrt{\frac{2}{k}}\frac{\Gamma(\frac{k+1}{2})}{\Gamma(\frac{k}{2})} > 0$ (since $\Gamma(x) > 0$ for all $x > 0$). (4.105) now follows immediately from (4.100). Put $s_k := \frac{\Gamma(\frac{k+1}{2})}{\Gamma(\frac{k}{2})}$, where $k \in \mathbb{N}$. Recall that the function $\ln \circ \Gamma\big|_{(0,\infty)} : (0,\infty) \longrightarrow \mathbb{R}$ is convex, implying that in particular

$$\Gamma(\tfrac{k+1}{2}) = \Gamma(\tfrac{1}{2}\,x_k + \tfrac{1}{2}\,y_k) \le \sqrt{\Gamma(x_k)}\,\sqrt{\Gamma(y_k)} = \sqrt{\Gamma(\tfrac{k}{2})}\,\sqrt{\Gamma(\tfrac{k+2}{2})},$$

where $x_k := \frac{k}{2}$ and $y_k := \frac{k+2}{2} = \frac{k}{2}+1$. Thus, $s_k \le s_{k+1}$ for all $k \in \mathbb{N}$. However, since $s_k\,s_{k+1} = \frac{k}{2}$ for all $k \in \mathbb{N}$, it consequently follows that for all $k \in \mathbb{N}_2$

$$\tfrac{k-1}{2} = s_{k-1}\,s_k \le s_k^2 \le s_k s_{k+1} = \tfrac{k}{2},$$

whence $\lim\limits_{k\to\infty} c_k^2 = \lim\limits_{k\to\infty} \frac{2}{k} s_k^2 = 1$. Finally, since

$$\frac{1}{c_k^2} - 1 = {}_2F_1(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{k+2}{2}; 1) - 1 = \frac{\Gamma(\frac{k+2}{2})}{\pi}\sum_{\nu=1}^{\infty}\frac{\Gamma^2(\nu+\frac{1}{2})}{\Gamma(\nu+\frac{k+2}{2})\,\nu!} > 0 \text{ for all } k \in \mathbb{N}.$$

it follows that in fact $0 < c_k < 1$ for all $k \in \mathbb{N}$. □

In the context of Theorem 1.3, the one-dimensional special cases of (4.100) and (4.101) disclose a unification of the real and complex Gaussian structure, encoded at least in the *little* Grothendieck constant:

Corollary 4.8. *Let $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$. Then the little Grothendieck constant $k_G^{\mathbb{F}}$ can be written as*

$$k_G^{\mathbb{F}} = {}_2F_1(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{d_{\mathbb{F}}+2}{2}; 1) = \begin{cases} \pi/2 & \text{if } \mathbb{F} = \mathbb{R} \text{ and } d_{\mathbb{R}} = 1 \\ 4/\pi & \text{if } \mathbb{F} = \mathbb{C} \text{ and } d_{\mathbb{C}} = 2 \end{cases}.$$

Corollary 4.9 (**Krivine, 1979**). *Let $f \in C([-1,1])$, $k \in \mathbb{N}_2$ and $u \in \mathbb{S}^{k-1}$. Then*

$$\int_{\mathbb{S}^{k-1}} f(\langle u, v\rangle_{\mathbb{R}_2^k}) \mathrm{d}\sigma_{k-1}(v) = \int_{-1}^{1} f(t)\, \mathrm{d}\mathbb{Q}_k(t) = \sqrt{\frac{k-1}{2\pi}}\, c_{k-1} \int_{-1}^{1} f(t)(1-t^2)^{\frac{k-3}{2}}\, \mathrm{d}t\,,$$

where $\mathbb{Q}_k(\mathrm{d}s) := \frac{\Gamma(k/2)}{\sqrt{\pi}\,\Gamma((k-1)/2)}\,(1-t^2)^{\frac{k-3}{2}}\,\mathrm{d}s$ is a probability measure on $[-1,1]$.

Proof. We just have to link (4.105) with the (unindexed) equality on page 27 of [91]. □

Remark 4.10 (**Absolutely p-summing operators and GT in matrix form**). Recall that $T \in \mathcal{L}(E,F)$ between Banach spaces E and F is called absolutely p-summing ($1 \leq p < \infty$) if there exists a constant $c \geq 0$ such that for all $n \in \mathbb{N}$ and $x_1, \ldots, x_n \in E$

$$\Big(\sum_{i=1}^{n} \|Tx_i\|^p\Big)^{1/p} \leq c\, w_p(x_1, \ldots, x_n)\,, \tag{4.107}$$

where $w_p(x_1, \ldots, x_n) := \sup\limits_{\psi \in B_{E'}} \Big(\sum_{i=1}^{n} |\langle x_i, \psi\rangle|^p\Big)^{1/p}$. The p-summing norm $\|T\|_{\mathcal{P}_p}$ is defined as the infimum of all constants $c \geq 0$ which satisfy (4.107) (cf., e.g., [33, Chapter 11] or [79, Chapter 2]). Expressed in the terminology of absolutely 1-summing operators, Grothendieck proved that his inequality in particular is *equivalent* to

$$\|T\|_{\mathcal{P}_1} \leq K_G^{\mathbb{F}}\, \|T\| \tag{4.108}$$

for all $\mathbb{F}$-Hilbert spaces H, $n \in \mathbb{N}$ and finite rank operators $T \in \mathcal{L}(l_1^n, H)$ (cf. [100, 116] and [77, Theorem 10.7]). Actually, the proof of (4.108) in the finite rank case is quite simple. It is based on the following two facts. Firstly, since $(l_1^n)' \cong l_\infty^n$, it follows that for all $a_1, \ldots, a_m \in l_1^n$ ($a_i \equiv (a_{i1}, \ldots, a_{in})^\top$), $\|A\|_{\infty,1} = w_1(a_1, \ldots, a_m)$ and $\|A^*A\|_{\infty,1} = (w_2(a_1, \ldots, a_m))^2$, where

$$A := (a_1 \,\vdots\, a_2 \,\vdots\, \cdots \,\vdots\, a_m)^\top \equiv (a_{ij}) \in \mathbb{M}_{m,n}(\mathbb{F}).$$

Secondly, since $H' \cong H$ (Riesz), we obtain that

$$\sum_{i=1}^{m} \|T\,a_i\|_H = \sum_{i=1}^{m} \Big\| \sum_{j=1}^{n} a_{ij}\, Te_j \Big\|_H = \mathrm{tr}(A^*\Gamma_H(u, z_T)) \leq K_G^{\mathbb{F}}\, \|T\|\, \|A\|_{\infty,1} = K_G^{\mathbb{F}}\, \|T\|\, w_1(a_1, \ldots, a_m),$$

for some $u \in B_H^m$ and $z_T \in H^n$, where the latter is defined as $(z_T)_j := Te_j \in \|T\|\, S_{l_1^n}$ ($j \in [n]$). Similarly, we obtain the well-known $\mathcal{P}_2$-representation of the little Grothendieck inequality ("little GT"), which even is *equivalent* to little GT in matrix form, since the use of $(\mathcal{P}_2, \|\cdot\|_{\mathcal{P}_2})$ in fact naturally implies the emergence of the *positive semidefinite* matrix $A^*A \in \mathbb{M}_n(\mathbb{F})^+$:

$$\sum_{i=1}^{m} \|T\,a_i\|_H^2 = \sum_{l=1}^{n}\sum_{j=1}^{n}\Big(\sum_{i=1}^{m} \overline{a_{il}}\,a_{ij}\Big)\Big\langle (z_T)_j, (z_T)_l\Big\rangle_H = \operatorname{tr}((A^*A)\Gamma_H(z_T, z_T))$$
$$\leq k_G^{\mathbb{F}}\,\|T\|^2\,\|A^*A\|_{\infty,1} = k_G^{\mathbb{F}}\,\|T\|^2(w_2(a_1,\ldots,a_m))^2,$$

In other words,

$$\|T\|_{\mathcal{P}_2} \leq \sqrt{k_G^{\mathbb{F}}}\,\|T\| \tag{4.109}$$

for all $\mathbb{F}$-Hilbert spaces H, $n \in \mathbb{N}$ and (finite rank operators) $T \in \mathcal{L}(l_1^n, H)$. It is surprising that no attention seems to have been paid to the equivalence of the psd matrix version of little GT and the absolutely 2-summing version of little GT so far. So, its worth to state it here. Moreover, if we combine [33, Theorem 11.10], (4.100) and (4.101), we can somewhat simplify the representation of the 1-summing norm of $Id_{\mathbb{F}_2^k}$ for any $k \in \mathbb{N}$. We namely have

$$\|Id_{\mathbb{R}_2^k}\|_{\mathcal{P}_1} = \sqrt{\frac{\pi}{2}}\,\mathbb{E}[\|\mathbf{X}\|_{\mathbb{R}_2^k}] = \sqrt{\frac{\pi}{2}}\,a_k\,\frac{(k-1)!!}{(k-2)!!} \overset{(4.105)}{=} \sqrt{k}\Big(\sqrt{\frac{\pi}{2}}\,c_k\Big) \quad \text{for all } k \in \mathbb{N}$$

and

$$\|Id_{\mathbb{C}_2^k}\|_{\mathcal{P}_1} = \sqrt{\frac{4}{\pi}}\,\mathbb{E}[\|\mathbf{Z}\|_{\mathbb{C}_2^k}] = \frac{2}{\pi}\,\|Id_{\mathbb{R}_2^{2k}}\|_{\mathcal{P}_1} = \frac{(2k-1)!!}{(2k-2)!!} \overset{(4.106)}{=} \sqrt{k}\Big(\sqrt{\frac{4}{\pi}}\,c_{2k}\Big) \quad \text{for all } k \in \mathbb{N}\,,$$

where $a_k := a_k(1)$ satisfies (4.103). Consequently, Lemma 4.7 recovers [77, Proposition 8.8], respectively [33, Corollary 11.10] and reveals a link between norms of certain absolutely 1-summing operators and values of Gaussian hypergeometric functions (since $\lim\limits_{\nu\to\infty} c_\nu = 1$):

$$\lim_{k\to\infty}\frac{1}{k}\|Id_{\mathbb{F}_2^k}\|_{\mathcal{P}_1}^2 = k_G^{\mathbb{F}} = {}_2F_1\Big(\frac{1}{2},\frac{1}{2},\frac{d_{\mathbb{F}}+2}{2};1\Big).$$

That is,

$$\lim_{k\to\infty}\frac{1}{k}\|Id_{\mathbb{R}_2^k}\|_{\mathcal{P}_1}^2 = \frac{\pi}{2} = {}_2F_1\Big(\frac{1}{2},\frac{1}{2},\frac{3}{2};1\Big) \text{ and } \lim_{k\to\infty}\frac{1}{k}\|Id_{\mathbb{C}_2^k}\|_{\mathcal{P}_1}^2 = \frac{4}{\pi} = {}_2F_1\Big(\frac{1}{2},\frac{1}{2},2;1\Big),$$

implying a further facet of a link between (Euclidean norms of) Gaussian random vectors and the 1-Banach ideal of absolutely 1-summing operators.

Proposition 4.4 also allows us to give a straightforward, simple proof of the following important well-known surface integral characterisation of the trace of a matrix:

Corollary 4.11. *Let* $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$, $m, n \in \mathbb{N}$, $A \in \mathbb{M}_{m,m}(\mathbb{F}), B \in \mathbb{M}_{m,n}(\mathbb{F}), C \in \mathbb{M}_{n,m}(\mathbb{F})$ *and* $D \in \mathbb{M}_{n,n}(\mathbb{F})$. *Let* $\boldsymbol{Z} \sim \mathbb{F}N_m(0, I_m)$. *Then the following properties hold:*

(i)
$$tr(\operatorname{Re}(A)) + i\,tr(\operatorname{Im}(A)) = tr(A) = \mathbb{E}[f_A(\boldsymbol{Z})],$$
where $\mathbb{F}^m \ni z \mapsto f_A(z) := z^*Az = tr(Azz^*)$.

(ii)

$$tr(A) = m\Big(\int\limits_{\mathbb{S}^{m-1}} u^\top \mathrm{Re}(A) u \,\mathrm{d}\sigma_{m-1}(u) + i \int\limits_{\mathbb{S}^{m-1}} u^\top \mathrm{Im}(A) u \,\mathrm{d}\sigma_{m-1}(u)\Big).$$

In particular,

$$\int\limits_{\mathbb{S}^{m+n-1}} tr(B\Gamma_{\mathbb{R}}(u,v))\,\mathrm{d}\sigma_{m+n-1}(vec(u,v)) = \int\limits_{\mathbb{S}^{m+n-1}} u^\top B v \,\mathrm{d}\sigma_{m+n-1}(vec(u,v)) = 0.$$

Proof. (i) Since $\mathbf{Z} \sim \mathbb{F}N_m(0, I_m)$, it follows that $\mathbb{E}[\mathbf{Z}\mathbf{Z}^*] = I_m$. Consequently, the linearity of $\mathbb{E}$ implies that

$$\mathrm{tr}(A) = \mathrm{tr}(A\mathbb{E}[\mathbf{Z}\mathbf{Z}^*]) = \mathbb{E}[\mathrm{tr}(A\mathbf{Z}\mathbf{Z}^*)] = \mathbb{E}[\mathrm{tr}(\mathbf{Z}^* A\mathbf{Z})] = \mathbb{E}[f_A(\mathbf{Z})].$$

(ii) Obviously, we may assume that $A \in \mathbb{M}_m(\mathbb{R})$. Since then $f_A(rx) = r^2 f_A(x)$ for all $(r,x) \in (0,\infty) \times \mathbb{R}^m$, we may apply Proposition 4.4 to $p = 2$, implying that

$$\mathrm{tr}(A) = 2\,\frac{\Gamma\big(\frac{m}{2}+1\big)}{\Gamma\big(\frac{m}{2}\big)} \int\limits_{\mathbb{S}^{m-1}} f_A(u)\,\mathrm{d}\sigma_{m-1}(u) = m \int\limits_{\mathbb{S}^{m-1}} u^\top A u \,\mathrm{d}\sigma_{m-1}(u)$$

(since $\Gamma\big(\frac{m}{2}+1\big) = \frac{m}{2}\Gamma\big(\frac{m}{2}\big)$). Finally, if we put $w := \mathrm{vec}(u,v)$ and $\Delta(B) := \frac{1}{2}\begin{pmatrix} 0 & B \\ B^\top & 0 \end{pmatrix} \in \mathbb{M}_{m+n,m+n}(\mathbb{R})$, it obviously follows that $w^\top \Delta(B) w = u^\top B v$ and $\mathrm{tr}(\Delta(B)) = 0$. Consequently, we obtain

$$0 = \mathrm{tr}(\Delta(B)) = (m+n) \int\limits_{\mathbb{S}^{m+n-1}} u^\top B v \,\mathrm{d}\sigma_{m+n-1}(w).$$

□

4.3. Integrating powers of inner products of random vectors, uniformly distributed on $\mathbb{S}^{n-1}$

Let us recall the (real, respectively complex) correlation matrices

$$\Sigma_{2n}(z) := \begin{pmatrix} I_n & z\,I_n \\ \bar{z}\,I_n & I_n \end{pmatrix} = \begin{pmatrix} 1 & z \\ \bar{z} & 1 \end{pmatrix} \otimes I_n\,,$$

where $|z| \leq 1$ and $n \in \mathbb{N}$ (cf. (2.31) and Proposition 2.12). Moreover, if $\mathbf{X} \sim N_n(0, I_n)$ and $A \in \mathcal{B}(\mathbb{S}^{n-1})$ is an arbitrary Borel subset of the unit sphere $\mathbb{S}^{n-1} \subseteq \mathbb{R}^n$ ($n \geq 2$), (4.98), applied to the function $\mathbb{R}^n \setminus \{0\} \ni x \mapsto f_A(x) := \mathbb{1}_A(\frac{x}{\|x\|_{\mathbb{R}^n_2}})$ (and $p = 0$) implies that in particular

$$\mathbb{P}\Big(\frac{\mathbf{X}}{\|\mathbf{X}\|_{\mathbb{R}^n}} \in A\Big) = \mathbb{E}[f_A(\mathbf{X})] = \int\limits_{\mathbb{S}^{n-1}} \mathbb{1}_A(\xi)\,\mathrm{d}\sigma_{n-1}(\xi) = \sigma_{n-1}(A)$$

(since $\mathbf{X} \neq 0$ $\mathbb{P}$-a.s.). Thus, we get again the well-known fact that $\frac{\mathbf{X}}{\|\mathbf{X}\|_{\mathbb{R}^n}}$ is uniformly distributed on the unit sphere $\mathbb{S}^{n-1}$ if $\mathbf{X} \sim N_n(0, I_n)$. Note that, in addition, for any $X \sim N_1(0,1)$, it is true that

$$\mathbb{P}\Big(\frac{X}{|X|} = \varepsilon\Big) = \mathbb{P}(X > 0 \text{ and } \varepsilon = 1) + \mathbb{P}(X \leq 0 \text{ and } \varepsilon = -1) = \frac{1}{2} \text{ for all } \varepsilon \in \{-1, 1\}\,,$$

so that we could also say that the random variable $\frac{X}{|X|}$ is uniformly distributed on the "unit sphere" $S^0 := \{-1, 1\} \subseteq \mathbb{R}^1$ if $X \sim N_1(0, 1)$.

Theorem 4.12. *Let $m, n \in \mathbb{N}$, $\rho \in (-1, 1)$ and $vec(\boldsymbol{X}, \boldsymbol{Y}) = vec(X_1, \ldots, X_n, Y_1, \ldots, Y_n) \sim N_{2n}\big(0, \Sigma_{2n}(\rho)\big)$.*

(i) *If m is odd then*

$$\mathbb{E}\Big[\Big\langle \frac{\boldsymbol{X}}{\|\boldsymbol{X}\|_{\mathbb{R}_2^n}}, \frac{\boldsymbol{Y}}{\|\boldsymbol{Y}\|_{\mathbb{R}_2^n}} \Big\rangle_{\mathbb{R}_2^n}^m\Big] = c_{odd}(m, n)\, \rho\, (1-\rho^2)^{\frac{n}{2}}\, {}_3F_2\Big(\frac{n+1}{2}, \frac{n+1}{2}, \frac{m+2}{2}; \frac{3}{2}, \frac{m+n+1}{2}; \rho^2\Big),$$

where

$$c_{odd}(m, n) := \frac{m}{\sqrt{\pi}} \frac{\Gamma^2(\frac{n+1}{2})\, \Gamma(\frac{m}{2})}{\Gamma(\frac{n}{2})\Gamma(\frac{m+n+1}{2})}.$$

(ii) *If m is even then*

$$\mathbb{E}\Big[\Big\langle \frac{\boldsymbol{X}}{\|\boldsymbol{X}\|_{\mathbb{R}_2^n}}, \frac{\boldsymbol{Y}}{\|\boldsymbol{Y}\|_{\mathbb{R}_2^n}} \Big\rangle_{\mathbb{R}_2^n}^m\Big] = c_{even}(m, n)\, (1-\rho^2)^{\frac{n}{2}}\, {}_3F_2\Big(\frac{n}{2}, \frac{n}{2}, \frac{m+1}{2}; \frac{1}{2}, \frac{m+n}{2}; \rho^2\Big),$$

where

$$c_{even}(m, n) := \frac{1}{\sqrt{\pi}} \frac{\Gamma(\frac{n}{2})\, \Gamma(\frac{m+1}{2})}{\Gamma(\frac{m+n}{2})}.$$

In particular,

$$\begin{aligned}\mathbb{E}\Big[\Big\langle \frac{\boldsymbol{X}}{\|\boldsymbol{X}\|_{\mathbb{R}_2^n}}, \frac{\boldsymbol{Y}}{\|\boldsymbol{Y}\|_{\mathbb{R}_2^n}} \Big\rangle_{\mathbb{R}_2^n}\Big] &= c_n^2\, (1-\rho^2)^{\frac{n}{2}}\, \rho\, {}_2F_1\Big(\frac{n+1}{2}, \frac{n+1}{2}; \frac{n+2}{2}; \rho^2\Big) \\ &= c_n^2\, \rho\, {}_2F_1\Big(\frac{1}{2}, \frac{1}{2}; \frac{n+2}{2}; \rho^2\Big),\end{aligned} \tag{4.110}$$

where $c_n := c_{odd}(1, n) = \sqrt{\frac{2}{n}} \frac{\Gamma(\frac{n+1}{2})}{\Gamma(\frac{n}{2})}$.

Proof. Fix $m \in \mathbb{N}$ and $\rho \in (-1, 1)$. Firstly, let $n = 1$. Observe that $\mathbb{R}_2^1 = (\mathbb{R}, |\cdot|)$, implying that the inner product on $\mathbb{R}_2^1$ is given by the standard product of real numbers. Moreover, note that $c_{\text{odd}}(m, 1) = \frac{2}{\pi}$ and $c_{\text{even}}(m, 1) = 1$. Thus, if $m = 2l + 1$ is odd, where $l \in \mathbb{N}_0$, the Grothendieck equality (cf. Corollary 4.2) implies that

$$\mathbb{E}\Big[\Big(\frac{X}{|X|} \cdot \frac{Y}{|Y|}\Big)^m\Big] = \mathbb{E}[\operatorname{sign}(X)\operatorname{sign}(Y)] = \frac{2}{\pi}\, \rho\, {}_2F_1\Big(\frac{1}{2}, \frac{1}{2}; \frac{3}{2}; \rho^2\Big) = \frac{2}{\pi} \arcsin(\rho).$$

On the other hand,

$$\begin{aligned}&c_{\text{odd}}(m, 1)\, \sqrt{1-\rho^2}\, \rho\, {}_3F_2\Big(1, 1, \frac{m+2}{2}; \frac{3}{2}, \frac{m+2}{2}; \rho^2\Big) \\ &= \frac{2}{\pi}\, \rho\, \Big(\sqrt{1-\rho^2}\, {}_2F_1\Big(1, 1; \frac{3}{2}; \rho^2\Big)\Big) \\ &= \frac{2}{\pi}\, \rho\, {}_2F_1\Big(\frac{1}{2}, \frac{1}{2}; \frac{3}{2}; \rho^2\Big) = \frac{2}{\pi} \arcsin(\rho),\end{aligned}$$

(where the penultimate equality follows from Euler's transformation formula of hypergeometric functions (cf., e.g., [6, Theorem 2.2.5, formula (2.2.7)]).
If $m = 2l$ is even ($l \in \mathbb{N}_0$), then

$$c_{\text{even}}(m,1)\sqrt{1-\rho^2}\,{}_3F_2\Big(\frac{1}{2},\frac{1}{2},\frac{m+1}{2};\frac{1}{2},\frac{m+1}{2};\rho^2\Big) = \sqrt{1-\rho^2}\,{}_2F_1\Big(\frac{1}{2},\frac{1}{2};\frac{1}{2};\rho^2\Big) = 1$$

(since ${}_2F_1\big(\frac{1}{2},\frac{1}{2},\frac{1}{2};\rho^2\big) = \arcsin'(\rho) = \frac{1}{\sqrt{1-\rho^2}}$). This concludes the proof for the case $n = 1$.
So, let now $n \geq 2$ be given. We have to calculate the following well-defined (Lebesgue) integral

$$I := c_n^{(1)}(\rho)\int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\Big\langle\frac{x}{\|x\|},\frac{y}{\|y\|}\Big\rangle_{\mathbb{R}_2^n}^m \exp\Big(-\frac{\|x\|^2+\|y\|^2-2\rho\langle x,y\rangle_2}{2(1-\rho^2)}\Big)\mathrm{d}^n x\,\mathrm{d}^n y\,,$$

where $c_n^{(1)}(\rho) := \frac{1}{(2\pi)^n\,(1-\rho^2)^{n/2}}$ (cf. (2.33)). The main idea is to calculate I by a two-fold application of the n-dimensional polar coordinates formula, implying the appearance of a double integral of type $\int_0^\infty\int_0^\infty F(r,s)\mathrm{d}r\,\mathrm{d}s$ and a decoupled spherical integral of type $\int_{\mathbb{S}^{n-1}} G(u,v)\mathrm{d}\sigma_{n-1}(v)$, where the latter actually does not depend on u. Despite the entanglement of the radius integrand parts $r \in (0,\infty)$ and $s \in (0,\infty)$ and the spherical integrand parts $u \in \mathbb{S}^{n-1}$ and $v \in \mathbb{S}^{n-1}$ in the density function, that decoupling can be obtained, simply by making use of the Maclaurin series representation of the entangled part of the density function $(0,\infty)^2 \times (\mathbb{S}^{n-1})^2 \ni (r,s,u,v) \mapsto \exp\Big(\frac{rs\rho\langle u,v\rangle_{\mathbb{R}_2^n}}{1-\rho^2}\Big)$. Due to (4.104), the resulting integrals can then be calculated easily. We will also recognise the need for the even/odd case-distinction at this point. To concretise the calculation steps, put

$$c_n^{(2)}(\rho) := c_n^{(1)}(\rho)(\omega_n(\mathbb{S}^{n-1}))^2 = \frac{1}{(2\pi)^n\,(1-\rho^2)^{n/2}}\Big(\frac{2\,\pi^{n/2}}{\Gamma(n/2)}\Big)^2 = \frac{1}{2^{n-2}\,\Gamma^2(n/2)\,(1-\rho^2)^{n/2}}\,. \tag{4.111}$$

A two-fold application of the n-dimensional polar coordinates, together with Fubini's theorem implies that

$$I = c_n^{(2)}(\rho)\int_0^\infty\int_0^\infty\int_{\mathbb{S}^{n-1}}\int_{\mathbb{S}^{n-1}}\langle u,v\rangle_{l_n^2}^m \exp\Big(-\frac{1}{2}\Big(\frac{r^2+s^2}{1-\rho^2}\Big)\Big)\exp\Big(\frac{rs\rho\langle u,v\rangle_2}{1-\rho^2}\Big)r^{n-1}s^{n-1}\,\mathrm{d}\sigma_{n-1}(v)\,\mathrm{d}\sigma_{n-1}(u).$$

Since $\exp\Big(\frac{rs\rho\langle u,v\rangle_2}{1-\rho^2}\Big) = \sum\limits_{\nu=0}^{\infty}\frac{1}{\nu!}\frac{\rho^\nu}{(1-\rho^2)^\nu}r^\nu\,s^\nu\langle u,v\rangle_{l_n^2}^\nu$, it consequently follows that

$$I = c_n^{(2)}(\rho)\sum_{\nu=0}^{\infty}\frac{1}{\nu!}\,\frac{\rho^\nu}{(1-\rho^2)^\nu}\,I_\nu(\rho)\,J_\nu(m), \tag{4.112}$$

where

$$I_\nu(\rho) := \int_0^\infty\int_0^\infty r^{\nu+n-1}s^{\nu+n-1}\exp\Big(-\frac{1}{2}\Big(\frac{r^2+s^2}{1-\rho^2}\Big)\Big)\mathrm{d}r\,\mathrm{d}s = \Big(\int_0^\infty r^{\nu+n-1}\exp\Big(-\frac{1}{2}\Big(\frac{r}{\sqrt{1-\rho^2}}\Big)^2\Big)\,\mathrm{d}r\Big)^2$$

and

$$J_\nu(m) := \int_{\mathbb{S}^{n-1}}\int_{\mathbb{S}^{n-1}}\langle u,v\rangle_{l_n^2}^{m+\nu}\,\mathrm{d}\sigma_{n-1}(v)\,\mathrm{d}\sigma_{n-1}(u)\,.$$

A simple change of variables in $I_\nu(\rho)$ ($r \mapsto \frac{r}{\sqrt{1-\rho^2}}$) therefore implies that

$$I_\nu(\rho) = \frac{\pi}{2}(1-\rho^2)^{n+\nu}\Big(2\int_0^\infty x^{n-1+\nu}\gamma_1(\mathrm{d}x)\Big)^2 \overset{(4.96)}{=} \big(2^{n-2}\,(1-\rho^2)^n\big)\, 2^\nu\,(1-\rho^2)^\nu\,\Gamma^2\Big(\frac{\nu+n}{2}\Big)$$
$$\overset{(4.111)}{=} \frac{(1-\rho^2)^{n/2}}{c_n^{(2)}(\rho)\,\Gamma^2(n/2)}\, 2^\nu\,(1-\rho^2)^\nu\,\Gamma^2\Big(\frac{\nu+n}{2}\Big).$$

Because of (4.104), it follows that

$$J_\nu(m) = \int_{\mathbb{S}^{n-1}} \langle u, v\rangle_{l_n^2}^{m+\nu}\,\mathrm{d}\sigma_{n-1}(v) = \frac{1+(-1)^{m+\nu}}{2}\Big(\frac{\Gamma(\frac{\nu+m+1}{2})\Gamma(\frac{n}{2})}{\sqrt{\pi}\,\Gamma(\frac{\nu+m+n}{2})}\Big).$$

Hence,

$$I \overset{(4.112)}{=} \frac{1}{\Gamma(n/2)}\,(1-\rho^2)^{n/2}\sum_{\nu=0}^\infty \frac{1+(-1)^{m+\nu}}{2}\,\frac{2^\nu}{\nu!\,\sqrt{\pi}}\,\frac{\Gamma^2\big(\frac{\nu+n}{2}\big)\Gamma(\frac{\nu+m+1}{2})}{\Gamma(\frac{\nu+m+n}{2})}\,\rho^\nu$$

It is no coincidence that the factor $\frac{2^\nu}{\nu!\,\sqrt{\pi}}$ emerges. If we namely apply Legendre's duplication formula to $\Gamma(2a)$, where $a := \frac{\nu+1}{2}$ (cf., e.g., [6, Theorem 1.5.1]), it follows that $\frac{2^\nu}{\nu!\,\sqrt{\pi}} = \frac{1}{\Gamma(\frac{\nu+1}{2})\Gamma(\frac{\nu+2}{2})}$, whence

$$I = \frac{1}{\Gamma(n/2)}\,(1-\rho^2)^{n/2}\sum_{\nu=0}^\infty \frac{1+(-1)^{m+\nu}}{2}\,\frac{\Gamma^2\big(\frac{\nu+n}{2}\big)\Gamma(\frac{\nu+m+1}{2})}{\Gamma(\frac{\nu+1}{2})\Gamma(\frac{\nu+2}{2})\Gamma(\frac{\nu+m+n}{2})}\,\rho^\nu\,.$$

Obviously, we only have to consider the set of all $\nu \in \mathbb{N}_0$, such that $\nu + m$ is even. So, we need to distinguish between the odd case and the even case, relative to m. Firstly, let m be odd. Then $\nu \in \{2l+1 : l \in \mathbb{N}_0\}$. Due to the definition of the constant $c_{\mathrm{odd}}(m,n)$ and the structure of the special function ${}_3F_2$, it follows immediately that

$$I = (1-\rho^2)^{n/2}\,\frac{1}{\Gamma(n/2)}\,\rho\sum_{l=0}^\infty \frac{\Gamma^2\big(l+\frac{n+1}{2}\big)\Gamma(l+\frac{m+2}{2})}{\Gamma(l+\frac{m+n+1}{2})\Gamma(l+\frac{3}{2})}\,\frac{(\rho^2)^l}{l!}$$
$$= c_{\mathrm{odd}}(m,n)\,(1-\rho^2)^{\frac{n}{2}}\,\rho\,{}_3F_2\Big(\frac{n+1}{2},\frac{n+1}{2},\frac{m+2}{2};\frac{3}{2},\frac{m+n+1}{2};\rho^2\Big),$$

which concludes the proof of (i).

Similary, the representation (ii) can be derived if m is even. Finally, the last equality in (4.110) again is an implication of Euler's transformation formula of hypergeometric functions (cf., e.g., [6, Theorem 2.2.5, formula (2.2.7)]). □

Remark 4.13. The special case (4.110) is contained in (the proof of) [24, Lemma 2.1].

Remark 4.14. Let $p \in (-1,\infty)$ and $f \in L^2(\gamma_1)$, satisfying $f(ry) = r^p\,f(y)$ for all $(r,y) \in (0,\infty)\times\mathbb{R}$. A natural question is, whether $I_f := \mathbb{E}\Big[\Big\langle f\Big(\frac{\mathbf{X}}{\|\mathbf{X}\|_{\mathbb{R}_2^n}}, \frac{\mathbf{Y}}{\|\mathbf{Y}\|_{\mathbb{R}_2^n}}\Big)\Big\rangle_{\mathbb{R}_2^n}\Big]$ can be similarly represented as $I = I_{f_m}$? In general, it seems that a closed-form representation of I_f is not possible. However, our proof of Theorem 4.12 clearly reveals that

$$I_f = \frac{\sqrt{\pi}}{2^{p/2}\,\Gamma(n/2)}\,(1-\rho^2)^{n/2}\sum_{\nu=0}^\infty \frac{\Gamma^2\big(\frac{\nu+n}{2}\big)}{2^{\nu/2}\,\Gamma(\frac{\nu+1}{2})\Gamma(\frac{\nu+2}{2})\Gamma(\frac{\nu+p+n}{2})}\,\mathbb{E}[f(X)X^\nu]\,\rho^\nu$$
$$= \mathbb{E}\Big[f(X)\,\frac{\sqrt{\pi}}{2^{p/2}\,\Gamma(n/2)}\,(1-\rho^2)^{n/2}\sum_{\nu=0}^\infty \frac{\Gamma^2\big(\frac{\nu+n}{2}\big)}{2^{\nu/2}\,\Gamma(\frac{\nu+1}{2})\Gamma(\frac{\nu+2}{2})\Gamma(\frac{\nu+p+n}{2})}\,(\rho X)^\nu\Big],$$

where $X \sim N_1(0,1)$. Observe that the factor $2^{\nu/2}$ in the denominator cancels out in the f_m-case (i.e., if $f = f_m$)! It originates from the integral

$$\int_{\mathbb{S}^{n-1}} f(\langle u, v\rangle_{l_n^2})\, \langle u, v\rangle_{l_n^2}^{\nu}\, \mathrm{d}\sigma_{n-1}(v) = 2^{-p/2}\, 2^{-\nu/2}\, \frac{\Gamma(\frac{n}{2})}{\Gamma(\frac{\nu+p+n}{2})}\, \mathbb{E}[f(X)X^{\nu}]$$

(cf. Corollary 4.6). In general, that important reduction of the fraction cannot be maintained, though. Hence, if we represent the latter series as the sum of the even series part and the odd series part, we obtain

$$I_f = I_f^{\text{even}} + I_f^{\text{odd}}\,,$$

where

$$I_f^{\text{even}} := \mathbb{E}\Big[f(X)\, \frac{\sqrt{\pi}}{2^{p/2}\,\Gamma(n/2)}\,(1-\rho^2)^{n/2} \sum_{l=0}^{\infty} \frac{\Gamma^2\big(l+\frac{n}{2}\big)}{\Gamma(l+\frac{1}{2})\Gamma(l+\frac{p+n}{2})}\, \frac{(\frac{1}{2}\rho^2X^2)^l}{l!}\Big]$$

and

$$I_f^{\text{odd}} := \mathbb{E}\Big[Xf(X)\, \frac{\sqrt{\pi}}{2^{(p+1)/2}\,\Gamma(n/2)}\,\rho(1-\rho^2)^{n/2} \sum_{l=0}^{\infty} \frac{\Gamma^2\big(l+\frac{1+n}{2}\big)}{\Gamma(l+\frac{3}{2})\Gamma(l+\frac{p+n+1}{2})}\, \frac{(\frac{1}{2}\rho^2X^2)^l}{l!}\Big].$$

A straightforward calculation shows that

$$I_f^{\text{even}} = c_+(p,n)\sqrt{\frac{\pi}{2}}\frac{1}{(p-1)!!\,b_{p+1}}\,(1-\rho^2)^{n/2}\mathbb{E}\Big[f(X)\,{}_2F_2\Big(\frac{n}{2},\frac{n}{2};\frac{1}{2},\frac{p+n}{2};(\tfrac{1}{\sqrt{2}}\rho X)^2\Big)\Big]$$

and

$$I_f^{\text{odd}} = c_-(p,n)\sqrt{\frac{\pi}{2}}\frac{1}{p!!\,b_{p+2}}\,\rho(1-\rho^2)^{n/2}\mathbb{E}\Big[Xf(X)\,{}_2F_2\Big(\frac{n+1}{2},\frac{n+1}{2};\frac{3}{2},\frac{p+n+1}{2};(\tfrac{1}{\sqrt{2}}\rho X)^2\Big)\Big]\,,$$

where b_n satisfies (4.93) ($n \in \{p+1, p+2\}$).

5. Completely correlation preserving functions

5.1. Completely real analytic functions and the entrywise matrix functional calculus

Already while looking for the smallest upper bound of both, $K_G^{\mathbb{R}}$ and $K_G^{\mathbb{C}}$, we are lead to a deep interplay of different subfields of mathematics (both, pure and applied) including Gaussian harmonic analysis and Malliavin calculus (Mehler kernel, Ornstein-Uhlenbeck semigroup, Hermite polynomials, Gegenbauer polynomials (also known as *ultraspherical polynomials*), integration over spheres in $\mathbb{R}^n$), complex analysis (analytic continuation and biholomorphic mappings, special functions), combinatorial analysis (inversion of Taylor series and ordinary partial Bell polynomials), matrix analysis (positive semidefinite matrices, block matrices) and multivariate statistics and high-dimensional Gaussian dependence modelling (correlation matrices, real and complex Gaussian random vectors, Gaussian measure).

In particular, we have to look for those functions which map correlation matrices of any size and any rank entrywise into a correlation matrix of the same size again, by means of the so-called *Hadamard product* of matrices:

Definition 5.1 (**Hadamard product**)**.** Let $m, n \in \mathbb{N}$. Let $A = (a_{ij}) \in \mathbb{M}_{m,n}(\mathbb{F})$ and $B = (b_{ij}) \in \mathbb{M}_{m,n}(\mathbb{F})$. The Hadamard product $A * B \in \mathbb{M}_{m,n}(\mathbb{F})$ is defined as

$$(A * B)_{ij} := a_{ij}\, b_{ij} \quad ((i,j) \in [m] \times [n])\,.$$

The Hadamard product is sometimes called the *entrywise product*, for obvious reasons, or the *Schur product*, because of some early and basic results about the product obtained by Issai Schur (cf. [68]). Like the usual matrix product, the distributive law also holds for the Hadamard product: $A * (B + C) = A * B + A * C$. Unlike the usual matrix product, the Hadamard product is commutative: $A * B = B * A$.

Remark 5.2. Very often, the Hadamard product is denoted by the symbol $\circ$. However, given our view, the symbolic notation $\circ$ perhaps could lead to a minor ambiguity, since quite regularly, $\circ$ denotes composition of mappings. This is why we adopt the symbol $*$ instead, used for the definition of the Schur product in [114, p 29 ff].

Remark 5.3 (**Hadamard product as subordinated Kronecker product**)**.** Fix $m, n \in \mathbb{N}$ and $A, B \in \mathbb{M}_{m,n}(\mathbb{F})$. There exists an interesting link between the Hadamard product $A * B$ and the Kronecker product $A \otimes B$, induced by (1.5) and (3.71). In order to recognise this, let $(i,j) \in [m] \times [n]$ be given arbitrarily. Then

$$\begin{aligned}(A * B)_{ij} &= (e_i^\top A e_j)(e_i^\top B e_j) \overset{(!)}{=} e_i^\top \otimes e_i^\top (A \otimes B) e_j \otimes e_j \\ &\overset{(3.71)}{=} e^{(m^2)\top}_{(i-1)m+i}(A \otimes B) e^{(n^2)}_{(j-1)n+i} = (A \otimes B)_{\Psi_m(i,i), \Psi_n(j,j)}\,.\end{aligned}$$

Consequently,

$$A * B = (A \otimes B)_\psi\,,$$

where $\psi(i,j) := (\Psi_m(i,i), \Psi_n(j,j)) = ((i-1)m + i, (j-1)n + j)$ for all $(i,j) \in [m] \times [n]$.

If we combine the latter fact and Proposition 3.26, we immediately obtain (cf. also (5.114)):

Proposition 5.4. *Let $m, n \in \mathbb{N}$, $S \in \mathbb{M}_{m,n}(\mathbb{F})$ and $R \in \mathbb{M}_{m,n}(\mathbb{F})$. If $S \in \mathcal{Q}_{m,n}(\mathbb{F})$ and $R \in \mathcal{Q}_{m,n}(\mathbb{F})$, then $S * R \in \mathcal{Q}_{m,n}(\mathbb{F})$. Note again that the Hadamard product is commutative.*

Although, the proof of the following two facts are just a consequent application of the definition of the Schur product, they are of interest on their own, and they help us strongly to support, inter alia, a quick proof of Theorem 5.8. In this context, diagonal matrices play an important role: if $a = (a_1, \ldots, a_p)^\top \in \mathbb{F}^p$, then $D_a \in \mathbb{M}_p(\mathbb{F})$ denotes the matrix, whose (i,j)'th entry is given by $\delta_{ij}\, a_j$. Moreover, we need the matrix $J^{(m,n)} \in \mathbb{M}_{m,n}(\mathbb{F})$, whose (i,j)'th entry is given by 1: $J^{(m,n)} := \sum_{i=1}^m \sum_{j=1}^n e_i e_j^\top$.

Lemma 5.5. *Let $m, n \in \mathbb{N}$, $B \in \mathbb{M}_{m,n}(\mathbb{F})$ and $(x,y) \in \mathbb{F}^m \times \mathbb{F}^n$. Then*

$$\Gamma_{\mathbb{F}}(x,y) * B = \overline{x} y^\top * B = D_x^* B D_y\,.$$

In particular,

$$\Gamma_{\mathbb{F}}(y,y) * A \in \mathbb{M}_n(\mathbb{F})^+ \textit{ for all } A \in \mathbb{M}_n(\mathbb{F})^+\,.$$

Lemma 5.6 (Hadamard product factor shifting). *Let $m, n \in \mathbb{N}$ and $A, B, C \in \mathbb{M}_{m,n}(\mathbb{F})$. Then*

$$\langle A * \overline{B}, J^{(m,n)} \rangle_F = \langle A, B \rangle_F = \langle J^{(m,n)}, \overline{A} * B \rangle_F . \tag{5.113}$$

In particular,

$$\langle A * B, C \rangle_F = \langle B, \overline{A} * C \rangle_F .$$

Remark 5.7. Lemma 5.6 implies that for any $A \in \mathbb{M}_n(\mathbb{F})$ the adjoint of the Schur multiplier $S_A : \mathbb{M}_{m,n}(\mathbb{F}) \longrightarrow \mathbb{M}_{m,n}(\mathbb{F})$, $B \mapsto A * B$ coincides with the Schur multiplier $S_{\overline{A}}$ (cf. [114, p. 29 ff]):

$$S_A^* = S_{\overline{A}} .$$

The usefulness of the structure of the Hadamard product is reflected in the Schur product theorem which states that the (closed, convex and self-dual) cone of all positive semidefinite matrices is stable under Schur multiplication. We give a short and completely self-contained proof:

Theorem 5.8 (Schur, 1911). *Let $n \in \mathbb{N}$. Let $A \in \mathbb{M}_n(\mathbb{F})^+$ and $B \in \mathbb{M}_n(\mathbb{F})^+$ be positive semidefinite. Then $A * B \in \mathbb{M}_n(\mathbb{F})^+$. In particular,*

$$C(n; \mathbb{F}) * C(n; \mathbb{F}) \subseteq C(n; \mathbb{F}). \tag{5.114}$$

Proof. Fix $y \in \mathbb{F}^n$, and put $M := \Gamma_{\mathbb{F}}(\overline{y}, \overline{y}) * \overline{B} = yy^* * \overline{B}$. Because of Lemma 5.5, $M^* = M \in \mathbb{M}_n(\mathbb{F})^+$ (since also $\overline{B} \in \mathbb{M}_n(\mathbb{F})^+$). Consequently, Lemma 5.6 implies that

$$\begin{aligned} y^*(A * B)y &= \mathrm{tr}(yy^*(A * B)) = \langle A * B, yy^* \rangle_F = \langle A, M \rangle_F = \mathrm{tr}\Big(M^{1/2} M^{1/2} A^{1/2} A^{1/2}\Big) \\ &= \mathrm{tr}\Big((M^{1/2} A^{1/2})(A^{1/2} M^{1/2})\Big) = \| A^{1/2} M^{1/2} \|_F^2 \geq 0 , \end{aligned}$$

and the claim follows. □

Definition 5.9 (Entrywise functional calculus). Let $m, n \in \mathbb{N}$. Given $\emptyset \neq U \subseteq \mathbb{F}$, a function $f : U \longrightarrow \mathbb{F}$ and a matrix $A = (a_{ij}) \in \mathbb{M}_{m,n}(U)$ put

$$f[A] := (f(a_{ij})) \quad ((i, j) \in [m] \times [n]) .$$

In particular, if $f(x) = \sum_{n=0}^{\infty} c_n \, x^n, x \in U$, where $c_n \in \mathbb{F}$ for all $n \in \mathbb{N}$, we have

$$f[A]_{ij} = \sum_{n=1}^{\infty} c_n \, a_{ij}^n \text{ for all } (i, j) \in [m] \times [n] .$$

Functions of the latter type, where $c_n \geq 0$ for all $n \in \mathbb{N}$ play a significant role, also with respect to an analysis of $K_G^{\mathbb{R}}$ and $K_G^{\mathbb{C}}$. This is particularly reflected in the next two results with respect to the real field, which however also play a key role in the complex case (cf. Theorem 7.2 and Corollary 7.4). Recall that a function $\psi : I \longrightarrow \mathbb{R}$, defined on an open interval $I \subseteq \mathbb{R}$, is *absolutely monotonic*, if $\psi \in C^\infty(I)$ and $\psi^{(n)} \geq 0$ on I for all $n \in \mathbb{N}_0$ (cf. e.g. [82, Chapter 19] and [149, Chapter IV] regarding a rigorous reassessment of that crucial and very rich concept, coined by S. N. Bernstein in 1929). Regarding a refresher of complex analysis of functions of one complex variable, we recommend to place the rich source [135] next to our paper.

Lemma 5.10. *Let $r \in (0,\infty)$ and $\psi : (-r,r) \longrightarrow \mathbb{R}$ be real analytic. Suppose that $b := \left(\frac{\psi^{(n)}(0)}{n!}\, r^n\right)_{n\in\mathbb{N}_0} \in l_1$. Then $\psi = \widetilde{\psi}\Big|_{(-r,r)}$, where the complex, bounded function $\widetilde{\psi} : r\overline{\mathbb{D}} \longrightarrow \|b\|_1\overline{\mathbb{D}}$ is defined as*

$$\widetilde{\psi}(z) := \sum_{n=0}^{\infty} \frac{\psi^{(n)}(0)}{n!}\, z^n \text{ for all } z \in r\overline{\mathbb{D}}.$$

The real function $\psi_{abs} : [-r,r] \longrightarrow [-\|b\|_1, \|b\|_1], x \mapsto \sum_{n=0}^{\infty} \frac{|\psi^{(n)}(0)|}{n!}\, x^n$ is continuous and bounded, such as the complex-valued function $\widetilde{\psi}$. $\psi_{abs}\Big|_{(-r,r)}$ is real analytic, and $\psi_{abs}\Big|_{(0,r)}$ is absolutely monotonic on $(0,r)$. $\|b\|_1 = \psi_{abs}(r)$ and

$$|\widetilde{\psi}(z)| \leq \psi_{abs}(|z|) \leq \psi_{abs}(r) \text{ for all } z \in r\overline{\mathbb{D}}\,. \tag{5.115}$$

In particular, ψ_{abs} can be extended to the continuous complex function $\widetilde{\psi}_{abs} : r\overline{\mathbb{D}} \longrightarrow \|b\|_1\overline{\mathbb{D}}$, defined as

$$\psi_{abs}(z) \equiv \widetilde{\psi}_{abs}(z) := \sum_{n=0}^{\infty} \frac{|\psi^{(n)}(0)|}{n!}\, z^n \text{ for all } z \in r\overline{\mathbb{D}}.$$

$\widetilde{\psi}\Big|_{r\mathbb{D}}$ (respectively $\psi_{abs}\Big|_{r\mathbb{D}}$) is the unique holomorphic extension of ψ (respectively $\psi_{abs}\Big|_{(-r,r)}$) on the domain $r\mathbb{D}$.

Proof. Since ψ on $(-r,r)$ is real analytic, it follows that (locally, around 0)

$$\psi(x) = \sum_{n=0}^{\infty} b_n\, x^n \text{ for all } x \in (-s,s),$$

for some $0 < s \leq r$, where $b_n := \frac{\psi^{(n)}(0)}{n!} \in \mathbb{R}$ for all $n \in \mathbb{N}_0$. By assumption, $r > 0$, and $\sum_{n=0}^{\infty} |b_n| r^n = \|b\|_1 < \infty$, whence $\sum_{n=0}^{\infty} |b_n||x|^n \leq \|b\|_1 < \infty$ for all $x \in [-r,r]$. Thus, $(-r,r) \ni x \mapsto \sum_{n=0}^{\infty} b_n\, x^n$ is a well-defined real analytic function which coincides with the real analytic function ψ on the open subset $(-s,s)$ of the open interval $(-r,r)$. Consequently, both real analytic functions on $(-s,s)$ have to coincide on $(-r,r)$ (cf. [88, Corollary 1.2.4 and Corollary 1.2.6]). Clearly, $\widetilde{\psi}$ is well-defined and satisfies $\psi = \widetilde{\psi}\Big|_{(-r,r)}$. Since $\|b\|_1 < \infty$ (by assumption), it follows that the series of continuous functions $\sum_{n=0}^{\infty} |b_n| x^n$ converges normally in $[-r,r]$ (with respect to the supremum norm) and hence uniformly in $[-r,r]$ (due to the majorant criterium (or M-test) of Weierstrass). Consequently, the function

$$[-r,r] \ni x \mapsto \psi_{\text{abs}}(x) = \sum_{n=0}^{\infty} |b_n| x^n$$

is well-defined, real analytic on $(-r,r)$ and continuous on $[-r,r]$. Similarly, it follows that the function $\widetilde{\psi}$ is continuous. Finally, given the construction of ψ_{abs}, the existence of $\widetilde{\psi_{\text{abs}}}$ is trivial. □

Since that class of real analytic functions plays a recurring and decisive role in our paper (particularly for $r = 1$), and since real (and complex) analyticity of a function actually is a local property, it is justifiable to introduce the following definition:

Definition 5.11. Let $r \in (0, \infty)$. Put

$$W_+^\omega((-r,r)) := \{\psi : \psi \in C^\omega((-r,r)) \text{ and } \Big(\frac{\psi^{(n)}(0)}{n!} r^n\Big)_{n \in \mathbb{N}_0} \in l_1\}.$$

Any element in $\psi \in W_+^\omega((-r,r))$ is said to be *completely real analytic on* $(-r,r)$ *at* 0.

Observe that by definition any function in $W_+^\omega((-r,r))$ coincides with its own Taylor series at 0 "completely" (i.e., *everywhere*) on its domain of definition $(-r,r)$ (and not "locally, around" 0 only). Moreover, due to Lemma 5.10, it follows that for any $\psi \in W_+^\omega((-r,r))$ also $\psi_{\text{abs}}\big|_{(-r,r)} \in W_+^\omega((-r,r))$, and

$$\psi_{\text{abs}}^{(n)}(0) = |\psi^{(n)}(0)| \text{ for all } n \in \mathbb{N}_0 \,. \tag{5.116}$$

Let us explicitly highlight three facts, implied by Lemma 5.10. To this end, if $\alpha \in \mathbb{T}$ is given, we consider the biholomorphic function $M_\alpha : \mathbb{C} \longrightarrow \mathbb{C}$, defined as $M_\alpha(z) := \alpha z$. Obviously, $M_\alpha^{-1} = M_{\overline{\alpha}}$ and $M_\alpha(\mathbb{D}) = \mathbb{D}$.

Remark 5.12 (Sign condition). Let ψ and $\widetilde{\psi}$ be given as in Lemma 5.10. If ψ is odd and $\text{sign}(\psi^{(2n+1)}(0)) = (-1)^n$ for all $n \in \mathbb{N}_0$, then

$$\psi_{\text{abs}}(z) = \frac{1}{i}\widetilde{\psi}(iz) = (M_{-i} \circ \widetilde{\psi} \circ M_i)(z) \text{ for all } z \in r\overline{\mathbb{D}}$$

and

$$\psi_{\text{abs}}^{(2n+1)}(\zeta) = (-1)^n\, \widetilde{\psi}^{(2n+1)}(i\zeta) \text{ for all } \zeta \in r\mathbb{D} \text{ and } n \in \mathbb{N}_0$$

(since $i^{2n} = (-1)^n$ for all $n \in \mathbb{N}_0$).

Remark 5.13 (Wiener algebra). Let ψ be given as in Lemma 5.10. Assume that $r = 1$. Then $\widetilde{\psi}\big|_{\mathbb{D}}$ and $\psi_{\text{abs}}\big|_{\mathbb{D}}$ are elements of

$$W^+(\mathbb{D}) := \{f : f(z) = \sum_{n=0}^{\infty} b_n z^n \text{ is holomorphic on } \mathbb{D} \text{ and satisfies } \sum_{n=0}^{\infty} |b_n| < \infty\}\,.$$

$W^+(\mathbb{D})$ is known as the *Wiener algebra*. It is a unital commutative (complex) Banach algebra with respect to the norm $\| \sum_{n=0}^{\infty} b_n z^n \|_{W^+(\mathbb{D})} := \sum_{n=0}^{\infty} |b_n|$, where multiplication is defined as that one of analytic functions, via the Cauchy product formula (cf. [104]). In particular, $\|\widetilde{\psi}\big|_{\mathbb{D}}\|_{W^+(\mathbb{D})} = \psi_{\text{abs}}(1) = \|\psi_{\text{abs}}\big|_{\mathbb{D}}\|_{W^+(\mathbb{D})}$. Since by construction of $W^+(\mathbb{D})$ the series $f = \sum_{n=0}^{\infty} f_n$ is normally convergent in $\overline{\mathbb{D}}$ (with respect to the supremum norm), where $\overline{\mathbb{D}} \ni z \mapsto f_n(z) := b_n z^n$, the series f is uniformly convergent in $\overline{\mathbb{D}}$, and it follows that every element of $W^+(\mathbb{D})$ can be continuously extended to an element of the unital commutative Banach algebra $A(\mathbb{D})$, where

$$A(\mathbb{D}) := \{g : g \in C(\overline{\mathbb{D}}) \text{ such that } g\big|_{\mathbb{D}} \text{ is holomorphic on } \mathbb{D}\}$$

is equipped with the supremum norm and the usual pointwise algebraic operations. $A(\mathbb{D})$ denotes the well-known *disc algebra* (cf. [47, V.1., Example 4] and [150, Chapter III.E.]). Thus, $W^+(\mathbb{D})$ could be viewed as a subalgebra of the disc algebra $A(\mathbb{D})$. Since $A(\mathbb{D}) \subseteq H^\infty \subseteq H^2 \subseteq H^1$, it is likely that a further link to the very rich theory of Hardy spaces might open up here (cf., e.g., [47, 81, 125, 126]) .

Remark 5.14 (**Inversion and complete real analyticity**)**.** Like a common thread, the following highly non-trivial problem - which is decisive for the determination of upper bounds of $K_G^{\mathbb{F}}$ - runs through our entire paper. Very generally formulated, let $\psi \in W_+^\omega((-1,1))$ be odd and completely real analytic on $(-1,1)$ at 0. Assume that $\psi = \psi_{\text{abs}}\big|_{(-1,1)}$ and that $\psi : (-1,1) \overset{\cong}{\longrightarrow} (-1,1)$ is bijective. Assume further that ψ^{-1} is real analytic on $(-1,1)$. Does $\psi^{-1} \in W_+^\omega((-1,1))$ already apply then; i.e., is then also $(\psi^{-1})_{\text{abs}}$ well-defined (cf., e.g., Lemma 6.11, Corollary 6.34, Theorem 6.45, Example 6.48 and Example 7.15)? Both, [22] and [57] present multi-page proofs, each one built on rather advanced complex analysis (including tricky holomorphic extension techniques), to answer that problem to the positive for key functions $\psi \in W_+^\omega((-1,1))$ in relation to the determination of the values of $K_G^{\mathbb{C}}$, respectively $K_G^{\mathbb{R}}$!

5.2. Completely correlation preserving functions and Schoenberg's theorem

Let $0 < c \leq r$ and ψ be given as in Lemma 5.10. Assume that $\psi \neq 0$. Since $\psi \in W_+^\omega((-r,r))$, it follows that $\psi^{(n_0)}(0) \neq 0$ for some $n_0 \in \mathbb{N}_0$, implying that $\psi_{\text{abs}}(c) \geq \frac{|\psi^{(n_0)}(0)|}{n_0\,!}\, c^{n_0} > 0$. Thus, the function

$$(-1,1) \ni \rho \mapsto \psi_c(\rho) := \frac{\psi(c\rho)}{\psi_{\text{abs}}(c)} \tag{5.117}$$

is well-defined, continuous, bounded and satisfies $0 \neq \psi_c \in W_+^\omega((-1,1))$. In Theorem 6.32 we will shed light on the hidden structure of these functions ψ_c. Let $n \in \mathbb{N}$. Since $(\psi_c)_{\text{abs}}(1) = 1$, it even follows that $(\psi_c)_{\text{abs}} = \frac{\psi_{\text{abs}}(c\,\cdot)}{\psi_{\text{abs}}(c)} : [-1,1] \longrightarrow [-1,1]$ transforms any real $n \times n$-correlation matrix entrywise into a real $n \times n$-correlation matrix; i.e.,

$$(\psi_c)_{\text{abs}}[A] \in C(n;\mathbb{R}) \text{ for all } A \in C(n;\mathbb{R}), \text{ for all } n \in \mathbb{N} \tag{5.118}$$

(due to Theorem 5.8). Within the scope of our paper, functions $f \in C([-1,1])$, satisfying $f\big|_{(-1,1)} \in W_+^\omega((-1,1))$ and $f\big|_{(-1,1)}(\rho) = \Big(f\big|_{(-1,1)}\Big)_{\text{abs}}(\rho)$ for all $\rho \in (-1,1)$, are of particular importance, due to the following version of a fundamental result of I. J. Schoenberg (cf. [82, Theorem 16.2] and [131]):

Theorem 5.15 (**Schoenberg, 1942**)**.** *Let $f : [-1,1] \longrightarrow \mathbb{R}$ be a continuous function. Then the following statements are equivalent:*

(i) *$f[A]$ is positive semidefinite for all $A \in \bigcup_{n=1}^\infty \mathbb{M}_n([-1,1])^+$.*

(ii) *$f[\Sigma]$ is positive semidefinite for all $\Sigma \in \bigcup_{n=1}^\infty C(n;\mathbb{R})$.*

(iii) *$f(x)$ equals a convergent series $\sum_{n=0}^\infty a_n\, x^n$ for all $x \in [-1,1]$, where $a_n \geq 0$ for all $n \in \mathbb{N}_0$.*

(iv) *$f\big|_{(-1,1)} \in W_+^\omega((-1,1))$ and $f = \Big(f\big|_{(-1,1)}\Big)_{abs}$.*

(v) *$f\big|_{(-1,1)} \in W_+^\omega((-1,1))$ and $f\big|_{(0,1)}$ is absolutely monotonic.*

(vi) $f\big|_{(-1,1)}$ *can be extended to a holomorphic function* $\mathbb{D} \ni z \mapsto \widetilde{f}(z) := \sum_{n=0}^{\infty} a_n z^n$, *where* $a_n \geq 0$ *for all* $n \in \mathbb{N}_0$ *and* $f(1) = \sum_{n=0}^{\infty} a_n < \infty$.

In particular, if (iii) or (vi) holds, then $a_n = \frac{f^{(n)}(0)}{n!} \geq 0$ *for all* $n \in \mathbb{N}_0$, *and the series* $\sum_{n=0}^{\infty} a_n x^n$ *converges uniformly on* $[0, 1]$.

Proof. $(i) \Rightarrow (ii)$: trivial (since $C(n;\mathbb{R}) \subseteq \mathbb{M}_n([-1,1])^+$ for all $n \in \mathbb{N}$).
$(ii) \Leftrightarrow (iii)$: See [82, Theorem 16.24, p. 107 and remarks below].
$(iii) \Rightarrow (iv)$: Since $f\big|_{(-1,1)}$ coincides with a real analytic function on $(-1, 1)$ (namely the series $\sum_{n=0}^{\infty} a_n x^n$), it follows that $a_n = \frac{f^{(n)}(0)}{n!} \geq 0$ (cf. [88, Corollary 1.1.16]).
$(iv) \Rightarrow (v)$: Given an arbitrary $n \in \mathbb{N}_0$, the assumption (iv) implies that we only have to calculate the n-th derivative of the series on $(0, 1)$.
$(v) \Rightarrow (vi)$: Firstly, Bernstein's Theorem (cf. e. g. [149, Theorem 3a, p. 146]) implies that $f\big|_{(0,1)}$ has the holomorphic extension $\mathbb{D} \ni z \mapsto \widetilde{f}(z) := \sum_{n=0}^{\infty} a_n z^n$, where $a_n := \frac{f^{(n)}(0)}{n!} \geq 0$ for all $n \in \mathbb{N}_0$. Since $f\big|_{(-1,1)} \in C^{\omega}((-1, 1))$ in particular is real analytic, it follows that $f\big|_{(-1,1)} = \widetilde{f}\big|_{(-1,1)}$ (cf. [88, Corollary 1.1.16]). Since f is continuous (by assumption), it therefore follows that $f(1) = \lim_{x\uparrow 1} \widetilde{f}(x) = \sum_{n=0}^{\infty} a_n$, where the latter equality follows from Abel's theorem on power series.
$(vi) \Rightarrow (iii)$: Since $f(1) = \sum_{n=0}^{\infty} a_n < \infty$ and $a_n \geq 0$ for all $n \in \mathbb{N}_0$, it clearly follows that $\sum_{n=0}^{\infty}(-1)^n a_n \leq f(1) < \infty$. Since f is continuous (by assumption), Abel's theorem on power series therefore implies that $f(-1) = \lim_{x\downarrow -1} \widetilde{f}(x) = \sum_{n=0}^{\infty}(-1)^n a_n$, and (iii) follows.
$(iii) \Rightarrow (i)$: Nothing is to show if $f = 0$. If $f \neq 0$, assumption (iii), together with Lemma 5.10 (applied to $r = 1 = c$) implies that $0 \neq f = \left(f\big|_{(-1,1)}\right)_{\text{abs}}$ and $f(1) = f_{\text{abs}}(1) > 0$. Hence, we may apply Lemma 5.10 to the well-defined function $f_1 := \frac{f_{\text{abs}}}{f_{\text{abs}}(1)} = \frac{f}{f(1)}$, and (i) follows.
Finally, since every real analytic function has a unique power series representation (cf. [88, Corollary 1.1.16]), it follows that $a_n = \frac{f^{(n)}(0)}{n!}$ for all $n \in \mathbb{N}_0$. The uniform convergence of the series $\sum_{n=0}^{\infty} a_n x^n$ on $[0, 1]$ follows from [88, Proposition 1.1.3]. $\square$

Fix $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$. Looking for common sources of the real and complex cases, we put $D_{\mathbb{F}} := \{a \in \mathbb{F} : |a| < 1\}$, so that $D_{\mathbb{R}} = (-1, 1)$ and $D_{\mathbb{C}} = \mathbb{D}$. Property (5.118) in Lemma 5.10 deserves an autonomous and far-reaching

Definition 5.16 (**Completely correlation preserving function**). Fix $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$. Let $h : D_{\mathbb{F}} \longrightarrow \mathbb{F}$ be a function.

(i) Given $n \in \mathbb{N}$, h is n-correlation-preserving (short: n-CP) if for any $n \times n$ correlation matrix $\Sigma \in C(n;\mathbb{F})$ also $h[\Sigma] \in C(n;\mathbb{F})$ is an $n \times n$ correlation matrix.

(ii) h is called completely correlation-preserving (short: CCP) if h is n-correlation-preserving for all $n \in \mathbb{N}$.

Since every CCP function h is 2-CP, Definition 5.16 directly implies that $h(\overline{D_{\mathbb{F}}}) \subseteq \overline{D_{\mathbb{F}}}$ and $h(1) = 1$. If $h : \overline{D_{\mathbb{F}}} \longrightarrow \mathbb{F}$ satisfies $h(1) > 0$, then $h[\Sigma] \in \mathbb{M}_n(\overline{D_{\mathbb{F}}})^+$ for all $\Sigma \in C(n;\mathbb{F})$ if and only if $\frac{1}{h(1)}h$ is n-CP. If h_1 and h_2 are two CCP functions (respectively two n-CP functions), and if $\lambda \geq 0$, Definition 5.16 immediately implies that also $h_2 \circ h_1$, $h_1 \circ h_2$ and $\lambda h_1 + (1-\lambda)h_2$ are CCP functions (respectively n-CP functions). Furthermore, since $h_1 h_2[A] = h_1[A] * h_2[A]$ for all matrices $A \in \mathbb{M}_{m,n}(\mathbb{F}), m, n \in \mathbb{N}$, it follows from (5.114) that also the product $h_1 h_2$ of two CCP functions (respectively two n-CP functions) again is CCP (respectively n-CP). Much less trivial is the fact (which involves the Grothendieck constant!) that in general, the inverse function h^{-1} of an invertible CCP function h is *not* a CCP function (cf. Corollary 6.10, Remark 6.44 and Theorem 6.45-(i)), such as the inverse of $h := \frac{2}{\pi}\arcsin$, given by $[-1,1] \ni y \mapsto h^{-1}(y) = \sin(\frac{\pi}{2}y) = \sum_{n=0}^{\infty} b_n \frac{y^n}{n!}$, where $b_n := (-1)^{\lfloor n/2 \rfloor} \cdot \frac{1-(-1)^n}{2} \cdot (\frac{\pi}{2})^n$.

In the real case, Theorem 5.15 immediately leads to a full characterisation of continuous CCP functions, since:

Theorem 5.17. *Let $h : [-1,1] \longrightarrow \mathbb{R}$ be a continuous function. Then the following statements are equivalent:*

(i) *h is CCP.*

(ii) *$h[A]$ is positive semidefinite for all $A \in \bigcup_{n=1}^{\infty} \mathbb{M}_n([-1,1])^+$ and $h(1) = 1$.*

(iii) *$h(x)$ has the unique series representation $h(x) = \sum_{n=0}^{\infty} a_n x^n$ for all $x \in [-1,1]$, where $a_n \geq 0$ for all $n \in \mathbb{N}_0$ and $\sum_{n=0}^{\infty} a_n = 1$.*

(iv) *$[-1,1] \ni \rho \mapsto h(\rho) = \mathbb{E}_{\mathbb{P}}[\rho^X] = \sum_{n=0}^{\infty} \mathbb{P}(X = n)\rho^n$ is the probability generating function of some discrete random variable X.*

(v) *$h\big|_{(-1,1)} \in W_+^{\omega}((-1,1))$, $h = \left(h\big|_{(-1,1)}\right)_{abs}$ and $h(1) = 1$.*

(vi) *$h\big|_{(-1,1)} \in W_+^{\omega}((-1,1))$, $h\big|_{(0,1)}$ is absolutely monotonic and $h(1) = 1$.*

(vii) *$h\big|_{(-1,1)}$ can be extended to a holomorphic function $\mathbb{D} \ni z \mapsto \widetilde{h}(z) := \sum_{n=0}^{\infty} a_n z^n$, where $a_n \geq 0$ for all $n \in \mathbb{N}_0$ and $\sum_{n=0}^{\infty} a_n = 1$.*

(viii) *$h\big|_{(-1,1)}$ can be extended to a complex function $\widetilde{H} : \overline{\mathbb{D}} \longrightarrow \overline{\mathbb{D}}, z \mapsto \sum_{n=0}^{\infty} a_n z^n$, where $a_n \geq 0$ for all $n \in \mathbb{N}_0$ and $\sum_{n=0}^{\infty} a_n = 1$.*

If (iii) *or* (vii) *or* (viii) *is given, the series $\sum_{n=0}^{\infty} a_n z^n$ converges then absolutely on $\overline{\mathbb{D}}$ and $\sum_{n=0}^{\infty} a_n x^n$ converges uniformly on $[0,1]$.*

Remark 5.18 (CCP versus RKHS). Theorem 5.17-(iii) also reveals a direct link to representing kernel Hilbert spaces (RKHS). [115, Theorem 4.12.], together with the remark on complexification in [115, Chapter 5.1] namely implies that

$$(-1,1) \times (-1,1) \ni (s,t) \mapsto K_h(s,t) := \sum_{n=0}^{\infty} a_n (st)^n = \sum_{n=0}^{\infty} f_n(s) f_n(t)$$

is a well-defined kernel function for a real RKHS $H(K_h)$ of real-analytic functions on $(-1,1)$ (cf. [115, Definition 2.12]), where $f_n(\rho) := \sqrt{a_n}\,\rho^n$. The set of functions f_n for which $a_n \neq 0$ is an orthonormal basis for $H(K_h)$.

It is quite instructive to analyse how n-CP functions in particular relate to properties of Schoenberg's kernel functions $\mathcal{P}(\mathbb{S}^d)$, $d \in \mathbb{N}$. Schoenberg's approach was revisited by the geostatistician T. Gneiting in his impressive paper [49], where $\mathcal{P}(\mathbb{S}^d)$ is denoted as Ψ_d. So, let us recall the concept of a positive definite function on a metric space (which in particular is a kernel function (cf. [115, Definition 2.12.]), originally coined by Schoenberg in [131]. Supported by Lemma 3.2, these kernel functions result in a further characterisation of real-valued n-CP functions. In order to recognise this observation, let (X, d) be a metric space. Fix $d \in \mathbb{N}_2$. A function $f : [0, \infty) \longrightarrow \mathbb{R}$ is positive definite on X if f is continuous, and if *for any* $n \in \mathbb{N}$ and any $(x_1, x_2, \ldots, x_n) \in X^\nu$, the matrix $f[d(x_i, x_j)_{i,j=1}^n]$ is positive semidefinite (cf. [82, Definition 16.15] and [49, 131]). Consequently, if we apply Schoenberg's definition to the unit sphere $\mathbb{S}^{d-1}$, where the metric on $\mathbb{S}^{d-1}$ is induced by the geodesic distance $\mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \ni (x, y) \mapsto \arccos(\langle x, y\rangle)$, Lemma 3.2 implies that any continuous function $f : [-1, 1] \longrightarrow \mathbb{R}$ which satisfies that $f \circ \cos : [0, \pi] \longrightarrow \mathbb{R} \in \mathcal{P}(\mathbb{S}^{d-1}) \equiv \Psi_{d-1}$ in particular is d-CP. Thus, [49, Table 1] shows us a wealth of non-trivial d-CCP functions, where $d \in [3]$. Similarly, we recognise that a continuous function $h : [-1, 1] \longrightarrow \mathbb{R}$ is CCP if and only if $h \circ \cos \in \Psi_\infty = \bigcap_{d=1}^\infty \Psi_d$.

If we combine these facts with [49, Theorem 7], we are rewarded with a large class of (even) CCP functions. To this end, recall that a continuous function $\psi : [0, \infty) \longrightarrow \mathbb{R}$ is called *completely monotone* if $\psi\big|_{(0,\infty)} \in C^\infty((0, \infty))$ and $(-1)^n \psi^{(n)}(x) \geq 0$ for all $n \in \mathbb{N}_0$ and all $x > 0$ (cf., e.g., [82, Definition 27.18] and [149, Definition 2c]). Many explicit examples of completely monotone functions are listed in [103]. They play a significant role in various subfields of probability theory including theory and applications of Lévy processes and infinite divisibility.

Theorem 5.19. *Let $\psi : [0, \infty) \longrightarrow \mathbb{R}$ be completely monotone and non-constant. Suppose that $\psi(0) = 1$, then*

$$\psi \circ \arccos : [-1, 1] \longrightarrow \mathbb{R} \textit{ is a CCP function.}$$

In particular, $\psi([0, \pi]) \subseteq [-1, 1]$.

If we apply the complex analogue of Schoenberg's Theorem, coined by J.P.R. Christensen and P. Ressel in 1982 (cf. [82, Theorem 16.7]) to complex CCP functions, we obtain

Theorem 5.20. *Let $h : \overline{\mathbb{D}} \longrightarrow \mathbb{C}$ be a continuous complex function. Then the following statements are equivalent:*

(i) *h is CCP.*

(ii) *$h(z)$ has the unique series representation $h(z) = \sum_{k=0}^\infty \sum_{l=0}^\infty a_{kl}\, z^k\, \overline{z}^l$ for all $z \in \overline{\mathbb{D}}$, where $a_{kl} \geq 0$ for all $k, l \in \mathbb{N}_0$ and $\sum_{k=0}^\infty (\sum_{l=0}^\infty a_{kl}) = 1$.*

Observe that a significant implication of Theorem 5.20 is that in general *complex* CCP functions are not holomorphic, respectively analytic. Theorem 5.17, together with Lemma 5.10 immediately implies how one can easily construct complex CCP functions out of real ones:

Remark 5.21. Let $h = h_{f,f} : [-1, 1] \longrightarrow [-1, 1]$ be a real CCP function ($\|f\|_{\gamma_k} = 1$) and $\widetilde{h} : \overline{\mathbb{D}} \longrightarrow \overline{\mathbb{D}}$ be as in Lemma 5.10. Then the following functions are all complex CCP functions: $\widetilde{h}$, $\overline{\widetilde{h}}$ and $\widetilde{h} \cdot \overline{\widetilde{h}} = |\widetilde{h}|^2$.

6. The real case: towards extending Krivine's approach

6.1. Some facts about real multivariate Hermite polynomials

Another important estimation (even with upper bound 1) which might help to support our search for a "suitable" CCP function which is different from the CCP function $\frac{2}{\pi}\arcsin$ in the real case, is included in the next two results. We start with the real case first. To this end, recall e.g. from [20, Chapter 1.3] that for fixed $k \in \mathbb{N}$ $\{H_\alpha : \alpha \in \mathbb{N}_0^k\}$ is an ortho*normal* basis in $L^2(\gamma_k)$, where the k-variate Hermite polynomial $H_\alpha : \mathbb{R}^k \longrightarrow \mathbb{R}$ is defined by

$$H_\alpha(x_1, x_2, \ldots, x_k) := \prod_{i=1}^{k} H_{\alpha_i}(x_i) = \frac{(-1)^{|\alpha|}}{\sqrt{\alpha!}} \frac{D^\alpha \varphi_k(x)}{\varphi_k(x)} \,. \tag{6.119}$$

Here, $\varphi_k(x_1, x_2, \ldots, x_k) := \prod_{i=1}^{k} \varphi(x_i)$, $D^\alpha := (\frac{\partial}{\partial x_1})^{\alpha_1} \cdots (\frac{\partial}{\partial x_k})^{\alpha_k}$, $\alpha! := \prod_{i=1}^{k} \alpha_i!$ and $|\alpha| := \sum_{i=1}^{k} \alpha_i$ ($n \in \mathbb{N}_0$, $y \in \mathbb{R}, x = (x_1, \ldots, x_k)^\top \in \mathbb{R}^k$), and

$$\begin{aligned} H_n(y) &:= \frac{1}{\sqrt{n!}}(-1)^n \exp\Big(\frac{y^2}{2}\Big) \frac{\mathrm{d}^n}{\mathrm{d}y^n} \exp\Big(-\frac{y^2}{2}\Big) = \frac{(-1)^n}{\sqrt{n!}} \frac{\varphi^{(n)}(y)}{\varphi(y)} \\ &= \frac{1}{\sqrt{n!}} \sum_{k=0}^{\lfloor n/2 \rfloor} H_{n,k}\, (-1)^k\, y^{n-2k} = (-1)^n H_n(-y). \end{aligned} \tag{6.120}$$

H_n denotes the (probabilist's version of the) one-dimensional Hermite polynomial, where

$$H_{n,k} := \binom{n}{2k} (2k-1)!! = \frac{n!}{2^k k! (n-2k)!} \,.$$

Thus,

$$H_\alpha\, \varphi_k = \frac{(-1)^{|\alpha|}}{\sqrt{\alpha!}} \frac{D^\alpha \varphi_k}{\varphi_k} \,. \tag{6.121}$$

Since $(y + i\, z)^n = \sum_{l=0}^{n} \binom{n}{l} i^l\, z^l\, y^{n-l}$ and $\mathbb{E}[X^m] = \frac{(-1)^m + 1}{2} (m-1)!!$ for all $m, n \in \mathbb{N}_0$, $y, z \in \mathbb{R}$ and $X \sim N_1(0,1)$, it follows that

$$\mathbb{E}[(y + i\, X)^n] = \sum_{l=0}^{n} \binom{n}{l} i^l\, \mathbb{E}[X^l]\, y^{n-l} = \sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n}{2k} (-1)^k\, (2k-1)!!\, y^{n-2k} = \sqrt{n!}\, H_n(y)$$

for all $n \in \mathbb{N}_0$, $y \in \mathbb{R}$ and $X \sim N_1(0,1)$. In particular, we reobtain the numbers

$$H_{2l}(0) = (-1)^l \frac{1}{\sqrt{(2l)!}} (2l-1)!! = (-1)^l \sqrt{\frac{(2l-1)!!}{(2l)!!}} = (-1)^l \frac{\sqrt{(2l)!}}{2^l\, l!} \text{ and } H_{2l+1}(0) = 0 \tag{6.122}$$

for all $l \in \mathbb{N}_0$ (cf. also (6.165)). Recall that the generating function of the one-dimensional Hermite polynomials is given by (cf. [20, (1.3.1)])

$$\mathbb{R} \times \mathbb{R} \ni (\lambda, x) \mapsto \exp\Big(\lambda x - \frac{1}{2}\lambda^2\Big) = \sum_{\nu=0}^{\infty} \frac{\lambda^\nu}{\sqrt{\nu!}} H_\nu(x)$$

implying that in the k-dimensional case the equality

$$\exp\left(\lambda^\top x - \frac{1}{2}\|\lambda\|^2\right) = \prod_{i=1}^{k} \exp\left(\lambda_i\, x_i - \frac{1}{2}\lambda_i^2\right) = \sum_{m\in\mathbb{N}_0^k} \frac{1}{\sqrt{m!}}\, H_m(x)\lambda^m = \sum_{\nu=0}^{\infty}\Big(\sum_{m\in C(\nu,k)} \frac{H_\alpha(x)}{\sqrt{m!}}\Big)\lambda^m \tag{6.123}$$

holds for all $\lambda, x \in \mathbb{R}^k$, where $C(\nu,k) := \{m \in \mathbb{N}_0^k : |m| = \nu\}$. Namely, since $|H_m(x)| \leq (2\pi)^{k/4}\exp\left(\frac{1}{4}\|x\|_2^2\right)$ for all $m \in \mathbb{N}_0^k$ and $x \in \mathbb{R}^k$ (see [36, Lemma 1], respectively [73, Proposition 2.3 (i)]), the quotient test implies that $\sum_{\nu=0}^{\infty} \frac{1}{\sqrt{\nu!}}\, H_\nu(x)\lambda^\nu$ even converges absolutely. Hence, each one of the k families $\left(\frac{1}{\sqrt{\nu!}}\, H_\nu(x_i)\lambda_i^\nu\right)_{\nu\in\mathbb{N}_0}$ is summable ($i \in [k]$). Consequently, it follows that also the family $\Big(\prod_{i=1}^{k} \frac{1}{\sqrt{m_i!}}\, H_{m_i}(x_i)\lambda_i^{m_i}\Big)_{m\in\mathbb{N}_0^k} = \left(\frac{1}{\sqrt{m!}}\, H_m(x)\lambda^m\right)_{m\in\mathbb{N}_0^k}$ is summable. (6.123) now follows from the reiteration of the double summation principle and the associativity formula for summable families. Consequently, we obtain (see also [20, Lemma 1.3.2 (iii)]):

$$\sqrt{m!}\, H_m(x) = D^m \exp(\lambda^\top x - \tfrac{1}{2}\|\lambda\|^2)\Big|_{\lambda=0} = \prod_{\nu=1}^{k} (\tfrac{\partial}{\partial\lambda_\nu})^{m_\nu} \exp(\lambda_\nu x - \tfrac{1}{2}\lambda_\nu^2)\Big|_{\lambda_\nu=0} \tag{6.124}$$

for all $m \in \mathbb{N}_0^k$ and $x \in \mathbb{R}^k$.
In fact, (6.124) allows a further (purely analytic) proof of the Grothendieck *equality* and its multi-dimensional generalisation. As a by-product, we provide a closed-form analytical representation of the multvariate distribution function of a Gaussian random vector $\mathbf{X} \sim N_{2k}(0, \Sigma_{2k}(\rho))$ (cf. Proposition 6.21). In general, closed-form analytical representations of general multivariate Gaussian distribution functions are not available (cf., e.g., [62]). All that can be derived from the calculation of the following vital "Fourier-Hermite coefficients", which include sign as a particular case (cf. Corollary 6.2 below):

Theorem 6.1. *Let $k \in \mathbb{N}$, $m = (m_1, \ldots, m_k)^\top \in \mathbb{N}_0^k$, $a = (a_1, \ldots, a_k)^\top \in \mathbb{R}^k$ and $b = (b_1, \ldots, b_k)^\top \in \mathbb{R}^k$. Put $I_a := \prod_{i=1}^{k}[a_i, \infty)$ and $J_b := \prod_{i=1}^{k}(-\infty, b_i]$. Then*

$$\int_{I_a} H_m\, \mathrm{d}\gamma_k = \langle \mathbb{1}_{I_a}, H_m\rangle_{\gamma_k} = \prod_{\substack{i=1\\ m_i=0}}^{k} (1 - \Phi(a_i)) \prod_{\substack{i=1\\ m_i\neq 0}}^{k} \frac{1}{\sqrt{m_i}}\varphi(a_i) H_{m_i-1}(a_i) \tag{6.125}$$

and

$$\int_{J_b} H_m\, \mathrm{d}\gamma_k = \langle \mathbb{1}_{J_b}, H_m\rangle_{\gamma_k} = (-1)^{c(k,m)} \prod_{\substack{i=1\\ m_i=0}}^{k} \Phi(b_i) \prod_{\substack{i=1\\ m_i\neq 0}}^{k} \frac{1}{\sqrt{m_i}}\varphi(b_i) H_{m_i-1}(b_i), \tag{6.126}$$

where $c(k,m) := k - \sum_{i=1}^{k} \delta_{m_i\, 0} \in \{0, 1, \ldots, k\}$ counts the number of non-zero components of the vector m.

Proof. Firstly, note that

$$\int_{\mathbb{M}} H_m\, \mathrm{d}\gamma_k = \prod_{i=1}^{k} \int_{\mathbb{M}_i} H_{m_i}\, \mathrm{d}\gamma_1 = \prod_{\substack{i=1\\ m_i=0}}^{k} \int_{\mathbb{M}_i} H_{m_i}\, \mathrm{d}\gamma_1 \prod_{\substack{i=1\\ m_i\neq 0}}^{k} \int_{\mathbb{M}_i} H_{m_i}\, \mathrm{d}\gamma_1\,,$$

where $\mathbb{M} \in \{I_a, J_b\}$, $\mathbb{M}_i := [a_i, \infty)$ if $\mathbb{M} = I_a$ and $\mathbb{M}_i := (-\infty, b_i]$ if $\mathbb{M} = J_b$. Consequently, we only have to compute the one-dimensional integral factors

$$\int_{[a_i,\infty)} H_{m_i}\,\mathrm{d}\gamma_1 = \delta_{m_i\,0} - \int_{(-\infty,a_i]} H_{m_i}\,\mathrm{d}\gamma_1\,.$$

To this end, fix $(m, a) \in \mathbb{N}_0 \times \mathbb{R}$. If $m = 0$, then $H_m = 1$, whence

$$\int_{[a,\infty)} H_m\,\mathrm{d}\gamma_1 = \gamma_1([a,\infty)) = \int_a^\infty \varphi(x)\mathrm{d}x = 1 - \Phi(a) = 1 - \int_{(-\infty,a]} H_m\,\mathrm{d}\gamma_1.$$

If $m \neq 0$, (6.124), together with the Leibniz integral rule, applied to the parameter-dependent integral $\int_{[a,\infty)}(\frac{\partial}{\partial\lambda})^m \exp(\lambda x - \frac{1}{2}\lambda^2)\gamma_1(\mathrm{d}x) = 2\pi \int_{[a,\infty)}(\frac{\partial}{\partial\lambda})^m \varphi(x-\lambda)\mathrm{d}x$, imply that

$$\begin{aligned}
-\int_{(-\infty,a]} H_m\,\mathrm{d}\gamma_1 = \int_{[a,\infty)} H_m\,\mathrm{d}\gamma_1 &= \tfrac{1}{\sqrt{m!}}((\tfrac{\partial}{\partial\lambda})^m \int_{[a,\infty)} \varphi(x-\lambda)\mathrm{d}x)\Big|_{\lambda=0}\\
&= \tfrac{1}{\sqrt{m!}}(\tfrac{\partial}{\partial\lambda})^m(1-\Phi(a-\lambda))\Big|_{\lambda=0} = \tfrac{1}{\sqrt{m!}}(\tfrac{\partial}{\partial\lambda})^m\Phi(\lambda-a)\Big|_{\lambda=0}\\
&= \tfrac{1}{\sqrt{m!}}\,\varphi^{(m-1)}(-a) \overset{(6.120)}{=} \tfrac{1}{\sqrt{m}}\varphi(a)H_{m-1}(a).
\end{aligned}$$

□

Corollary 6.2. *Let $k \in \mathbb{N}$, $m = (m_1, \ldots, m_k)^\top \in \mathbb{N}_0^k$, $a = (a_1, \ldots, a_k)^\top \in \mathbb{R}^k$ and $b = (b_1, \ldots, b_k)^\top \in \mathbb{R}^k$. Put $I_a := \prod_{i=1}^k [a_i, \infty)$ and $J_b := \prod_{i=1}^k (-\infty, b_i]$. Let $\chi_a : \mathbb{R}^k \longrightarrow \{-1, 1\}$ and $\psi_b : \mathbb{R}^k \longrightarrow \{-1, 1\}$ be defined as*

$$\chi_a(x) := 2\mathbb{1}_{I_a}(x) - 1 \;\; and \;\; \psi_b(x) := 1 - 2\mathbb{1}_{J_b}(x) = -\chi_{-b}(-x).$$

$$\langle\chi_a, H_0\rangle_{\gamma_k} = 2\prod_{i=1}^k (1-\Phi(a_i)) - 1 \;\; and \;\; \langle\psi_b, H_0\rangle_{\gamma_k} = 1 - 2\prod_{i=1}^k \Phi(b_i). \tag{6.127}$$

If $m \neq 0$, then

$$\begin{aligned}
&\langle\chi_a, H_m\rangle_{\gamma_k} = 2 \prod_{\substack{i=1\\ m_i=0}}^k (1-\Phi(a_i)) \prod_{\substack{i=1\\ m_i\neq0}}^k \frac{1}{\sqrt{m_i}}\varphi(a_i)H_{m_i-1}(a_i)\\
&and\\
&\langle\psi_b, H_m\rangle_{\gamma_k} = 2(-1)^{c(k,m)+1} \prod_{\substack{i=1\\ m_i=0}}^k \Phi(b_i) \prod_{\substack{i=1\\ m_i\neq0}}^k \frac{1}{\sqrt{m_i}}\varphi(b_i)H_{m_i-1}(b_i),
\end{aligned} \tag{6.128}$$

where $c(k,m) := k - \sum_{i=1}^k \delta_{m_i\,0} \in \{0, 1, \ldots, k\}$. In particular,

$$\langle sign, H_{2n}\rangle_{\gamma_1} = 0 \;\; and \;\; \langle sign, H_{2n+1}\rangle_{\gamma_1} = (-1)^n\sqrt{\frac{2}{\pi}}\,\frac{(2n-1)!!}{\sqrt{(2n+1)!}} = \frac{(-1)^n}{2^n}\sqrt{\frac{2}{\pi}}\,\frac{(n+1)!}{\sqrt{(2n+1)!}}\,C_n \tag{6.129}$$

for any $n \in \mathbb{N}_0$, where $C_n := \frac{1}{n+1}\binom{2n}{n}$ denotes the n'th Catalan number.

Moreover, because of the fact that $H_\nu(-x) = (-1)^\nu H_\nu(x)$ (respectively, $H_\nu(|x|) = (\text{sign}(x))^\nu H_\nu(x)$) for all $\nu \in \mathbb{N}_0$ and $x \in \mathbb{R}$, a k-fold multiplication of (the values of) one-dimensional Hermite polynomials implies that

$$H_n(-x) = (-1)^{|n|} H_n(x) \text{ for all } n \in \mathbb{N}_0^k \text{ and } x \in \mathbb{R}^k .$$

Hence,

$$\langle g_\rho, H_n\rangle_{\gamma_k} = \langle g, (H_n)_\rho\rangle_{\gamma_k} = \rho^{|n|}\langle g, H_n\rangle_{\gamma_k} \text{ for all } g \in L^2(\gamma_k) \text{ and } \rho \in \{-1, 1\}, \tag{6.130}$$

where $\mathbb{R}^k \ni y \mapsto f_\rho(y) := f(\text{sign}(\rho)y) = f(\rho\, y)$ satisfies $\|f_\rho\|_{\gamma_k} = \|f\|_{\gamma_k}$ for $f \in \{g, H_n\}$ (which follows from a simple change of variables and the trivial fact that $|\rho^k| = 1$ for all $\rho \in \{-1, 1\}$). Obviously, dependent on the smoothness structure of $g \in L^2(\gamma_k)$, it's quite a challenge to calculate the "Fourier-Hermite coefficients" $\langle g, (H_n)_\rho\rangle_{\gamma_k} = \int_{\mathbb{R}^k} g(x)H_n(x)\gamma_k(\mathrm{d}x)$ explicitly. Regarding that particular problem, let us note a first important fact (cf. also Proposition 6.28):

Proposition 6.3. *Let $k \in \mathbb{N}$, $\boldsymbol{X} \sim N_k(0, I_k)$ and $g \in L^2(\gamma_k)$. Then the function $\mathbb{R}^k \ni \lambda \mapsto \mathbb{E}[g(\boldsymbol{X} + \lambda)]$ is smooth around 0. It satisfies*

$$D^\alpha\, \mathbb{E}[g(\boldsymbol{X} + \lambda)]\Big|_{\lambda=0} = \sqrt{\alpha!}\,\langle g, H_\alpha\rangle_{\gamma_k} = \sqrt{\alpha!}\,\mathbb{E}[g(\boldsymbol{X})H_\alpha(\boldsymbol{X})] \textit{ for all } \alpha \in \mathbb{N}_0^k . \tag{6.131}$$

In particular, if in addition g is smooth, then

$$\langle g, H_\alpha\rangle_{\gamma_k} = \mathbb{E}[g(\boldsymbol{X})H_\alpha(\boldsymbol{X})] = \frac{1}{\sqrt{\alpha!}}\,\mathbb{E}[D^\alpha\, g(\boldsymbol{X})]$$

for all $\alpha \in \mathbb{N}_0^k$.

Proof. Consider the function $\mathbb{R}^k \times \mathbb{R}^k \ni (x, \lambda) \mapsto F(x, \lambda) := \exp(\langle x, \lambda\rangle_2 - \frac{1}{2}\|\lambda\|_2)$. A straightforward application of the k-dimensional change of variables formula implies that $I_g(\lambda) := \mathbb{E}[g(\mathbf{X} + \lambda)] = \mathbb{E}[g(\mathbf{X})F(\mathbf{X}, \lambda)]$. Consequently, due to (6.123), it follows that

$$I_g(\lambda) = \sum_{\alpha \in \mathbb{N}_0^k} \frac{\mathbb{E}[g(\mathbf{X})H_\alpha^*(\mathbf{X})]}{\alpha!}\lambda^\alpha ,$$

where we put $H_\alpha^*(x) := \sqrt{\alpha!}\, H_\alpha(x)$ for all $\alpha \in \mathbb{N}_0^k$ and $x \in \mathbb{R}^k$. Thus, the multi-indices version of the k-dimensional Taylor formula (cf. [40, Theorem 2.8.4]) implies that

$$D^\alpha\, \mathbb{E}[g(\mathbf{X} + \lambda)]\Big|_{\lambda=0} = D^\alpha\, I_g(\lambda)\Big|_{\lambda=0} = \mathbb{E}[g(\mathbf{X})H_\alpha^*(\mathbf{X})] = \sqrt{\alpha!}\,\mathbb{E}[g(\mathbf{X})H_\alpha(\mathbf{X})].$$

□

6.2. Real CCP functions and covariances: a Fourier-Hermite analysis approach

Fix $f, g \in L^2(\mathbb{R}^k, \gamma_k), \nu \in \mathbb{N}_0$ and $k \in \mathbb{N}$. Put $C(\nu, k) := \{n \in \mathbb{N}_0^k : |n| = \nu\}$ and

$$p_\nu(f, g) := \sum_{n \in C(\nu,k)} \langle f, H_n\rangle_{\gamma_k}\,\langle g, H_n\rangle_{\gamma_k} = p_\nu(g, f) . \tag{6.132}$$

Since the inequality of arithmetic and geometric means in particular holds for any pair of elements, indexed by elements of the set of finitely many elements $C(\nu, k)$, it allows (the proof of) a direct transfer of Hölder's inequality by means of summation over $C(\nu, k)$, whence

$$|p_\nu(f,g)| \leq \sqrt{p_\nu(f,f)}\sqrt{p_\nu(g,g)} \text{ for all } \nu \in \mathbb{N}_0 . \tag{6.133}$$

Since $\{C(\nu,k) : \nu \in \mathbb{N}_0\}$ obviously is a partition of the set $\mathbb{N}_0^k$ and $\{H_\alpha : \alpha \in \mathbb{N}_0^k\}$ is an orthonormal basis in $L^2(\gamma_k)$, Hölder's inequality again implies that

$$[-1,1] \ni \rho \mapsto h_{f,g}(\rho) := \sum_{n\in\mathbb{N}_0^k} \langle f, H_n\rangle_{\gamma_k} \langle g, H_n\rangle_{\gamma_k} \rho^{|n|} = \sum_{\nu=0}^{\infty} p_\nu(f,g)\,\rho^\nu \tag{6.134}$$

converges absolutely, and

$$h_{f,g}(\rho) \leq \sum_{\nu=0}^{\infty} |p_\nu(f,g)| \leq \|f\|_{\gamma_k}\|g\|_{\gamma_k} .$$

Hence, since $h_{f,g} = \frac{1}{4}(h_{f+g,f+g} - h_{f-g,f-g})$ (due to the polarisation equality) and $|h_{p,p}(\rho)| \leq \sum_{n\in\mathbb{N}_0^k}\langle p, H_n\rangle_{\gamma_k}^2 |\rho|^{|n|} \leq \|p\|_{\gamma_k}^2$ for all $p \in L^2(\mathbb{R}^k,\gamma_k)$ and $\rho \in [-1,1]$, $h_{f,g}$ is well-defined and bounded. Note also that by construction $h_{f,g} = h_{g,f}$. Since $p_\nu(f,g) = \frac{1}{4}(p_\nu(f+g,f+g) - p_\nu(f-g,f-g))$ for all $\nu \in \mathbb{N}_0$, it even follows that

$$\sum_{\nu=0}^{\infty} |p_\nu(f,g)| \leq \frac{1}{4}(h_{f+g,f+g}(1) + h_{f-g,f-g}(1)) = \frac{1}{4}(\|f+g\|_{\gamma_k}^2 + \|f-g\|_{\gamma_k}^2) < \infty.$$

Consequently, $h_{f,g}\big|_{(-1,1)} \in W_+^\omega((-1,1))$.

Observe also that *for any* $f = \sum_{n\in\mathbb{N}_0^k} a_n H_n \in L^2(\gamma_k)$ and *any* $g = \sum_{n\in\mathbb{N}_0^k} b_n H_n \in L^2(\gamma_k)$, it follows that $a_n = x_n(f) := \langle f, H_n\rangle_{\gamma_k}$ and $b_n = x_n(g) = \langle g, H_n\rangle_{\gamma_k}$ for all $n \in \mathbb{N}_0^k$, implying that $p_\nu(f,g) = \sum_{n\in C(\nu,k)} a_n b_n$, whence

$$h_{f,g}(\rho) = \sum_{\nu=0}^{\infty}\Big(\sum_{n\in C(\nu,k)} a_n b_n\Big)\rho^\nu \text{ for all } \rho \in [-1,1]$$

and $\sum_{\nu=0}^{\infty}\Big(\sum_{n\in C(\nu,k)} a_n^2\Big) = \sum_{n\in\mathbb{N}_0^k} a_n^2 = \|f\|_{\gamma_k}^2$. In particular,

$$h_{f,f}(\rho) = \sum_{\nu=0}^{\infty}\Big(\sum_{n\in C(\nu,k)} a_n^2\Big)\rho^\nu \text{ for all } \rho \in [-1,1] .$$

This immediately results in another important statement which should be compared with [91, Proposition 5 and Théorème 3] and (6.176):

Proposition 6.4. *Let $k \in \mathbb{N}$ and $f, g \in S_{L^2(\gamma_k)}$. If H is a real Hilbert space, then there exists a real Hilbert space $\mathbb{H}$ such that for any $u, v \in S_H$,*

$$h_{f,g}(\langle u, v\rangle_H) = \langle \psi_u(f), \psi_v(g)\rangle_{\mathbb{H}} ,$$

where $\psi_w : L^2(\gamma_k) \longrightarrow \mathbb{H}$ is a mapping which satisfies $\psi_w(S_{L^2(\gamma_k)}) \subseteq S_{\mathbb{H}}$ for any $w \in S_H$. In particular, for any $m, n \in \mathbb{N}$, the following statements hold:

$$h_{f,g}[S] \in \mathcal{Q}_{m,n} \textit{ for all } S \in \mathcal{Q}_{m,n}$$

and

$$h_{f,g}[A] \in \mathbb{M}_n(\mathbb{R})^+ \textit{ for all } A \in \mathbb{M}_n(\mathbb{R})^+ .$$

Proof. Firstly, based on the construction of the tensor product of Hilbert spaces (cf. S. K. Berberian's beautiful explanation of this concept in `https://web.ma.utexas.edu/mp_arc/c/14/14-2.pdf`), it follows that for any $\nu \in \mathbb{N}_0$, there exist mappings $w_\nu : H \longrightarrow H_\nu$, such that $w_\nu(S_H) \subseteq S_{H_\nu}$ and

$$\langle x, y \rangle_H^\nu = \langle w_\nu(x), w_\nu(y) \rangle_{H_\nu} \text{ for all } x, y \in \mathbb{R}^n, \tag{6.135}$$

where the Hilbert space $H_\nu := \bigotimes_{l=1}^{\nu} H$ denotes the ν-fold tensor product of H, $w_\nu(x) := \bigotimes_{l=1}^{\nu} x$ and $w_\nu(y) := \bigotimes_{l=1}^{\nu} y$. If $H \equiv \mathbb{R}_2^m$ is finite-dimensional, the structure of the (real) Gaussian measure in fact allows an explicit construction of such mappings $w_\nu : \mathbb{R}_2^m \longrightarrow L^2(\mathbb{R}_2^{\nu m}, \gamma_{\nu m})$ (without having to make use of abstract tensor products of Hilbert spaces), via

$$w_\nu(x)(\text{vec}(\xi_1, \ldots, \xi_\nu)) := \prod_{i=1}^{\nu} \langle x, \xi_i \rangle_{\mathbb{R}_2^m}$$

(cf. also [77, Lemma 10.4]). We only have to implement the well-known fact that $\gamma_{\nu m}$ coincides with the product measure $\bigotimes_{i=1}^{\nu} \gamma_m$. Hence,

$$\begin{aligned} h_{f,g}(\langle u, v \rangle_H) &= \sum_{\nu=0}^{\infty} \Big(\sum_{n \in C(\nu,k)} x_n(f) x_n(g) \Big) \Big\langle w_\nu(u), w_\nu(v) \Big\rangle_{H_\nu} \\ &= \sum_{\nu=0}^{\infty} \Big(\sum_{n \in C(\nu,k)} \Big\langle x_n(f) w_\nu(u),\, x_n(g) w_\nu(v) \Big\rangle_{H_\nu} \Big). \end{aligned}$$

Consequently, the definition of the (l_2-)direct product of Hilbert spaces leads us instantly to the desired Hilbert space $\mathbb{H} := \bigoplus_{\nu=0}^{\infty} \Big(\bigoplus_{n \in C(\nu,k)} H_\nu \Big)$ and the mappings ψ_u and ψ_v (cf. proof of [78, Theorem 17.2.9]). □

We will recognise soon that an *additional boundedness assumption* on $f = \sum_{n \in \mathbb{N}_0^k} a_n H_n \in L^2(\gamma_k)$ itself is of utmost importance in relation to an approximation of the smallest upper bound of $K_G^{\mathbb{F}}$ (cf. Theorem 6.40, Theorem 6.45 and Theorem 7.14). To perform this highly non-trivial task, we have to look strongly for "suitable" $f = \sum_{n \in \mathbb{N}_0^k} a_n H_n \in L^2(\gamma_k)$ which in addition are bounded (a.s.); i.e., we have to look for some $M > 0$ such that (pointwise!) for (γ_k-almost) all $x \in \mathbb{R}^k$,

$$|f(x)| \leq M \tag{6.136}$$

(as is the case with (6.166)).

We are now fully prepared to extend these important facts to one of our key results in this paper. In particular, we provide a multi-dimensional generalisation of the one-dimensional case $k = 1$ (cf. [18, Section 3.1]) and specify a non-obvious tightening of the upper bound of $h_{f,g}$. Here, it should be noted that the inclusion of Proposition 2.13 would allow to view Theorem 6.5 as a straightforward simple implication of the key results in [110, Chapter 11], including the consideration of [110, Definition 11.10] (cf. also [17, Chapter 5.6.1], [121, Lemma 2.2] and Remark 6.14). However, we give a self-contained proof, built on the well-established Ornstein-Uhlenbeck semigroup (whose construction is recalled in the proof) and which sheds light also on the impact of the negative correlation case $-1 < \rho < 0$ in shape of an alternating sign change in the related power series.

Theorem 6.5. *Let $k \in \mathbb{N}, f, g \in L^2(\mathbb{R}^k, \gamma_k)$, $\boldsymbol{S} \sim N_k(0, I_k)$, $\rho \in [-1,1]$ and $vec(\boldsymbol{X}, \boldsymbol{Y}) \sim N_{2k}(0, \Sigma_{2k}(\rho))$. Then the following properties hold:*

(i) $h_{f,g}\Big|_{(-1,1)} \in W_+^\omega((-1,1))$,

$$h_{f,g}(0) = \mathbb{E}[f(\boldsymbol{S})]\,\mathbb{E}[g(\boldsymbol{S})] \text{ and } h_{f,g}(\rho) = \mathbb{E}[f(\boldsymbol{X})g(\boldsymbol{Y})] = Cov(f(\boldsymbol{X}), g(\boldsymbol{Y})) + h_{f,g}(0). \tag{6.137}$$

In particular, $h_{f,g}(1) = \mathbb{E}[f(\boldsymbol{S})g(\boldsymbol{S})] = \langle f, g\rangle_{\gamma_k}$, $h_{f,f}(1) = \|f\|^2_{\gamma_k}$ and $h_{f,g}(-1) = \mathbb{E}[f(\boldsymbol{S})g(\boldsymbol{-S})] = \langle f, g_{-1}\rangle_{\gamma_k}$.

(ii) *$h_{f,g} : [-1,1] \longrightarrow \mathbb{R}$ is bounded and satisfies*

$$|h_{f,g}(\rho)| \leq \|f\|_{\gamma_k}\,\|g\|_{\gamma_k} \text{ for all } \rho \in [-1,1]\,. \tag{6.138}$$

(iii) *If $\rho \in (-1,1)$, then*

$$h_{f,g}(\rho) = \frac{1}{(2\pi)^k(1-\rho^2)^{k/2}} \int_{\mathbb{R}^k}\int_{\mathbb{R}^k} f(x)g(y)\exp\Big(-\frac{\|x\|^2+\|y\|^2-2\rho\langle x,y\rangle}{2(1-\rho^2)}\Big)\mathrm{d}^k x\,\mathrm{d}^k y. \tag{6.139}$$

(iv) *If H is a real separable Hilbert space and $u, v \in S_H$, there exists a family $\{\boldsymbol{X}_w : w \in S_H\}$ of $\mathbb{R}^k$-valued random vectors, such that $vec(\boldsymbol{X}_u, \boldsymbol{X}_v) \sim N_{2k}(0, \Sigma_{2k}(\langle u, v\rangle_H))$ and*

$$h_{f,g}(\langle u,v\rangle_H) = \mathbb{E}[f(\boldsymbol{X}_u)g(\boldsymbol{X}_v)]. \tag{6.140}$$

(v) *If either f or g is odd, then $p_{2\nu}(f,g) = 0$ for all $\nu \in \mathbb{N}_0$ and*

$$cov(f(\boldsymbol{X}), g(\boldsymbol{Y})) = \mathbb{E}[f(\boldsymbol{X})\,g(\boldsymbol{Y})] = h_{f,g}(\rho) = \rho\sum_{\nu=0}^{\infty} p_{2\nu+1}(f,g)\rho^{2\nu}\,.$$

In particular, $h_{f,g}$ is odd.

Proof. (i) Firstly, since $H_0 = 1$, it follows that $h_{f,g}(0) = p_0(f,g) = \langle f, 1\rangle_{\gamma_k}\,\langle g, 1\rangle_{\gamma_k}$. Therefore, we have to consider the remaining cases $|\rho| = 1$, $0 < \rho < 1$ and $-1 < \rho < 0$. Firstly, let $|\rho| = 1$. Observe that in this case a probability density function does not exist since $\Sigma_{2k}(\rho)$ is singular (see Proposition 2.12). However, $\mathrm{vec}(\mathbf{S}, \rho\,\mathbf{S}) = A_\rho\mathbf{S} \sim N_{2k}(0, \Sigma_{2k}(\rho))$, where $\mathbb{M}_{2k,k}(\mathbb{R}) \ni A_\rho := (I_k, \rho I_k)^\top$ (since $\mathbf{S} \sim N_k(0, I_k)$ and $A_\rho A_\rho^\top = \Sigma_{2k}$). Consequently, $\mathbb{P}_{\mathrm{vec}(\mathbf{X},\mathbf{Y})} = \mathbb{P}_{\mathrm{vec}(\mathbf{S},\rho\mathbf{S})} = (A_\rho)_*\mathbb{P}_{\mathbf{S}}$ (image measure), whence

$$\mathbb{E}[f(\mathbf{S})g(\rho\mathbf{S})] = \int_{\mathbb{R}^{2k}} f\otimes g\,\mathrm{d}((A_\rho)_*\mathbb{P}_{\mathbf{S}}) = \int_{\mathbb{R}^k}(f\otimes g)\circ A_\rho\,\mathrm{d}\mathbb{P}_{\mathbf{S}} = \int_{\mathbb{R}^k} f(x)g(\rho\, x)\mathbb{P}_{\mathbf{S}}(\mathrm{d}x) = \langle f, g_\rho\rangle_{\gamma_k}\,,$$

where $g_\rho \in L^2(\gamma_k)$ is given as in (6.130). Thus, since $\{H_\nu : \nu \in \mathbb{N}_0^k\}$ is an orthonormal basis in the Hilbert space $L^2(\gamma_k)$, and $\mathbb{N}_0^k$ is partitioned according to $\mathbb{N}_0^k = \biguplus_{\nu=0}^\infty C(\nu,k)$, the associativity formula for summable families leads to

$$\begin{aligned}\mathbb{E}[f(\mathbf{X})g(\mathbf{Y})] = \mathbb{E}[f(\mathbf{S})g_\rho(\mathbf{S})] = \langle f, g_\rho\rangle_{\gamma_k} &= \sum_{\nu=0}^{\infty}\sum_{n\in C(\nu,k)}\langle f, H_n\rangle_{\gamma_k}\,\langle g_\rho, H_n\rangle_{\gamma_k}\\ &= \sum_{\nu=0}^{\infty}\Big(\sum_{n\in C(\nu,k)}\langle f, H_n\rangle_{\gamma_k}\,\langle g, H_n\rangle_{\gamma_k}\Big)\rho^\nu = h_{f,g}(\rho)\,,\end{aligned}$$

whereby the penultimate equality follows from (6.130). Next, let $0 < \rho < 1$. Then $\vartheta(\rho) := -\ln(\rho) = \ln(1/\rho) > 0$, implying that the linear operator $T_{\vartheta(\rho)} \in \mathcal{L}(L^2(\gamma_k))$ is well-defined, where $(T_t)_{t\geq 0}$ denotes the strongly continuous Ornstein-Uhlenbeck semigroup of bounded non-negative symmetric linear operators on $L^2(\gamma_k)$ (see [20, Theorem 1.4.1.]). Thus, by construction of the Ornstein-Uhlenbeck semigroup, and since $\mathbf{S} \sim N_k(0, I_k)$, it follows that

$$\mathbb{E}[f(\rho\, y + \sqrt{1-\rho^2}\,\mathbf{S}] = \mathbb{E}[f(e^{-\vartheta(\rho)}\, y + \sqrt{1-e^{-2\vartheta(\rho)}}\,\mathbf{S}] = T_{\vartheta(\rho)}f(y) \text{ for all } y \in \mathbb{R}^k\,. \tag{6.141}$$

A straightforward change of variables calculation leads to

$$\mathbb{E}[f(\rho\, y + \sqrt{1-\rho^2}\,\mathbf{S}] = \mathbb{E}[f(\mathbf{S})M_\rho(\mathbf{S}, y; k)] \text{ for all } y \in \mathbb{R}^k\,,$$

where $\mathbb{R}^k \times \mathbb{R}^k \ni (x, y) \mapsto M_\rho(x, y; k)$ denotes the k-dimensional Mehler kernel (cf. (2.34)). The latter is well-defined, since $\rho^2 \neq 1$ by assumption. Consequently, we may apply (2.33), and obtain

$$\begin{aligned}\mathbb{E}[f(\mathbf{X})g(\mathbf{Y})] &= \frac{1}{(2\pi)^k(1-\rho^2)^{k/2}} \int_{\mathbb{R}^{2k}} f(x)g(y)\exp\Big(-\frac{\|x\|^2+\|y\|^2-2\rho\langle x,y\rangle}{2(1-\rho^2)}\Big)\mathrm{d}^{2k}(x,y)\\ &= \int_{\mathbb{R}^k} \mathbb{E}[f(\mathbf{S})M_\rho(\mathbf{S}, y; k)]\, g(y)\gamma_k(\mathrm{d}y) = \langle T_{\vartheta(\rho)}f, g\rangle_{\gamma_k}\,.\end{aligned} \tag{6.142}$$

Moreover, an application of [20, Theorem 1.4.4.] and the construction of ϑ imply that

$$T_{\vartheta(\rho)}f = \sum_{\nu=0}^{\infty} \rho^\nu \big(\sum_{n\in C(\nu,k)} \langle f, H_n\rangle_{\gamma_k} H_n\big)$$

on $L^2(\gamma_k)$. Consequently, it follows that

$$\begin{aligned}\mathbb{E}[f(\mathbf{X})g(\mathbf{Y})] &= \Big\langle \sum_{\nu=0}^{\infty} \rho^\nu \Big(\sum_{n\in C(\nu,k)} \langle f, H_n\rangle_{\gamma_k} H_n\Big), g\Big\rangle_{\gamma_k}\\ &= \sum_{\nu=0}^{\infty}\Big(\sum_{n\in C(\nu,k)} \langle f, H_n\rangle_{\gamma_k}\langle H_n, g\rangle_{\gamma_k}\Big)\rho^\nu = h_{f,g}(\rho),\end{aligned} \tag{6.143}$$

which finishes the prove of (i) for the case $0 < \rho < 1$. So, let us consider the remaining case $-1 < \rho < 0$. Since $\mathrm{vec}(\mathbf{X}, \mathbf{Y}) \sim N_{2k}(0, \Sigma_{2k}(\rho))$ by assumption, it follows that $\mathrm{vec}(-\mathbf{X}, \mathbf{Y}) \sim N_{2k}(0, \Sigma_{2k}(|\rho|))$ (since $0 < |\rho| = -\rho < 1$). Thus,

$$\mathbb{E}[f(\mathbf{X})g(\mathbf{Y})] = \mathbb{E}[f_{-1}(-\mathbf{X})g(\mathbf{Y})] \overset{(6.143)}{=} h_{f_{-1},g}(|\rho|) = \sum_{\nu=0}^{\infty} p_\nu(f_{-1}, g)|\rho|^\nu \overset{(6.130)}{=} \sum_{\nu=0}^{\infty} p_\nu(f, g)\rho^\nu\,,$$

which also finishes the proof of (i) for the remaining case $-1 < \rho < 0$. To sum up, given an arbitrary $\rho \in (-1, 1) \setminus \{0\}$ and any $\mathrm{vec}(\mathbf{X}, \mathbf{Y}) \sim N_{2k}(0, \Sigma_{2k}(\rho))$, we have:

$$\begin{aligned}\mathbb{E}[f(\mathbf{X})g(\mathbf{Y})] &= \frac{1}{(2\pi)^k(1-\rho^2)^{k/2}} \int_{\mathbb{R}^{2k}} f(x)g(y)\exp\Big(-\frac{\|x\|^2+\|y\|^2-2\rho\langle x,y\rangle}{2(1-\rho^2)}\Big)\mathrm{d}^{2k}(x,y)\\ &= h_{f,g}(\rho) = h_{f_\rho,g}(|\rho|) = \langle T_{\vartheta(|\rho|)}f_\rho, g\rangle_{\gamma_k}\,.\end{aligned} \tag{6.144}$$

Actually, if we put $\vartheta(1) := 0$, we have shown that

$$\mathbb{E}[f(\mathbf{X})g(\mathbf{Y})] = h_{f,g}(\rho) = \langle T_{\vartheta(|\rho|)} f_\rho, g\rangle_{\gamma_k} = \langle f_\rho, T_{\vartheta(|\rho|)} g\rangle_{\gamma_k} \text{ for all } \rho \in [-1,1] \setminus \{0\}. \tag{6.145}$$

Since $\|T_t\|_{\mathcal{L}\left(L^2(\gamma_k)\right)} = 1$ for all $t \geq 0$ (cf. [20, Theorem 1.4.1]), it therefore follows that

$$|h_{f,g}(\rho)| \leq \|T_{\vartheta(|\rho|)} f_\rho\|_{\gamma_k} \|g\|_{\gamma_k} \leq \|f\|_{\gamma_k} \|g\|_{\gamma_k}$$

for all $\rho \in [-1,1] \setminus \{0\}$. Moreover, $\left|h_{f,g}(0)\right| = \left|\mathbb{E}[f(\mathbf{S})]\,\mathbb{E}[g(\mathbf{S})]\right| \leq \|f\|_{\gamma_k} \|g\|_{\gamma_k}$ for all $\mathbf{S} \sim N_k(0, I_k)$. Finally, since $\operatorname{vec}(\mathbf{Y},\mathbf{X}) \stackrel{d}{=} \operatorname{vec}(\mathbf{X},\mathbf{Y})$, (i), (ii) and (iii) are completely proven.
(iv) Let $u, v \in S_H$. Consider the real $2k$-dimensional Gaussian random vector $\operatorname{vec}(\mathbf{Z}_u, \mathbf{Z}_v) \sim N_{2k}(0, \Sigma_{2k}(\langle u, v\rangle_H))$ (which exists, due to Proposition 3.36). Hence, if we put $\rho_{u,v} := \langle u, v\rangle_H \in [-1,1]$, it follows that $h_{f,g}(\rho_{u,v}) = \mathbb{E}[f(\mathbf{Z}_u)g(\mathbf{Z}_v)]$, which concludes claim (iv).
(v) Without loss of generality, we may assume that f is odd. Then

$$\langle f, H_n\rangle_{\gamma_k} = -\langle f_{-1}, H_n\rangle_{\gamma_k} \stackrel{(6.130)}{=} (-1)^{1+|n|}\langle f, H_n\rangle_{\gamma_k}$$

for all $n \in \mathbb{N}_0^k$, so that $(1-(-1)^{1+|n|})\langle f, H_n\rangle_{\gamma_k} = 0$ for all $n \in \mathbb{N}_0^k$. Consequently, it follows that

$$\langle f, H_n\rangle_{\gamma_k} = 0 \text{ for all } n \in \{m \in \mathbb{N}_0^k : |m| \text{ is even}\}. \tag{6.146}$$

In particular, $\mathbb{E}[f(\mathbf{X})] = \langle f, H_0\rangle_{\gamma_k} = 0$. Thus,

$$\operatorname{cov}(f(\mathbf{X}), g(\mathbf{Y})) = \mathbb{E}[f(\mathbf{X})g(\mathbf{Y})] = h_{f,g}(\rho) \stackrel{(6.146)}{=} \rho \sum_{\nu=0}^{\infty} p_{2\nu+1}(f,g)\rho^{2\nu}.$$

□

Expressed in matrix notation, Theorem 6.5-(iv) leads directly to a further crucial result:

Corollary 6.6. *Let $k, m, n \in \mathbb{N}$ and $f, g \in L^2(\gamma_k)$. Then the following matrix representations hold:*

(i) *For any $S \equiv (s_{ij}) \in \mathcal{Q}_{m,n}$ there exist a random vector $\boldsymbol{P}_f = (f(\boldsymbol{X}_1), \ldots, f(\boldsymbol{X}_m))^\top$ in $\mathbb{R}^m$ and a random vector $\boldsymbol{Q}_g = (g(\boldsymbol{Y}_1), \ldots, g(\boldsymbol{Y}_n))^\top$ in $\mathbb{R}^n$, such that $(\boldsymbol{X}_i, \boldsymbol{Y}_j) \sim N_{2k}(0, \Sigma_{2k}(s_{ij}))$ for all $(i,j) \in [m] \times [n]$ and*

$$h_{f,g}[S] = \mathbb{E}[\boldsymbol{P}_f \boldsymbol{Q}_g^\top] = \Big(\mathbb{E}[f(\boldsymbol{X}_i)g(\boldsymbol{Y}_j)]\Big)_{ij}. \tag{6.147}$$

(ii) *For any correlation matrix $\Sigma \equiv (\sigma_{ij}) \in C(n;\mathbb{R})$ there exists a random vector $\boldsymbol{R}_f = (f(\boldsymbol{Z}_1), \ldots, f(\boldsymbol{Z}_n))^\top$ in $\mathbb{R}^n \setminus \{0\}$, such that $(\boldsymbol{Z}_i, \boldsymbol{Z}_j) \sim N_{2k}(0, \Sigma_{2k}(\sigma_{ij}))$ for all $(i,j) \in [m] \times [n]$ and*

$$h_{f,f}[\Sigma] = \mathbb{E}[\Theta_{f,f}] = \mathbb{E}[\boldsymbol{R}_f \boldsymbol{R}_f^\top] = \Big(\mathbb{E}[f(\boldsymbol{Z}_i)f(\boldsymbol{Z}_j)]\Big)_{ij}, \tag{6.148}$$

where $\Theta_{f,f} := \boldsymbol{R}_f \boldsymbol{R}_f^\top \in \mathbb{M}_n(\mathbb{R})^+$ is a positive semidefinite random matrix of rank 1.

Corollary 6.7. *Let $k \in \mathbb{N}$, $f, g \in L^2(\mathbb{R}^k, \gamma_k)$, $r \in [-1,1]$, $\boldsymbol{S} \sim N_k(0, I_k)$ and $vec(\boldsymbol{X}, \boldsymbol{Y}) \sim N_{2k}(0, \Sigma_{2k}(r))$. If $\|f\|_{\gamma_k} = 1$, $\|g\|_{\gamma_k} = 1$ and $\mathbb{E}[f(\boldsymbol{S})] = \mathbb{E}[g(\boldsymbol{S})] = 0$, then*

$$h_{f,g}(r) = \rho(f(\boldsymbol{X}), g(\boldsymbol{Y}))$$

coincides with the Pearson correlation coefficient between the real random variables $f(\boldsymbol{X})$ and $g(\boldsymbol{Y})$.

In case of $f = g$ some important extra analytical facts emerge; particularly if in addition f is odd (which is the relevant case for the topic of this paper):

Theorem 6.8. *Let $k \in \mathbb{N}$ and $f \in L^2(\mathbb{R}^k, \gamma_k)$ be odd, such that $r := \|f\|^2_{\gamma_k} > 0$. Then the following properties hold:*

(i) $h_{f,f}\big|_{(-1,1)} \in W^\omega_+((-1,1))$.

(ii) *$h_{f,f}$ is a CCP function if and only if $r = 1$.*

(iii) *$h_{f,f} : [-1,1] \longrightarrow [-r, r]$ is an odd strictly increasing homeomorphism, which satisfies $h_{f,f}((-1,0)) = (-r, 0)$ and $h_{f,f}((0,1)) = (0, r)$. Moreover,*

$$0 \leq h'_{f,f}(0) = \sum_{i=1}^k \Big(\int_{\mathbb{R}^k} f(x) x_i \gamma_k(\mathrm{d}x)\Big)^2 = \int_{\mathbb{R}^{2k}} f(x) f(y) \langle x, y \rangle_{\mathbb{R}^k_2} \gamma_{2k}(\mathrm{d}(x,y)). \quad (6.149)$$

(iv) *If $h'_{f,f}(0) > 0$, then $h'_{f,f}(\rho) > 0$ for all $\rho \in (-1,1)$. In particular, $h^{-1}_{f,f}\big|_{(-r,r)} = \Big(h_{f,f}\big|_{(-r,r)}\Big)^{-1}$ is real analytic on $(-r, r)$ if and only if $h'_{f,f}(0) > 0$.*

(v) *If $h^{-1}_{f,f}\big|_{(-r,r)} \in W^\omega_+((-r,r))$, then*

$$\Big(h^{-1}_{f,f}\big|_{(-r,r)}\Big)_{abs}(y) \geq \frac{1}{h'_{f,f}(0)}\, y \text{ for all } y \in [0, r]\,. \quad (6.150)$$

In particular, $s(r,f) := \Big(h^{-1}_{f,f}\big|_{(-r,r)}\Big)_{abs}(r) > 0$. If $\alpha > 0$ and $h'_{f,f}(0) < \frac{r}{\alpha}$, then $s(r,f) > \alpha$. Moreover,

$$[-1,1] \ni t \mapsto \psi(t) := \frac{1}{s(r,f)} \Big(h^{-1}_{f,f}\big|_{(-r,r)}\Big)_{abs}(r\, t)$$

is an odd, strictly increasing and homeomorphic CCP function. In particular, the function $\Big(h^{-1}_{f,f}\big|_{(-r,r)}\Big)_{abs} : [-r, r] \xrightarrow{\cong} [-s(r,f), s(r,f)]$ is strictly increasing, odd and homeomorphic, as well as its inverse. $\Big(h^{-1}_{f,f}\big|_{(-r,r)}\Big)_{abs}(y) = s(r,f)\, \psi(\frac{y}{r})$ for all $y \in [-r, r]$ and $\Big(\Big(h^{-1}_{f,f}\big|_{(-r,r)}\Big)_{abs}\Big)^{-1}(x) = r\, \psi^{-1}(\frac{x}{s(r,f)})$ for all $x \in [-s(r,f), s(r,f)]$.

Proof. (ii) The claim follows from the power series representation of $h_{f,f}$ and condition (iii) of Theorem 5.17. Regarding the latter, we only have to perform Parseval's equality, applied to the Hilbert space $L^2(\gamma_k)$, since

$$r = \sum_{n \in \mathbb{N}_0^k} \langle f, H_n \rangle^2_{\gamma_k} = \sum_{\nu=0}^\infty \Big(\sum_{n \in C(\nu,k)} \langle f, H_n \rangle^2_{\gamma_k}\Big) = h_{f,f}(1) = \sum_{\nu=0}^\infty a_\nu, \quad (6.151)$$

where $0 \le a_\nu := p_\nu(f,f) = \sum_{n \in C(\nu,k)} \langle f, H_n \rangle^2_{\gamma_k}$ for all $\nu \in \mathbb{N}_0$.
From now on, we may assume without loss of generality that $r = 1$ in the remaining part of the proof (since $h_{f,f} = r\, h_{f^\circ, f^\circ}$, where $f^\circ := \frac{1}{\sqrt{r}} f$).
(iii) Since $h_{f,f}$ is odd, it follows that $0 < 1 = h_{f,f}(1) = \sum_{\nu=0}^\infty p_{2\nu+1}(f,f)$. Hence, $p_{2\mu+1}(f,f) > 0$ for some $\mu \in \mathbb{N}_0$. Let $-1 \le \rho_1 < \rho_2 \le 1$. Recall that $\mathbb{R} \ni s \mapsto s^{2v+1}$ is strictly increasing for all $\nu \in \mathbb{N}_0$. Thus, $p_{2\mu+1}(f,f)\rho_1^{2\mu+1} < p_{2\mu+1}(f,f)\rho_2^{2\mu+1}$. Hence,

$$h_{f,f}(\rho_1) = p_{2\mu+1}(f,f)\rho_1^{2\mu+1} + \sum_{\nu \ne \mu} p_{2\nu+1}(f,f)\rho_1^{2\nu+1} < p_{2\mu+1}(f,f)\rho_2^{2\mu+1} + \sum_{\nu \ne \mu} p_{2\nu+1}(f,f)\rho_1^{2\nu+1} \le h_{f,f}(\rho_2).$$

Due to (6.151), we may apply the M-test of Weierstrass, and it consequently follows that the strictly increasing odd function $h_{f,f} : [-1,1] \longrightarrow [1,1]$ is continuous and hence invertible (due to Bolzano's intermediate value theorem of calculus). Finally, since $[-1,1]$ is compact, it follows that the bijective continuous function $h_{f,f}$ already is a homeomorphism which satisfies $h_{f,f}(0) = 0$, $h_{f,f}(1) = 1$, and hence $h_{f,f}((-1,0)) = (-1,0)$ and $h_{f,f}((0,1)) = (0,1)$. Since $h'(0) = p_1(f,f) = \sum_{i=1}^k \langle f, H_{e_i} \rangle^2_{\gamma_k}$ and $H_1(a) = a$ for all $a \in \mathbb{R}$, it follows that $h'_{f,f}(0) = \sum_{i=1}^k \left(\int_{\mathbb{R}^k} f(x) x_i \gamma_k(\mathrm{d}x) \right)^2$. Moreover, since $\gamma_{2k} = \gamma_k \otimes \gamma_k$, the latter integral obviously coincides with $\int_{\mathbb{R}^{2k}} f(x) f(y) \langle x, y \rangle_{\mathbb{R}^k_2} \gamma_{2k}(\mathrm{d}(x,y))$, which implies (6.149).
(iv) Since $h_{f,f}$ is odd, it follows that

$$h_{f,f}(\rho) = \sum_{\nu=0}^\infty p_{2\nu+1}(f,f)\rho^{2\nu+1} \text{ for all } \rho \in [-1,1].$$

Thus,

$$h'_{f,f}(\rho) = p_1(f,f) + \sum_{\nu=1}^\infty (2\nu+1) p_{2\nu+1}(f,f)\rho^{2\nu} \ge p_1(f,f) = h'_{f,f}(0) \text{ for all } \rho \in (-1,1).$$

Since $h'_{f,f}(0) > 0$ (by assumption), $h'_{f,f}$ is nonvanishing on $(-1,1)$: $h'_{f,f}(\rho) > 0$ for all $\rho \in (-1,1)$. Therefore, we may apply the Real Analytic Inverse Function Theorem (cf. [88, Theorem 1.5.3]), implying that also $\left(h_{f,f}\big|_{(-1,1)} \right)^{-1}$ is real analytic on $(-1,1)$. The converse implication follows from the simple fact that $h'_{f,f}(0) \ge 0$ and $0 < 1 = (h_{f,f} \circ h^{-1}_{f,f})'(0) = h'_{f,f}(0) \cdot (h^{-1}_{f,f})'(0)$.
(v) Let $0 \le y \le 1$. Since $\left(\left(h_{f,f}\big|_{(-1,1)} \right)^{-1}_{\text{abs}} \right)'(0) = \left| \left(h^{-1}_{f,f} \right)'(0) \right| = \left| \frac{1}{h'_{f,f}(0)} \right| = \frac{1}{h'_{f,f}(0)}$, it follows that

$$\left(h_{f,f}\big|_{(-1,1)} \right)^{-1}_{\text{abs}}(y) = \left(\left(h_{f,f}\big|_{(-1,1)} \right)^{-1}_{\text{abs}} \right)'(0)\, y + \sum_{\nu=1}^\infty b_{2\nu+1}\, y^{2\nu+1} \ge \frac{1}{h'_{f,f}(0)}\, y\,.$$

Theorem 5.17 implies that the function ψ is an odd CCP function, so that Lemma 5.10 and a similar approach as in the proof of (iii) conclude the proof of statement (v) (since $s_1 = \left(h^{-1}_{f,f}\big|_{(-1,1)} \right)_{\text{abs}}(1) > 0$). □

A first implication for *odd* CCP functions is a strong improvement of the boundedness condition in Theorem 6.5-(ii); induced by the Schwarz lemma from complex analysis:

Proposition 6.9. *Let $k \in \mathbb{N}$ and $f \in S_{L^2(\gamma_k)}$ be odd. Assume that $h_{f,f}(r) \neq r$ for some $r \in (0,1)$. Then*

$$h_{f,f}(\rho) < \rho \text{ for all } \rho \in (0,1) \text{ and } h_{f,f}(\tau) > \tau \text{ for all } \tau \in (-1,0). \tag{6.152}$$

Moreover, $0 \leq h'_{f,f}(0) < 1$. If in addition, $h_{f,f}^{-1}\big|_{(-1,1)} \in W_+^{\omega}((-1,1))$, then

$$\Big(h_{f,f}^{-1}\big|_{(-1,1)}\Big)_{abs}(1) > 1\,. \tag{6.153}$$

Proof. Due to Theorem 6.8, $[-1,1] \ni \rho \mapsto h_{f,f}(\rho) = \sum_{\nu=0}^{\infty} p_{2\nu+1}(f,f)\,\rho^{2\nu+1}$ is an odd, strictly increasing CCP function, which satisfies $h_{f,f}\big|_{(-1,1)} = \widetilde{h}\big|_{(-1,1)}$, where $\mathbb{D} \ni z \mapsto \widetilde{h}(z) := \sum_{\nu=0}^{\infty} p_{2\nu+1}(f,f)\, z^{2\nu+1}$ is holomorphic (cf. Lemma 5.10). Thus, for any $z \in \mathbb{D}$ it follows that

$$|\widetilde{h}(z)| \leq h_{f,f}(|z|) < h_{f,f}(1) = 1\,,$$

whence $\widetilde{h}(\mathbb{D}) \subseteq \mathbb{D}$. Since $\widetilde{h}(0) = h_{f,f}(0) = 0$, we consequently may apply the Schwarz lemma to the holomorphic function $\widetilde{h}$, implying that

$$|h_{f,f}(\rho)| = |\widetilde{h}(\rho)| \leq |\rho| \text{ for all } \rho \in (-1,1)$$

and $h'_{f,f}(0) \leq 1$. Assume by contradiction that $|\widetilde{h}(\rho_0)| = |h_{f,f}(\rho_0)| = |\rho_0|$ for some $\rho_0 \in (-1,1) \setminus \{0\}$ or $h'_{f,f}(0) = 1$. In each case, the Schwarz lemma implies that there exists $q \in \mathbb{Z}$, such that $h_{f,f}(\rho) = (-1)^q \rho$ for all $\rho \in (-1,1)$ (since $e^{in\pi} = \cos(n\pi) = (-1)^n$ for all $n \in \mathbb{N}_0$). However, since e.g. $0 \leq h_{f,f}(1/2) \neq -1/2$, it follows that $h_{f,f}(\rho) = \rho$ for all $\rho \in [-1,1]$, which contradicts the assumption. Consequently, an application of Theorem 6.8-(v) and the assumption implies that in fact $\Big(h_{f,f}^{-1}\big|_{(-1,1)}\Big)_{\text{abs}}(1) > 1$ (since $\Big(h_{f,f}^{-1}\big|_{(-1,1)}\Big)_{\text{abs}}$ is well-defined). □

All of a sudden we end up with an important general and non-obvious structural statement about *odd* CCP functions; namely:

Corollary 6.10. *Let $k \in \mathbb{N}$ and $f \in S_{L^2(\gamma_k)}$ be odd. Assume that $h_{f,f}(r) \neq r$ for some $r \in (0,1)$. Then $h_{f,f}^{-1}$ is not a CCP function.*

Proof. We just have to link Theorem 5.17-(v) and (6.153). □

We will recognise soon that Theorem 6.8 is strongly linked with the value of the Grothendieck constant $K_G^{\mathbb{F}}$ (cf. Theorem 6.45). We namely obtain in a natural way another significant new definition; the so-called "hyperbolic CCP transform". To make this concept understandable, recall Lemma 5.10 and Remark 5.12 and reconsider the odd CCP function $\psi := h_{\text{sign},\text{sign}} = \frac{2}{\pi}\arcsin$; i.e., the Grothendieck function. Since $\psi^{-1} = \sin(\frac{\pi}{2}\,\cdot)$ on $[-1,1]$, it follows that $\Big(\psi^{-1}\big|_{(-1,1)}\Big)_{\text{abs}}(\tau) = \sinh(\frac{\pi}{2}\tau) = \frac{1}{i}\sin(\frac{\pi}{2}\,i\tau)$ for all $\tau \in [-1,1]$. Note that $\Big(\psi^{-1}\big|_{(-1,1)}\Big)_{\text{abs}}(1) = \sinh(\pi/2) > 1$, implying that $[-1,1] \subseteq (-\sinh(\pi/2), \sinh(\pi/2))$. Thus,

$$\begin{aligned}\frac{2}{\pi}\,\ln(y + \sqrt{y^2+1}) &= \frac{2}{\pi}\sinh^{-1}(y) = \Big(\Big(\psi^{-1}\big|_{(-1,1)}\Big)_{\text{abs}}\Big)^{-1}(y) \\ &= \frac{2}{\pi}\Big(\frac{1}{i}\,\sin^{-1}(i\,y)\Big) = \frac{1}{i}\,\widetilde{\psi}(iy)\end{aligned} \tag{6.154}$$

for all $y \in [-1,1]$. The Maclaurin series representation of the real CCP function ψ therefore implies the Maclaurin series of $y \mapsto \frac{1}{i}\,\widetilde{\psi}(iy)$ on (the whole of) $\mathbb{R}$ is given by

$$\frac{1}{i}\,\widetilde{\psi}(iy) \overset{(6.165)}{=} \frac{2}{\pi}\sum_{\nu=0}^{\infty}(-1)^{\nu}\,\frac{((2\nu-1)!!)^2}{(2\nu+1)!}y^{2\nu+1} = -\frac{1}{3\pi} + \sum_{\substack{\nu=0\\ \nu\neq 1}}^{\infty}(-1)^{\nu}\,\frac{((2\nu-1)!!)^2}{(2\nu+1)!}y^{2\nu+1}\,.$$

Consequently, it follows that

$$\Big(\big(\psi^{-1}\big|_{(-1,1)}\big)_{\text{abs}}\Big)^{-1}(\rho) = \frac{1}{i}\,\widetilde{\psi}(i\rho) < \psi(\rho) < \rho \ \text{ for all } \ \rho \in (0,1)\,.$$

Theorem 6.8 and Proposition 6.9, together with Remark 5.12 imply that the Grothendieck function is a special case of

Lemma 6.11 (Hyperbolic CCP transform). *Let $k \in \mathbb{N}$ and $\psi = h_{f,f}$, where $f \in S_{L^2(\gamma_k)}$ is odd. Assume that $\psi^{-1}|_{(-1,1)} \in W_{+}^{\omega}((-1,1))$ and $\psi(r) \neq r$ for some $r \in (0,1)$. Let the complex function $F := \widetilde{\psi|_{(-1,1)}} : \overline{\mathbb{D}} \longrightarrow \overline{\mathbb{D}}$ be defined as in Lemma 5.10. Then $F(\mathbb{D}) \subseteq \mathbb{D}$ and*

$$F(z) = \sum_{\nu=0}^{\infty} p_{2\nu+1}(f,f)\,z^{2\nu+1} \ \textit{ for all } \ z \in \overline{\mathbb{D}}\,,$$

where each $p_{2\nu+1}(f,f) \in [0,\infty)$ satisfies (6.132). Put $s^* := (\psi^{-1}|_{(-1,1)})_{abs}(1)$. Then $s^* > 1$ and

$$\psi^{hyp} := ((\psi^{-1}|_{(-1,1)})_{abs})^{-1} : [-s^*, s^*] \xrightarrow{\cong} [-1,1]$$

is an odd, strictly increasing homeomorphism, which satisfies $[-1,1] \subseteq (-s^*, s^*)$, $\psi^{hyp}((0,1]) \subseteq (0,1)$ and $\psi^{hyp}([-1,0)) \subseteq (-1,0)$. Moreover,

$$0 < \psi^{hyp}(1) \leq \psi'(0) < 1\,, \tag{6.155}$$

and the following two statements hold:

(i)
$$|\psi^{hyp}(\rho)| < \psi(|\rho|) < |\rho| \ \textit{ for all } \ \rho \in (-1,1)\setminus\{0\}\,.$$

(ii) *If $sign((\psi^{-1}|_{(-1,1)})^{(2n+1)}(0)) = (-1)^n$ for all $n \in \mathbb{N}_0$, then*

$$\psi^{hyp}(x) = \sum_{\nu=0}^{\infty}(-1)^{\nu}\,p_{2\nu+1}(f,f)\,x^{2\nu+1} = \frac{1}{i}\,F(ix) = (M_{-i}\circ F\circ M_i)(x) \ \textit{ for all } \ x \in [-1,1]\,.$$

Proof. Since also $\psi^{\text{hyp}} = ((\psi^{-1}|_{(-1,1)})_{\text{abs}})^{-1}$ is strictly increasing and odd (such as $(\psi^{-1}|_{(-1,1)})_{\text{abs}}$), Proposition 6.9 implies that $\psi^{\text{hyp}}((0,1]) \subseteq (0,1)$ and $\psi^{\text{hyp}}([-1,0)) \subseteq (-1,0)$ (since $s^* > 1$). Recall from Proposition 6.9 that $0 < \psi'(0) < 1$. To verify (6.155), it therefore suffices to show that

$$(\psi^{-1}|_{(-1,1)})_{\text{abs}}(\psi'(0)) \overset{!}{\geq} 1\,. \tag{6.156}$$

Remember also that $|(\psi^{-1})'(0)| = \frac{1}{\psi'(0)}$. Thus, $(\psi^{-1}|_{(-1,1)})_{\text{abs}}(\psi'(0)) = 1 + \sum_{l=1}^{\infty}\alpha_{2l+1}(\psi'(0))^{2l+1}$, where $\alpha_{2l+1} \geq 0$ for all $l \in \mathbb{N}$, and (6.156) follows at once.

(i) Since also ψ^{hyp} is odd, we only have to verify that the claim holds for any $\rho \in (0,1)$. So, fix $0 < \rho < 1$. Due to Proposition 6.9, it is sufficient to show that

$$(\psi^{-1}|_{(-1,1)})_{\text{abs}}(\psi(\rho)) \overset{!}{>} \rho \tag{6.157}$$

To this end, put $\sigma := \psi(\rho)$. Then $\sigma > \psi(0) = 0$. Since ψ is an odd CCP function, it follows that

$$\psi(x) = \psi'(0)x + \sum_{l=1}^{\infty} a_{2l+1}\, x^{2l+1} \text{ for all } x \in [-1,1]\,,$$

where $a_{2l+1} \geq 0$ for all $m \in \mathbb{N}$. Assume by contradiction that $a_{2l+1} = 0$ for all $l \in \mathbb{N}$. Then $\psi(x) = \psi'(0)x$ for all $x \in [-1,1]$. In particular, $1 = \psi(1) = \psi'(0) < 1$, which is absurd. Thus, an $l_0 \in \mathbb{N}$ exists, such that $a_{2l_0+1} > 0$, implying that in particular $\sigma = \psi(\rho) > \psi'(0)\rho$. Given the assumption on $\psi^{-1}|_{(-1,1)}$, we therefore obtain that

$$(\psi^{-1}|_{(-1,1)})_{\text{abs}}(\sigma) = \frac{\sigma}{\psi'(0)} + \sum_{m=1}^{\infty} b_{2m+1}\sigma^{2m+1} > \rho + \sum_{m=1}^{\infty} b_{2m+1}\sigma^{2m+1} \geq \rho\,,$$

where $b_{2m+1} \geq 0$ for all $m \in \mathbb{N}$. Since $\rho \in (0,1)$ was arbitrarily chosen, (6.157) and hence (i) follows.

(ii) Let $G := \widetilde{\psi^{-1}|_{(-1,1)}} : \overline{\mathbb{D}} \longrightarrow \overline{\mathbb{D}}$ be defined as in Lemma 5.10. Since ψ is strictly increasing, (5.115) implies that $|F(z)| \leq \psi(|z|) < \psi(1) = 1$ for all $z \in \mathbb{D}$, whence $F(\mathbb{D}) \subseteq \mathbb{D}$. Similarly, we obtain that $G(\mathbb{D}) \subseteq \mathbb{D}$ (since $\psi^{-1}|_{(-1,1)} \in W_{+}^{\omega}((-1,1))$ by assumption). $F|_{\mathbb{D}}$ is the unique holomorphic extension of $\psi|_{(-1,1)}$ (since $\mathbb{D}$ is a domain; i.e., a non-empty connected open set). $F|_{\mathbb{D}}$ is invertible, and $(F|_{\mathbb{D}})^{-1} = G|_{\mathbb{D}}$ is the unique holomorphic extension of $\psi^{-1}|_{(-1,1)}$. Let $x \in (-1,1)$. Then $ix \in \mathbb{D}$, implying that

$$(M_{-i} \circ F \circ M_i)^{-1}(x) = (M_{-i} \circ G \circ M_i)(x).$$

However, since $\text{sign}((\psi^{-1}|_{(-1,1)})^{(2n+1)}(0)) = (-1)^n$ for all $n \in \mathbb{N}_0$ (by assumption), Remark 5.12 implies that

$$(M_{-i} \circ G \circ M_i)(x) = (\psi^{-1}|_{(-1,1)})_{\text{abs}}(x)\,.$$

Hence, $\psi^{\text{hyp}} = ((\psi^{-1}|_{(-1,1)})_{\text{abs}})^{-1} = M_{-i} \circ F \circ M_i$ on $(-1,1)$. Since ψ^{hyp} is continuous on $[-1,1]$ and the holomorphic function $F|_{\mathbb{D}}$ in particular is continuous on $(-1,1) \subseteq \mathbb{D} = M_i(\mathbb{D})$, a standard limit argument implies that $\psi^{\text{hyp}}(1) = (M_{-i} \circ F \circ M_i)(1)$ and $\psi^{\text{hyp}}(-1) = (M_{-i} \circ F \circ M_i)(-1)$. $\square$

Next, consider for example, the function $a := \frac{1}{\sqrt{2}}(1 + H_2) : \mathbb{R} \longrightarrow \mathbb{R}$. Then $a \in S_{L^2(\gamma_1)}$ and $[-1,1] \ni \rho \mapsto h_{a,a}(\rho) = \frac{1}{2}(1+\rho^2)$ defines an *even* CCP function, such that $h_{a,a}(0) = \frac{1}{2} > 0$. With this example in mind, the assumption in the second part of the following result is not empty.

Proposition 6.12. *Let $k \in \mathbb{N}$, $\rho \in [-1,1]$ and $a, b, f, g \in L^2(\mathbb{R}^k, \gamma_k)$. Then $a \otimes f \in L^2(\mathbb{R}^{2k}, \gamma_{2k})$ and $b \otimes g \in L^2(\mathbb{R}^{2k}, \gamma_{2k})$, and*

$$h_{a\otimes f, b\otimes g} = h_{a,b} \cdot h_{f,g}\,.$$

In particular, the product $h^{ev\otimes\circ} := h^{ev} h^{odd}$ of an even and odd CCP function is an odd, strictly increasing homeomorphic CCP function. If $(h^{odd})'(0) > 0$ and $h^{ev}(0) > 0$, then $(h^{ev\otimes\, odd})^{-1}\big|_{(-1,1)}$ is real analytic. A product of two odd CCP functions is an even CCP function.

Proof. Let $\rho \in [-1,1]$ and $\mathrm{vec}\big(\mathbf{X}_1, \mathbf{Y}_1, \mathbf{X}_2, \mathbf{Y}_2\big) = \mathrm{vec}(\mathbf{S}_1, \mathbf{S}_2) \sim N_{4k}\big(0, \Sigma_{4k}(\rho)\big)$, where $\mathbf{S}_i := \mathrm{vec}(\mathbf{X}_i, \mathbf{Y}_i)$, $i = 1, 2$. Put $\mathbf{X} := \mathrm{vec}(\mathbf{X}_1, \mathbf{X}_2)$ and $\mathbf{Y} := \mathrm{vec}(\mathbf{Y}_1, \mathbf{Y}_2)$. Then Corollary 2.15 implies that $\mathbf{X} \stackrel{d}{=} \mathbf{Y} \sim N_{2k}\big(0, \Sigma_{2k}(\rho)\big)$ are independent. Let $G \in O(4n)$ be the matrix, introduced in (1.9). Then $\mathrm{vec}(x_1, y_1, x_2, y_2) = G\,\mathrm{vec}(x_1, x_2, y_1, y_2)$ for all $x_1, x_2, y_1, y_2 \in \mathbb{R}^k$. Thus, $\mathbb{P}_{\mathrm{vec}(\mathbf{S}_1, \mathbf{S}_2)} = G_* \mathbb{P}_{\mathrm{vec}(\mathbf{X}, \mathbf{Y})}$ (image measure), and

$$\begin{aligned}
h_{a\otimes f, b\otimes g}(\rho) &= \mathbb{E}\Big[a \otimes f(\mathbf{S}_1)\, b \otimes g(\mathbf{S}_2)\Big] = \mathbb{E}_{\mathbb{P}_{\mathrm{vec}(\mathbf{S}_1,\mathbf{S}_2)}}\Big[(a \otimes f) \otimes (b \otimes g)\Big] \\
&= \mathbb{E}_{\mathbb{P}_{\mathrm{vec}(\mathbf{X},\mathbf{Y})}}\Big[\Big((a \otimes f) \otimes (b \otimes g)\Big) \circ G\Big] = \mathbb{E}_{\mathbb{P}_{\mathrm{vec}(\mathbf{X},\mathbf{Y})}}\Big[(a \otimes b) \otimes (f \otimes g)\Big] \\
&= \mathbb{E}\Big[(a \otimes b)(\mathbf{X})\,(f \otimes g))(\mathbf{Y})\Big] = \mathbb{E}\Big[a \otimes b(\mathbf{X})\Big]\mathbb{E}\Big[f \otimes g(\mathbf{Y})\Big] \\
&= h_{a,b}(\rho) h_{f,g}(\rho).
\end{aligned}$$

Since $(h^{\mathrm{ev} \otimes \mathrm{odd}})' = (h^{\mathrm{ev}})'\, h^{\mathrm{odd}} + h^{\mathrm{ev}}(h^{\mathrm{odd}})'$, $(h^{\mathrm{odd}})'(0) > 0$ and $h^{\mathrm{ev}}(0) > 0$ (by assumption), it follows that $(h^{\mathrm{ev}\otimes\mathrm{odd}})'(0) > 0$. The claim now follows from Theorem 6.8-(iv). $\square$

If we apply Theorem 6.5 to a pair of k-dimensional Hermite polynomials and recall that $\{H_\alpha : \alpha \in \mathbb{N}_0^k\}$ actually is an orthonormal basis in $L^2(\gamma_k)$ (cf. (6.119)), we immediately reobtain another remarkable property of Hermite polynomials (cf. [109, Lemma 1.1.1] and [110, Proposition 11.33]).

Corollary 6.13. *Let $k \in \mathbb{N}$, $\rho \in [-1,1]$, $\alpha = (\alpha_1, \ldots, \alpha_k) \in \mathbb{N}_0^k$ and $\beta = (\beta_1, \ldots, \beta_k)^\top \in \mathbb{N}_0^k$. If $\mathrm{vec}(\boldsymbol{X}, \boldsymbol{Y}) \sim N_{2k}(0, \Sigma_{2k}(\rho))$, then*

$$h_{H_\alpha, H_\beta}(\rho) = \mathbb{E}[H_\alpha(\boldsymbol{X})\, H_\beta(\boldsymbol{Y})] = \delta_{\alpha,\beta}\rho^{|\alpha|} = \prod_{i=1}^{k} \delta_{\alpha_i,\beta_i}\, \rho^{\alpha_i}.$$

Remark 6.14 (Noise stability). Fix $k \in \mathbb{N}$. Let $f \in L^2(\gamma_k)$ and A, B Borel sets in $\mathbb{R}^k$. Let $\rho \in [-1,1] \setminus \{0\}$ and $\mathrm{vec}(\mathbf{X}, \mathbf{Y}) \sim N_{2k}(0, \Sigma_{2k}(\rho))$. Then $\mathrm{sign}(\rho)\mathbf{X} \sim N_k(0, I_k)$. Consequently, (6.141) implies that

$$T_{\vartheta(|\rho|)} f_\rho(y) = \mathbb{E}[f(\rho\, y + \sqrt{1-\rho^2}\,\mathbf{X})] = \int_{\mathbb{R}^k} f(\rho\, y + \sqrt{1-\rho^2}\, x)\gamma_k(\mathrm{d}x) = U_\rho f(y) \tag{6.158}$$

for all $y \in \mathbb{R}^k$, where U_ρ is the Gaussian noise operator (cf. [110, Definition 11.12]). U_ρ also is well-defined for $\rho = 0$, with constant value $U_0 f = \mathbb{E}[f(\mathbf{X})]$. Observe that (6.158) implies that $U_\rho = T_{\vartheta(|\rho|)} M_\rho$, where the isometry $M_\rho = M_\rho^{-1} \in \mathcal{L}(L^2(\gamma_k), L^2(\gamma_k))$ is given by $M_\rho f := f_\rho$. A special case of (6.144) is given by

$$\mathbb{P}(\mathbf{X} \in A, \mathbf{Y} \in B) = \mathbb{E}[\mathbb{1}_A(\mathbf{X})\mathbb{1}_B(\mathbf{Y})] = h_{\mathbb{1}_A, \mathbb{1}_B}(\rho) = \langle \mathbb{1}_A, U_\rho \mathbb{1}_B \rangle_{\gamma_k}.$$

Therefore, Theorem 6.5 (under inclusion of Proposition 2.13) encompasses the key concept of Gaussian noise stability, most commonly introduced as $\mathbf{Stab}_\rho[f] := \langle f, U_\rho f\rangle_{\gamma_k}$ ($\rho \in [-1,1]$, $f \in L^2(\gamma_k)$). Gaussian noise stability also comprises deep connections to geometry of minimal surfaces, hypercontractivity, isoperimetric inequalities, communication complexity and Gaussian copulas. A very comprehensive introductory processing of these topics can be found in [110, Chapter 11] and the cited references therein, including the central results of E. Mossel and J. Neeman.

In fact, it can be verified that T_t (and hence $U_\rho = T_{\vartheta(|\rho|)}M_\rho$) is even a *nuclear* operator, implying that each T_t (and each U_ρ) in particular is a *compact* Hilbert-Schmidt operator! More precisely, we have

Proposition 6.15. *Let $k \in \mathbb{N}$, $t \geq 0$ and $\rho \in (-1,1)\setminus\{0\}$. Then both, $T_t \in \mathcal{L}(L^2(\gamma_k), L^2(\gamma_k))$, and $U_\rho \in \mathcal{L}(L^2(\gamma_k), L^2(\gamma_k))$ are Hilbert-Schmidt operators, satisfying*

$$\|T_t\|_{\mathcal{S}_2} = \frac{1}{(1-e^{-2t})^{k/2}} \text{ and } \|U_\rho\|_{\mathcal{S}_2} = \frac{1}{(1-\rho^2)^{k/2}}.$$

T_t as well as U_ρ are even nuclear, and

(i) $\|T_t\|_{\mathcal{N}} \leq \frac{1}{(1-e^{-t})^k}$.

(ii) $\|U_\rho\|_{\mathcal{N}} \leq \frac{1}{(1-|\rho|)^k}$.

Proof. Fix $t \geq 0$. Put $K := L^2(\gamma_k)$ and $\rho(t) := e^{-t}$. Then $t = \vartheta(\rho(t))$. Since $\|M_\rho\| = 1 = \|M_\rho^{-1}\|$ and $U_\rho = T_{\vartheta(|\rho|)}M_\rho$ (respectively, $M_\rho^{-1}U_\rho = T_{\vartheta(|\rho|)}$), the ideal property of the Banach ideal $\big(\mathcal{S}_2, \|\cdot\|_{\mathcal{S}_2}\big)$ implies that we only have to verify the claim for T_t. For this purpose, we use the orthonormal basis $\{H_\alpha : \alpha \in \mathbb{N}_0^k\}$ of k-dimensional Hermite polynomials in $L^2(\gamma_k)$ (cf. (6.119)). The semigroup property implies that $T_t = T_{t/2}^2 = T_{t/2}^* T_{t/2}$. Corollary 6.13, together with (6.145) therefore leads to

$$\begin{aligned}\sum_{\alpha\in\mathbb{N}_0^k} \|T_{t/2}H_\alpha\|_K^2 &= \sum_{\alpha\in\mathbb{N}_0^k} \langle T_t H_\alpha, H_\alpha\rangle_K = \sum_{\alpha\in\mathbb{N}_0^k} h_{H_\alpha,H_\alpha}(\rho(t)) = \sum_{\alpha\in\mathbb{N}_0^k} \rho(t)^{|\alpha|} \\ &= \sum_{\alpha\in\mathbb{N}_0^k} \prod_{i=1}^k \rho(t)^{\alpha_i} = \prod_{i=1}^k \sum_{\alpha_i=0}^\infty \rho(t)^{\alpha_i} = \frac{1}{(1-\rho(t))^k}.\end{aligned}$$

Hence, $\big(\|T_{t/2}H_\alpha\|_K\big)_{\alpha\in\mathbb{N}_0^k} \in l^2(\mathbb{N}_0^k)$. So, we may apply [78, Proposition 20.2.7] (which holds in particular for the index set $I := \mathbb{N}_0^k$), and it follows that for any $r \geq 0$, T_r is a Hilbert-Schmidt operator with Hilbert-Schmidt norm

$$\|T_r\|_{\mathcal{S}_2} = \Big(\sum_{\alpha\in\mathbb{N}_0^k} \|T_r H_\alpha\|_K^2\Big)^{1/2} = \frac{1}{(1-\rho(2r))^{k/2}}.$$

Consequently, $T_t = T_{t/2}^2$ is the composition of two Hilbert-Schmidt operators, which allows us to apply [78, Proposition 20.2.8]. It follows that $T_t \in \mathcal{N}(K,K)$ and

$$\|T_t\|_{\mathcal{N}} \leq \|T_{t/2}\|_{\mathcal{S}_2}^2 = \frac{1}{(1-\rho(t))^k}.$$

□

6.3. Examples of real CCP functions, Gaussian copulas and an extension of Stein's lemma

As was to be expected, Theorem 6.5 and Theorem 6.8 give us first non-trivial examples, such as

$$h_{\text{sign},\text{sign}} : [-1,1] \longrightarrow [-1,1], x \mapsto \frac{2}{\pi}\arcsin(x) = \frac{2}{\pi}\, x\, {}_2F_1\Big(\frac{1}{2}, \frac{1}{2}, \frac{3}{2}; x^2\Big)$$

in the one-dimensional real case (implying the Grothendieck equality) and

$$h_{f_2,f_2} : [-1,1] \longrightarrow [-1,1], \tau \mapsto \frac{\pi}{4}\tau\, {}_2F_1\Big(\frac{1}{2}, \frac{1}{2}, 2; \tau^2\Big)$$

in the one-dimensional complex case (implying the Haagerup equality), where

$$\mathbb{R}^2 \ni x \mapsto f_2(x) := \begin{cases} \sqrt{2}\, \frac{x_1}{\|x\|_2} & \text{if } x \neq 0 \\ 0 & \text{if } x = 0 \end{cases}.$$

(cf. [57, Lemma 3.2. and Proof of Theorem 3.1] and Example 7.15). If we namely apply Theorem 4.12 to $m = 1$ and arbitrary $k \in \mathbb{N}$, we will recognise that Theorem 6.5 and Theorem 6.8 lead us to CCP functions $h_{f,f}$, where $f \in S_{L^2(\gamma_k)}$ is *bounded a.e.*. These examples also include [24, Lemma 2.1] as a special case. More precisely, we have:

Proposition 6.16. *Let $k \in \mathbb{N}$, $\rho \in [-1,1]$ and vec$(\boldsymbol{X}, \boldsymbol{Y}) \equiv (X_1, \ldots, X_k, Y_1, \ldots, Y_k)^\top \sim N_{2k}(0, \Sigma_{2k}(\rho))$. Consider the odd function*

$$\mathbb{R}^k \ni x \mapsto f_k(x) := \begin{cases} \sqrt{k}\, \frac{x_1}{\|x\|_{\mathbb{R}_2^k}} & \text{if } x \neq 0 \\ 0 & \text{if } x = 0 \end{cases}.$$

Then $f_k \in S_{L^2(\gamma_k)} \cap L^\infty(\gamma_k)$ and $\|f_k\|_\infty = \sqrt{k}$. The function $h_{f_k,f_k} : [-1,1] \longrightarrow [-1,1]$ is an odd strictly increasing homeomorphism which is CCP and satisfies $h_{f_k,f_k}\big|_{(-1,1)} \in W_+^\omega((-1,1))$. Let c_k be defined as in Lemma 4.7. Then $0 < h'_{f_k,f_k}(0) = c_k^2 < 1$. $h^{-1}_{f_k,f_k}\big|_{(-1,1)}$ is real analytic, and

$$\begin{aligned} h_{f_k,f_k}(\rho) &= k\,\mathbb{E}\Big[\frac{X_1 Y_1}{\|\boldsymbol{X}\|_{\mathbb{R}_2^k}\, \|\boldsymbol{Y}\|_{\mathbb{R}_2^k}}\Big] = \mathbb{E}\Big[\Big\langle \frac{\boldsymbol{X}}{\|\boldsymbol{X}\|_{\mathbb{R}_2^k}}, \frac{\boldsymbol{Y}}{\|\boldsymbol{Y}\|_{\mathbb{R}_2^k}} \Big\rangle_{\mathbb{R}_2^k}\Big] \\ &= c_k^2\, \rho\, {}_2F_1\Big(\frac{1}{2}, \frac{1}{2}, \frac{k+2}{2}; \rho^2\Big) = c_k^2\, k\,!!\sum_{n=0}^\infty \frac{((2n-1)!!)^2}{(2n)!!\,(2n+k)!!}\, \rho^{2n+1} \end{aligned} \tag{6.159}$$

In particular, the function $[-1,1] \ni \rho \mapsto h_{f_k,f_k}(\rho) - c_k^2\, \rho$ is CCP as well. If $|\rho| < 1$, then

$$h_{f_k,f_k}(\rho) = \sqrt{\frac{2k}{\pi}}\, c_k\, \rho \int_0^1 \frac{(\sqrt{1-t^2})^{k-1}}{\sqrt{1-\rho^2 t^2}}\, \mathrm{d}t\,. \tag{6.160}$$

Moreover,

$$\mathbb{E}\Big[\frac{X_i Y_i}{\|\boldsymbol{X}\|_{\mathbb{R}_2^k}\, \|\boldsymbol{Y}\|_{\mathbb{R}_2^k}}\Big] = \frac{c_k^2}{k}\, \rho\, {}_2F_1\Big(\frac{1}{2}, \frac{1}{2}, \frac{k+2}{2}; \rho^2\Big) \ \text{ and } \ \mathbb{E}\Big[\frac{X_i^2}{\|\boldsymbol{X}\|^2_{\mathbb{R}_2^k}}\Big] = \frac{1}{k}$$

for all $i \in [k]$.

Proof. If $k = 1$, (6.159) precisely coincides with the Grothendieck equality (Corollary 4.2). Thus, in order to prove (6.159), we may assume that $k \geq 2$. We just have to prove the second equality only (due to (4.110) and (4.95)). To this end, fix $i \in [k] \setminus \{1\}$. Consider the partitioned random vector vec$(\mathbf{X}', \mathbf{Y}')$, defined as $\mathbf{X}' := P_i^1\, \mathbf{X}$ and $\mathbf{Y}' := P_i^1\, \mathbf{Y}$, where

$P_i^1 := e_1\, e_i^\top + e_i\, e_1^\top + \frac{1}{2}\sum_{j\in[k]\setminus\{1,i\}} e_j\, e_j^\top = (P_i^1)^\top = (P_i^1)^{-1}$. So, if we swap the 1'st row and the i'th row of the equality matrix I_k, we obtain P_i^1, implying that $X_1' = X_i, X_i' = X_1$ and $X_j' = X_j$ for all $j \in [k] \setminus \{1, i\}$. Due to the construction of the random vector $\text{vec}(\mathbf{X}', \mathbf{Y}')$ and the structure of the correlation matrix $\Sigma_{2k}(\rho)$, it follows that

$$\begin{pmatrix} \mathbf{X}' \\ \mathbf{Y}' \end{pmatrix} = \begin{pmatrix} P_i^1 & 0 \\ 0 & P_i^1 \end{pmatrix} \begin{pmatrix} \mathbf{X} \\ \mathbf{Y} \end{pmatrix}$$

and

$$\begin{pmatrix} P_i^1 & 0 \\ 0 & P_i^1 \end{pmatrix} \begin{pmatrix} I_k & \rho\, I_k \\ \rho\, I_k & I_k \end{pmatrix} \begin{pmatrix} P_i^1 & 0 \\ 0 & P_i^1 \end{pmatrix} = \begin{pmatrix} I_k & \rho\, I_k \\ \rho\, I_k & I_k \end{pmatrix}.$$

Hence, $\text{vec}(\mathbf{X}', \mathbf{Y}') \stackrel{d}{=} \text{vec}(\mathbf{X}, \mathbf{Y}) \sim N_{2k}(0, \Sigma_{2k}(\rho))$. Consequently, we obtain

$$\mathbb{E}\Big[\frac{X_1\, Y_1}{\|\mathbf{X}\|_{\mathbb{R}_2^k}\, \|\mathbf{Y}\|_{\mathbb{R}_2^k}}\Big] = \mathbb{E}\Big[\frac{X_i'\, Y_i'}{\|\mathbf{X}'\|_{\mathbb{R}_2^k}\, \|\mathbf{Y}'\|_{\mathbb{R}_2^k}}\Big] = \mathbb{E}\Big[\frac{X_i\, Y_i}{\|\mathbf{X}\|_{\mathbb{R}_2^k}\, \|\mathbf{Y}\|_{\mathbb{R}_2^k}}\Big].$$

Since $h_{f_k,f_k}(\rho) = c_k^2\, \rho + c_k^2\, k\,!!\sum_{n=1}^\infty \frac{((2n-1)!!)^2}{(2n)!!\,(2n+k)!!}\, \rho^{2n+1}$ for all $\rho \in [-1, 1]$, it follows that $h'_{f_k,f_k}(0) = c_k^2 > 0$, implying that $h^{-1}_{f_k,f_k}\Big|_{(-1,1)}$ is real analytic (due to Theorem 6.8-(iii)). (6.160) follows from Euler's integral representation of the function $(-1, 1) \ni \rho \mapsto {}_2F_1\Big(\frac{1}{2}, \frac{1}{2}, \frac{k+2}{2}; \rho^2\Big)$ (cf. e.g. [6, Theorem 2.2.1]). Theorem 6.8 now completes the proof. □

Remark 6.17. Let $k \in \mathbb{N}$ and c_k be defined as in Lemma 4.7. Then [23, Theorem 1] in fact implies that

$$\frac{\pi}{2}\, c_d^2 \le K_G^{\mathbb{R}}(d) \text{ for all } d \in \mathbb{N}_3\,.$$

Remark 6.18 (**Krivine rounding scheme reconsidered**)**.** Fix $k \in \mathbb{N}$. Due to Proposition 6.16, the following set of real-valued functions is non-empty:

$$\mathcal{G}_k := \Big\{ f : f \in S_{L^2(\gamma_k)}, f \text{ is odd}, h'_{f,f}(0) > 0 \Big\}. \tag{6.161}$$

Let $f \in \mathcal{G}_k$. If in addition, $|f| = 1$ and $h^{-1}_{f,f}\Big|_{(-1,1)} \in W_+^\omega((-1, 1))$ Lemma 6.11 implies that $\{f \circ \sqrt{2}, f \circ \sqrt{2}\}$ is a Krivine rounding scheme, introduced in [22, Definition 2.1] (since $h_{f,f}$ coincides with the function $H_{f\circ\sqrt{2}, f\circ\sqrt{2}}$, introduced in [22, Definition 2.1] and $c(f \circ \sqrt{2}, f \circ \sqrt{2}) = h^{\text{hyp}}_{f,f}(1) \in (0, 1)$). The latter fact should be compared with Theorem 6.45!

Now it is no longer surprising that Proposition 6.16 encompasses the Grothendieck equality and the Haagerup equality as particular cases.

Example 6.19 ($k = 1$ **- Grothendieck**)**.** Fix $\rho \in [-1, 1]$. It is well-known that $\arcsin(\rho) = \rho\, {}_2F_1\Big(\frac{1}{2}, \frac{1}{2}, \frac{3}{2}; \rho^2\Big)$, whence $h_{f_1,f_1}(\rho) = \frac{2}{\pi} \arcsin(\rho)$.

Example 6.20 ($k = 2$ **- Haagerup**)**.** Let $n \in \mathbb{N}$, $u, v \in \mathbb{C}^n$ such that $\|u\| = 1$ and $\|v\| = 1$. Let $Z \sim \mathbb{C}N_n(0, I_n)$. The Haagerup equality (4.89), together with (4.90) implies that

$$\mathbb{E}[\text{sign}(u^* Z)\overline{\text{sign}(v^* Z)}] = \text{sign}(u^* v)\, h_{f_2,f_2}(|u^* v|).$$

In the following, we shed some light on the underlying structure of the function h_{ψ_a,ψ_b}, where $\psi_p := 1 - 2\mathbb{1}_{J_p} \in S_{L^2(\gamma_k)}$ and $J_p := \prod_{i=1}^{k}(-\infty, p_i]$ for all $p \equiv (p_1, \ldots, p_k)^\top \in \mathbb{R}^k$ (introduced in Corollary 6.2). Recall here that for any $n \in \mathbb{N}$, $\Sigma \in \mathbb{M}_n(\mathbb{R})^+$ and $\mathbf{X} \equiv (X_1, \ldots, X_n)^\top \sim N_n(0, \Sigma)$, $\Phi_{0,\Sigma} : \mathbb{R}^n \longrightarrow [0, 1]$ denotes the n-variate distribution function of $\mathbf{X}$, i.e.,

$$\Phi_{0,\Sigma}(x) := F_{\mathbf{X}}(x) = \mathbb{P}\Big(\bigcap_{i=1}^{n}\{X_i \leq x_i\}\Big) \text{ for all } x \equiv (x_1, \ldots, x_n)^\top \in \mathbb{R}^n .$$

Proposition 6.21. *Let $k \in \mathbb{N}$, $\rho \in [-1, 1]$ and $\boldsymbol{X} \equiv (X_1, \ldots, X_{2k})^\top \sim N_{2k}(0, \Sigma_{2k}(\rho))$. Let $a, b \in \mathbb{R}^k$ and $x \equiv (x_1, \ldots, x_{2k})^\top = vec(a, b)$. Then*

$$h_{\psi_a,\psi_b}(\rho) = 4\Phi_{0,\Sigma_{2k}(\rho)}(x) + 1 - 2\Phi_{0,I_k}(a) - 2\Phi_{0,I_k}(b). \tag{6.162}$$

Furthermore,

$$\Phi_{0,\Sigma_{2k}(\rho)}(x) = \Phi_{0,I_k}(a)\Phi_{0,I_k}(b) + \sum_{\nu=1}^{\infty} d_\nu(x; k)\, \rho^\nu ,$$

where

$$d_\nu(x; k) := \sum_{m \in C(\nu,k)} \Big(\prod_{\substack{i=1 \\ m_i=0}}^{2k} \Phi(x_i) \prod_{\substack{i=1 \\ m_i \neq 0}}^{2k} \frac{1}{\sqrt{m_i}} \varphi(x_i) H_{m_i-1}(x_i)\Big).$$

Proof. Fix $\mathbf{X} \equiv (X_1, \ldots, X_{2k})^\top \sim N_{2k}(0, \Sigma_{2k}(\rho))$ and $x = \text{vec}(a, b)$. Since $\psi_a(x_1)\, \psi_b(x_2) = (1-2\mathbb{1}_{J_a}(x_1))(1-2\mathbb{1}_{J_b}(x_2)) = 1-2\mathbb{1}_{J_a}(x_1)-2\mathbb{1}_{J_b}(x_2)+4\mathbb{1}_{J_a}(x_1)\mathbb{1}_{J_b}(x_2)$ for all $x_1, x_2 \in \mathbb{R}^k$ and $\mathbf{X} = \text{vec}(\mathbf{X}_1, \mathbf{X}_2)$, where $\mathbf{X}_1 := (X_1, \ldots, X_k)^\top \sim N_k(0, I_k)$ and $\mathbf{X}_2 := (X_{k+1}, \ldots, X_{2k})^\top \sim N_k(0, I_k)$, an application of Theorem 6.5 to the function h_{ψ_a,ψ_b} implies that

$$\begin{aligned}
F_{\mathbf{X}}(x) &= \mathbb{P}\Big(\bigcap_{i=1}^{2k}\{X_i \leq x_i\}\Big) = \mathbb{E}[\mathbb{1}_{J_a}(\mathbf{X}_1)\mathbb{1}_{J_b}(\mathbf{X}_2)] = \frac{1}{4}(h_{\psi_a,\psi_b}(\rho) - 1 + 2\Phi_{0,I_k}(a) + 2\Phi_{0,I_k}(b)) \\
&= \frac{1}{4}\Big((1 - 2\Phi_{0,I_k}(a))(1 - 2\Phi_{0,I_k}(b)) + \sum_{\nu=1}^{\infty} p_\nu(\psi_a, \psi_b)\rho^\nu - 1 + 2\Phi_{0,I_k}(a) + 2\Phi_{0,I_k}(b)\Big) \\
&= \Phi_{0,I_k}(a)\Phi_{0,I_k}(b) + \frac{1}{4}\sum_{\nu=1}^{\infty}\Big(\sum_{m \in C(\nu,k)} \langle\psi_a, H_m\rangle_{\gamma_k} \langle\psi_b, H_m\rangle_{\gamma_k}\Big)\rho^\nu .
\end{aligned}$$

The third equality is equivalent to (6.162). Corollary 6.2 clearly finishes the proof. □

Proposition 6.21 immediately gives us another significant example - which contains the Grothendieck equality as a special case again. Due to the famous Theorem of Sklar, it emerges from a lurking multivariate Gaussian copula; i.e., from a certain finite-dimensional distribution function with uniformly distributed marginals (cf., e.g., [111] and the references therein).

Example 6.22 **(A lurking $\Sigma_{2k}(\rho)$-Gaussian copula).** Let $k \in \mathbb{N}$, $m = (m_1, \ldots, m_k)^\top \in \mathbb{N}_0^k$, $\alpha = (\alpha_1, \ldots, \alpha_k)^\top \in (0, 1)^k$ and $\beta = (\beta_1, \ldots, \beta_k)^\top \in (0, 1)^k$. Let $a = (a_1, \ldots, a_k)^\top \in \mathbb{R}^k$ and $b = (b_1, \ldots, b_k)^\top \in \mathbb{R}^k$, where $a_i := \Phi^{-1}(\alpha_i)$ and $b_i := \Phi^{-1}(\beta_i)$ for all $i \in [k]$. Then

$$h_{\psi_a,\psi_b}(\rho) = 1 - 2\Big(\prod_{i=1}^{k}\alpha_i + \prod_{i=1}^{k}\beta_i\Big) + 4\, c_{\Sigma_{2k}(\rho)}(\alpha, \beta) \text{ for all } \rho \in [-1, 1],$$

where

$$(0,1)^k \ni (u_1,\ldots,u_k) \mapsto c_{\Sigma_{2k}(\rho)}(u_1,\ldots,u_k) := \Phi_{0,\Sigma_{2k}(\rho)}(\Phi^{-1}(u_1),\ldots,\Phi^{-1}(u_k))$$

denotes the $2k$-dimensional Gaussian copula with respect to the correlation matrix $\Sigma_{2k}(\rho)$ (cf., e.g., [111]). Consequently, if $(\alpha,\beta) = (\frac{1}{2},\frac{1}{2})$, it follows that $a = 0$, $b = 0$ and

$$h_{\psi_0,\psi_0}(\rho) = 1 - \tfrac{1}{2^{k-2}} + 4\Phi_{0,\Sigma_{2k}(\rho)}(0) = 1 - \tfrac{1}{2^{k-2}} + 4\mathbb{P}\Big(\bigcap_{i=1}^{2k}\{X_i \leq 0\}\Big) \tag{6.163}$$

for all $\rho \in [-1,1]$ and $\mathbf{X} = (X_1,\ldots,X_{2k})^\top \sim N_{2k}(0,\Sigma_{2k}(\rho))$ (since $\Phi(0) = \frac{1}{2}$). In fact, if $(\alpha,\beta) = (\frac{1}{2},\frac{1}{2})$ and $k = 1$, then $\psi_0 = \mathrm{sign} - \mathbb{1}_{\{0\}}$, implying that (6.163) even reduces to the Grothendieck equality. In order to recognise this, recall first that $(2l)! = 2^l\, l!\,(2l-1)!!$ for any $l \in \mathbb{N}_0$, whence

$$((2l-1)!!)^2 = \binom{2l}{l}\frac{(2l)!}{4^l}\,. \tag{6.164}$$

Consequently, the power series representation of the function h_{ψ_0,ψ_0}, together with Corollary 6.2 and (6.122) implies that

$$\begin{aligned}
4\mathbb{P}(X_1 \leq 0, X_2 \leq 0) - 1 = h_{\mathrm{sign},\mathrm{sign}}(\rho) &= h_{\psi_0,\psi_0}(\rho) \\
&= \sum_{n=0}^{\infty}(\langle \psi_0, H_n\rangle_{\gamma_1})^2\,\rho^n = \frac{2}{\pi}\sum_{l=0}^{\infty}\frac{1}{2l+1}H_{2l}^2(0)\,\rho^{2l+1} \\
&\overset{(6.122)}{=} \frac{2}{\pi}\sum_{l=0}^{\infty}((2l-1)!!)^2\,\frac{\rho^{2l+1}}{(2l+1)!} \overset{(6.164)}{=} \frac{2}{\pi}\arcsin(\rho)
\end{aligned} \tag{6.165}$$

for all $\rho \in [-1,1]$ and $(X_1,X_2)^\top \sim N_2(0,I_2)$ (cf. also [62, 101]). Again, we recognise that the Hermite expansion of the function sign - in $L^2(\gamma_1)$ - is given by

$$\mathrm{sign} = \psi_0 = \sqrt{\frac{2}{\pi}}\sum_{l=0}^{\infty}(-1)^l\,\frac{(2l-1)!!}{\sqrt{(2l+1)!}}\,H_{2l+1} \tag{6.166}$$

(cf. (6.129)).

A further interesting one-dimensional example ($k = 1$) is given by the function $h_{\Phi,\Phi}$, where $\Phi = F_X$ is the (continuous) distribution function of a standard normally distributed random variable $X \sim N_1(0,1)$. To this end, recall that the (continuous) random variable $U := \Phi(X) \sim U(0,1)$ is uniformly distributed on $[0,1]$, implying that $\Phi \in L^2(\gamma_1)$, with $\langle \Phi, 1\rangle_{\gamma_1} = \mathbb{E}[U] = \frac{1}{2}$ and $\|\Phi\|_{\gamma_1}^2 = \mathbb{E}[U^2] = Var(U) + \mathbb{E}^2[U] = \frac{1}{12} + \frac{1}{4} = \frac{1}{3}$ (cf. [111, Remark 2.17.]). In particular, $\mathbb{E}[\kappa(X)] = 0$, where $\kappa := 2\sqrt{3}\Phi - \sqrt{3} = \sqrt{3}(2\Phi - 1)$. Now, we are ready to prove

Proposition 6.23. *Let $X \sim N_1(0,1)$ and $\kappa := \sqrt{3}\big(2\Phi - 1\big)$. Then the following properties hold:*

(i)

$$\frac{\mathrm{d}^n}{\mathrm{d}t^n}\mathbb{E}[\Phi(X+t)] = 2^{-n/2}\,\varphi^{(n-1)}\Big(\frac{t}{\sqrt{2}}\Big) \textit{ for all } n \in \mathbb{N} \textit{ and } t \in \mathbb{R}\,.$$

(ii)

$$\mathbb{E}[\Phi(X+t)] = \Phi\Big(\frac{t}{\sqrt{2}}\Big) \textit{ for all } n \in \mathbb{N} \textit{ and } t \in \mathbb{R}\,.$$

(iii) $\mathbb{E}[\Phi(X)\,H_{2n+1}(X)] = (-1)^n \sqrt{\frac{1}{2\pi}}\sqrt{\frac{1}{4^n}\frac{1}{2n+1}\binom{2n}{n}}\sqrt{(\frac{1}{2})^{2n+1}}$ *for all* $n \in \mathbb{N}_0$. *In particular,* $\mathbb{E}[\kappa(X)\,H_{2n+1}(X)] = (-1)^n \sqrt{\frac{6}{\pi}}\sqrt{\frac{1}{4^n}\frac{1}{2n+1}\binom{2n}{n}}\sqrt{(\frac{1}{2})^{2n+1}}$ *for all* $n \in \mathbb{N}_0$.

(iv) $h_{\Phi,\Phi}(\rho) = \frac{1}{4} + \frac{1}{2\pi}\arcsin(\frac{\rho}{2})$ *and* $h_{\kappa,\kappa}(\rho) = \frac{6}{\pi}\arcsin(\frac{\rho}{2})$ *for all* $\rho \in [-1,1]$.

(v) $h_{\sqrt{3}\,\Phi,\sqrt{3}\,\Phi} = 3\,h_{\Phi,\Phi} = \frac{3}{4}(1+\frac{2}{\pi}\arcsin(\frac{1}{2}\cdot))$ *is a strictly increasing homeomorphic CCP function which maps* $[-1,1]$ *onto* $[\frac{1}{2},1]$ *and is neither odd nor even.* $h_{\kappa,\kappa}$ *is an odd, strictly increasing homeomorphic CCP function.* $h^{-1}_{\sqrt{3}\,\Phi,\sqrt{3}\,\Phi}(t) = -2\cos(\frac{2\pi}{3}t)$ *for all* $t \in [\frac{1}{2},1]$, $h^{-1}_{\kappa,\kappa}(s) = 2\sin(\frac{\pi}{6}s)$ *and* $\big(h^{-1}_{\kappa,\kappa}\big)_{abs}(s) = 2\sinh(\frac{\pi}{6}s)$ *for all* $s \in [-1,1]$. *In particular,* $\big(h^{-1}_{\kappa,\kappa}\big)_{abs}(1) > 1$. $h^{hyp}_{\kappa,\kappa}(\rho) = \frac{6}{\pi}\sinh^{-1}(\frac{\rho}{2})$ *for all* $\rho \in [-1,1]$.

(vi) κ *is odd,* $\|\kappa\|_{\gamma_1} = 1$ *and* $h'_{\kappa,\kappa}(0) = \frac{3}{\pi} > 0$. *Moreover,* $\kappa \in L^\infty(\gamma_1)$, *and* $\|\kappa\|_\infty = \sqrt{3}$.

Proof. (i) Fix $t \in \mathbb{R}$. We prove this result by induction on n. Obviously, we have to verify the base case only ($n = 1$). To this end, we apply a few Fourier transform techniques including the well-known fact that $\widehat{\varphi} = \varphi$ is its own Fourier transform. So, let $n = 1$. Then

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbb{E}[\Phi(X+t)] = \int_{\mathbb{R}}(\tau_{-t}\varphi)(x)\widehat{\varphi}(x)\mathrm{d}x = \int_{\mathbb{R}}\widehat{(\tau_{-t}\varphi)}(x)\varphi(x)\mathrm{d}x\,,$$

where $\tau_{-t}\varphi(x) := \varphi(x-(-t))$ denotes the translation operator (here, applied to φ). Since $\widehat{(\tau_{-t}\varphi)}(x) = \widehat{\varphi}(x)\exp(itx) = \varphi(x)\exp(itx)$ for all $x \in \mathbb{R}$, it follows that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbb{E}[\Phi(X+t)] = \frac{1}{2\pi}\int_{\mathbb{R}}\exp(-x^2)\exp(itx)\mathrm{d}x = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\varphi(y)\exp\Big(i\frac{t}{\sqrt{2}}y\Big)\mathrm{d}y$$
$$= \frac{1}{\sqrt{2}}\widehat{\varphi}(-\frac{t}{\sqrt{2}}) = \frac{1}{\sqrt{2}}\varphi(-\frac{t}{\sqrt{2}}) = \frac{1}{\sqrt{2}}\varphi^{(0)}(\frac{t}{\sqrt{2}}),$$

which finishes the verification of the base case.

(ii) We just have to integrate the base case on both sides (from 0 to t, say).

(iii) Since the Taylor series representation of φ obviously is given by

$$\varphi(x) = \frac{1}{\sqrt{2\pi}}\exp(-\frac{x^2}{2}) = \frac{1}{\sqrt{2\pi}}\sum_{m=0}^{\infty}\frac{(-1)^m}{2^m\,m!}\,x^{2m}$$

for all $x \in \mathbb{R}$, it follows that $\varphi^{(2m)}(0) = (2m)!\Big(\frac{1}{\sqrt{2\pi}}\frac{(-1)^m}{2^m\,m!}\Big) = \frac{1}{\sqrt{2\pi}}\frac{(-1)^m\,m!}{2^m}\binom{2m}{m}$ and $\varphi^{(2m+1)}(0) = 0$ for all $m \in \mathbb{N}_0$. (iii) now follows directly from (i) and (the one-dimensional case of) the equality (6.131), respectively Proposition 6.3.

(iv) follows directly from (iii).

(v) follows from (iv), Theorem 6.5, Lemma 6.11 and the fact that for example, $h_{\sqrt{3}\,\Phi,\sqrt{3}\,\Phi}(-1) = \frac{1}{2} \notin \{-1,1\}$.

(vi) Since $\Phi(x) + \Phi(-x) = 1$ for all $x \in \mathbb{R}$, it follows that κ is odd. (iv), applied to $\rho = 1$ implies that $\|\kappa\|^2_{\gamma_k} = h_{\kappa,\kappa}(1) = 1$. Moreover, (iv) clearly implies that $h'_{\kappa,\kappa}(0) = \frac{3}{\pi} > 0$. Finally, since $\Phi : \mathbb{R} \longrightarrow [0,1]$ is a distribution function, it follows that κ is bounded and $|\kappa(x)| \leq \sqrt{3} = \sqrt{3} \lim\limits_{x\to\infty}(2\Phi(x) - 1) = \lim\limits_{x\to\infty} \kappa(x)$ for all $x \in \mathbb{R}$. □

We will soon realise that Theorem 6.5 actually reflects a characterisation of the class of all real continuous CCP functions (see Theorem 6.33).

Within the scope of our analysis of the Grothendieck constants, we need *invertible* CCP functions, implying that we may ignore even CCP functions, defined on $[-1,1]$ (since these are non-injective). However, thanks to Theorem 5.17, $[-1,1] \ni \rho \mapsto \rho\, h(\rho)$ is an odd CCP function for any even CCP function h. In fact, we will recognise next that in particular any CCP function $h_{f,f}$, which satisfies $h_{f,f}(-1) < 1$ induces canonically an odd CCP function $h_{f^\times,f^\times}$, where $f^\times \in S_H$ is odd, $H := L^2(\mathbb{R}^k, \gamma_k)$. In the complex case it seems that we even have to use odd functions, to avoid calculations with non-positive semidefinite entrywise absolute values of correlation matrices (cf. (7.218) and Theorem 7.14, (ii)).

Proposition 6.24 (**Odd CCP transform**). *Let $k \in \mathbb{N}$ and $f \in L^2(\mathbb{R}^k, \gamma_k)$. Consider the odd function $\mathbb{R}^k \ni x \mapsto f^{odd}(x) := \frac{f(x)-f(-x)}{2}$ (the odd part of f). Then f is odd if and only if $f^{odd} = f$. In particular, $(f^{odd})^{odd} = f^{odd}$. f is even if and only if $f^{odd} = 0$. Moreover, $f^{odd} \in L^2(\mathbb{R}^k, \gamma_k)$ and*

(i)

$$\|f^{odd}\|^2_{\gamma_k} = \frac{h_{f,f}(1) - h_{f,f}(-1)}{2} \geq 0\,.$$

(ii) *f is even λ_k-a.s. if and only if $h_{f,f}(-1) = h_{f,f}(1)$.*

(iii) *f is odd λ_k-a.s. if and only if $h_{f,f}(-1) = -h_{f,f}(1)$.*

(iv) *Assume that $h_{f,f}(1) > h_{f,f}(-1)$. Put*

$$f^\times := \sqrt{\frac{2}{h_{f,f}(1) - h_{f,f}(-1)}}\, f^{odd}\,. \tag{6.167}$$

Then f is not even, $\|f^\times\|_{\gamma_k} = 1$, and $h_{f^\times,f^\times} = \frac{2}{h_{f,f}(1)-h_{f,f}(-1)} h_{f^{odd},f^{odd}}$ is an odd CCP function.

Proof. Due to Theorem 6.5, respectively Theorem 6.8, we just have to verify the non-trivial parts of the claims (i), (ii) and (iii).

(i) Fix $\mathbf{X} \sim N_k(0, I_k)$. Then

$$\|f^{\mathrm{odd}}\|^2_{\gamma_k} = \frac{1}{4}\,\mathbb{E}[(f^\circ)^2(\mathbf{X})] = \frac{1}{4}\Big(\mathbb{E}[f^2(\mathbf{X})] - 2\,\mathbb{E}[f(\mathbf{X})f(\text{-}\mathbf{X})] + \mathbb{E}[f^2(\text{-}\mathbf{X})]\Big).$$

Since $\text{-}\mathbf{X} \stackrel{d}{=} \mathbf{X} \sim N_k(0, I_k)$ and $\mathrm{vec}(\mathbf{X}, \text{-}\mathbf{X}) \sim N_{2k}(0, \Sigma_{2k}(-1))$, it follows from Theorem 6.5 that

$$\|f^{\mathrm{odd}}\|^2_{\gamma_k} = \frac{1}{2}\Big(\|f\|^2_{\gamma_k} - \mathbb{E}[f(\mathbf{X})f(\text{-}\mathbf{X})]\Big) = \frac{1}{2}(h_{f,f}(1) - h_{f,f}(-1)).$$

(ii) follows directly from (i).
(iii) Consider the even function $f^{\text{ev}} := f - f^{\text{odd}} \in L^2(\mathbb{R}^k, \gamma_k)$; i.e., the even part of f. By construction, $f^{\text{ev}}(x) = \frac{f(x)+f(-x)}{2}$ for all $x \in \mathbb{R}^k$. Similarly, as in the proof of (i), we therefore obtain

$$\|f^{\text{ev}}\|_{\gamma_k}^2 = \frac{h_{f,f}(1) + h_{f,f}(-1)}{2},$$

wherefrom claim (iii) obviously follows. □

Example 6.25. Since $\arcsin(\frac{1}{2}) = \frac{\pi}{6}$, Proposition 6.23-(iv) implies that $h_{\Phi,\Phi}(1) = \frac{1}{3}$ and $h_{\Phi,\Phi}(-1) = \frac{1}{6}$, whence

$$\Phi^{\times} = \sqrt{3}(2\Phi - 1) = \kappa\,.$$

Example 6.26. Let $[-1,1] \ni \rho \mapsto C^{\text{Ga}}(\frac{1}{2}, \frac{1}{2}; \rho)$ denote the bivariate Gaussian copula with Pearson's correlation coefficient ρ as parameter, evaluated at $(\frac{1}{2}, \frac{1}{2})$. Then

$$C^{\text{Ga}}(\frac{1}{2}, \frac{1}{2}; \rho) = \Phi_{\Sigma_2(\rho)}(\Phi^{-1}(\frac{1}{2}), \Phi^{-1}(\frac{1}{2})) = \mathbb{P}(X \leq 0, Y \leq 0) = h_{g,g}(\rho)\,,$$

where $\Phi_{\Sigma_2(\rho)}$ denotes the bivariate distribution function of the random vector $(X,Y)^\top \sim N_2(0, \Sigma_2(\rho))$ and $g := \mathbb{1}_{(-\infty,0]}$. Thus, $g^{\text{odd}} = -\frac{1}{2}\,\text{sign}$, $h_{g,g}(1) = \mathbb{P}(X \leq 0) = \Phi(0) = \frac{1}{2}$ and $h_{g,g}(-1) = \mathbb{P}(X \leq 0, -X \leq 0) = \mathbb{P}(X = 0) = 0$. Consequently,

$$g^{\times} = -\text{sign} = 2\,\mathbb{1}_{(-\infty,0)} - 1 + \mathbb{1}_{\{0\}}\,,$$

and it follows that $h_{g^{\times},g^{\times}} = \frac{2}{\pi}\arcsin$ (on $[-1,1]$).

Regarding an explicit calculation of the correlation coefficients $\mathbb{E}[f(\mathbf{X})g(\mathbf{Y})]$, induced by a pair of non-linearly transformed Gaussian random vectors and given "sufficiently smooth" functions f and g, we implement a few facts from the theory of distributions and test function spaces. A detailed in-depth introduction to these "generalised functions" and test function spaces and their analysis is provided by e. g. [61, 76, 127]. To this end, let $k \in \mathbb{N}$, $f \in L^1_{\text{loc}}(\mathbb{R}^k)$ (i.e., f is locally integrable) and $\psi \in \mathcal{S}_k$ be an arbitrary test function, where $\mathcal{S}_k$ denotes the Schwartz space of rapidly decreasing test functions on $\mathbb{R}^k$. Put

$$\langle \psi, \Lambda_f \rangle := \int_{\mathbb{R}^k} f(x)\psi(x)\mathrm{d}^k x\,.$$

Observe that the latter symbol $\langle \cdot, \cdot \rangle$ denotes the duality bracket on $\mathcal{S}_k \times \mathcal{S}_k'$ and not an inner product of Hilbert space elements. When there is no ambiguity, we adopt the common habit to identify the tempered distribution $\Lambda_f \in \mathcal{S}_k'$ with $f \in L^1_{\text{loc}}(\mathbb{R}^k)$ itself. More generally, recall that tempered distributions and their derivatives are elements of the dual space $\mathcal{S}_k'$ of $\mathcal{S}_k$, such as the Dirac delta distribution $\delta_0 = \delta$, defined via $\langle \psi, \delta \rangle := \psi(0)$ for any $\psi \in \mathcal{S}_k$. Observe that there is no $g \in L^1_{\text{loc}}(\mathbb{R}^k)$ such that $\delta = \Lambda_g$.

Let us quickly recall how differentiation of tempered distributions is defined. It originates from a reiteration of the integration by parts formula and is also known as "weak differentiation" (cf. e. g. [127, Chapter 6.12]):

$$\langle \psi, D^n u \rangle := (-1)^{|n|}\langle D^n\psi, u \rangle = (-1)^{|n|}\langle \psi, D^{n-1}(Du) \rangle \tag{6.168}$$

for all $\psi \in \mathcal{S}_k, u \in \mathcal{S}_k'$ and $n \in \mathbb{N}_0^k$. Consequently, since $H_n\,\varphi_k \in \mathcal{S}_k$ for all $n \in \mathbb{N}_0^k$ and $D^n u \in \mathcal{S}_k'$ for all $u \in \mathcal{S}_k$, (6.121) in particular implies:

$$\langle H_n\,\varphi_k, u\rangle = \frac{1}{\sqrt{n!}}\langle \varphi_k, D^n u\rangle \text{ for all } u \in \mathcal{S}_k' \text{ and } n \in \mathbb{N}_0^k\,.$$

Given an arbitrary compact subset $K \subseteq \mathbb{R}^k$ and $f \in L^2(\gamma_k)$, it follows that

$$\int_K |f|\,\mathrm{d}\lambda_k = \sqrt{2\pi}\int_{\mathbb{R}^k} \mathbb{1}_K(x)\exp(\frac{1}{2}\|x\|^2)\,|f(x)|\,\gamma_k(\mathrm{d}x) \leq c_K\,\|f\|_{\gamma_k}\,,$$

where $c_K := \sqrt{2\pi}\int_K e^{\|x\|^2}\,\gamma_k(\mathrm{d}x) = \sqrt{2\pi}\int_K \exp(\frac{1}{2}\|x\|^2)\lambda_k(\mathrm{d}x) < \infty$. Consequently, $L^2(\gamma_k) \subseteq L^1_{\mathrm{loc}}(\mathbb{R}^k)$, implying that for any $\mathbf{X} \sim N_k(0, I_k)$

$$\mathbb{E}[H_n(\mathbf{X})f(\mathbf{X})] = \langle H_n, f\rangle_{\gamma_k} = \langle H_n\,\varphi_k, \Lambda_f\rangle = \frac{1}{\sqrt{n!}}\langle \varphi_k, D^n\Lambda_f\rangle \text{ for all } f \in L^2(\gamma_k) \text{ and } n \in \mathbb{N}_0^k\,. \tag{6.169}$$

Example 6.27 (**n'th weak derivative of $\Lambda_{\mathbb{1}_{[0,\infty)}}$**). Let $k = 1$ and $n \in \mathbb{N}_0$. A very easy proof by induction on n, based on (6.168), together with (6.120) firstly reveals that

$$\langle \varphi, D^n\delta\rangle = (-1)^n\,\varphi^{(n)}(0) = \frac{\sqrt{n!}}{\sqrt{2\pi}}\,H_n(0)\,.$$

(6.122) therefore implies that

$$\langle \varphi, D^{2l}\delta\rangle = (-1)^l\,\frac{1}{\sqrt{2\pi}}\,(2l-1)!! \text{ for all } l \in \mathbb{N}_0\,.$$

Similarly, (6.168) implies that $D\Lambda_{\mathbb{1}_{[0,\infty)}} = \delta$. Since $\mathrm{sign} = 2\,\mathbb{1}_{[0,\infty)} - 1$ (γ_1-almost surely) and $\langle H_{2l+1}, 1\rangle_{\gamma_1} = \langle H_{2l+1}, H_0\rangle_{\gamma_1} = \delta_{2l+1,0} = 0$, it follows that

$$\begin{aligned}\langle H_{2l+1}, \mathrm{sign}\rangle_{\gamma_1} = 2\langle H_{2l+1}, \mathbb{1}_{[0,\infty)}\rangle_{\gamma_1} &\overset{(6.169)}{=} \frac{2}{\sqrt{(2l+1)!}}\langle \varphi, D^{2l+1}\Lambda_{\mathbb{1}_{[0,\infty)}}\rangle \\ &= \frac{2}{\sqrt{(2l+1)!}}\langle \varphi, D^{2l}\delta\rangle = (-1)^l\sqrt{\frac{2}{\pi}}\,\frac{(2l-1)!!}{\sqrt{(2l+1)!}}\end{aligned}$$

for all $l \in \mathbb{N}_0$. This outcome – which is solely based on a multiple weak differentiation of $\Lambda_{\mathbb{1}_{[0,\infty)}}$ – should be compared now with (the derivation of) (6.165)!

(6.169) can be strongly simplified if f is smooth (cf. also Proposition 6.3). More precisely, if $N \in \mathbb{N}_0, D^n f \in L^2(\gamma_k) \cap C(\mathbb{R}^k)$ for all $n \in \mathbb{N}_0^k$, satisfying $0 \leq |n| \leq N$, and if $\mathbf{X} \sim N_k(0, I_k)$, then $D^n\Lambda_f = \Lambda_{D^n f}$ (cf. [127, Chapter 6.13]), and

$$\mathbb{E}[H_n(\mathbf{X})f(\mathbf{X})] = \langle H_n, f\rangle_{\gamma_k} = \frac{1}{\sqrt{n!}}\mathbb{E}[D^n f(\mathbf{X})] \text{ for all } n \in \mathbb{N}_0^k\,, \text{ with } |n| \leq N\,. \tag{6.170}$$

In fact, even more can be said. Recall that (by construction of Sobolev spaces) the latter equality also holds without the smoothness assumption, if we just assume that $f \in L^2(\gamma_k) \cap W^{N,1}_{\mathrm{loc}}(\mathbb{R}^k)$, so that in this case $D^n f$ denotes the distributional n'th derivative in

$L^1_{\mathrm{loc}}(\mathbb{R}^k)$ instead (cf. e.g. [61, Chapter 3.1]). Independent of an application of Theorem 6.5 to the primary topic of our paper, it implies further non-trivial consequences including a generalisation of Stein's Lemma (cf. [92, Theorem 1 and Example 1]) and a certain "decorrelation property" of harmonic functions. We only have to combine (6.170) and Theorem 6.5, resulting at once in

Proposition 6.28. *Let $k \in \mathbb{N}$, $\rho \in [-1,1]$ and $vec(\boldsymbol{X}, \boldsymbol{Y}) \sim N_{2k}(0, \Sigma_{2k}(\rho))$. Let $f, g \in L^2(\gamma_k)$. Then*

$$cov(f(\boldsymbol{X}), g(\boldsymbol{Y})) = \sum_{\nu=1}^{\infty} \Big(\sum_{n \in C(\nu,k)} \frac{1}{n!} \langle \varphi_k, D^n \Lambda_f \rangle \langle \varphi_k, D^n \Lambda_g \rangle \Big) \rho^\nu .$$

If in addition $(f,g) \in W^{N,1}_{loc}(\mathbb{R}^k) \times W^{N,1}_{loc}(\mathbb{R}^k)$, or if $(D^n f, D^n g) \in (L^2(\gamma_k) \cap C(\mathbb{R}^k)) \times (L^2(\gamma_k) \cap C(\mathbb{R}^k))$ for all $n \in \mathbb{N}_0^k$, satisfying $0 \leq |n| \leq N$ for some $N \in \mathbb{N}$, then

$$cov(f(\boldsymbol{X}), g(\boldsymbol{Y})) = \sum_{\nu=1}^{N} \Big(\sum_{n \in C(\nu,k)} \frac{1}{n!} \mathbb{E}[D^n f(\boldsymbol{X})] \mathbb{E}[D^n g(\boldsymbol{Y})] \Big) \rho^\nu + \sum_{\nu=N+1}^{\infty} \Big(\sum_{n \in C(\nu,k)} \frac{1}{n!} \langle \varphi_k, D^n \Lambda_f \rangle \langle \varphi_k, D^n \Lambda_g \rangle \Big) \rho^\nu .$$

In particular, if $N = 1$, then

$$cov(f(\boldsymbol{X}), Y_i) = \rho\, \mathbb{E}[\frac{\partial f}{\partial x_i}(\boldsymbol{X})]$$

for all $i \in [k]$, respectively

$$\mathbb{E}[f(\boldsymbol{X})\, \boldsymbol{Y}] = \rho\, \mathbb{E}[\nabla f(\boldsymbol{X})].$$

If $N = 2$, then

$$cov(f(\boldsymbol{X}), \|\boldsymbol{Y}\|^2) = \rho^2\, \mathbb{E}[\triangle f(\boldsymbol{X})].$$

In the one-dimensional case (i.e., $k = 1$), a direct application of Proposition 6.28, respectively (6.170), implies two further results which are of their own interest. In particular, our approach enables the provision of a quick and short proof of the following generalisation of Stein's Lemma to standard Gaussian random powers (cf. [99, Theorem 1]):

Corollary 6.29. *Let $m \in \mathbb{N}_0$, $f \in L^2(\gamma_1)$ and $X \sim N_1(0,1)$ be given. If $D^l f \equiv f^{(l)} \in L^2(\gamma_1) \cap C(\mathbb{R})$ for all $0 \leq l \leq m$, then*

$$\mathbb{E}[f(X) X^m] = \mathbb{E}[(-i)^m H_m(iD)(f(X))] = \sum_{\nu=0}^{\lfloor m/2 \rfloor} \binom{m}{2\nu} (2\nu - 1)!!\, \mathbb{E}[D^{m-2\nu} f(X)] .$$

Proof. Fix $m \in \mathbb{N}_0$. Put $f_m(x) := x^m$ $(x \in \mathbb{R})$. Firstly, recall the well-known result that

$$\mathbb{E}[f_\nu(X)] = \mathbb{E}[X^\nu] = \frac{1 + (-1)^\nu}{2} (\nu - 1)!! \text{ for all } \nu \in \mathbb{N}_0 ,$$

implying that

$$\langle f_m, H_l \rangle_{\gamma_1} \overset{(6.170)}{=} \frac{1}{\sqrt{l!}} \mathbb{E}[D^l f_m(X)] = \begin{cases} \frac{1+(-1)^{m-l}}{2} \sqrt{l!} \binom{m}{l} (m-l-1)!! & \text{if } l \leq m \\ 0 & \text{if } l > m \end{cases}$$

Consequently,

$$\mathbb{E}[f(X)f_m(X)] = h_{f,f_m}(1) = \sum_{l=0}^{m} \langle f, H_l\rangle_{\gamma_1} \langle f_m, H_l\rangle_{\gamma_1} = \sum_{l=0}^{m} \frac{1+(-1)^{m-l}}{2} \mathbb{E}[D^l f(X)] \binom{m}{l} (m-l-1)!!\,.$$

If m is even, it therefore follows that

$$\mathbb{E}[f(X)f_m(X)] = \sum_{k=0}^{m/2} \mathbb{E}[D^{2k} f(X)] \binom{m}{2k} (m-2k-1)!! = \sum_{\nu=0}^{m/2} \mathbb{E}[D^{m-2\nu} f(X)] \binom{m}{2\nu} (2\nu-1)!!\,.$$

Similarly, if m is odd, we obtain

$$\mathbb{E}[f(X)f_m(X)] = \sum_{\nu=0}^{(m-1)/2} \mathbb{E}[D^{m-2\nu} f(X)] \binom{m}{2\nu} (2\nu-1)!!\,.$$

However, since $\binom{m}{2\nu}(2\nu-1)!! = H_{m,\nu}$ (due to (6.120)), the claim clearly follows. $\square$

Corollary 6.30. *Let $\nu \in \mathbb{N}_0$, $f, g \in L^2(\gamma_1)$ and $\rho \in (-1,1)$. Then*

$$h_{f,g}^{(\nu)}(\rho) = \sum_{n=0}^{\infty} \frac{1}{n!} \langle \varphi, D^n(D^\nu \Lambda_f)\rangle \langle \varphi, D^n(D^\nu \Lambda_g)\rangle \rho^n\,.$$

In particular, if in addition $(f,g) \in C^\infty(\mathbb{R}^k) \times C^\infty(\mathbb{R}^k)$, then

$$h_{f,g}^{(\nu)}(\rho) = h_{f^{(\nu)},g^{(\nu)}}(\rho) \text{ for all } \rho \in (-1,1).$$

Proof. Since $h_{f,g}$ is real analytic, $h_{f,g}^{(\nu)}$ is well-defined (where $h_{f,g}^{(0)} := h_{f,g}$, of course). Due to (6.169) and Theorem 6.5, applied to $k=1$, the remaining part of the proof is a straightforward proof by induction on $\nu \in \mathbb{N}_0$. $\square$

Remark 6.31. Firstly, observe that the strong impact of the standard (multivariate) *Gaussian* law, is reflected in (6.169), primarily implied by the fact that the Gaussian density function φ_k and hence each $H_n\,\varphi_k$, is rapidly decreasing: $H_n\,\varphi_k \in \mathcal{S}_k$ for all $n \in \mathbb{N}_0^k$ (since each H_n is a polynomial). This fact and the structure of the (multivariate) Hermite polynomials (which itself is also induced by the structure of φ_k) namely enables a reiterated use of the integration by parts formula in the smooth case, respectively a use of the Sobolev space $W_{\text{loc}}^{N,1}(\mathbb{R}^k)$ in the non-smooth case, implying the transition of each inner product $\langle H_n, f\rangle_{\gamma_k}$ on the Hilbert space $L^2(\gamma_k)$ into the duality bracket $\langle \varphi_k, D^n \Lambda_f\rangle$ on $\mathcal{S}_k \times \mathcal{S}_k'$. The latter, however, seems to be more convenient for performing specific computations.

6.4. Upper bounds of $K_G^{\mathbb{R}}$ and inversion of real CCP functions

Our next step is to embed Grothendieck's original approach as well as Krivine's improvement into a general framework. We are going to show that we may *substitute* the Grothendieck function $h_{\text{sign},\text{sign}} = \frac{2}{\pi}\arcsin$ through *invertible* CCP functions $h_{f,f}$, generated by *bounded* functions $f : \mathbb{R}^k \longrightarrow \mathbb{R}$ (see Theorem 6.40 and Theorem 6.45). Various proofs of Krivine's main result ($K_G^{\mathbb{R}} \leq \frac{\pi}{2\ln(1+\sqrt{2})} \approx 1,782$) are set out in detail in [70, Section 5], [77, proof of Lemma 10.5] and [151]. We will recognise soon that inverses of odd CCP functions also lead to a further crucial construction of correlation matrices, lurking in the following important implication of Lemma 5.10:

Theorem 6.32. *Let $r > 0$, $0 < c \leq r$ and $0 \neq \psi \in W_+^\omega((-r,r))$. Then $\psi_{abs}\Big|_{[0,r]}$ is strictly increasing and $\psi_{abs}(c) > 0$. For any $k \in \mathbb{N}$ there exist $\alpha_k \equiv \alpha_k^{\psi,c} \in S_{L^2(\gamma_k)}$ and $\beta_k \equiv \beta_k^{\psi,c} \in S_{L^2(\gamma_k)}$, such that the following properties hold:*

(i) *If $\boldsymbol{X} \sim N_k(0, I_k)$, then $\sqrt{\psi_{abs}(c)}\,\mathbb{E}[\alpha_k(\boldsymbol{X})] = sign(\psi(0))\sqrt{|\psi(0)|}$ and $\sqrt{\psi_{abs}(c)}\,\mathbb{E}[\beta_k(\boldsymbol{X})] = \sqrt{|\psi(0)|}$. In particular, $\mathbb{E}[\alpha_k(\boldsymbol{X})] = sign(\psi(0))\mathbb{E}[\beta_k(\boldsymbol{X})]$.*

(ii) *If $c < r$, then $[-c, c] \subseteq (-r, r)$ and*

$$\psi(c\rho) = \psi_{abs}(c) h_{\alpha_k,\beta_k}(\rho) \text{ for all } \rho \in [-1,1]. \tag{6.171}$$

In particular, $\psi(c) = \psi_{abs}(c)\langle\alpha_k, \beta_k\rangle_{\gamma_k}$.

(iii) *If $c \leq r$, then*

$$\psi_{abs}(c\rho) = \psi_{abs}(c)\, h_{\alpha_k,\alpha_k}(\rho) = \psi_{abs}(c)\, h_{\beta_k,\beta_k}(\rho) \text{ for all } \rho \in [-1,1].$$

(iv) *If $c < r$, H is an arbitrary $\mathbb{R}$-Hilbert space, then there exists a $\mathbb{R}$-Hilbert space $\mathbb{H}$ such that for any $u, v \in S_H$*

$$\psi(c\langle u, v\rangle_H) = \psi_{abs}(c)\langle\psi_u(\alpha_k), \psi_v(\beta_k)\rangle_{\mathbb{H}} = \langle a_u, b_v\rangle_{\mathbb{H}}\,, \tag{6.172}$$

where for any $w \in S_H$, $\|a_w\|^2_{\mathbb{H}} = \|b_w\|^2_{\mathbb{H}} = \psi_{abs}(c)$ and $\psi_w : L^2(\gamma_k) \longrightarrow \mathbb{H}$ is a mapping which satisfies $\psi_w(S_{L^2(\gamma_k)}) \subseteq S_{\mathbb{H}}$. In particular, $\psi(c) = \langle a_w, b_w\rangle_{\mathbb{H}}$ for all $w \in S_H$.
If $c \leq r$, then

$$\begin{aligned}\psi_{abs}(c\langle u, v\rangle_H) &= \psi_{abs}(c)\langle\psi_u(\alpha_k), \psi_v(\alpha_k)\rangle_{\mathbb{H}} = \psi_{abs}(c)\langle\psi_u(\beta_k), \psi_v(\beta_k)\rangle_{\mathbb{H}} \\ &= \langle a_u, a_v\rangle_{\mathbb{H}} = \langle b_u, b_v\rangle_{\mathbb{H}}\,,\end{aligned}$$

Proof. Let $0 < c \leq r$. Put $b_\nu := \frac{\psi^{(\nu)}(0)}{\nu!}$ ($\nu \in \mathbb{N}_0$). Consider the family $\{q_n : n \in \mathbb{N}_0^k\}$, defined as $q_0 := \sqrt{|\psi(0)|} = \sqrt{|b_0|}$ and

$$q_n \equiv q_n(k) := \sqrt{\frac{|\psi^{(|n|)}(0)|}{n!\,k^{|n|}}} = \sqrt{\frac{|n|\,!\,|b_{|n|}|}{n!\,k^{|n|}}} = \sqrt{\frac{|n|\,!}{n!}\,a_{|n|}^{|n|}} = \sqrt{\frac{|n|\,!}{n!}\prod_{i=1}^{k} a_{|n|}^{n_i}}$$

for $n \in \mathbb{N}_0^k \setminus \{0\}$, where $a_\nu \equiv a_\nu(k) := \left(\frac{|b_\nu|}{k^\nu}\right)^{1/\nu}$ ($\nu \neq 0$). As before, let $C(\nu; k) := \{n \in \mathbb{N}_0^k : |n| = \nu\}$, where $\nu \in \mathbb{N}_0$. A straightforward application of the multinomial theorem implies that for all $\nu \in \mathbb{N}$ the following equality holds:

$$\sum_{n \in C(\nu;k)} q_n^2(k) = \sum_{n \in C(\nu;k)} \frac{\nu!}{n!}\prod_{i=1}^{k} a_\nu^{n_i} = \sum_{n \in C(\nu;k)} \binom{\nu}{n_1, n_2, \ldots, n_k}\prod_{i=1}^{k} a_\nu^{n_i} = \Big(\sum_{i=1}^{k} a_\nu\Big)^\nu = k^\nu a_\nu^\nu = |b_\nu|\,. \tag{6.173}$$

It should be noted here, that by construction also $\sum_{n \in C(0;k)} q_n^2 = q_0^2 = |b_0|$ holds. Consequently, since $\{H_\alpha : \alpha \in \mathbb{N}_0^k\}$ is an orthonormal basis in $L^2(\gamma_k)$, it follows that

$$\alpha_k^{\psi,c} := \frac{1}{\sqrt{\psi_{\text{abs}}(c)}}\sum_{n \in \mathbb{N}_0^k} \text{sign}(b_{|n|})\, q_n(k)(\sqrt{c})^{|n|} H_n \in S_{L^2(\gamma_k)}$$

and

$$\beta_k^{\psi,c} := \frac{1}{\sqrt{\psi_{\text{abs}}(c)}} \sum_{n \in \mathbb{N}_0^k} q_n(k)(\sqrt{c})^{|n|} H_n \in S_{L^2(\gamma_k)}$$

are well-defined (including the case $c = r$), from which the assertions (i), (ii) and (iii) follow (due to (6.173)). (iv) follows from (ii), (iii) and Proposition 6.4, with $\rho := \langle u, v \rangle_H$, and (v) is an implication of Lemma 5.10 and the construction of α_k and β_k. □

If we combine Theorem 5.17, Theorem 6.5, Proposition 6.24 and Theorem 6.32, (iii), a further significant characterisation of continuous odd CCP functions follows at once:

Theorem 6.33 (**CCP representation theorem**). *Let $\psi : [-1, 1] \longrightarrow \mathbb{R}$ be a continuous odd function and $k \in \mathbb{N}$. Then the following statements are equivalent:*

(i) *ψ is a CCP function.*

(ii) *$\psi = h_{f,f}$ for some odd $f \in S_{L^2(\gamma_k)}$.*

Theorem 6.32-(iv), together with Lemma 6.11 directly enriches us with another crucial result, related to a construction of real quantum correlation matrices which actually include lurking upper bounds of $K_G^{\mathbb{R}}$:

Corollary 6.34. *Let $m, n, k \in \mathbb{N}$ and $f \in S_{L^2(\gamma_k)}$ be odd. Assume that $h_{f,f}^{-1}\big|_{(-1,1)} \in W_+^{\omega}((-1, 1))$. Put*

$$c(f) := h_{f,f}^{hyp}(1)\,.$$

Then $c(f) \in (0, 1)$ and

$$h_{f,f}^{-1}[c(f)S] \in \mathcal{Q}_{m,n} \text{ for all } S \in \mathcal{Q}_{m,n}\,.$$

If $\Sigma = \begin{pmatrix} M & S \\ S^\top & N \end{pmatrix} \in C(m + n; \mathbb{R})$ is an arbitrary real $(m + n) \times (m + n)$ correlation matrix (with block elements $M \in C(m; \mathbb{R}), N \in C(n; \mathbb{R})$ and $S \in \mathcal{Q}_{m,n}$), then

$$\begin{pmatrix} (h_{f,f}^{-1})_{abs}[c(f)M] & h_{f,f}^{-1}[c(f)S] \\ h_{f,f}^{-1}[c(f)S^\top] & (h_{f,f}^{-1})_{abs}[c(f)N] \end{pmatrix} \in C(m + n; \mathbb{R}) \tag{6.174}$$

again is an $(m + n) \times (m + n)$ correlation matrix with real entries.

Proof. We just have to apply Theorem 6.32, (iv), including (6.172), to the function $\psi := h_{f,f}^{-1}\big|_{(-1,1)}$ and the constant $c := h_{f,f}^{\text{hyp}}(1)$ $(0 < c < 1$, due to Lemma 6.11). □

If $\psi : D_{\mathbb{F}} \longrightarrow D_{\mathbb{F}}$ is an arbitrary CCP function and $\Sigma \in C(m + n; \mathbb{F})$ is an arbitrary $m + n$-correlation matrix, then

$$\psi[\Sigma] = \begin{pmatrix} \psi[\Gamma_H(u, u)] & \psi[\Gamma_H(u, v)] \\ \psi[\Gamma_H(u, v)^*] & \psi[\Gamma_H(v, v)] \end{pmatrix} \in C(m + n; \mathbb{F})$$

again is a correlation matrix. Consequently, it follows that $\psi[\Gamma_H(u, u)] = \Gamma_K(x, x) \in C(m; \mathbb{F})$, $\psi[\Gamma_H(v, v)] = \Gamma_K(y, y) \in C(n; \mathbb{F})$ and $\psi[\Gamma_H(u, v)] = \Gamma_K(x, y) \in \mathcal{Q}_{m,n}(\mathbb{F})$ for some Hilbert space K over $\mathbb{F}$ and some $(x, y) \in S_K^m \times S_K^n$ (due to Corollary 3.5). However, a considerably stronger result holds (cf. also (6.174)):

Theorem 6.35. *Let $m, n \in \mathbb{N}$ and $M := \begin{pmatrix} A & S \\ S^\top & B \end{pmatrix} \in \mathbb{M}_{m+n}(\mathbb{R})$, where $A \in \mathbb{M}_m(\mathbb{R})$, $S \in \mathbb{M}_{m,n}(\mathbb{R})$ and $B \in \mathbb{M}_n(\mathbb{R})$. Let $0 < r < \infty$ and $f, g : (-r, r) \longrightarrow \mathbb{R}$ be two functions, such that $(-r, r) \ni x \mapsto f(x) = \sum_{\nu=0}^{\infty} a_\nu x^\nu \in W_+^\omega((-r, r))$ and $(-r, r) \ni x \mapsto g(x) = \sum_{\nu=0}^{\infty} b_\nu x^\nu \in W_+^\omega((-r, r)) \in W_+^\omega((-r, r))$. Let $q \in C^\omega((-r, r))$, such that*

$$|c_\nu| \leq \sqrt{|a_\nu|\,|b_\nu|} \text{ for all } \nu \in \mathbb{N}_0\,, \tag{6.175}$$

where $c_\nu := \frac{q^{(\nu)}(0)}{\nu!}$. Then $q \in W_+^\omega((-r, r))$, and the following properties hold:

(i) *If $M \in \mathbb{M}_{m+n}([-r, r])^+$ is positive semidefinite, and if any entry of the matrices A, S and B is an element of $[-r, r]$, then also*

$$\begin{pmatrix} f_{abs}[A] & \tilde{q}[S] \\ \tilde{q}[S]^\top & g_{abs}[B] \end{pmatrix} \in \mathbb{M}_{m+n}([-r, r])^+$$

is positive semidefinite, where $\tilde{q}$ is defined as in Lemma 5.10. In particular, if $0 < c^* \leq r$ is a root of $f_{abs} - 1$, then

$$\tilde{q}[c^*\Gamma] \in \mathcal{Q}_{m,n} \text{ for all } \Gamma \in \mathcal{Q}_{m,n}\,.$$

(ii) *If $M \in C(m + n; \mathbb{R})$ is a real correlation matrix, then also*

$$\begin{pmatrix} h_{\alpha,\alpha}[A] & h_{\alpha,\beta}[S] \\ h_{\alpha,\beta}[S^\top] & h_{\beta,\beta}[B] \end{pmatrix} \in C(m + n; \mathbb{R})$$

is a real correlation matrix for all $\alpha, \beta \in S_{L^2(\gamma_k)}$. In particular,

$$h_{\alpha,\beta}[\cdot] : \mathcal{Q}_{m,n} \longrightarrow \mathcal{Q}_{m,n} \text{ for all } \alpha, \beta \in S_{L^2(\gamma_k)}. \tag{6.176}$$

(iii) *For all $\alpha, \beta \in S_{L^2(\gamma_k)}$, for all Hilbert spaces H and $u, v \in S_H$ there exist $d \in \mathbb{N}$ and $x, y \in \mathbb{S}^{d-1}$, such that*

$$h_{\alpha,\beta}(\langle u, v\rangle_H) = \langle x, y\rangle_{\mathbb{R}_2^d} = x^\top y\,.$$

Proof. (i) Our proof is built on a sufficient and necessary characterisation of positive semidefinite block matrices, Schur multiplication of matrices, and a straightforward application of Hölder's inequality in l_2. Due to [56, Lemma 1.1.13, statement 2], it suffices to show that the following inequality is satisfied and well-defined:

$$|h^\top q[S]k| \leq \sqrt{(h^\top f_{\text{abs}}[A]h)}\sqrt{(k^\top g_{\text{abs}}[B]k)} \text{ for all } (h, k) \in \mathbb{R}^m \times \mathbb{R}^n\,. \tag{6.177}$$

So, fix $h \in \mathbb{R}^m$ and $k \in \mathbb{R}^n$. Given the assumption that M is positive semidefinite, it follows that also A and B are positive semidefinite matrices. Since $M^{*0} = \mathbf{1}_{m+n}\mathbf{1}_{m+n}^\top$, $A^{*0} = \mathbf{1}_m\mathbf{1}_m^\top$, $B^{*0} = \mathbf{1}_n\mathbf{1}_n^\top$ and $S^{*0} = \mathbf{1}_m\mathbf{1}_n^\top$, the Schur multiplication theorem therefore implies that in fact for any $\nu \in \mathbb{N}_0$

$$M^{*\nu} = \begin{pmatrix} A^{*\nu} & S^{*\nu} \\ \left(S^{*\nu}\right)^\top & B^{*\nu} \end{pmatrix}$$

is positive semidefinite, such as $A^{*\nu}$ and $B^{*\nu}$. Hence,

$$|h^\top S^{*\nu} k| \leq \sqrt{h^\top A^{*\nu} h}\,\sqrt{k^\top B^{*\nu} k} \text{ for all } \nu \in \mathbb{N}_0$$

(due to [56, Lemma 1.1.13.2]). Put $\alpha_\nu := \sqrt{|a_\nu|}\,\sqrt{h^\top (A^{*\nu}) h} = \sqrt{h^\top (|a_\nu| A^{*\nu}) h}$ and $\beta_\nu := \sqrt{|b_\nu|}\,\sqrt{h^\top (B^{*\nu}) h} = \sqrt{k^\top (|b_\nu| B^{*\nu}) k}$. An application of Hölder's inequality in l_2 implies that

$$\sum_{\nu=0}^{\infty} \alpha_\nu \beta_\nu \leq \Big(\sum_{\nu=0}^{\infty} \alpha_\nu^2\Big)^{\frac{1}{2}} \Big(\sum_{\nu=0}^{\infty} \beta_\nu^2\Big)^{\frac{1}{2}} = \sqrt{(h^\top f_{\text{abs}}[A] h)}\sqrt{(k^\top g_{\text{abs}}[B] k)}. \tag{6.178}$$

Due to (7.222), a further application of Hölder's inequality in l_2 implies that

$$\sum_{\nu=0}^{\infty} |c_\nu|\, r^\nu \overset{(7.222)}{\leq} \sum_{\nu=0}^{\infty} \sqrt{|a_\nu|\, r^\nu}\,\sqrt{|b_\nu|\, r^\nu} \leq \Big(\sum_{\nu=0}^{\infty} |a_\nu|\, r^\nu\Big)^{\frac{1}{2}} \Big(\sum_{\nu=0}^{\infty} |b_\nu|\, r^\nu\Big)^{\frac{1}{2}} = \sqrt{f_{\text{abs}}(r)\, g_{\text{abs}}(r)} < \infty\,.$$

Thus, $q \in W_+^\omega((-r, r))$. Hence,

$$\begin{aligned} |h^\top \tilde{q}[S]\, k| &= \Big|h^\top \Big(\sum_{\nu=0}^{\infty} c_\nu\, S^{*\nu}\Big) k\Big| \leq \sum_{\nu=0}^{\infty} |c_\nu| |h^\top S^{*\nu} k| \\ &\leq \sum_{\nu=0}^{\infty} \sqrt{|a_\nu|\, |b_\nu|}\, \sqrt{h^\top A^{*\nu} h}\, \sqrt{k^\top B^{*\nu} k} = \sum_{\nu=0}^{\infty} \alpha_\nu\, \beta_\nu\,. \end{aligned}$$

Thus, (6.178) implies (6.177). Suppose that $f_{\text{abs}}(c^*) = 1$ for some $0 < c^* \leq r$. Let $S \in \mathcal{Q}_{m,n}$. Due to Corollary 3.5, we may assume without loss of generality that $A \in C(m; \mathbb{R})$ and $B \in C(n; \mathbb{R})$, implying that $M \in C(m+n; \mathbb{R})$. In particular, $c^* M = \begin{pmatrix} c^* A & c^* S \\ (c^* S)^\top & c^* B \end{pmatrix}$ is positive semidefinite. Lemma 3.2-(ii) therefore implies that

$${}_{f,g}M_q := \begin{pmatrix} f_{\text{abs}}[c^* A] & \tilde{q}[c^* S] \\ \tilde{q}[c^* S]^\top & g_{\text{abs}}[c^* B] \end{pmatrix}$$

is already a correlation matrix (since $f_{\text{abs}}(c^* a_{ii}) = f_{\text{abs}}(c^*) = 1 = f_{\text{abs}}(c^* b_{ii})$). Corollary 3.5 therefore concludes the proof of (i).
(ii) Put $f := h_{\alpha,\alpha}, g := h_{\beta,\beta}$ and $q := h_{\alpha,\beta}$. Observe that $h_{\alpha,\beta} = q = \tilde{q}\big|_{[-1,1]}$ (since $h_{\alpha,\beta}$ is continuous). Firstly, since $\alpha, \beta \in S_{L^2(\gamma_k)}$, Theorem 6.5-(i) implies that $f(1) = 1 = g(1)$, so that the diagonal of the matrix ${}_{f,g}M_q$ is occupied with $m+n$ 1's. It remains to prove that ${}_{f,g}M_q$ is positive semidefinite. Recall that $|p_\nu(\alpha, \beta)| \leq \sqrt{p_\nu(\alpha, \alpha)}\sqrt{p_\nu(\beta, \beta)}$ for all $\nu \in \mathbb{N}_0$, where $p_\nu(\psi, \kappa) := \sum_{n \in C(\nu,k)} \langle \psi, H_n \rangle_{\gamma_k} \langle \kappa, H_n \rangle_{\gamma_k} = \frac{h^{(\nu)}_{\psi,\kappa}(0)}{\nu!}, \psi, \kappa \in \{\alpha, \beta\}$ (cf. (6.133)). Theorem 6.5 and Theorem 6.33 therefore imply that all assumptions of (i) are satisfied for the so defined functions f, g and q (including (7.222)), so that we may apply statement (i) also to these functions. Finally, (6.176) and hence (iii) follows from Corollary 3.5 and Proposition 3.13. □

However, we will recognise that Theorem 6.35 cannot be fully transferred to the complex field, so that we have to distinguish carefully between the real case and the complex case here (cf. Proposition 7.7). If we link (5.116) and Theorem 6.35, we obtain

Corollary 6.36. *Let $m, n \in \mathbb{N}, A \in \mathbb{M}_{m,n}(\mathbb{R})$ and*

$$\Sigma = \begin{pmatrix} M & S \\ S^\top & N \end{pmatrix} \in C(m+n;\mathbb{R})$$

be an arbitrary real $(m+n)\times(m+n)$ correlation matrix (with block elements $M \in C(m;\mathbb{R}), N \in C(n;\mathbb{R})$ and $S \in \mathcal{Q}_{m,n}$). Let $r > 0$ and $0 \neq \psi \in W_+^\omega((-r,r))$. If $0 < c \leq r$, then

$$\frac{1}{\psi_{abs}(c)} \begin{pmatrix} \psi_{abs}[c\,M] & \widetilde{\psi}[c\,S] \\ \widetilde{\psi}[c\,S]^\top & \psi_{abs}[c\,N] \end{pmatrix} \in C(m+n;\mathbb{R}) \tag{6.179}$$

again is a correlation matrix with real entries. In particular,

$$\frac{1}{\psi_{abs}(c)}\widetilde{\psi}[cS] \in \mathcal{Q}_{m,n} \text{ for all } S \in \mathcal{Q}_{m,n}\,. \tag{6.180}$$

If we apply Theorem 6.32, (iv) and (6.180) to the *inverses* of invertible functions in $W_+^\omega((-1,1))$, Bolzano's intermediate value theorem from calculus immediately implies a further crucial result. To this end, recall also (5.115) and (5.116).

Theorem 6.37 (Real inner product rounding). *Let $\psi : [-1,1] \longrightarrow [-1,1]$ be a bijective real function. Assume that*

$$\psi|_{(-1,1)} \in W_+^\omega((-1,1)) \text{ and } \psi^{-1}|_{(-1,1)} \in W_+^\omega((-1,1)).$$

Then $|\psi^{-1}(0)| = (\psi^{-1}|_{(-1,1)})_{abs}(0) \leq (\psi^{-1}|_{(-1,1)})_{abs}(1)$. Assume that

$$|\psi^{-1}(0)| < 1 < (\psi^{-1}|_{(-1,1)})_{abs}(1).$$

Then there is a unique number $c^* \in (0,1)$, such that $(\psi^{-1})_{abs}(c^*) = 1$. Let $k \in \mathbb{N}$. There is $(\alpha, \beta) \in S_{L^2(\gamma_k)} \times S_{L^2(\gamma_k)}$ (dependent on c^* and k) such that for any separable $\mathbb{R}$-Hilbert space H and any $u, v \in S_H$, the following statements apply:

(i)

$$\langle u, v\rangle_H = \frac{1}{c^*}\psi(\rho_{u,v}) \tag{6.181}$$

where $\rho_{u,v} := h_{\alpha,\beta}(\langle u, v\rangle_H)$.

(ii)

$$c^* = \psi(\langle \alpha, \beta\rangle_{\gamma_1}).$$

(iii) *Suppose that $\psi = h_{f,g}$ for some $\nu \in \mathbb{N}$ and $f, g \in L^2(\gamma_\nu)$. If $\rho_{u,v} \in (-1,1)$, then*

$$c^*\,\langle u, v\rangle_H = \frac{1}{(2\pi)^\nu(1-\rho_{u,v}^2)^{\nu/2}} \int_{\mathbb{R}^\nu}\int_{\mathbb{R}^\nu} f(x)g(y)\exp\Big(-\frac{\|x\|^2 + \|y\|^2 - 2\rho_{u,v}\langle x, y\rangle_2}{2(1-\rho_{u,v}^2)}\Big)\mathrm{d}^\nu x\,\mathrm{d}^\nu y\,.$$

If $m, n \in \mathbb{N}$ and $(x, y) \in S_H^m \times S_H^n$, then there exist $m+n$ $\mathbb{R}^k$-valued random vectors $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_m$, $\boldsymbol{Y}_1, \ldots, \boldsymbol{Y}_n$, such that $vec(\boldsymbol{X}_i, \boldsymbol{Y}_j) \sim N_{2k}(0, \Sigma_{2k}(\rho_{ij}))$ for all $(i,j) \in [m] \times [n]$, and

$$\Gamma_H(x,y) = \frac{1}{c^*}h_{f,g}[R] = \frac{1}{c^*}\,\mathbb{E}[\boldsymbol{P}_f\,\boldsymbol{Q}_g^\top] = \frac{1}{c^*}\,\mathbb{E}[\Gamma_{\mathbb{R}}(\boldsymbol{P}_f, \boldsymbol{Q}_g)], \tag{6.182}$$

where $(\boldsymbol{P}_f)_i := f(\boldsymbol{X}_i)$, $(\boldsymbol{Q}_g)_j := g(\boldsymbol{Y}_j)$, $\rho_{ij} := h_{\alpha,\beta}(\langle x_i, y_j\rangle_H)$ and $R := h_{\alpha,\beta}[\Gamma_H(x,y)] = (\rho_{ij})_{(i,j)\in[m]\times[n]} \in \mathcal{Q}_{m,n}$.

(iv) *Moreover,* $c^*\langle u,v\rangle_H \in (-1,1)$ *for all* $u,v \in S_H$ *and*

$$tr(A^\top S) = \frac{1}{c^*}\, tr(A^\top\, \psi[Q_{c^*,\psi}]) \tag{6.183}$$

for all $m,n \in \mathbb{N}$, *for all* $A \in \mathbb{M}_{m,n}(\mathbb{R})$, *for all* $S \in \mathcal{Q}_{m,n}$, *where* $Q_{c^*,\psi} := \psi^{-1}[c^*\, S] \in \mathcal{Q}_{m,n}$.

It is far from being trivial that it is possible to transfer Theorem 6.37 from the real field $\mathbb{R}$ to the complex field $\mathbb{C}$; at least if $f = g$ is odd (cf. Theorem 7.13). In order to achieve this, we have to develop and implement certain non-trivial structural properties of the class of complex Hermite polynomials (cf. Theorem 7.11 and Theorem 7.12 below).

If $\nu \in \mathbb{N}_0$, $m,n \in \mathbb{N}$ and $A \in \mathbb{M}_{m,n}(\mathbb{F})$, then $A^{*\nu}$ denotes the ν-th entrywise power of the matrix A (in terms of Schur multiplication), where $A^{*0} := \mathbf{1}_m \mathbf{1}_n^*$ is the (rank 1) $m \times n$ matrix of all ones, where $\mathbf{1}_l := (1,1,\ldots,1)^\top \in \mathbb{F}^l, l \in \mathbb{N}$ (by adapting the convention that $0^0 := 1$ - cf. [82, Remark 9.2]).

Now, we are fully prepared to embed both, Grothendieck's original estimation $K_G^{\mathbb{R}} \leq \sinh(\frac{\pi}{2}) \approx 2.301$, and Krivine's original estimation $K_G^{\mathbb{R}} \leq \frac{\pi}{2\ln(1+\sqrt{2})} \approx 1,782$ into a general framework. In particular, we will provide a further proof of the Grothendieck inequality itself (see Theorem 6.40 below). Moreover, we will make a cute use of the little Grothendieck inequality, yielding a quite surprising outcome. To this end, we have to work with functions $h_{f,g}$, which are "generated" by *bounded functions* $f,g \in L^\infty(\mathbb{R}^k,\gamma_k) = L^\infty(\mathbb{R}^k,\lambda_k) \equiv L^\infty(\mathbb{R}^k)$, $k \in \mathbb{N}$. (6.138) obviously implies that

$$|h_{f,g}(\rho)| \leq \|f\|_\infty \, \|g\|_\infty \ \text{ for all } \ f,g \in L^\infty(\mathbb{R}^k) \ \text{ and } \ \rho \in [-1,1]\,.$$

Remark 6.38. In statistical machine learning a function $f : \mathbb{R}^k \longrightarrow \{-1,1\}, k \in \mathbb{N}$ is a particular example of a mapping from some general domain of definition to the set $\{-1,1\}$, where the latter is known as "concept" (cf. e.g. [138]). The concept f obviously satisfies the condition $\|f\|_{\gamma_k} = 1 = \|f\|_\infty$.

We also need the following important result which holds for both fields interchangeably.

Lemma 6.39. *Let* $\mathbb{F} \in \{\mathbb{R},\mathbb{C}\}$ *and* $m,n \in \mathbb{N}$. *Let* $\boldsymbol{R}$ *be a* m*-dimensional random vector in* $(\mathbb{F}\cap\overline{\mathbb{D}})^m$ *and* $\boldsymbol{S}$ *be a* n*-dimensional random vector in* $(\mathbb{F}\cap\overline{\mathbb{D}})^n$, *such that* $\mathbb{E}[\boldsymbol{R}\boldsymbol{S}^*]$ *exists. Then*

$$\|B * \mathbb{E}[\boldsymbol{R}\boldsymbol{S}^*]^{*\nu}\|_{\infty,1}^{\mathbb{F}} \leq \|B\|_{\infty,1}^{\mathbb{F}} \ \textit{for all } B \in \mathbb{M}_{m,n}(\mathbb{F}) \textit{ and } \nu \in \mathbb{N}\,.$$

Proof. Clearly, it is sufficient to verify the statement for $\nu = 1$. Without loss of generality, we may assume that $m = n$ (just to simplify the spelling). So, fix $B \in \mathbb{M}_n(\mathbb{F})$. Put $\mathbf{\Lambda} := \mathbf{R}\mathbf{S}^* = \Gamma_{\mathbb{F}}(\overline{\mathbf{R}},\overline{\mathbf{S}})$. Because of the structure of the operator norm $\|\cdot\|_{\infty,1}^{\mathbb{F}}$ and Lemma 5.6, it follows that

$$\|B * \mathbb{E}[\mathbf{\Lambda}]\|_{\infty,1}^{\mathbb{F}} = |\mathrm{tr}((B * \mathbb{E}[\mathbf{\Lambda}])^*\, p\, q^*)| = |\mathrm{tr}(B^*\, \mathbb{E}[(p\, q^*) * \overline{\mathbf{\Lambda}}])|$$

for some non-random vectors $p,q \in S_{\mathbb{F}}^n$. Given the assumed structure of the random matrix $\mathbf{\Lambda}$, it follows that $\overline{\mathbf{\Lambda}} = \overline{\mathbf{R}}\,\overline{\mathbf{S}}^*$. Consequently,

$$(p\, q^*) * \overline{\mathbf{\Lambda}} = (p\, q^*) * (\overline{\mathbf{R}}\,\overline{\mathbf{S}}^*) = (p * \overline{\mathbf{R}})(q * \overline{\mathbf{S}})^* = \Gamma_{\mathbb{F}}(\overline{p} * \mathbf{R}, \overline{q} * \mathbf{S})$$

is a random Gram matrix, such that both random vectors $\overline{p} * \mathbf{R}$, and $\overline{q} * \mathbf{S}$ map into $(\mathbb{F} \cap \overline{\mathbb{D}})^n$. Hence,

$$\|B * \mathbb{E}[\mathbf{\Lambda}]\|_{\infty,1}^{\mathbb{F}} = \Big|\mathrm{tr}(\mathbb{E}\Big[B^* \, \Gamma_{\mathbb{F}}(\overline{p} * \mathbf{R}, \overline{q} * \mathbf{S})\Big])\Big| \leq \mathbb{E}\Big[\Big|\mathrm{tr}(B^* \, \Gamma_{\mathbb{F}}(\overline{p} * \mathbf{R}, \overline{q} * \mathbf{S}))\Big|\Big] \leq \|B\|_{\infty,1}.$$

□

Theorem 6.40. *Let $k, m, n \in \mathbb{N}$ and $f, g \in L^\infty(\mathbb{R}^k)$. Put $r_\infty \equiv r_\infty(f, g) := \|f\|_\infty \|g\|_\infty$. Then:*

(i)

$$|tr(A^\top h_{f,g}[S])| \leq r_\infty \|A\|_{\infty,1} \text{ for all } A \in \mathbb{M}_{m,n}(\mathbb{R}) \text{ and } S \in \mathcal{Q}_{m,n} \tag{6.184}$$

and

$$|tr(A^\top h_{f,f}[\Sigma])| \leq \|f\|_\infty^2 \max_{x \in [-1,1]^n} |x^\top A x| \text{ for all } A \in \mathbb{M}_n(\mathbb{R}) \text{ and } \Sigma \in C(n; \mathbb{R}). \tag{6.185}$$

(ii) *Assume that $r_\infty > 0$ and f or g is odd. Let $h_{f,g} : [-1, 1] \longrightarrow \mathbb{R}$ be continuous and injective. Then $h_{f,g}$ is a homeomorphism which is either strictly increasing or strictly decreasing and satisfies $h_{f,g}([-1, 1]) = [-r, r]$, where $r \equiv r_k(f, g) := \max\{-h_{f,g}(1), h_{f,g}(1)\} = \max\{-\langle f, g\rangle_{\gamma_k}, \langle f, g\rangle_{\gamma_k}\}$. Moreover, $0 < r \leq r_\infty$. Assume that $h_{f,g}^{-1}\big|_{(-r,r)} \in W_+^\omega((-r, r))$. Then the following two statements hold:*

(ii-1) *If $\Big(h_{f,g}^{-1}\big|_{(-r,r)}\Big)_{abs}(r) > 1$, then there is exactly one number $0 < c_k^* \equiv c_k^*(f, g) < r$, such that $\Big(h_{f,g}^{-1}\big|_{(-r,r)}\Big)_{abs}(c_k^*) = 1$ and*

$$K_G^{\mathbb{R}} \leq \frac{r_\infty}{c_k^*}\,. \tag{6.186}$$

(ii-2) *If $r = r_\infty$, then there exists a unique number $0 < \gamma_k^* \equiv \gamma_k^*(f, g) \in (0, r]$, such that*

$$K_G^{\mathbb{R}} = \Big(h_{f,g}^{-1}\big|_{(-r,r)}\Big)_{abs}(\gamma_k^*) \leq \min\Big\{\frac{r}{c_k^*}, \Big(h_{f,g}^{-1}\big|_{(-r,r)}\Big)_{abs}(r)\Big\}. \tag{6.187}$$

Proof. Let $r_\infty > 0$. Put $f^\circ := \frac{f}{\|f\|_\infty}$ and $g^\circ := \frac{g}{\|g\|_\infty}$. If $h_{f,g} : [-1, 1] \longrightarrow [-a, a]$ is a well-defined and bijective, then also $h_{f^\circ,g^\circ} = \frac{1}{r_\infty} h_{f,g} : [-1, 1] \longrightarrow [-\frac{a}{r_\infty}, \frac{a}{r_\infty}]$ exists and is bijective. Since $h_{f^\circ,g^\circ}^{-1}(\frac{y}{r_\infty}) = h_{f,g}^{-1}(y)$ for all $y \in [-a, a]$ and $\max\{-h_{f,g}(1), h_{f,g}(1)\} = r_\infty \max\{-h_{f^\circ,g^\circ}(1), h_{f^\circ,g^\circ}(1)\}$, we may assume throughout the entire proof without loss of generality that $\|f\|_\infty = 1$ and $\|g\|_\infty = 1$, implying that $r_\infty = 1$.
Fix $A \in \mathbb{M}_{m,n}(\mathbb{R})$ and $S \in \mathcal{Q}_{m,n}$. Then $S = \Gamma_H(u, v)$ for some real finite-dimensional Hilbert space H and some $(u, v) \in S_H^m \times S_H^n$ (due to Proposition 3.13).
(i) Because of (6.147), it follows that

$$h_{f,g}[S] = h_{f,g}[\Gamma_H(u, v)] = \mathbb{E}[\mathbf{R}_f \, \mathbf{T}_g^\top] \tag{6.188}$$

where $(\mathbf{R}_f)_i := f(\mathbf{X}_{u_i})$ and $(\mathbf{T}_g)_j := g(\mathbf{X}_{v_j})$, for some $\mathrm{vec}(\mathbf{X}_{u_i}, \mathbf{X}_{v_j}) \sim N_{2k}(0, \Sigma_{2k}(\langle u_i, v_j\rangle_H))$ for all $(i,j) \in [m] \times [n]$. Since $\|f\|_\infty = 1 = \|g\|_\infty$, the stochastic inequality

$$|\mathrm{tr}(A^\top \mathbf{R}_f\, \mathbf{T}_g^\top)| \leq \|A\|_{\infty,1} \tag{6.189}$$

is satisfied (due to (3.41) and (3.42)). Hence,

$$\begin{aligned}|\mathrm{tr}(A^\top h_{f,g}[S])| &= |\mathrm{tr}(A^\top \mathbb{E}[\mathbf{R}_f\, \mathbf{T}_g^\top])| = |\mathbb{E}[\mathrm{tr}(A^\top \mathbf{R}_f\, \mathbf{T}_g^\top)]| \\ &\leq\ \mathbb{E}[|\mathrm{tr}(A^\top \mathbf{R}_f\, \mathbf{T}_g^\top)|] \overset{(6.189)}{\leq} \|A\|_{\infty,1}\,.\end{aligned}$$

Similarly, by making use of (6.148), the proof of (6.185) can be performed straightforwardly, so that (i) follows.

(ii) Firstly, since $h_{f,g}$ is odd, it follows that $-h_{f,g}(1) = h_{f,g}(-1)$. If $h_{f,g}$ is strictly decreasing, then $h_{f,g}(1) < h_{f,g}(-1) = -h_{f,g}(1)$, implying that $r = -h_{f,g}(1) = -\langle f, g\rangle_{\gamma_k} > -h_{f,g}(0) = 0$. Consequently, $0 < r = |h_{f,g}(1)| \leq \|f\|_{\gamma_k}\, \|g\|_{\gamma_k} \leq r_\infty$ (due to (6.137), respectively (6.138)). A similar proof obviously holds if $h_{f,g}$ is strictly increasing. All described topological properties of $h_{f,g}$ are an immediate application of well-known facts from classical real analysis.

(ii-1) Assume that $\left(h_{f,g}^{-1}\big|_{(-r,r)}\right)_{\mathrm{abs}}(r) > 1$. Since $h_{f,g}^{-1}(0) = 0 = \left(h_{f,g}^{-1}\big|_{(-r,r)}\right)_{\mathrm{abs}}(0)$, we may apply Theorem 6.37, (iv) to $\psi := \frac{1}{r}\, h_{f,g}$ (since $\left(\psi^{-1}\big|_{(-1,1)}\right)_{\mathrm{abs}} = \left(h_{f,g}^{-1}\big|_{(-r,r)}\right)_{\mathrm{abs}}(r\,\cdot)$). It follows that there exists a uniquely determined number $0 < \gamma_k^* \equiv \gamma_k^*(f,g) < 1$ such that $\left(\psi^{-1}\big|_{(-1,1)}\right)_{\mathrm{abs}}(\gamma_k^*) = 1$ and $\mathrm{tr}(A^\top S) = \frac{1}{\gamma_k^*}\,\mathrm{tr}(A^\top \psi[S_*]) = \frac{1}{r\,\gamma_k^*}\,\mathrm{tr}(A^\top h_{f,g}[S_*])$ for some $S_* \in \mathcal{Q}_{m,n}$. Put $0 < c_k^* := r\,\gamma_k^* < r$. Consequently, we may apply statement (i), and it follows that

$$|\mathrm{tr}(A^\top S)| = \frac{1}{c_k^*}|\mathrm{tr}(A^\top h_{f,g}[S_*])| \overset{(6.184)}{\leq} \frac{1}{c_k^*}\, \|A\|_{\infty,1}\,. \tag{6.190}$$

Proposition 3.15 therefore implies (6.186).

(ii-2) Assume that $r \geq r_\infty = 1$. Due to the existence of the inverse function $h_{f,g}^{-1} : [-r,r] \longrightarrow [-1,1]$, (6.188) implies that (algebraically)

$$S = h_{f,g}^{-1}[h_{f,g}[S]] = h_{f,g}^{-1}[\mathbb{E}[\mathbf{\Lambda}_{f,g}]],$$

where $\mathbf{\Lambda}_{f,g} := \mathbf{R}_f\, \mathbf{T}_g^\top$ Put $a_\nu := \frac{(h_{f,g}^{-1})^{(\nu)}(0)}{\nu!}$, $\nu \in \mathbb{N}$. Since by assumption $r \geq 1$, it follows that $\sum_{\nu=0}^\infty |a_\nu| \leq \sum_{\nu=0}^\infty |a_\nu| r^\nu = \left(h_{f,g}^{-1}\big|_{(-r,r)}\right)_{\mathrm{abs}}(r) < \infty$. Lemma 5.10, applied to the real analytic function $h_{f,g}^{-1}\big|_{(-r,r)}$ and the continuity of the function $h_{f,g}^{-1} : [-r,r] \longrightarrow [-1,1]$ therefore imply that

$$S = \sum_{\nu=0}^\infty a_\nu\, \mathbb{E}[\mathbf{\Lambda}_{f,g}]^{*\,\nu}\,,$$

where $*$ denotes entrywise multiplication on $M_{m,n}(\mathbb{R})$ (i.e., the Hadamard product of matrices). Since $\|f\|_\infty = \|g\|_\infty = 1$, it follows that

$$\|A_m\|_{\infty,1} \leq \|A\|_{\infty,1} \text{ for all } m \in \mathbb{N}_0, \tag{6.191}$$

where $A_m := A * \mathbb{E}[\mathbf{\Lambda}_{f,g}]^{*m}\,(m \in \mathbb{N}_0)$ (due to Lemma 6.39). Therefore, Lemma 5.6 leads to

$$
\begin{aligned}
|\mathrm{tr}(A^\top S)| &\leq \sum_{\nu=0}^{\infty} |a_\nu|\, |\mathrm{tr}(A^\top\, \mathbb{E}[\mathbf{\Lambda}_{f,g}]^{*\nu})| = |a_0||\mathrm{tr}(A^\top \mathbf{1}_m \mathbf{1}_n^*)| + \sum_{\nu=1}^{\infty} |a_\nu|\, |\mathrm{tr}(A_{\nu-1}^\top\, \mathbb{E}[\mathbf{\Lambda}_{f,g}])| \\
&\leq |a_0||\mathrm{tr}(A^\top \mathbf{1}_m \mathbf{1}_n^*)| + \sum_{\nu=1}^{\infty} |a_\nu|\, \mathbb{E}[|\mathrm{tr}(A_{\nu-1}^\top\, \mathbf{\Lambda}_{f,g})|] \\
&\overset{(6.189)}{\leq} |a_0|\|A\|_{\infty,1} + \sum_{\nu=1}^{\infty} |a_\nu|\, \|A_{\nu-1}\|_{\infty,1} \overset{(6.191)}{\leq} \Big(\sum_{\nu=0}^{\infty} |a_\nu|\Big)\|A\|_{\infty,1} \\
&\leq \Big(h_{f,g}^{-1}\big|_{(-r,r)}\Big)_{\mathrm{abs}}(r)\|A\|_{\infty,1}.
\end{aligned}
$$

Consequently, Proposition 3.15 implies that $1 < K_G^{\mathbb{R}} \leq \Big(h_{f,g}^{-1}\big|_{(-r,r)}\Big)_{\mathrm{abs}}(r)$. (6.187) now follows from (6.186) and Bolzano's intermediate value theorem, where the latter is applied to the strictly increasing function $\Big(h_{f,g}^{-1}\big|_{(-r,r)}\Big)_{\mathrm{abs}} - K_G^{\mathbb{R}}$ (cf. proof of Theorem 6.8-(iii)). □

Inequality (6.185), together with the equality (3.47) allows us to recover as special case (applied to $f = \mathrm{sign}$) an interesting result of Y. Nesterov, yet without having to make use of their random hyperplane rounding technique (cf. [106]):

Corollary 6.41. *Let $k, n \in \mathbb{N}$, $A \in \mathbb{M}_n(\mathbb{R})^+$ be positive semidefinite and $f \in L^\infty(\mathbb{R}^k)$ be odd. Then*

$$
h_{f,f}'(0) \sup_{\Sigma \in C(n;\mathbb{R})} tr(A\Sigma) \leq \sup_{\Sigma \in C(n;\mathbb{R})} tr(A\, h_{f,f}[\Sigma]) \leq \|f\|_\infty^2 \sup_{x \in \{-1,1\}^n} x^\top A x \leq \|f\|_\infty^2\, \|A\|_{\infty,1}\,.
$$

In particular,

$$
0 \leq h_{f,f}'(0) \leq \frac{2}{\pi}\, \|f\|_\infty^2\,. \tag{6.192}
$$

Proof. Let $\Sigma \in C(n;\mathbb{R})$. Put $h \equiv h_{f,f}$. Since f is odd, Theorem 6.5-(v) implies that

$$
h(\rho) = \sum_{\nu=0}^{\infty} b_{2\nu+1}\rho^{2\nu+1} = h'(0)\rho + \psi(\rho),
$$

for all $\rho \in [-1,1]$, where $\psi(\rho) := \sum_{\nu=1}^{\infty} b_{2\nu+1}\rho^{2\nu+1}$ and $b_{2\nu+1} \geq 0$ for all $\nu \in \mathbb{N}_0$. Hence, $\psi[\Sigma] = h[\Sigma] - h'(0)\Sigma \in \mathbb{M}_n(\mathbb{R})^+$ (due to Theorem 5.15), whence $\mathrm{tr}(\psi[\Sigma]) = \mathrm{tr}(A(h[\Sigma]) - h'(0)\,\mathrm{tr}(\Sigma)) \geq 0$ (since $\mathrm{tr}(AB) = \|B^{1/2}A^{1/2}\|_F^2 \geq 0$ for all $B \in \mathbb{M}_n(\mathbb{R})^+$). Thus,

$$
h'(0)\,\mathrm{tr}(A\Sigma) \leq \mathrm{tr}(A\, h[\Sigma]) \overset{(6.185)}{\leq} \|f\|_\infty^2 \sup_{x \in \{-1,1\}^n} x^\top A x = \|f\|_\infty^2 \sup_{x \in \{-1,1\}^n} \mathrm{tr}(A x x^\top) \leq \|f\|_\infty^2\, \|A\|_{\infty,1}.
$$

In order to verify (6.192), we are going to make use of the little Grothendieck inequality. Obviously, we may assume that $h'(0) > 0$, implying that

$$
\mathrm{tr}(B\Sigma) \leq \frac{1}{h'(0)}\, \|f\|_\infty^2\, \|B\|_{\infty,1} \text{ for all } B \in \mathbb{M}_n(\mathbb{R})^+ \text{ and } \Sigma \in C(n;\mathbb{R}).
$$

Consequently, the "correlation matrix version" of the little Grothendieck inequality (see (3.49)) implies

$$
\frac{\pi}{2} = k_G^{\mathbb{R}} \leq \frac{1}{h'(0)}\, \|f\|_\infty^2\,,
$$

and (6.192) follows. □

In a similar vain, we directly obtain a further (and very short) proof for the value of the real little Grothendieck constant $k_G^{\mathbb{R}}$. To this end, we only have to combine (6.184) and Proposition 6.16:

Corollary 6.42 (**Grothendieck, 1953**).

$$k_G^{\mathbb{R}} = \frac{\pi}{2}.$$

Proof. Let $A \in \mathbb{M}_n(\mathbb{R})^+$ and $\Sigma \in C(n;\mathbb{R})$ be arbitrary. We just have to work with the CCP function $[-1,1] \ni \rho \mapsto h_{f_1,f_1}(\rho) - c_1^2\,\rho = \frac{2}{\pi}\arcsin(\rho) - \frac{2}{\pi}\,\rho$. Because then

$$0 \leq \tfrac{2}{\pi}\,\mathrm{tr}(A\Sigma) = \mathrm{tr}(A(\tfrac{2}{\pi}\,\Sigma)) \leq \mathrm{tr}(Ah_{f_1,f_1}[\Sigma]) \overset{(6.184)}{\leq} \|A\|_{\infty,1}\,.$$

$\square$

Remark 6.43. A direct estimation of (6.149) leads to the upper bound $k\,\|f\|_\infty^2\,(\sqrt{\frac{2}{\pi}})^2 = \frac{2k}{\pi}\,\|f\|_\infty^2$, which, however, strongly depends on the dimension $k \in \mathbb{N}$. That upper bound, viewed as a function of k is even strictly increasing. Our application of the little Grothendieck inequality implies the non-trivial result that *for all* $k \in \mathbb{N}$, $h_{f,f}'(0)$ actually is bounded above by $\frac{2}{\pi}\|f\|_\infty^2$ "uniformly". Moreover, if f were an even function, then (6.192) would be trivial, since $h_{f,f}'(0) = 0$.

Theorem 6.40-(i) also implies a remarkable property of CCP functions. To this end, let $S \in \mathcal{Q}_{m,n}$ and $h = h_{f,f}$ be an arbitrary CCP function (not necessarily odd!), generated by some $f \in L^\infty(\mathbb{R}^k)$. Firstly, note that in any case,

$$\frac{\pi}{2}\frac{1}{K_G^{\mathbb{R}}} \overset{(1.1)}{<} 1 = \|f\|_{\gamma_k} \leq \|f\|_\infty \leq \|f\|_\infty^2\,.$$

If also $h_{f,f}^{-1}$ were a CCP function, then $\widetilde{S} := h_{f,f}^{-1}[S] \in \mathcal{Q}_{m,n}$ (due to (6.176)). Hence,

$$|\mathrm{tr}(A^\top S)| = |\mathrm{tr}(A^\top h_{f,f}[\widetilde{S}])| \leq \|f\|_\infty^2\,\|A\|_{\infty,1} \text{ for all } A \in \mathbb{M}_{m,n}(\mathbb{R}),$$

implying that $K_G^{\mathbb{R}} \leq \|f\|_\infty^2$. If we join the latter observation and Theorem 5.17-(v), we obtain another interesting fact (which should be carefully compared with Corollary 6.10):

Remark 6.44. Let $k, m, n \in \mathbb{R}$ and $h = h_{f,f}$ be CCP for some $f \in S_{L^2(\gamma_k)} \cap L^\infty(\mathbb{R}^k)$. If $\|f\|_\infty < \sqrt{K_G^{\mathbb{R}}}$, then the inverse function $h_{f,f}^{-1}$ is not CCP.

Next, we are going to summarise the remarkable properties of *odd CCP functions* which we found so far and shed some light on an additional, quite surprising estimate for odd CCP functions $h_{f,f}$ which emerges if we assume in addition that $f \in S_{L^2(\gamma_k)}$ is *bounded* (a.s.); i.e., if $f \in S_{L^2(\gamma_k)} \cap L^\infty(\mathbb{R}^k)$. In particular, if we combine Theorem 6.8-(ii), (v) and Theorem 6.40-(ii) in this case, we recover Grothendieck's upper bound as well as Krivine's upper bound at once. This follows from Example 6.48, which is a special case of our following key result for the real odd CCP case:

Theorem 6.45. *Let $k \in \mathbb{N}$ and $f \in S_{L^2(\gamma_k)} \cap L^\infty(\mathbb{R}^k)$ such that $\|f\|_{\gamma_k} = 1$. Then $\|f\|_\infty \geq 1$. Assume that f is odd and $h_{f,f}^{-1}\big|_{(-1,1)} \in W_+^\omega((-1,1))$. Then the following statements hold:*

(i)

$$\left(h_{f,f}^{-1}\big|_{(-1,1)}\right)_{abs}(y) \geq \frac{\pi}{2}\,\frac{1}{\|f\|_\infty^2}\, y \text{ for all } y \in [0,1]\,.$$

(ii)

$$K_G^{\mathbb{R}} \leq \frac{\|f\|_\infty^2}{h_{f,f}^{hyp}(1)}\,.$$

(iii) *Let $1 \leq c_* < K_G^{\mathbb{R}}$. If $\|f\|_\infty = 1$, then $0 < h_{f,f}^{hyp}(c_*) < 1$ and there is exactly one number $\gamma^*(f) \in (h_{f,f}^{hyp}(c_*), 1]$, such that*

$$K_G^{\mathbb{R}} = \left(h_{f,f}^{-1}\big|_{(-1,1)}\right)_{abs}(\gamma^*(f)) \leq \min\left\{\frac{1}{h_{f,f}^{hyp}(1)}, \left(h_{f,f}^{-1}\big|_{(-1,1)}\right)_{abs}(1)\right\}. \tag{6.193}$$

Proof. Since $f \in L^\infty$, it follows that $f \in L^2(\gamma_k)$ and $1 = \|f\|_{\gamma_k} \leq \|f\|_\infty$.
(i) and (ii) The claimed two inequalities directly follow from (5.115), (6.150), Lemma 6.11, Theorem 6.40, and (6.192).
(iii) Since $1 \leq c_* < K_G^{\mathbb{R}} \leq \left(h_{f,f}^{-1}\big|_{(-1,1)}\right)_{\text{abs}}(1)$ (due to Theorem 6.40), it follows from Lemma 6.11 that $0 < h_{f,f}^{\text{hyp}}(1) \leq h_{f,f}^{\text{hyp}}(c_*) < \gamma^*(f) := h_{f,f}^{\text{hyp}}(K_G^{\mathbb{R}}) \leq 1$. (iii) now follows from (ii). □

If we only assume that $f \in L^\infty(\mathbb{R}^k) \setminus \{0\}$, then an application of Theorem 6.45 to $\frac{1}{\|f\|_{\gamma_k}} f \in S_{L^2(\gamma_k)}$ directly leads to

Corollary 6.46. *Let $k \in \mathbb{N}$ and $f \in L^\infty(\mathbb{R}^k) \setminus \{0\}$. Then $0 < r \equiv r_k(f) := \|f\|_{\gamma_k}^2 < \infty$ and $\|f\|_\infty \geq \sqrt{r}$. Assume that f is odd and $h_{f,f}^{-1}\big|_{(-r,r)} \in W_+^\omega((-r,r))$. Then $\left(h_{f,f}^{-1}\big|_{(-r,r)}\right)_{abs}(r) > 1$, and the following statements hold:*

(i)

$$\left(h_{f,f}^{-1}\big|_{(-r,r)}\right)_{abs}(y) \geq \frac{\pi}{2}\,\frac{1}{\|f\|_\infty^2}\, y \text{ for all } y \in [0,r]\,.$$

(ii)

$$r\, K_G^{\mathbb{R}} \leq \frac{\|f\|_\infty^2}{h_{\frac{f}{\sqrt{r}},\frac{f}{\sqrt{r}}}^{hyp}(1)}\,. \tag{6.194}$$

(iii) *Let $1 \leq c_* < K_G^{\mathbb{R}}$. If $\|f\|_\infty = \sqrt{r}$, then $0 < h_{\frac{f}{\sqrt{r}},\frac{f}{\sqrt{r}}}^{hyp}(c_*) < 1$ and there is exactly one number number $\gamma^*(f) \in (h_{\frac{f}{\sqrt{r}},\frac{f}{\sqrt{r}}}^{hyp}(c_*), 1]$, such that*

$$K_G^{\mathbb{R}} = \left(h_{f,f}^{-1}\big|_{(-r,r)}\right)_{abs}(r\,\gamma^*(f)) \leq \min\left\{\frac{1}{h_{\frac{f}{\sqrt{r}},\frac{f}{\sqrt{r}}}^{hyp}(1)}, \left(h_{f,f}^{-1}\big|_{(-r,r)}\right)_{abs}(r)\right\}.$$

The proof of Theorem 6.45-(i) shows us that here we may circumvent the rather strong assumption of $h_{f,f}^{-1}\big|_{(-r,r)}$ being completely real analytic on $(-r,r)$ at 0; at least in the following sense (cf. Example 6.51 as application for this):

Proposition 6.47. *Let $k \in \mathbb{N}$ and $f \in L^\infty(\mathbb{R}^k) \setminus \{0\}$. Then $0 < r \equiv r_k := \|f\|_{\gamma_k}^2 < \infty$ and $\|f\|_\infty \geq \sqrt{r}$. Assume that f is odd, $h'_{f,f}(0) > 0$ and*

$$\sum_{n=0}^{\infty} \frac{|(h_{f,f}^{-1})^{(2n+1)}(0)|}{(2n+1)!}\,(c^*)^{2n+1} = 1\,, \tag{6.195}$$

for some $c^* \in (0,r]$. Then $h_{f,f}^{-1}\big|_{(-c^*,c^*)} \in W_+^\omega((-c^*,c^*))$, and the following statements hold:

(i)

$$\Big(h_{f,f}^{-1}\big|_{(-c^*,c^*)}\Big)_{abs}(y) \geq \frac{\pi}{2}\,\frac{1}{\|f\|_\infty^2}\,y \ \textit{ for all } y \in [0,c^*] \ \textit{ and } \ \Big(h_{f,f}^{-1}\big|_{(-c^*,c^*)}\Big)_{abs}(c^*) = 1\,.$$

(ii)

$$h_{f,f}^{-1}[c^*\,S] \in \mathcal{Q}_{m,n} \ \textit{ for all } S \in \mathcal{Q}_{m,n}\,. \tag{6.196}$$

(iii)

$$K_G^{\mathbb{R}} \leq \frac{\|f\|_\infty^2}{c^*}\,.$$

Proof. (i) The assumption clearly implies that $h_{f,f}^{-1}\big|_{(-c^*,c^*)} \in W_+^\omega((-c^*,c^*))$ and $\Big(h_{f,f}^{-1}\big|_{(-c^*,c^*)}\Big)_{\text{abs}}(c^*) = 1$.

(ii) and (iii) Observe that in particular the restriction $h_{f,f}^{-1}\big|_{[-c^*,c^*]} : [-c^*,c^*] \longrightarrow [-1,1]$ is continuous. Consequently, if $S \in \mathcal{Q}_{mn}$, then $S_0 := h_{f,f}^{-1}[c^*\,S] \in \mathcal{Q}_{mn}$ (due to (6.180)), and (ii) follows. Let $m,n \in \mathbb{N}$, $A \in \mathbb{M}_{m,n}(\mathbb{R})$ and $S \in \mathcal{Q}_{m,n}$ be arbitrarily given. Since $S_0 \in \mathcal{Q}_{mn}$, we therefore obtain

$$|\mathrm{tr}(A^\top S)| = \frac{1}{c^*}\,|\mathrm{tr}(A^\top h_{f,f}[S_0])| \overset{(6.184)}{\leq} \frac{1}{c^*}\,\|A\|_{\infty,1}\,,$$

and (iii) follows as well. ∎

Example 6.48 (Grothendieck and Krivine). Once again, we consider the CCP function $\psi := \frac{2}{\pi}\arcsin$. Recall that $\psi = h_{f,f}$, where $f := \mathrm{sign} \in S_{L^\infty(\mathbb{R})} \cap S_{L^2(\gamma_k)}$. Due to (6.154), it follows that

$$\psi^{\text{hyp}}(1) = \frac{2}{\pi}\,\sinh^{-1}(1) = \frac{2}{\pi}\,\ln(1+\sqrt{2}).$$

Hence,

$$K_G^{\mathbb{R}} \overset{(6.193)}{\leq} \min\Big\{\frac{1}{\psi^{\text{hyp}}(1)},\, \Big(\psi^{-1}\big|_{(-1,1)}\Big)_{\text{abs}}(1)\Big\} \leq \frac{\pi}{2\ln(1+\sqrt{2})}(\approx 1.78221) \leq \sinh(\frac{\pi}{2})(\approx 2.30129)$$

precisely reflects Krivine's upper bound of $K_G^{\mathbb{R}}$ as well as Grothendieck's (larger) upper bound of $K_G^{\mathbb{R}}$!

Example 6.49. Consider the CCP function $\kappa := \sqrt{3}(2\phi - 1)$ (cf. Proposition 6.23). Due to Theorem 6.45, (i), respectively (6.194), we obtain the following (weaker) estimation:

$$K_G^{\mathbb{R}} \leq \frac{\pi}{6\,\ln(\frac{1}{2}(1+\sqrt{5}))} \cdot \|\kappa\|_\infty^2 \leq \frac{\pi}{2\,\ln(\frac{1}{2}(1+\sqrt{5}))} (\approx 3.26425)\,.$$

We highly recommend the readers to check whether this estimation can be improved, if more generally the function $\kappa_\alpha := \alpha(2\phi - 1)$ is considered, where $0 < \alpha < \sqrt{3}$ is given (instead of the CCP function $\kappa = \kappa_{\sqrt{3}}$)! Observe also that $\|\kappa\|_\infty = \sqrt{3} \neq 1 = \|\kappa\|_{\gamma_k}$.

Example 6.50. Fix $k \in \mathbb{N}_3$ and consider the function $\psi := h_{f_k,f_k}$, introduced in Proposition 6.16. *Assume that* $\psi^{-1} \in W_+^\omega((-1,1))$. ψ then satisfies all assumptions, listed in Theorem 6.45, and it follows that $0 < c_k^* := h_{f_k,f_k}^{\mathrm{hyp}}(1) < 1$ satisfies

$$K_G^{\mathbb{R}} \leq \frac{k}{c_k^*} \tag{6.197}$$

(since $\|f_k\|_\infty^2 = k$). However, observe that the sequence $\left(\frac{k}{c_k^*}\right)_{k\in\mathbb{N}}$ is not bounded and hence cannot converge (since $0 < c_k^* \leq 1$). Moreover, in contrast to the previous two examples, we do not know whether also $\left(h_{f_k,f_k}^{-1}\Big|_{(-1,1)}\right)_{\mathrm{abs}}$ can be represented in a closed analytical form; one of the major open problems in our search for the smallest upper bound of $K_G^{\mathbb{R}}$ (cf. Subsection 9.1 and Example 7.15, where the latter includes the approximation of the constant $c_k^* \approx 0.71200$ if $k = 2$). A straightforward, yet a bit laborious calculation with fractions, based on the table (9.241) (similarly to the special case $k = 2$, treated in Example 7.15), yields that the Maclaurin series of $h_{f_k,f_k}^{-1}(s) \equiv \sum_{\nu=0}^\infty \beta_{2\nu+1}(k)\, s^{2\nu+1}$ can e.g. be approximated by the Taylor polynomial of degree 7 as:

$$\begin{aligned} h_{f_k,f_k}^{-1}(s) &= \beta_1(k)s + \beta_3(k)s^3 + \beta_5(k)s^5 + \beta_7(k)s^7 + o(|s|^7) \\ &= \frac{1}{c_k^2}\,s + \Big(-\frac{1}{c_k^6}\frac{1}{2(k+2)}\,s^2\Big)\Big(s + \frac{3}{4c_k^4}\,\frac{k-2}{(k+2)(k+4)}\,s^3 \\ &\quad + \frac{3}{8c_k^8}\,\frac{9(k+2)^2 - 48(k+2) + 64}{(k+2)^2\,(k+4)\,(k+6)}\,s^5\Big) + o(|s|^7). \end{aligned} \tag{6.198}$$

Observe also that $\beta_5(k) := -\frac{3}{8c_k^{10}}\,\frac{k-2}{(k+2)^2\,(k+4)} = 0$ if and only if $k = 2$ and that $\beta_5(k) \leq 0$ if and only if $k \geq 2$. Similarly, since the single (local) minimum of the function $\mathbb{R} \ni x \mapsto g(x) := 9x^2 - 48x + 64$ is attained at $x_* := \frac{8}{3}$ and $g(x_*) = 0$, it follows that $\beta_7(k) \leq 0$.

Example 6.51 (Shortening of the proof of [22, Theorem 1.1]). Our approach also allows to recover the strongest result to date, namely that $K_G^{\mathbb{R}} < \frac{\pi}{2\ln(1+\sqrt{2})}$; at least partially. What is certain, however, is that our approach also allows a non-negligible shortening of the proof of the key result [22, Theorem 1.1]. To this end, firstly observe that a simple change of variables reveals that *for any* $f, g \in L^2(\gamma_k)$, the corresponding generalised function $H_{f\circ\sqrt{2},g\circ\sqrt{2}}$, listed in [22, Definition 2.1], satisfies

$$H_{f\circ\sqrt{2},g\circ\sqrt{2}} = h_{f,g}\Big|_{(-1,1)} \tag{6.199}$$

(due to (6.139)). So, $H_{f\circ\sqrt{2},g\circ\sqrt{2}}$ is well-defined on $(-1,1)$. The Grothendieck function $\frac{2}{\pi}\arcsin$ is then generalised in [22] to the complex-valued function

$$F_{p,\eta} := (1-p)H_0 + pH_\eta\,, \tag{6.200}$$

where $0 \leq p \leq 1$, $0 \leq \eta < 1$ and $H_\eta : \mathbb{S} \longrightarrow \mathbb{C}$ is defined as in [22, (41)], where $\mathbb{S} := \{z \in \mathbb{C} : |\operatorname{Re}(z)| < 1\}$. Independent of any complex analysis a priori, the construction of H_η, together with (6.199) implies that

$$H_\eta\Big|_{\mathbb{S}\cap\mathbb{R}} = H_\eta\Big|_{(-1,1)} = H_{g_\eta\circ\sqrt{2},g_\eta\circ\sqrt{2}} \overset{(6.199)}{=} h_{g_\eta,g_\eta}\Big|_{(-1,1)}\,.$$

Here, the odd function $g_\eta : \mathbb{R}^2 \longrightarrow \mathbb{R}$ is defined as $g_\eta(x) := \sqrt{\frac{\pi}{2}}\, f_\eta(\frac{1}{\sqrt{2}}x)$, where the 2-dimensional sign concept $f_\eta : \mathbb{R}^2 \longrightarrow \{-1,1\}$ satisfies [22, (40)]. Consequently, the function $\frac{2}{\pi}\, H_\eta\Big|_{(-1,1)}$ actually is a restriction of the well-defined odd - and hence invertible - CCP function $\frac{2}{\pi}\, h_{g_\eta,g_\eta} = h_{\sqrt{2/\pi}\,g_\eta,\sqrt{2/\pi}\,g_\eta}$ to the open interval $(-1,1)$ (due to Theorem 6.33).

Let $\rho \in (-1,1)$ and $\operatorname{vec}(\mathbf{X},\mathbf{Y}) \sim N_4(0,\Sigma_4(\rho))$. Since $g_0(x) = \sqrt{\frac{\pi}{2}}\operatorname{sign}(x_2)$ for all $x = (x_1,x_2)^\top \in \mathbb{R}^2$, we may apply Proposition 2.13 to the partitioned Gaussian random vector $\operatorname{vec}(\mathbf{X},\mathbf{Y})$, and it follows that

$$H_0(\rho) = h_{g_0,g_0}(\rho) = \frac{\pi}{2}\,\mathbb{E}_{\mathbb{P}_{\operatorname{vec}(\mathbf{X},\mathbf{Y})}}[\operatorname{sign}(X_2)\operatorname{sign}(Y_2)] = \arcsin(\rho),$$

which already gives a one-line proof of [22, Lemma 4.3]. In particular, for any $p \in [0,1]$,

$$\frac{2}{\pi}\,F_{p,\eta}\Big|_{(-1,1)} = \psi_{p,\eta}\Big|_{(-1,1)} \tag{6.201}$$

emerges as a restriction of the odd and hence *strictly increasing, homeomorphic* CCP function $\psi_{p,\eta} := (1-p)\frac{2}{\pi}\arcsin + p\,\frac{2}{\pi}\,h_{g_\eta,g_\eta}$ on $(-1,1)$ (due to Theorem 5.17 and Theorem 6.8-(iii)). Observe that $\psi'_{p,\eta}(0) \geq (1-p)\frac{2}{\pi}$, implying that $\psi^{-1}_{p,\eta}\Big|_{(-1,1)} \in C^\omega((-1,1))$ if $p < 1$ (due to Theorem 6.8-(iv)). Because of the non-trivial result [22, Theorem 5.1] (including its technically demanding proof) it follows the existence of $(p_0,\eta_0) \in (0,1)\times(0,1)$ and $c^* \in (\frac{2}{\pi}\ln(1+\sqrt{2}), \frac{9}{5\pi})$, such that

$$\sum_{n=0}^{\infty}\frac{|(\psi^{-1}_{p_0,\eta_0})^{(2n+1)}(0)|}{(2n+1)!}\,(c^*)^{2n+1} = 1\,.$$

(Given the outcome of [22, Theorem 5.1], we only have to set $c^* := \frac{2\gamma}{\pi}$, where $\ln(1+\sqrt{2}) < \gamma < \frac{9}{10}$ satisfies [22, (63)].) Hence, $\psi^{-1}_{p_0,\eta_0}\Big|_{(-c^*,c^*)} \in W^\omega_+((-c^*,c^*))$. Since in particular $\psi^{-1}_{p_0,\eta_0}\Big|_{[-c^*,c^*]}$ is continuous, we may apply Proposition 6.47. Consequently, if $S \in \mathcal{Q}_{mn}$, then $S_0 := \psi^{-1}_{p_0,\eta_0}[c^*\,S] \in \mathcal{Q}_{mn}$ (due to (6.196)). Observe that for any $0 \leq \eta < 1$ the CCP function $\frac{2}{\pi}\,h_{g_\eta,g_\eta} = h_{\sqrt{2/\pi}\,g_\eta,\sqrt{2/\pi}\,g_\eta}$ actually originates from the *bounded* function $\sqrt{\frac{2}{\pi}}\,g_\eta \in S_{L^\infty}\cap S_{L^2(\gamma_2)}$, such as $\frac{2}{\pi}\arcsin = h_{\text{sign},\text{sign}}$. Let $S \in \mathcal{Q}_{m,n}$ be arbitrarily given. Since $S_0 \in \mathcal{Q}_{mn}$, we therefore obtain

$$\begin{aligned}|\operatorname{tr}(A^\top S)| &= \frac{1}{c^*}\,|\operatorname{tr}(A^\top\psi_{p_0,\eta_0}[S_0])| = \frac{1}{c^*}\,\Big|\operatorname{tr}\Big(A^\top\Big((1-p)\frac{2}{\pi}\arcsin[S_0] + p\,\frac{2}{\pi}\,h_{g_\eta,g_\eta}[S_0]\Big)\Big|\\ &\overset{(6.184)}{\leq} \frac{1}{c^*}\,((1-p)\|A\|_{\infty,1} + p\,\|A\|_{\infty,1}) = \frac{1}{c^*}\,\|A\|_{\infty,1}\,,\end{aligned}$$

whence

$$K_G^{\mathbb{R}} \leq \frac{1}{c^*} < \frac{\pi}{2\,\ln(1+\sqrt{2})}\,.$$

In summary, given the - crucial - result [22, Theorem 5.1], our general framework can be applied here as well, leading to a shortened proof of [22, Theorem 1.1].

Despite the quite remarkable outcome of Theorem 6.45, we should observe that its practical implementation seems to be quite difficult (at least without sufficiently large computer power). Primarily, as we already have seen, this is due to the following facts:

(i) Either we have to know a closed form representation (or at least a "close" approximation of the Maclaurin series) of $h_{f,f}$, $h_{f,f}^{-1}$ and $\big(h_{f,f}^{-1}\big)_{\text{abs}}$ if $f \in L^\infty(\mathbb{R}^k)$ is given (such as is the case for $k = 1$ and $f := \text{sign} \in L^\infty(\mathbb{R}^1) \cap S_{L^2(\gamma_1)}$), or we have to check, whether $h = h_{f,f}$ "originates" from some $f \in L^\infty(\mathbb{R}^k) \cap S_{L^2(\gamma_k)}$, if the functions h, h^{-1} and $\big(h^{-1}\big)_{\text{abs}}$ are known to us.

(ii) However, already in the one-dimensional case (i.e., for $k = 1$) that search requires rather complex calculation techniques, respectively some very helpful knowledge about Hermite polynomials. Moreover, if k increases, we are confronted with a "curse of combinatoric dimensionality", since for any $\nu \in \mathbb{N}_0$ and $n \in \mathbb{N}$ it can be easily shown by induction on k that the set $C(\nu, k) := \{n \in \mathbb{N}_0^k : |n| = \nu\}$ which determines the structure of $h_{f,f}$ (cf. Theorem 6.5) actually consists of $\binom{\nu+k-1}{k-1} = \frac{(\nu+k-1)!}{\nu!\,(k-1)!}$ elements. In particular, already $C(\nu, 2)$ consists of $\nu + 1$ elements ($\nu \in \mathbb{N}_0$). For example, to determine $C(2, 11)$ explicitly, we would have to know all of its 66 elements!

We will recognise how deep actually we are confronted with a "curse of combinatoric dimensionality" if only a Maclaurin series representation of the function $h_{f,f}$ is given to us (cf. Subsection 9.1).

7. The complex case: towards extending Haagerup's approach

7.1. Multivariate complex CCP functions and their relation to the real case

Next, we are going to transfer the main results in the previous section from the real field $\mathbb{R}$ to the complex field $\mathbb{C}$. In order to achieve this, we have to implement non-trivial structural properties of the class of *complex* Hermite polynomials (cf. Theorem 7.11 and Theorem 7.12). The complex versions of Theorem 6.5 and Theorem 6.8 also allow a generalisation of the Haagerup equality by transition from the $\Sigma_2(\zeta)$-correlated couple of two complex one-dimensional signum functions $\text{sign} : \mathbb{C} \longrightarrow \mathbb{T}$ to a $\Sigma_{2k}(\zeta)$-correlated couple of two (possibly different) arbitrary square-integrable functions $b, c : \mathbb{C}^k \longrightarrow \mathbb{C}$, where $k \in \mathbb{N}$ can be arbitrarily large (cf. Corollary 7.4 and Example 7.15). By definition (cf. [57, Lemma 3.2. and Proof of Theorem 3.1]), the complex sign-function is given as

$$\text{sign}(z) := \begin{cases} \frac{z}{|z|} & \text{if } z \in \mathbb{C}^* \\ 0 & \text{if } z = 0 \end{cases}.$$

We introduce the following helpful symbolic constructions and shortcuts. Fix $k, l \in \mathbb{N}$. Let $b : \mathbb{C}^k \longrightarrow \mathbb{C}$ and $c : \mathbb{C}^l \longrightarrow \mathbb{C}$ be two functions. Put

$$b_k \otimes_l c := (b \circ P_k)(c \circ Q_l),$$

where

$$P_k := \begin{pmatrix} 1 & 0 & \dots & 0 & 0 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 & 0 & 0 & \dots & 0 \end{pmatrix} = (I_k \,\vdots\, 0) \in \mathbb{M}_{k,k+l}(\mathbb{C})$$

and

$$Q_l := \begin{pmatrix} 0 & 0 & \dots & 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 & 0 & 0 & \dots & 1 \end{pmatrix} = (0 \,\vdots\, I_l) \in \mathbb{M}_{l,k+l}(\mathbb{C}),$$

implying that

$$b\,_k\otimes_l\, c(\mathrm{vec}(z \,\vdots\, w)) = b(z)c(w) \text{ for all } (z, w) \in \mathbb{C}^k \times \mathbb{C}^l\,. \tag{7.202}$$

Given the construction of $b\,_k\otimes_l\, c$ we may unambiguously shorten it simply to $b \otimes c$ (and suppress the listing of the dimensions of the domains of definition of b, respectively c). Let $d : \mathbb{C}^k \longrightarrow \mathbb{C}$ be a given function. Recall the induced functions $r(d) : \mathbb{R}^{2k} \longrightarrow \mathbb{R}$ and $s(d) : \mathbb{R}^{2k} \longrightarrow \mathbb{R}$, defined as $r(d) := \mathrm{Re}(d) \circ \frac{1}{\sqrt{2}} J_2^{-1}$ and $s(d) := \mathrm{Im}(d) \circ \frac{1}{\sqrt{2}} J_2^{-1}$ (cf. (2.24)). In order to facilitate reading, we put $d_\alpha(z) := d(\mathrm{sign}(\alpha)z)$, where $\alpha \in \mathbb{C}$ and $z \in \mathbb{C}^k$ (implying that $d_0 = d(0)$). Consequently, the construction of $b \otimes \overline{c}$ implies that

$$\begin{aligned} r(b \otimes \overline{c})(\mathrm{vec}(\mathrm{vec}(x_1, x_2), \mathrm{vec}(y_1, y_2))) &= r(b)(\mathrm{vec}(x_1, y_1))r(c)(\mathrm{vec}(x_2, y_2)) \\ &\quad + s(b)(\mathrm{vec}(x_1, y_1))s(c)(\mathrm{vec}(x_2, y_2)) \end{aligned}$$

and

$$\begin{aligned} s(b \otimes \overline{c})(\mathrm{vec}(\mathrm{vec}(x_1, x_2), \mathrm{vec}(y_1, y_2))) &= s(b)(\mathrm{vec}(x_1, y_1))r(c)(\mathrm{vec}(x_2, y_2)) \\ &\quad - r(b)(\mathrm{vec}(x_1, y_1))s(c)(\mathrm{vec}(x_2, y_2)) \end{aligned}$$

for all $x_1, x_2, y_1, y_2 \in \mathbb{R}^k$. In other words:

$$r(b \otimes \overline{c}) = (r(b) \otimes r(c)) \circ G + (s(b) \otimes s(c)) \circ G \tag{7.203}$$

on $\mathbb{R}^{4k}$, and

$$s(b \otimes \overline{c}) = (s(b) \otimes r(c)) \circ G - (r(b) \otimes s(c)) \circ G\,, \tag{7.204}$$

on $\mathbb{R}^{4k}$, where again $G = G^\top = G^{-1} \in O(4n)$ is the matrix, introduced in (1.9). Finally, d is odd (respectively, even) if and only if both, $r(d)$ and $s(d) = r(-i\,d)$ are odd (respectively, even).

Lemma 7.1. *Let $k \in \mathbb{N}$, $\rho \in [-1, 1]$, $\alpha \in \mathbb{C}$, $\theta \in \mathbb{R}$, $c, d : \mathbb{C}^k \longrightarrow \mathbb{C}$ and vec$(\boldsymbol{X}, \boldsymbol{Y}) \sim N_{4k}(0, \Sigma_{4k}(\rho))$. Then*

(i) $r(d_\alpha) = r(d) \circ R_2(sign(\alpha) I_k)$ *and* $r(d_\theta) = r(d) \circ sign(\theta) I_{2k}$.

(ii) *If* $\alpha \neq 0$*, then* $r(d) \in L^2(\mathbb{R}^{2k}, \gamma_{2k})$ *if and only if* $r(d_\alpha) \in L^2(\mathbb{R}^{2k}, \gamma_{2k})$*. In this case, the norms coincide:* $\|r(d)\|_{\gamma_{2k}} = \|r(d_\alpha)\|_{\gamma_{2k}}$.

(iii) *If* $\alpha \neq 0$, $h_{r(d),r(d)}(\rho) = \mathbb{E}[r(d)(\boldsymbol{X}) r(d)(\boldsymbol{Y})] = \mathbb{E}[r(d_\alpha)(\boldsymbol{X}) r(d_\alpha)(\boldsymbol{Y})] = h_{r(d_\alpha),r(d_\alpha)}(\rho)$.

(iv) $h_{r(c_r),r(d)}(|r|) = h_{r(c),r(d)}(r)$ *for all* $r \in [-1, 1]$.

Proof. (i) Put $\kappa := \text{sign}(\alpha)$. Fix $x \in \mathbb{R}^{2k}$. Since $J_2^{-1} \circ R_2(\kappa\, I_k) = (\kappa\, I_k) \circ J_2^{-1} = \kappa\, J_2^{-1}$ (cf. Figure 1), it follows that $d_\alpha\Big(\frac{1}{\sqrt{2}}\, J_2^{-1}(x)\Big) = d\Big(\frac{1}{\sqrt{2}} J_2^{-1}(R_2(\kappa\, I_k)x)\Big)$, whence $r(d_\alpha) = r(d) \circ R_2(\kappa I_k)$.
(ii) Let $\alpha \neq 0$. Since $\det(R_2(\kappa I_k)) = 1$ (due to (2.22)) and $\|R_2(\kappa I_k)a\|^2 = \langle a, R_2(\overline{\kappa} I_k) R_2(\kappa I_k) a\rangle_{\mathbb{R}_2^{2k}} = \|a\|^2$ for all $a \in \mathbb{R}^{2k}$ (due to (1.14)), an application of the change-of-variables formula implies that $r(d_\alpha) \in L^2(\mathbb{R}^{2k}, \gamma_{2k})$ if and only if $r(d) \in L^2(\mathbb{R}^{2k}, \gamma_{2k})$ and $\|r(d_\alpha)\|_2 = \|r(d)\|_2$.
(iii) Let $\alpha \neq 0$. Put $\kappa := \text{sign}(\alpha)$. Then $A_\kappa := R_2(\kappa I_k) \neq 0$. Put $\mathbf{X}_\kappa := A_\kappa \mathbf{X}$ and $\mathbf{Y}_\kappa := A_\kappa \mathbf{Y}$. Since

$$\begin{pmatrix} A_\kappa & 0 \\ 0 & A_\kappa \end{pmatrix} \begin{pmatrix} I_{2k} & \rho\, I_{2k} \\ \rho\, I_{2k} & I_{2k} \end{pmatrix} \begin{pmatrix} A_{\overline{\kappa}} & 0 \\ 0 & A_{\overline{\kappa}} \end{pmatrix} = \begin{pmatrix} I_{2k} & \rho\, I_{2k} \\ \rho\, I_{2k} & I_{2k} \end{pmatrix} = \Sigma_{4k}(\rho),$$

it follows that

$$\text{vec}(\mathbf{X}_\kappa, \mathbf{Y}_\kappa) = \begin{pmatrix} A_\kappa & 0 \\ 0 & A_\kappa \end{pmatrix} \text{vec}(\mathbf{X}, \mathbf{Y}) \sim N_{4k}(0, \Sigma_{4k}(\rho)).$$

Therefore, $\text{vec}(\mathbf{X}, \mathbf{Y}) \stackrel{d}{=} \text{vec}(\mathbf{X}_\kappa, \mathbf{Y}_\kappa)$, whence $\mathbb{E}[r(d_\alpha)(\mathbf{X}) r(d_\alpha)(\mathbf{Y})] \stackrel{(i)}{=} \mathbb{E}[r(d)(\mathbf{X}_\kappa) r(d)(\mathbf{Y}_\kappa)] = \mathbb{E}[r(d)(\mathbf{X}) r(d)(\mathbf{Y})]$ which proves (iii).
(iv) If $r = 0$, the claim immediately follows from the resulting independence of the standard Gaussian random vectors $\mathbf{X}$ and $\mathbf{Y}$. So, let $r \neq 0$. Let $\text{vec}(\mathbf{X}_1, \mathbf{X}_2) \sim N_{4k}(0, \Sigma_{4k}(|r|))$. Then $\text{vec}(\text{sign}(r)\mathbf{X}_1, \mathbf{X}_2) \sim N_{4k}(0, \Sigma_{4k}(r))$. The second equality of statement (i) therefore implies that

$$h_{r(c_r),r(d)}(|r|) = \mathbb{E}[r(c_r)(\mathbf{X}_1) r(d)(\mathbf{X}_2)] = \mathbb{E}[r(c)(\text{sign}(r)\mathbf{X}_1) r(d)(\mathbf{X}_2)] = h_{r(c),r(d)}(r).$$

□

Fix $\text{vec}(\mathbf{Z}, \mathbf{W}) \sim \mathbb{C}N_{2k}(0, \Sigma_{2k}(\zeta))$, where $\zeta \in \overline{\mathbb{D}} \setminus \{0\}$ and $k \in \mathbb{N}$. Let $b, c : \mathbb{C}^k \longrightarrow \mathbb{C}$, such that $b \otimes \overline{c} \in L^1(\mathbb{C}^{2k}, \mathbb{P}_{\text{vec}(\mathbf{Z},\mathbf{W})})$. We put

$$h^{\mathbb{C}}_{b,c}(\zeta) := h^{\mathbb{C}}(b, c; \zeta) := \mathbb{E}\Big[b(\mathbf{Z})\overline{c(\mathbf{W})}\Big] = \overline{h^{\mathbb{C}}_{c,b}(\overline{\zeta})}.$$

As in the real case (see (6.147)), the joint multivariate Gaussian splitting property (3.84) of inner products of vectors on the unit sphere and Lemma 2.14-(ii) imply the important observation that for any separable $\mathbb{C}$-Hilbert space H, for any $m, n \in \mathbb{N}$, and for any $(u, v) \in S_H^m \times S_H^n$, we have

$$h^{\mathbb{C}}_{b,c}[\Gamma_H(u, v)] = \mathbb{E}\Big[\overline{\mathbf{R}_c}\, \mathbf{S}_b{}^\top\Big] = \mathbb{E}[\Gamma_{\mathbb{C}}(\mathbf{R}_c, \mathbf{S}_b)], \qquad (7.205)$$

where the $\mathbb{C}^m$-valued random vector $\mathbf{R}_c$ and the $\mathbb{C}^n$-valued random vector $\mathbf{S}_b$ are defined as $(\mathbf{R}_c)_i := c(\mathbf{Z}_{u_i})$ and $(\mathbf{S}_b)_j := b(\mathbf{Z}_{v_j})$, respectively ($(i, j) \in [m] \times [n]$). Fix $f, g \in L^2(\mathbb{R}^k, \gamma_k)$ and put

$$H_{f,g} := h_{f,f} + h_{g,g}.$$

(6.139) implies a concrete integral representation of the function $H_{f,g}\big|_{(-1,1)}$, which particularly plays an important role in the complex case (cf. Corollary 7.4):

$$H_{f,g}(\rho) = \frac{1}{(2\pi)^k(1-\rho^2)^{k/2}} \int_{\mathbb{R}^k}\int_{\mathbb{R}^k} \Big\langle \begin{pmatrix} f(x) \\ g(x) \end{pmatrix}, \begin{pmatrix} f(y) \\ g(y) \end{pmatrix} \Big\rangle_{\mathbb{R}^2_2} \exp\Big(- \frac{\|x\|^2 + \|y\|^2 - 2\rho\langle x, y\rangle}{2(1-\rho^2)}\Big) \mathrm{d}^k x \, \mathrm{d}^k y \tag{7.206}$$

for all $\rho \in (-1, 1)$. Theorem 6.5 further implies that $H_{f,g}(\rho) = \sum_{\nu=0}^{\infty} a_\nu \, \rho^\nu$ for all $\rho \in [-1, 1]$, where $a_\nu := p_\nu(f, f) + p_\nu(g, g) \geq 0$ for all $\nu \in \mathbb{N}_0$. In particular, $H_{f,g}(1) = \|f\|^2_{\gamma_{2k}} + \|g\|^2_{\gamma_{2k}}$, implying that $H_{f,g}$ is real analytic on $(-1, 1)$, continuous on $[-1, 1]$ and absolutely monotonic on $[0, 1]$. Moreover, $H_{f,g}$ is bounded, and

$$|H_{f,g}(\rho)| \leq \|f\|^2_{\gamma_{2k}} + \|g\|^2_{\gamma_{2k}} = H_{f,g}(1) \tag{7.207}$$

for all $\rho \in [-1, 1]$. Hence, if $f \neq 0$ or $g \neq 0$, it follows that

$$H_{f,g} = H_{f,g}(1) \, \psi_{f,g}, \tag{7.208}$$

where the function $\psi_{f,g} := \frac{H_{f,g}}{H_{f,g}(1)} : [-1, 1] \longrightarrow [-1, 1]$ is CCP (due to Theorem 5.17). In particular, $H_{f,g}\big|_{(-1,1)} \in W^\omega_+((-1, 1))$. Thus, if $b \in L^2(\mathbb{C}^k, \gamma_k^{\mathbb{C}})$, then (2.27) implies that $r(b) \in L^2(\mathbb{R}^{2k}, \gamma_{2k})$ and $s(b) \in L^2(\mathbb{R}^{2k}, \gamma_{2k})$, and

$$H_{r(b),s(b)}(1) = \|r(b)\|^2_{\gamma_{2k}} + \|s(b)\|^2_{\gamma_{2k}} = \|b\|^2_{\gamma_k^{\mathbb{C}}}. \tag{7.209}$$

If - in addition - b is odd and $\|b\|^2_{\gamma_k^{\mathbb{C}}} > 0$, then also $r(b)$ and $s(b)$ are odd functions (such as $H_{r(b),s(b)}$), satisfying $r(b) \neq 0$ or $s(b) \neq 0$. Hence, we may apply Theorem 6.8 to the well-defined odd CCP function $\psi_{r(b),s(b)}$, and it follows that $H_{r(b),s(b)} : [-1, 1] \longrightarrow [-\|b\|^2_{\gamma_k^{\mathbb{C}}}, \|b\|^2_{\gamma_k^{\mathbb{C}}}]$ is a strictly increasing homeomorphism, such as the inverse function $(H_{r(b),s(b)})^{-1} : [-\|b\|^2_{\gamma_k^{\mathbb{C}}}, \|b\|^2_{\gamma_k^{\mathbb{C}}}] \longrightarrow [-1, 1]$ (due to (7.209) and (7.208)). Similarly, if we - further - assume that $H'_{r(b),s(b)}(0) > 0$, Theorem 6.8-(iv) shows that also $(H_{r(b),s(b)})^{-1}$ is real analytic on $(-\|b\|^2_{\gamma_k^{\mathbb{C}}}, \|b\|^2_{\gamma_k^{\mathbb{C}}})$. So, we could apply Lemma 5.10 to the real analytic function $(H_{r(b),s(b)})^{-1}\big|_{(-\|b\|^2_{\gamma_k^{\mathbb{C}}}, \|b\|^2_{\gamma_k^{\mathbb{C}}})}$ (if the assumptions are given) to check the existence of $(H^{-1}_{r(b),s(b)})_{\text{abs}} : [-\|b\|^2_{\gamma_k^{\mathbb{C}}}, \|b\|^2_{\gamma_k^{\mathbb{C}}}] \longrightarrow \mathbb{R}$ then (a crucial assumption in Theorem 7.13). Equipped with these facts, we arrive at the complex version of Theorem 6.5:

Theorem 7.2. *Let $k \in \mathbb{N}$, $\zeta \in \overline{\mathbb{D}}$, $\boldsymbol{L} \sim \mathbb{C}N_k(0, I_k)$ and $vec(\boldsymbol{Z}, \boldsymbol{W}) \sim \mathbb{C}N_{2k}(0, \Sigma_{2k}(\zeta))$. Let $b \in L^2(\mathbb{C}^k, \gamma_k^{\mathbb{C}})$ and $c \in L^2(\mathbb{C}^k, \gamma_k^{\mathbb{C}})$. Then $b \otimes \overline{c} \in L^1(\mathbb{C}^k \times \mathbb{C}^k, \mathbb{P}_{vec(\boldsymbol{Z},\boldsymbol{W})})$. If $\zeta = 0$, then*

$$\begin{aligned} \overline{h^{\mathbb{C}}_{c,b}(0)} = h^{\mathbb{C}}_{b,c}(0) &= \mathbb{E}[b(\boldsymbol{L})] \, \mathbb{E}[\overline{c}(\boldsymbol{L})] \\ &= h_{r(b),r(c)}(0) + h_{s(b),s(c)}(0) + i \, (h_{s(b),r(c)}(0) - h_{r(b),s(c)}(0)). \end{aligned} \tag{7.210}$$

If $\zeta \neq 0$, then

$$\overline{h^{\mathbb{C}}_{c,b}(\overline{\zeta})} = h^{\mathbb{C}}_{b,c}(\zeta) = h_{r(b_\zeta),r(c)}(|\zeta|) + h_{s(b_\zeta),s(c)}(|\zeta|) + i \, (h_{s(b_\zeta),r(c)}(|\zeta|) - h_{r(b_\zeta),s(c)}(|\zeta|)). \tag{7.211}$$

In particular,

$$0 \le h^{\mathbb{C}}_{b_{\overline{\zeta}},b}(\zeta) = H_{r(b),s(b)}(|\zeta|) \text{ and } h^{\mathbb{C}}_{b,c}(1) = \langle b, c\rangle_{\gamma^{\mathbb{C}}_k}. \tag{7.212}$$

$h^{\mathbb{C}}_{b,c} : \overline{\mathbb{D}} \longrightarrow \mathbb{C}$ is bounded and satisfies

$$|h^{\mathbb{C}}_{b,c}(\zeta)| \le \|b\|_{\gamma^{\mathbb{C}}_k} \|c\|_{\gamma^{\mathbb{C}}_k} \text{ for all } \zeta \in \overline{\mathbb{D}}. \tag{7.213}$$

Proof. Firstly, let $\zeta = 0$, implying that $\Sigma_{2k}(\zeta) = I_{2k}$. Thus, the partitioned random vector parts $\mathbf{Z} \sim \mathbb{C}N_k(0, I_k)$ and $\mathbf{W} \sim \mathbb{C}N_k(0, I_k)$ of the complex Gaussian random vector $\text{vec}(\mathbf{Z}, \mathbf{W}) \sim \mathbb{C}N_{2k}(0, I_{2k})$ are independent (cf. [5, Theorem 2.12]). If $\mathbf{X} \stackrel{d}{=} \sqrt{2}J_2(\mathbf{Z})$ and $\mathbf{Y} \stackrel{d}{=} \sqrt{2}J_2(\mathbf{W})$, then $\mathbf{X} \sim N_{2k}(0, I_{2k})$ and $\mathbf{Y} \sim N_{2k}(0, I_{2k})$. (2.25) therefore implies that

$$\begin{aligned}
\mathbb{E}\Big[b(\mathbf{Z})\overline{c(\mathbf{W})}\Big] &= \mathbb{E}[b(\mathbf{Z})]\mathbb{E}[\overline{c(\mathbf{W})}] \\
&= \mathbb{E}[r(b)(\mathbf{X})]\,\mathbb{E}[r(c)(\mathbf{Y})] + \mathbb{E}[s(b)(\mathbf{X})]\,\mathbb{E}[s(c)(\mathbf{Y})] \\
&+ i(\mathbb{E}[s(b)(\mathbf{X})]\,\mathbb{E}[r(c)(\mathbf{Y})] - \mathbb{E}[r(b)(\mathbf{X})]\,\mathbb{E}[s(c)(\mathbf{Y})]) \\
&= h_{r(b),r(c)}(0) + h_{s(b),s(c)}(0) + i(h_{s(b),r(c)}(0) - h_{r(b),s(c)}(0)),
\end{aligned} \tag{7.214}$$

where the last equality follows from Theorem 6.5-(i). Next, we consider the remaining case $\zeta \in \overline{\mathbb{D}} \setminus \{0\}$. Put $\sigma := \text{sign}(\overline{\zeta}) = \frac{\overline{\zeta}}{|\zeta|}$ and $\tau := \text{sign}(\zeta) = \frac{1}{\sigma}$. Lemma 7.1 implies that $r(b_\zeta) \in L^2(\mathbb{R}^{2k}, \gamma_{2k})$ and $\|r(b_\zeta)\|_2 = \|r(b)\|_2$. Similarly, it follows that $s(b_\zeta) \in L^2(\mathbb{R}^{2k}, \gamma_{2k})$, and $\|s(b_\zeta)\|_2 = \|s(b)\|_2$. The proof of (7.211) is built on Lemma 2.14-(v) and Lemma 7.1-(i). To this end, we have to consider the block matrix

$$G := \begin{pmatrix} I_k & 0 & 0 & 0 \\ 0 & 0 & I_k & 0 \\ 0 & I_k & 0 & 0 \\ 0 & 0 & 0 & I_k \end{pmatrix} = G^\top = G^{-1} \in O(4k)$$

again (cf. (1.9)). Lemma 2.14-(v) implies that $\text{vec}(\sigma\,\mathbf{Z}, \mathbf{W}) \sim \mathbb{C}N_{2k}(0, \Sigma_{2k}(|\zeta|))$ and

$$\mathbf{X} := \sqrt{2}\,G\,J_2(\text{vec}(\sigma\,\mathbf{Z}, \mathbf{W})) \stackrel{(1.8)}{=} \sqrt{2}\,\text{vec}(J_2(\sigma\,\mathbf{Z}), J_2(\mathbf{W})) \sim N_{4k}(0, \Sigma_{4k}(|\zeta|)). \tag{7.215}$$

Thus, Corollary 2.11, together with the equality $G^2 = I_{4k}$, yields

$$\mathbb{E}[b \otimes \overline{c}(\text{vec}(\mathbf{Z}, \mathbf{W}))] = \mathbb{E}[b_\zeta \otimes \overline{c}(\text{vec}(\sigma\,\mathbf{Z}, \mathbf{W}))] = \mathbb{E}[r(b_\zeta \otimes \overline{c})(G\,\mathbf{X})] + i\,\mathbb{E}[s(b_\zeta \otimes \overline{c})(G\,\mathbf{X})]. \tag{7.216}$$

Because of (7.203) and (7.204), it follows in particular that

$$r(b_\zeta \otimes \overline{c}) \circ G = r(b_\zeta) \otimes r(c) + s(b_\zeta) \otimes s(c)$$

on $\mathbb{R}^{2k} \times \mathbb{R}^{2k} \cong \mathbb{R}^{4k}$, and

$$s(b_\zeta \otimes \overline{c}) \circ G = s(b_\zeta) \otimes r(c) - r(b_\zeta) \otimes s(c)\,,$$

on $\mathbb{R}^{2k} \times \mathbb{R}^{2k} \cong \mathbb{R}^{4k}$. Linearity of the expectation and Theorem 6.5, together with the fact that by construction $\mathbf{X} = \text{vec}(\mathbf{X}_1, \mathbf{X}_2)$, (with $\mathbf{X}_1 := \sqrt{2}\,J_2(\sigma\mathbf{Z})$ and and $\mathbf{X}_2 := \sqrt{2}\,J_2(\mathbf{W})$)

now imply (7.211). Finally, to achieve the non-trivial boundedness statement (7.213) (which cannot simply be derived by making a standard use of the triangle inequality), we need to implement (a complexification of) the Ornstein-Uhlenbeck semigroup, respectively (6.145). Because of (7.210), the case $\zeta = 0$ is trivial, though. So, let us fix $0 \neq \zeta \in \overline{\mathbb{D}}$. Let $f \in \{r(b_\zeta), s(b_\zeta)\}$ and $g \in \{r(c), s(c)\}$. Then $h_{f,g}(|\zeta|) \overset{(6.145)}{=} \langle f, R_\zeta g\rangle_{\gamma_k}$, where $R_\zeta := T_{\vartheta(|\zeta|)}$. Consequently, since $r(R_\zeta g \circ \sqrt{2}J_2) = \mathrm{Re}(R_\zeta g \circ \sqrt{2}J_2) \circ \frac{1}{\sqrt{2}}J_2^{-1} = R_\zeta g = \mathrm{Im}(R_\zeta g \circ \sqrt{2}J_2) \circ \frac{1}{\sqrt{2}}J_2^{-1} = s(R_\zeta g \circ \sqrt{2}J_2)$, (2.30) leads to

$$\begin{aligned} h^{\mathbb{C}}_{b,c}(\zeta) &\overset{(7.211)}{=} h_{r(b_\zeta),r(c)}(|\zeta|) + h_{s(b_\zeta),s(c)}(|\zeta|) + i\,(h_{s(b_\zeta),r(c)}(|\zeta|) - h_{r(b_\zeta),s(c)}(|\zeta|)) \\ &= \langle b_\zeta, \psi(c;\zeta)\rangle_{\gamma_k^{\mathbb{C}}}, \end{aligned}$$

where $\psi(c;\zeta) := R_\zeta r(c) \circ \sqrt{2}J_2 + i\,(R_\zeta s(c) \circ \sqrt{2}J_2)$. Consequently, we may apply the Cauchy-Schwarz inequality, and Lemma 7.1-(ii) implies that

$$|h_{b,c}(\zeta)| \leq \|b_\zeta\|_{\gamma_k^{\mathbb{C}}}\, \|\psi(c;\zeta)\|_{\gamma_k^{\mathbb{C}}} = \|b\|_{\gamma_k^{\mathbb{C}}}\, \|\psi(c;\zeta)\|_{\gamma_k^{\mathbb{C}}}.$$

Since $\|T_\zeta\|_{\mathcal{L}(L^2(\gamma_{2k}))} = 1$ (see [20, Theorem 1.4.1]), a two-fold application of (2.27) implies that

$$\|\psi(c;\zeta)\|^2_{\gamma_k^{\mathbb{C}}} = \|R_\zeta r(c)\|^2_{\gamma_{2k}} + \|R_\zeta s(c)\|^2_{\gamma_{2k}} \leq \|r(c)\|^2_{\gamma_{2k}} + \|s(c)\|^2_{\gamma_{2k}} = \|c\|^2_{\gamma_k^{\mathbb{C}}}.$$

In conclusion, we finally obtain

$$|h_{b,c}(\zeta)| \leq \|b\|_{\gamma_k^{\mathbb{C}}}\, \|\psi(c;\zeta)\|_{\gamma_k^{\mathbb{C}}} \leq \|b\|_{\gamma_k^{\mathbb{C}}}\, \|c\|_{\gamma_k^{\mathbb{C}}}.$$

□

By taking into account that $\mathrm{sign}(\zeta)\,|\zeta|^{2\nu+1} = \zeta \cdot \zeta^\nu \cdot \overline{\zeta}^{\,\nu}$ for all $\zeta \in \mathbb{C}$ and $\nu \in \mathbb{N}_0$, Theorem 7.2 also leads to a straightforward generalisation of the Haagerup function (cf. [57, Proof of Theorem 3.1] and Example 7.15). To this end, we introduce a class of complex-valued functions which could be viewed as a transfer of the class of all odd real-valued functions to the complex field and contains the complex signum function $\mathrm{sign} : \mathbb{C} \longrightarrow \mathbb{C}$ as element.

Definition 7.3. Let $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$ and $k \in \mathbb{N}$. A function $b : \mathbb{F}^k \longrightarrow \mathbb{F}$ is circularly symmetric if

$$b(\alpha z) = \alpha b(z) \text{ for all } (\alpha, z) \in S_{\mathbb{F}} \times \mathbb{F}^k\,.$$

The set of all circularly symmetric functions is denoted by $CS_k(S_{\mathbb{F}})$.

Definition 7.3 obviously implies that $CS_k(S_{\mathbb{R}}) = CS_k(\{-1, 1\})$ coincides with the set of all odd real functions from $\mathbb{R}^k$ to $\mathbb{R}$ and that $CS_k(S_{\mathbb{C}}) = CS_k(\mathbb{T})$. Moreover, $(CS_k(S_{\mathbb{F}}), \circ, \mathrm{id})$ is a monoid (i.e., a semigroup, with unit element), where the binary operation $\circ$ is given by the composition of functions.

Corollary 7.4. *Let $k \in \mathbb{N}$ and $\zeta \in \overline{\mathbb{D}}$. Let $b, c \in L^2(\mathbb{C}^k, \gamma_k^{\mathbb{C}})$. Suppose that $b \in CS_k(\mathbb{T})$. Then*

(i)

$$h^{\mathbb{C}}_{b,c}(\zeta) = sign(\zeta)(h_{r(b),r(c)}(|\zeta|) + h_{s(b),s(c)}(|\zeta|) + i\,(h_{s(b),r(c)}(|\zeta|) - h_{r(b),s(c)}(|\zeta|)))\,. \tag{7.217}$$

$$h^{\mathbb{C}}_{b,b}(\zeta) = sign(\zeta) H_{r(b),s(b)}(|\zeta|) = \zeta \sum_{\nu=0}^{\infty} (p_{2\nu+1}(r(b), r(b)) + p_{2\nu+1}(s(b), s(b)))\zeta^{\nu}\,\overline{\zeta}^{\,\nu}\,. \tag{7.218}$$

In particular, we have:

(i-1) $h^{\mathbb{C}}_{b,b}\big|_{[-1,1]} = H_{r(b),s(b)} = h_{r(b),r(b)} + h_{s(b),s(b)}$ *and* $h^{\mathbb{C}}_{b,b}\big|_{(-1,1)} \in W^{\omega}_{+}((-1,1))$.

(i-2) *If* $|\zeta| = 1$, *then* $h^{\mathbb{C}}_{b,b}(\zeta) = \zeta\, \|b\|^2_{\gamma^{\mathbb{C}}_k}$.

(i-3) *If* $\zeta \in \mathbb{D}$ *and* $vec(\boldsymbol{X}, \boldsymbol{Y}) \sim N_{2k}(0, \Sigma_{2k}(|\zeta|))$, *then*

$$\begin{aligned} h^{\mathbb{C}}_{b,b}(\zeta) &= \frac{sign(\zeta)}{(2\pi)^{2k}(1-|\zeta|^2)^k} \int_{\mathbb{R}^{2k}} \int_{\mathbb{R}^{2k}} \Big\langle \begin{pmatrix} r(b)(x) \\ s(b)(x) \end{pmatrix}, \begin{pmatrix} r(b)(y) \\ s(b)(y) \end{pmatrix} \Big\rangle_{\mathbb{R}^2_2} \exp\Big(- \frac{\|x\|^2 + \|y\|^2 - 2|\zeta|\,\langle x, y\rangle}{2(1-|\zeta|^2)} \Big)\, \mathrm{d}^{2k}x\, \mathrm{d}^{2k}y \\ &= sign(\zeta)(\mathbb{E}[r(b)(\boldsymbol{X})r(b)(\boldsymbol{Y})] + \mathbb{E}[s(b)(\boldsymbol{X})s(b)(\boldsymbol{Y})]). \end{aligned} \tag{7.219}$$

(ii) $h^{\mathbb{C}}_{b,b}$ *is bounded, and*

$$|h^{\mathbb{C}}_{b,b}(\zeta)| \leq \|b\|^2_{\gamma^{\mathbb{C}}_k} \text{ for all } \zeta \in \overline{\mathbb{D}}. \tag{7.220}$$

(iii) *If* $b \neq 0$, *then* $\frac{1}{\|b\|^2_{\gamma^{\mathbb{C}}_k}} H_{r(b),s(b)}$ *as well as* $\frac{1}{\|b\|^2_{\gamma^{\mathbb{C}}_k}} h^{\mathbb{C}}_{b,b}$ *are CCP functions. Both,* $H_{r(b),s(b)} : [-1,1] \longrightarrow [-\|b\|^2_{\gamma^{\mathbb{C}}_k}, \|b\|^2_{\gamma^{\mathbb{C}}_k}]$ *and* $h^{\mathbb{C}}_{b,b} : \overline{\mathbb{D}} \longrightarrow \|b\|^2_{\gamma^{\mathbb{C}}_k}\overline{\mathbb{D}}$ *are circularly symmetric homeomorphisms.* $H_{r(b),s(b)}$ *is strictly increasing and satisfies* $H_{r(b),s(b)}((-1,0)) = (-\|b\|^2_{\gamma^{\mathbb{C}}_k}, 0)$ *and* $H_{r(b),s(b)}((0,1)) = (0, \|b\|^2_{\gamma^{\mathbb{C}}_k})$. *Moreover,* $h^{\mathbb{C}}_{b,b}(\mathbb{D}) = \mathbb{D}$ *and*

$$(h^{\mathbb{C}}_{b,b})^{-1}(w) = sign(w) H^{-1}_{r(b),s(b)}(|w|) \text{ for all } w \in \|b\|^2_{\gamma^{\mathbb{C}}_k}\overline{\mathbb{D}}\,. \tag{7.221}$$

(iv) $h'_{r(b),r(b)}(0) > 0$ *or* $h'_{s(b),s(b)}(0) > 0$ *if and only if* $H^{-1}_{r(b),s(b)}|_{(-\|b\|^2_{\gamma^{\mathbb{C}}_k}, \|b\|^2_{\gamma^{\mathbb{C}}_k})} = (H_{r(b),s(b)}\big|_{(-1,1)})^{-1}$ *is real analytic on* $(-\|b\|^2_{\gamma^{\mathbb{C}}_k}, \|b\|^2_{\gamma^{\mathbb{C}}_k})$.

Proof. (i): Firstly, since $b \in CS_k(\mathbb{T})$, b in particular is an odd function; i.e., $b(-z) = -b(z)$ for all $z \in \mathbb{C}^k$. Thus, also $r(b)$ and $s(b)$ are odd (since $2\,\mathrm{Re}(b) = b + \overline{b}$ and $2i\,\mathrm{Im}(b) = b - \overline{b}$), such as $h_{r(b),r(b)}$, $h_{s(b),s(b)}$ and $H_{r(b),s(b)}$.
Fix $\zeta \in \overline{\mathbb{D}}$. Since $b \in CS_k(\mathbb{T})$, it follows that

$$h^{\mathbb{C}}_{b,c}(\zeta) = \mathrm{sign}(\zeta) h^{\mathbb{C}}_{b_{\overline{\zeta}},c}(\zeta)$$

(which also holds for $\zeta = 0$ due to (7.214)). (7.217) now follows from Lemma 7.1-(ii), (2.27) and (7.211), where the latter is applied to the well-defined function $\overline{\mathbb{D}} \setminus \{0\} \ni z \mapsto h^{\mathbb{C}}_{b_{\overline{\zeta}},c}(z)$. In particular,

$$h^{\mathbb{C}}_{b,b}(\zeta) = \mathrm{sign}(\zeta) H_{r(b),s(b)}(|\zeta|)$$

(due to (7.212)). Therefore, Theorem 6.5, (iii), applied to the odd functions $h_{r(b),r(b)}$ and $h_{s(b),s(b)}$ immediately lead to the power series representation (7.218) of $h^{\mathbb{C}}_{b,b}$, which holds on $\overline{\mathbb{D}}$. (7.219) now follows from (2.33) and (7.206).

(ii) (7.220) is an implication of (7.213).

(iii) Assume that $b \neq 0$. Then $H_{r(b),s(b)} = \|b\|^2_{\gamma_k^{\mathbb{C}}} \psi_{r(b),s(b)}$, where $\psi_{r(b),s(b)} := \frac{H_{r(b),s(b)}}{\|b\|^2_{\gamma_k^{\mathbb{C}}}}$ is CCP (due to (7.208) and (7.209)). (7.218), together with Theorem 5.20 (where the latter is applied to the coefficients $a_{kl} := (p_{2\nu+1}(r(b), r(b)) + p_{2\nu+1}(s(b), s(b)))\delta_{k,l+1}$, $k, l \in \mathbb{N}_0$) implies that $\frac{1}{\|b\|^2_{\gamma_k^{\mathbb{C}}}} h^{\mathbb{C}}_{b,b} : \overline{\mathbb{D}} \longrightarrow \overline{\mathbb{D}}$ is a CCP function. (7.208) and Theorem 6.8-(iii) imply that both, $H_{r(b),s(b)}$ and $h^{\mathbb{C}}_{b,b}$ are homeomorphisms. The representation (7.221) of $(h^{\mathbb{C}}_{b,b})^{-1}$ follows at once. (i-2) and Theorem 6.8-(iii) obviously conclude the proof of (iii).

(iv) Since $h'_{r(b),r(b)}(0) > 0$ or $h'_{s(b),s(b)}(0) > 0$ if and only if $H'_{r(b),s(b)}(0) > 0$, and since $H_{r(b),s(b)}$ is odd, we may adopt the underlying idea of the proof of Theorem 6.8,(iv), implying statement (iv). □

Remark 7.5. Already the trivial example $b := 1$, $c := 1$ and $\zeta := i$ shows us that the additional assumption $b \in CS_k(\mathbb{T})$ in Corollary 7.4 cannot be dropped.

Recall (2.29), including the construction of the function $g^{\mathbb{C}}$ therein. Due to Proposition 6.12 and Corollary 7.4 we obtain

Remark 7.6. Let $k \in \mathbb{N}$ and $f \in L^2(\mathbb{R}^k, \gamma_k)$. Then $r(f^{\mathbb{C}}) = f \otimes 1$ and $s(f^{\mathbb{C}}) = 0$. Moreover,

$$h_{f,f} = h_{f\otimes 1, f\otimes 1} = H_{r(f^{\mathbb{C}}),s(f^{\mathbb{C}})} .$$

If in addition $f^{\mathbb{C}} \in CS_k(\mathbb{T})$, then $h_{f,f} = h^{\mathbb{C}}_{f^{\mathbb{C}},f^{\mathbb{C}}}\Big|_{[-1,1]}$.

At this point, it is very useful to recall Theorem 6.35 and its proof, where we also implemented Abel's theorem on *real* power series. From complex analysis it is well-known that in general Abel's theorem on power series in this form does not hold for $\mathbb{F} = \mathbb{C}$. Moreover, already the structure of the somewhat "simpler" complex-valued odd functions $h_{b,c}$ (cf. (7.217) and (7.218)) seemingly does not allow a transfer of Theorem 6.35-(ii) and (iii) to the complex case (due to Theorem 5.20). However, since [56, Lemma 1.1.13, statement 2] also holds also for the complex field, the proof of Theorem 6.35 can be easily adapted, as well as the proof of Corollary 6.36, so that at least the following versions of a complex hybrid correlation transform can be stated at once:

Proposition 7.7. *Let $m, n \in \mathbb{N}$, $0 < r < \infty$ and*

$$M := \begin{pmatrix} A & S \\ S^* & B \end{pmatrix} \in M_{m+n}(r\,\overline{\mathbb{D}})^+$$

be positive semidefinite, where any entry of the matrices A, S and B is an element of $r\,\overline{\mathbb{D}}$. Let $f, g : (-r, r) \longrightarrow \mathbb{R}$ be two functions, such that $(-r, r) \ni x \mapsto f(x) = \sum_{\nu=0}^{\infty} a_\nu x^\nu \in W^{\omega}_{+}((-r, r))$ and $(-r, r) \ni x \mapsto g(x) = \sum_{\nu=0}^{\infty} b_\nu x^\nu \in W^{\omega}_{+}((-r, r))$. Let $q : r\mathbb{D} \longrightarrow \mathbb{C}$ be a holomorphic function, such that

$$|c_\nu| \leq \sqrt{|a_\nu|\,|b_\nu|} \text{ for all } \nu \in \mathbb{N}_0\,, \tag{7.222}$$

where $c_\nu := \frac{q^{(\nu)}(0)}{\nu!}$. *Then* $q_r \in W^+(\mathbb{D})$, *where* $q_r(\zeta) := q(r\zeta)$ *for all* $\zeta \in \mathbb{D}$. *Put* $r\,\overline{\mathbb{D}} \ni z \mapsto \tilde{q}(z) := \sum_{\nu=0}^\infty c_\nu z^\nu$, $r\,\overline{\mathbb{D}} \ni z \mapsto f_{abs}(z) := \sum_{\nu=0}^\infty |a_\nu| z^\nu$ *and* $r\,\overline{\mathbb{D}} \ni z \mapsto g_{abs}(z) := \sum_{\nu=0}^\infty |b_\nu| z^\nu$. *Then* $\tilde{q_r}(\frac{z}{r}) = \tilde{q}(z)$ *for all* $z \in r\,\overline{\mathbb{D}}$ *and* $\tilde{q}\Big|_{r\,\mathbb{D}} = q$, *where* $\tilde{q_r} \in A(\mathbb{D})$ *is the continuous extension of* q_r. *Moreover, the following properties hold:*

(i)
$$\begin{pmatrix} f_{abs}[A] & \tilde{q}[S] \\ \tilde{q}[S]^* & g_{abs}[B] \end{pmatrix} \in M_{m+n}(r\,\overline{\mathbb{D}})^+$$
is positive semidefinite.

(ii) *If* $0 < c_* \leq r$ *is a root of* $f_{abs} - 1$, *then*
$$\tilde{q}[c_*\,\Gamma] \in \mathcal{Q}_{m,n}(\mathbb{C}) \text{ for all } \Gamma \in \mathcal{Q}_{m,n}(\mathbb{C}) .$$

Thus, an application of Lemma 5.10 immediately leads us to

Corollary 7.8. *Let* $m, n \in \mathbb{N}, A \in \mathbb{M}_{m,n}(\mathbb{C})$ *and*
$$\Sigma = \begin{pmatrix} M & S \\ S^\top & N \end{pmatrix} \in C(m+n;\mathbb{C})$$
be an arbitrary complex $(m+n)\times(m+n)$ *correlation matrix (with block elements* $M \in C(m;\mathbb{C}), N \in C(n;\mathbb{C})$ *and* $S \in \mathcal{Q}_{m,n}(\mathbb{C})$*). Let* $r > 0$ *and* $0 \neq \psi \in W_+^\omega((-r,r))$. *Put* $r\,\overline{\mathbb{D}} \ni z \mapsto \tilde{\psi}(z) := \sum_{\nu=0}^\infty a_\nu z^\nu$, *where* $a_\nu := \frac{\psi^{(\nu)}(0)}{\nu!}$. *If* $0 < c \leq r$, *then*
$$\frac{1}{\psi_{abs}(c)} \begin{pmatrix} \psi_{abs}[c\,M] & \tilde{\psi}[c\,S] \\ \tilde{\psi}[c\,S^*] & \psi_{abs}[c\,N] \end{pmatrix} \in C(m+n;\mathbb{C})$$
again is a correlation matrix with complex entries. In particular,
$$\frac{1}{\psi_{abs}(c)} \tilde{\psi}[cS] \in \mathcal{Q}_{m,n}(\mathbb{C}) \text{ for all } S \in \mathcal{Q}_{m,n}(\mathbb{C}) . \tag{7.223}$$

7.2. On complex bivariate Hermite polynomials

Our next aim is to reveal in detail that it is possible to transfer the content of Theorem 6.40 from the real case to the complex one, while maintaining our constructive proof (including the intended avoidance of the tensor product language). However, we cannot simply copy the proof of Theorem 6.40. Nevertheless, we are going to unfurl that in fact it is possible to transfer (6.186) and (6.187) from the real case to the complex one. To this end, we are going to work with a particular case of the rich class of complex bivariate Hermite polynomials, first considered by K. Itô while working with complex multiple Wiener integrals (cf. [75]). Similarly to the real case, we need to verify a convenient correlation property of a random version of these polynomials, which to the best of our knowledge have not been published before (see Theorem 7.11 below). A detailed introductory discussion of complex Hermite polynomials and their structure (which would exceed the topic of our paper by far) can be studied in [48, 74]. Firstly, we have to recall the following general construction:

Definition 7.9 (**Complex Hermite polynomial**)**.** Let $m, n \in \mathbb{N}_0$ and $z, w \in \mathbb{C}$. The complex Hermite polynomial $H_{m,n} : \mathbb{C}^2 \longrightarrow \mathbb{C}$ is defined as

$$H_{m,n}(z, w) := \frac{1}{\sqrt{m!n!}} \sum_{j=0}^{m \wedge n} (-1)^j j! \binom{m}{j} \binom{n}{j} z^{m-j} \, w^{n-j} \, .$$

Within the scope of our work, we need the particular case of Itô's complex Hermite polynomials

$$\begin{aligned} \mathbb{C} \ni z \mapsto H_{m,n} \circ \kappa(z) &:= H_{m,n}(z, \overline{z}) \\ &= i^{m+n} \sum_{j=0}^{m} \sum_{k=0}^{n} i^{j+k} (-1)^{j+n} \sqrt{\binom{m}{j}\binom{n}{k}} s(j,k) H_{j+k}(\sqrt{2}\,\mathrm{Re}(z))\, s(m-j, n-k) H_{m-j+n-k}(\sqrt{2}\,\mathrm{Im}(z)), \end{aligned}$$

where $\kappa(z) := \mathrm{vec}(z, \overline{z})$ and $s(\nu, \mu) := \sqrt{\frac{(\nu+\mu)!}{\nu!\mu!}}$ for all $\nu, \mu \in \mathbb{N}_0$, including the following facts, which we give without proof (cf. [75, 74]).

Theorem 7.10. *Let $m, n \in \mathbb{N}_0$ and $z, w \in \mathbb{C}$. Then*

(i) *$\{H_{m,n} \circ \kappa : m, n \in \mathbb{N}_0\}$ is an orthonormal basis in the complex Hilbert space $L^2(\gamma_1^{\mathbb{C}})$.*

(ii) *The exponential generating function of $\{H_{m,n} \circ \kappa : m, n \in \mathbb{N}_0\}$ is given as*

$$\sum_{m,n=0}^{\infty} H_{m,n}(z, \overline{z}) \frac{u^m}{\sqrt{m!}} \frac{v^n}{\sqrt{n!}} = \exp(uz + v\overline{z} - uv) \text{ for all } u, v \in \mathbb{C}.$$

Lemma 2.7-(ii) allows us to transfer (the special case $k = 1$ of) Corollary 6.13 to the complex case. More precisely, we have

Theorem 7.11. *Let $m, n, \nu, \mu \in \mathbb{N}_0$ and $\zeta \in \overline{\mathbb{D}}$. If $vec(Z, W) \sim \mathbb{C}N_2(0, \Sigma_2(\zeta))$, then*

$$\mathbb{E}\Big[H_{m,n}(Z, \overline{Z})\overline{H_{\nu,\mu}(W, \overline{W})}\Big] = \delta_{m,\nu}\, \delta_{n,\mu}\, \zeta^m \,\overline{\zeta}^{\,n} = \delta_{(m,n),(\nu,\mu)}\, \zeta^m \overline{\zeta}^{\,n}.$$

Proof. Let $u, v, a, b \in \mathbb{C}$. Due to Theorem 7.10-(ii), a multiplication of the two (random) exponential generating functions leads to

$$\sum_{m,n=0}^{\infty} \sum_{\nu,\mu=0}^{\infty} H_{m,n}(Z, \overline{Z})\overline{H_{\nu,\mu}(W, \overline{W})} \frac{u^m}{\sqrt{m!}} \frac{v^n}{\sqrt{n!}} \frac{\overline{a}^\nu}{\sqrt{\nu!}} \frac{\overline{b}^\mu}{\sqrt{\mu!}} = \exp\Big(\binom{\overline{u}}{b}^* \binom{Z}{W} + \binom{\overline{v}}{a}^* \overline{\binom{Z}{W}}\Big) \exp(-uv - \overline{a}\overline{b}).$$

Thus, if we put $\alpha_{m,n,\nu,\mu}(\zeta) := \mathbb{E}\Big[H_{m,n}(Z, \overline{Z})\overline{H_{\nu,\mu}(W, \overline{W})}\Big]$, then Lemma 2.7-(ii) implies that

$$\sum_{m,n=0}^{\infty} \sum_{\nu,\mu=0}^{\infty} \alpha_{m,n,\nu,\mu}(\zeta) \frac{u^m v^n \overline{a}^\nu \overline{b}^\mu}{\sqrt{m!n!\nu!\mu!}} = \exp\Big((u, \overline{b})\Sigma_2(\zeta)\binom{v}{\overline{a}}\Big) \exp(-uv - \overline{a}\overline{b}) = \exp(u\overline{a}\zeta + \overline{b}v\overline{\zeta}).$$

Since $u, v, a, b \in \mathbb{C}$ were arbitrarily chosen, the multi-index notation shows us, that we actually have proven that

$$\sum_{n \in \mathbb{N}_0^4} \frac{\beta_n(\zeta)}{n!} (z_1, z_2, z_3, z_4)^n = \exp(z_1 z_3\, \zeta + z_2 z_4\, \overline{\zeta}) = \exp(z_1 z_3\, \zeta) \exp(z_2 z_4\, \overline{\zeta}) \text{ for all } z_1, z_2, z_3, z_4 \in \mathbb{C},$$

where $\beta_n(\zeta) := \sqrt{n!}\,\alpha_n(\zeta)$. Consequently, it follows that

$$\sum_{n\in\mathbb{N}_0^4} \Big(\frac{\beta_n(\zeta) - \sqrt{n!}\,\delta_{n_1,n_3}\,\delta_{n_2,n_4}\,\zeta^{n_1}\,\overline{\zeta}^{n_2}}{n!}\Big) z^n = 0 \text{ for all } z \in \mathbb{C}^4\,,$$

wherefrom the claim follows (by uniqueness of the multi-dimensional power series expansion for the entire function $f = 0$ around 0 [125, Ch. 1.2.2.]). $\square$

7.3. Upper bounds of $K_G^{\mathbb{C}}$ and inversion of complex CCP functions

Equipped with the complex Hermite polynomials and Theorem 7.11, it is possible to transfer Theorem 6.32 from the real field $\mathbb{R}$ to the complex field $\mathbb{C}$; at least in the odd case. We "just" have to construct the mappings $\alpha_1^{\psi,c} \in S_{L^2(\gamma_1^{\mathbb{C}})}$ and $\beta_1^{\psi,c} \in S_{L^2(\gamma_1^{\mathbb{C}})}$ properly.

Theorem 7.12. *Let $k \in \mathbb{N}$ and $0 < c \leq 1$. Let $0 \neq \psi \in W_+^{\omega}((-1,1))$ be odd. Then there exist $\alpha \equiv \alpha_{\psi,c}, \beta \equiv \beta_{\psi,c} \in S_{L^2(\gamma_1^{\mathbb{C}})}$, which satisfy the following properties:*

(i) $\mathbb{E}[\alpha(Z)] = \mathbb{E}[\beta(Z)] = 0$ *for all* $Z \sim \mathbb{C}N_1(0,1)$.

(ii) *If $c\,\zeta \in \mathbb{D}$, then*

$$sign(\zeta)\psi(c|\zeta|) = \psi_{abs}(c)\, h_{\alpha,\beta}^{\mathbb{C}}(\zeta)$$

and

$$sign(\zeta)\psi_{abs}(c|\zeta|) = h_{\alpha,\alpha}^{\mathbb{C}}(\zeta)\psi_{abs}(c) = h_{\beta,\beta}^{\mathbb{C}}(\zeta)\psi_{abs}(c).$$

In particular,

$$\psi(c) = \psi_{abs}(c)\,\langle\alpha,\beta\rangle_{\gamma_1^{\mathbb{C}}}\,. \tag{7.224}$$

(iii) *If $c \neq 1$ and H is an arbitrary $\mathbb{C}$-Hilbert space, then*

$$sign(\langle u,v\rangle_H)\psi(c|\langle u,v\rangle_H|) = \psi_{abs}(c)\, h_{\alpha,\beta}^{\mathbb{C}}(\langle u,v\rangle_H)$$

and

$$sign(\langle u,v\rangle_H)\psi_{abs}(c\,|\langle u,v\rangle_H|) = \psi_{abs}(c)\, h_{\alpha,\alpha}^{\mathbb{C}}(\langle u,v\rangle_H) = \psi_{abs}(c)\, h_{\beta,\beta}^{\mathbb{C}}(\langle u,v\rangle_H)$$

for all $u, v \in S_H$.

Proof. Let $0 < c \leq 1$ and $\zeta \in \overline{\mathbb{D}}$. Since $0 \neq \psi \in W_+^{\omega}((-1,1))$, it follows that $\psi^{(n_0)}(0) \neq 0$ for some $n_0 \in \mathbb{N}_0$, implying that $\psi_{\text{abs}}(x) > 0$ for all $x \in (0,1]$. Thus, $\psi_{\text{abs}}(c) > 0$. Put $\widetilde{b_n} \equiv \widetilde{b_{n_1,n_2}} := \frac{\psi^{(2n_1+1)}(0)}{(2n_1+1)!}\delta_{n_1,n_2}$, where $n = (n_1,n_2) \in \mathbb{N}_0^2$. Because of (3.84) and (3.85), we may choose complex random variables $Z_\zeta \sim \mathbb{C}N_1(0,1)$ and $Z_1 \sim \mathbb{C}N_1(0,1)$, such that $\text{vec}(Z_\zeta, Z_1) \sim \mathbb{C}N_2(0,\Sigma_2(\zeta))$, $\text{vec}(Z_\zeta, Z_\zeta) \sim \mathbb{C}N_2(0,\Sigma_2(1))$ and $\text{vec}(Z_1, Z_1) \sim \mathbb{C}N_2(0,\Sigma_2(\zeta))$. Theorem 7.11 therefore in particular implies that

$$\mathbb{E}\Big[H_{k+1,l}(Z_\zeta,\overline{Z_\zeta})\overline{H_{\nu+1,\mu}(Z_1,\overline{Z_1})}\Big] = \delta_{(k,l),(\nu,\mu)}\,\zeta^k\overline{\zeta}^l. \tag{7.225}$$

and

$$\mathbb{E}\Big[H_{k+1,l}(Z_\zeta,\overline{Z_\zeta})\overline{H_{\nu+1,\mu}(Z_\zeta,\overline{Z_\zeta})}\Big] = \delta_{(k,l),(\nu,\mu)} = \mathbb{E}\Big[H_{k+1,l}(Z_1,\overline{Z_1})\overline{H_{\nu+1,\mu}(Z_1,\overline{Z_1})}\Big] \tag{7.226}$$

for all $k, l, \nu, \mu \in \mathbb{N}_0$. Consequently, since ψ is odd by assumption, a straightforward calculation (including the definition of the real numbers $\widetilde{b_n}$ and (2.27) and (7.226)) implies that

$$\mathbb{C} \ni z \mapsto \alpha(z) \equiv \alpha_{\psi,c}(z) := \frac{1}{\sqrt{\psi_{\text{abs}}(c)}} \sum_{n \in \mathbb{N}_0^2} \text{sign}(\widetilde{b_n}) \sqrt{|\widetilde{b_n}|} H_{n_1+1,n_2}(z, \overline{z})(\sqrt{c})^{|n|+1}$$

and

$$\mathbb{C} \ni z \mapsto \beta(z) \equiv \beta_{\psi,c}(z) := \frac{1}{\sqrt{\psi_{\text{abs}}(c)}} \sum_{n \in \mathbb{N}_0^2} \sqrt{|\widetilde{b_n}|} H_{m_1+1,m_2}(z, \overline{z})(\sqrt{c})^{|m|+1}$$

both lead to well-defined elements $\alpha \in L^2(\gamma_1^{\mathbb{C}})$ and $\beta \in L^2(\gamma_1^{\mathbb{C}})$.

(i) Let $Z \sim \mathbb{C}N_1(0,1)$. Then $(Z, Z)^\top \sim \mathbb{C}N_2(0, \Sigma_2(1))$ (due to (2.23)). Since $H_{0,0} = 1$, Theorem 7.11 therefore implies that

$$\mathbb{E}\Big[H_{l_1+1,l_2}(Z, \overline{Z})\Big] = \mathbb{E}\Big[H_{l_1+1,l_2}(Z, \overline{Z})\overline{H_{0,0}(Z, \overline{Z})}\Big] = 0 \text{ for all } (l_1, l_2) \in \mathbb{N}_0^2,$$

and (i) follows.

(ii) Similarly, as explained above, (7.225), together with the construction of the real numbers $\widetilde{b_n}$ and the fact that $\zeta^{l+1}\overline{\zeta}^l = |\zeta|^{2l}\zeta = \text{sign}(\zeta)|\zeta|^{2l+1}$ for all $l \in \mathbb{N}_0$ implies that

$$\psi_{\text{abs}}(c)\mathbb{E}[\alpha(Z_\zeta)\overline{\alpha(Z_1)}] = \text{sign}(\zeta)\psi_{\text{abs}}(c|\zeta|) = \psi_{\text{abs}}(c)\mathbb{E}[\beta(Z_\zeta)\overline{\beta(Z_1)}].$$

and

$$\psi_{\text{abs}}(c)\mathbb{E}[\alpha(Z_\zeta)\overline{\beta(Z_1)}] = \text{sign}(\zeta)\psi(|c\,\zeta|).$$

However, $\mathbb{E}[\alpha(Z_\zeta)\overline{\beta(Z_1)}] = h^{\mathbb{C}}_{\alpha,\beta}(\zeta)$, $\mathbb{E}[\alpha(Z_\zeta)\overline{\alpha(Z_1)}] = h^{\mathbb{C}}_{\alpha,\alpha}(\zeta)$ and $\mathbb{E}[\beta(Z_\zeta)\overline{\beta(Z_1)}] = h^{\mathbb{C}}_{\beta,\beta}(\zeta)$, which proves (ii).

(iii) We just have to apply (ii) to $\overline{\mathbb{D}} \ni \zeta := \langle u, v\rangle_H$. □

Recall Corollary 7.4 including the structure of $h^{\mathbb{C}}_{b,b}$, strongly built on the odd homeomorphic real CCP function $\frac{1}{\|b\|^2_{\gamma_k^{\mathbb{C}}}} H_{r(b),s(b)} : [-1,1] \longrightarrow [-1,1]$. Thus, if we link (7.218), (7.221) and Theorem 7.12 (where the latter is applied to the function $\psi := \Big(\frac{1}{\|b\|^2_{\gamma_k^{\mathbb{C}}}} H_{r(b),s(b)}\Big)^{-1} = H^{-1}_{r(b),s(b)}(\|b\|^2_{\gamma_k^{\mathbb{C}}} \cdot)$), we are able to prove

Theorem 7.13 (Complex inner product rounding). *Let $k \in \mathbb{N}$ and $b \in S_{L^2(\gamma_k^{\mathbb{C}})}$. If $b \in CS_k(\mathbb{T})$ and $(H_{r(b),s(b)})^{-1}\big|_{(-1,1)} \in W^{\omega}_{+}((-1,1))$, then $\Big(H^{-1}_{r(b),s(b)}\Big)_{abs}(1) > 1$, and there exist $\alpha_b \in L^2(\gamma_1^{\mathbb{C}})$ and $\beta_b \in L^2(\gamma_1^{\mathbb{C}})$, satisfying $0 < \langle \alpha_b, \beta_b\rangle_{\gamma_1^{\mathbb{C}}} < 1$, such that for all $\mathbb{C}$-Hilbert spaces H and $u, v \in S_H$ the following properties are satisfied:*

(i)

$$\langle u, v\rangle_H = \frac{1}{c^*} h^{\mathbb{C}}_{b,b}(\zeta_{u,v}(b)), \tag{7.227}$$

where $0 < c^* \equiv c^*(b) := H^{hyp}_{r(b),s(b)}(1) < 1$ and $\zeta_{u,v}(b) := h^{\mathbb{C}}_{\alpha_b,\beta_b}(\langle u, v\rangle_H) \in \mathbb{D}$.

(ii)

$$c^* = H_{r(b),s(b)}(\langle \alpha_b, \beta_b \rangle_{\gamma_1^{\mathbb{C}}}) = h^{\mathbb{C}}_{b,b}(\langle \alpha_b, \beta_b \rangle_{\gamma_1^{\mathbb{C}}}).$$

(iii) *If* $vec(\boldsymbol{X}, \boldsymbol{Y}) \sim N_{2k}(0, \Sigma_{2k}(|\zeta_{u,v}(b)|))$, *then*

$$c^* \langle u, v \rangle_H = \frac{sign(\zeta_{u,v})}{(2\pi)^{2k}(1 - |\zeta_{u,v}|^2)^k} \int_{\mathbb{R}^{2k}} \int_{\mathbb{R}^{2k}} \Big\langle \begin{pmatrix} r(b)(x) \\ s(b)(x) \end{pmatrix}, \begin{pmatrix} r(b)(y) \\ s(b)(y) \end{pmatrix} \Big\rangle_{\mathbb{R}^2_2} \exp\Big(-\frac{\|x\|^2 + \|y\|^2 - 2|\zeta_{u,v}(b)| \langle x, y \rangle}{2(1 - |\zeta_{u,v}(b)|^2)}\Big) \mathrm{d}^{2k}x \, \mathrm{d}^{2k}y$$

$$= sign(\zeta_{u,v}) \Big(\mathbb{E}[r(b)(\boldsymbol{X}) r(b)(\boldsymbol{Y})] + \mathbb{E}[s(b)(\boldsymbol{X}) s(b)(\boldsymbol{Y})] \Big),$$

(iv) *If* $m, n \in \mathbb{N}$ *and* $(z, w) \in S_H^m \times S_H^n$, *then there exist* $m + n$ $\mathbb{C}^k$*-valued random vectors* $\boldsymbol{Z}_1, \dots, \boldsymbol{Z}_m, \boldsymbol{W}_1, \dots, \boldsymbol{W}_n$, *such that* $vec(\boldsymbol{Z}_i, \boldsymbol{W}_j) \sim \mathbb{C}N_{2k}(0, \Sigma_{2k}(\zeta_{ij}(b)))$ *for all* $(i, j) \in [m] \times [n]$, *and*

$$\Gamma_H(z, w) = \frac{1}{c^*} \mathbb{E}[\overline{\boldsymbol{P}_b} \boldsymbol{Q}_b^\top], \tag{7.228}$$

where $(\boldsymbol{P}_b)_i := b(\boldsymbol{Z}_i)$, $(\boldsymbol{Q}_b)_j := b(\boldsymbol{W}_j)$ *and* $\zeta_{ij}(b) := h^{\mathbb{C}}_{\alpha_b,\beta_b}(\langle z_i, w_j \rangle_H) \in \mathbb{D}$, $(i, j) \in [m] \times [n]$.

Proof. (i) Fix $u, v \in S_H$. Put $\psi := H^{-1}_{r(b),s(b)}$ and $\zeta := \langle u, v \rangle_H$. Since $b \in CS_k(\mathbb{T})$, it follows that both, $r(b)$ and $s(b)$ are odd. Hence, the CCP function $H_{r(b),s(b)} = h_{r(b),r(b)} + h_{s(b),s(b)}$ is odd as well (Corollary 7.4), implying that also its inverse ψ is an odd function. So, we may apply Proposition 6.9, together with Theorem 6.33, and it follows that $0 < c^* = H^{\text{hyp}}_{r(b),s(b)}(1) < 1$ is well-defined and satisfies $\psi_{\text{abs}}(c^*) = 1$. (7.221), together with Theorem 7.12 therefore implies that

$$(h^{\mathbb{C}}_{b,b})^{-1}(c^* \zeta) = \text{sign}(c^* \zeta) \psi(|c^* \zeta|) = \text{sign}(\zeta) \, \psi(c^* |\zeta|) = \psi_{\text{abs}}(c^*) \, \zeta_{u,v}(b) = \zeta_{u,v}(b),$$

where $\alpha_b := \alpha_{\psi,c^*}, \beta_b := \beta_{\psi,c^*}$ and $\zeta_{u,v}(b) := h^{\mathbb{C}}_{\alpha_b,\beta_b}(\zeta) \in \overline{\mathbb{D}}$ (due to (7.213)). Hence, $c^* \zeta = h^{\mathbb{C}}_{b,b}(\zeta_{u,v}(b))$. However, since $c^* \zeta \in \mathbb{D}$, it follows that $\zeta_{u,v}(b) \in \mathbb{D}$ (due to Corollary 7.4, (i)).

(ii) Since $H_{r(b),s(b)}(0) = 0 < c^* < 1 = \|b\|^2_{\gamma_k^{\mathbb{C}}} = H_{r(b),s(b)}(1)$ and $\psi_{\text{abs}}(c^*) = 1$, the strict monotonicity of the odd function $\psi = H^{-1}_{r(b),s(b)}$ implies that $0 = \psi(0) < \psi(c^*) \overset{(7.224)}{=} \langle \alpha_b, \beta_b \rangle_{\gamma_1^{\mathbb{C}}} < \psi(1) = 1$. Thus, $\text{sign}(\langle \alpha_b, \beta_b \rangle_{\gamma_1^{\mathbb{C}}}) = 1$, and we obtain

$$c^* = H_{r(b),s(b)}(\langle \alpha_b, \beta_b \rangle_{\gamma_1^{\mathbb{C}}}) \overset{(7.218)}{=} h^{\mathbb{C}}_{b,b}(\langle \alpha_b, \beta_b \rangle_{\gamma_1^{\mathbb{C}}}).$$

(iii) This is an immediate application of (i) and Corollary 7.4 (since $\zeta_{u,v}(b) \in \mathbb{D}$).

(iv) Let $(z, w) \in S_H^m \times S_H^n$ and $(i, j) \in [m] \times [n]$. Because of (i), there exists $\text{vec}(\mathbf{Z}_i, \mathbf{W}_j) \sim \mathbb{C}N_{2k}(0, \Sigma_{2k}(\zeta_{ij}(b)))$ (where $\zeta_{ij}(b) \equiv \zeta_{z_i,w_j}(b)$), such that

$$\Gamma_H(z, w)_{ij} = \langle w_j, z_i \rangle_H = \overline{\langle z_i, w_j \rangle_H} \overset{(i)}{=} \frac{1}{c^*} \overline{h_{b,b}(\zeta_{ij}(b))}$$
$$= \frac{1}{c^*} \mathbb{E}[\overline{b(\mathbf{Z}_i)} b(\mathbf{W}_j)] = \frac{1}{c^*} \mathbb{E}[\overline{(\mathbf{P}_b)_i} (\mathbf{Q}_b)_j] = \frac{1}{c^*} \mathbb{E}[\overline{\mathbf{P}_b} \mathbf{Q}_b^\top]_{ij}.$$

□

Our next result shows that in fact also Theorem 6.45, respectively Corollary 6.46 can be transferred to the complex case:

Theorem 7.14. *Let $k, m, n \in \mathbb{N}$ and $b, c \in L^\infty(\mathbb{C}^k)$. Then $0 \leq r \equiv r_k(b) := \|b\|^2_{\gamma_k^{\mathbb{C}}} < \infty$ and $\|b\|_\infty \geq \sqrt{r}$. Moreover, the following statements hold:*

(i)
$$|tr(A^* h^{\mathbb{C}}_{b,c}[S])| \leq \|b\|_\infty \, \|c\|_\infty \, \|A\|^{\mathbb{C}}_{\infty,1} \text{ for all } A \in \mathbb{M}_{m,n}(\mathbb{C}) \text{ and } S \in \mathcal{Q}_{m,n}(\mathbb{C}).$$

(ii) *Assume that $b \in CS_k(\mathbb{T}) \setminus \{0\}$ and $H^{-1}_{r(b),s(b)}\big|_{(-r,r)} \in W^\omega_+((-r,r))$. Put $c^* \equiv c^*(b) := H^{hyp}_{\frac{r(b)}{\sqrt{r}},\frac{s(b)}{\sqrt{r}}}(1)$. Then $c^* \in (0,1)$, and the following properties are satisfied:*

(ii-1)
$$r\, K_G^{\mathbb{C}} \leq \frac{\|b\|^2_\infty}{c^*}\,. \tag{7.229}$$

(ii-2) *Let $1 \leq \kappa_* < K_G^{\mathbb{C}}$. If $\|b\|_\infty = \sqrt{r}$, then $0 < H^{hyp}_{\frac{r(b)}{\sqrt{r}},\frac{s(b)}{\sqrt{r}}}(\kappa_*) < 1$ and there is exactly one number number $\gamma^* \equiv \gamma^*(b) \in (H^{hyp}_{\frac{r(b)}{\sqrt{r}},\frac{s(b)}{\sqrt{r}}}(\kappa_*), 1]$, such that*

$$K_G^{\mathbb{C}} = \Big(H^{-1}_{r(b),s(b)}\big|_{(-r,r)}\Big)_{abs}(r\,\gamma^*) \leq \min\Big\{\frac{1}{c^*}, \Big(H^{-1}_{r(b),s(b)}\big|_{(-r,r)}\Big)_{abs}(r)\Big\}\,. \tag{7.230}$$

Proof. Without loss of generality, as in the proof of the real case (Theorem 6.40), we may assume throughout the proof that $\|b\|_\infty = 1$ and $\|c\|_\infty = 1$ if $\|b\|_\infty > 0$ and $\|c\|_\infty > 0$ (else, we just have to rescale the pair (b, c) to the pair $\big(\frac{1}{\|b\|_\infty}\, b, \frac{1}{\|c\|_\infty}\, c\big)$). In particular, $\|b\|^2_\infty = 1$.
(i) Because of (7.205), we may fully adopt the proof of Theorem 6.40-(i).
(ii) Recall from Corollary 7.4 that both, $H_{r(b),s(b)} : [-1,1] \longrightarrow [-r,r]$ and $h^{\mathbb{C}}_{b,b} : \overline{\mathbb{D}} \longrightarrow r\overline{\mathbb{D}}$ are circularly symmetric homeomorphisms. Put $\psi_b := H^{-1}_{r(b),s(b)} : [-r,r] \longrightarrow [-1,1]$ and $a_m := \frac{|\psi_b^{(m)}(0)|}{m!}$, $m \in \mathbb{N}$.
(ii-1) Given our assumptions, we may apply Theorem 7.13 to the function $H^{-1}_{r(b^\circ),s(b^\circ)} = \big(\frac{1}{r}\, H_{r(b),s(b)}\big)^{-1} = \psi_b(r\,\cdot)$, where $b^\circ := \frac{b}{\sqrt{r}} \in S_{L^2(\gamma_k^{\mathbb{C}})}$ is an element of the unit sphere of $L^2(\gamma_k^{\mathbb{C}})$. Put $\alpha^* := rc^*$. Thus, if $S \in \mathcal{Q}_{m,n}(\mathbb{C})$ is arbitrarily given, then

$$S \overset{(7.228)}{=} \frac{1}{c^*}\,\mathbb{E}\big[\overline{\mathbf{P}_{b^\circ}}\mathbf{Q}^\top_{b^\circ}\big] = \frac{1}{\alpha^*}\,\mathbb{E}\big[\overline{\mathbf{P}_b}\mathbf{Q}^\top_b\big],$$

where the m-dimensional complex random vector $\mathbf{P}_b$ maps into $\overline{\mathbb{D}}^m$ and the n-dimensional complex random vector $\mathbf{Q}_b$ maps into $\overline{\mathbb{D}}^n$ (since $\|b\|_\infty = 1$). Hence,

$$|\mathrm{tr}(A^*S)| = \frac{1}{\alpha^*}|\mathrm{tr}(A^*\mathbb{E}[\overline{\mathbf{P}_b}\,\mathbf{Q}^\top_b])| \leq \frac{1}{\alpha^*}\,\mathbb{E}[|\mathrm{tr}(A^*\overline{\mathbf{P}_b}\mathbf{Q}^\top_b)|] \leq \frac{1}{\alpha^*}\,\|A\|_{\infty,1},$$

and (7.229) follows.

(ii-2) Since $r = \|b\|_\infty^2 = 1$ (by assumption), it follows that $\sum_{\nu=0}^\infty a_{2\nu+1} = (\psi_b\big|_{(-1,1)})_{\text{abs}}(1) < \infty$. So, we may apply Lemma 5.10 to the odd real analytic function $\psi_b\big|_{(-1,1)}$, whence

$$\psi_b(|w|) = \sum_{\nu=0}^\infty a_{2\nu+1}|w|^{2\nu+1} = |w| \sum_{\nu=0}^\infty a_{2\nu+1}\, w^\nu\, \overline{w}^\nu \text{ for all } w \in \overline{\mathbb{D}} = h_{b,b}^{\mathbb{C}}(\mathbb{D}).$$

Thus, (7.221) implies that

$$\overline{\mathbb{D}} \ni (h_{b,b}^{\mathbb{C}})^{-1}(w) = \text{sign}(w)\psi_b(|w|) = w \sum_{\nu=0}^\infty a_{2\nu+1}\, w^\nu\, \overline{w}^\nu \text{ for all } w \in \overline{\mathbb{D}}.$$

Consequently, the matrix equality (7.205) leads to

$$S = (h_{b,b}^{\mathbb{C}})^{-1}[h_{b,b}^{\mathbb{C}}[S]] = (h_{b,b}^{\mathbb{C}})^{-1}[\mathbb{E}[\mathbf{\Lambda}_b]] = \sum_{\nu=0}^\infty a_{2\nu+1}\mathbb{E}[\mathbf{\Lambda}_b]^{*\nu} * \mathbb{E}[\overline{\mathbf{\Lambda}_b}]^{*\nu} * \mathbb{E}[\mathbf{\Lambda}_b],$$

where $*$ denotes entrywise multiplication on $M_n(\mathbb{F})$ (i.e., the Hadamard product of matrices) and $\mathbf{\Lambda}_b := \overline{\mathbf{R}_b}\,\mathbf{S}_b{}^\top$. Put $M_\nu := \mathbb{E}[\mathbf{\Lambda}_b]^{*\nu} * \mathbb{E}[\overline{\mathbf{\Lambda}_b}]^{*\nu} = \overline{M_\nu}$. Since $\|b\|_\infty = 1$, we may apply Lemma 6.39 to the random matrix $\mathbf{\Lambda}_b$, and it follows that

$$|\text{tr}(A^*S)| \leq \sum_{\nu=0}^\infty a_{2\nu+1}\,|\langle M_\nu*\mathbb{E}[\mathbf{\Lambda}_b], A\rangle_2| = \sum_{\nu=0}^\infty a_{2\nu+1}\,|\langle \mathbb{E}[\mathbf{\Lambda}_b], A*M_\nu\rangle_2| \leq \sum_{\nu=1}^\infty a_{2\nu+1}\,\|A*M_\nu\|_{\infty,1}\,,$$

whereby the last inequality follows from the construction of the random Gram matrix $\mathbf{\Lambda}_b$. Next, we may apply Lemma 6.39 twice, so that

$$\|A * M_\nu\|_{\infty,1} \leq \|A * \mathbb{E}[\mathbf{\Lambda}_b]^{*\nu}\|_{\infty,1} \leq \|A\|_{\infty,1}.$$

Altogether, it follows that

$$|\text{tr}(A^*S)| \leq \|A\|_{\infty,1} \sum_{\nu=0}^\infty a_{2\nu+1} = (\psi_b|_{(-1,1)})_{\text{abs}}(1)\,\|A\|_{\infty,1}\,.$$

Consequently, $K_G^{\mathbb{C}} \leq (\psi_b|_{(-1,1)})^{\text{abs}}(1) = \Big(H_{r(b),s(b)}^{-1}\big|_{(-r,r)}\Big)_{\text{abs}}(r)$. Hence, if we put $\gamma^* := H^{\text{hyp}}_{\frac{r(b)}{\sqrt{r}},\frac{s(b)}{\sqrt{r}}}(K_G^{\mathbb{C}})$, then $0 < H^{\text{hyp}}_{\frac{r(b)}{\sqrt{r}},\frac{s(b)}{\sqrt{r}}}(1) \leq H^{\text{hyp}}_{\frac{r(b)}{\sqrt{r}},\frac{s(b)}{\sqrt{r}}}(\kappa_*) < \gamma^* \leq 1$, and (ii-1) concludes the proof of (7.230). □

Recall again from Theorem 5.20 that in general complex CCP functions need not be analytic. Due to this fact and the structure of the complex-valued (circularly symmetric) functions $h_{b,b}$, which is built on absolute values and signs of complex numbers (cf. Corollary 7.4, including (7.218)), it seems that Proposition 6.47 cannot be easily transferred to the complex case (if at all).

Example 7.15 (**Haagerup function**)**.** Both, Corollary 7.4 and Proposition 6.16 enable us to recover quickly a direct power series representation of Haagerup's CCP function $h_{b,b} : \mathbb{D} \longrightarrow \mathbb{D}$, where $b :=$ sign. (Retranslated into the language of Haagerup, $h_{b,b} = \Phi$ and $H_{r(b),s(b)} = \varphi$ (cf. [57, Lemma 3.5 and Theorem 3.1])). To this end, let $0 \neq \zeta \in \overline{\mathbb{D}}$ and $\rho := |\zeta|$. As shown on [57, p. 200], the function $h_{b,b}$ can then be written in terms of sign(ζ)

and the two complete elliptic integrals $E(\rho)$ and $K(\rho)$. However, in our approach (by which Haagerup's CCP function is obtained as a special case), we don't have to work with elliptic integration. Firstly note that

$$r(b)(x_1, x_2) = r(b)(x) = \frac{x_1}{\|x\|_2} \text{ and } s(b)(x) = r(b)(x_2, x_1) = \frac{x_2}{\|x\|_2}$$

for all $x = \text{vec}(x_1, x_2) \in \mathbb{R}^2 \setminus \{0\}$. Thus, if $\tau \in [-1, 1]$ and $\text{vec}(\mathbf{X}, \mathbf{Y}) \sim N_{2k}(0, \Sigma_{2k}(\tau))$, $k := 2$ are given, then

$$\begin{aligned}
H_{r(b),s(b)}(\tau) &= h_{r(b),r(b)}(\tau) + h_{s(b),s(b)}(\tau) \\
&= \mathbb{E}[r(b)(\mathbf{X})r(b)(\mathbf{Y})] + \mathbb{E}[s(b)(\mathbf{X})s(b)(\mathbf{Y})] \\
&= \mathbb{E}[r(b)(X_1, X_2)r(b)(Y_1, Y_2)] + \mathbb{E}[r(b)(X_2, X_1)r(b)(Y_2, Y_1)] \\
&= \mathbb{E}\Big[\frac{X_1 Y_1}{\|\mathbf{X}\|_2 \, \|\mathbf{Y}\|_2}\Big] + \mathbb{E}\Big[\frac{X_2 Y_2}{\|\mathbf{X}\|_2 \, \|\mathbf{Y}\|_2}\Big] \\
&= \mathbb{E}\Big[\Big\langle \frac{\mathbf{X}}{\|\mathbf{Y}\|_2}, \frac{\mathbf{Y}}{\|\mathbf{X}\|_2} \Big\rangle\Big] \\
&= \frac{\pi}{4} \tau \, {}_2F_1\Big(\frac{1}{2}, \frac{1}{2}, 2; \tau^2\Big) = h_{f_2,f_2}(\tau),
\end{aligned}$$

whereby the equalities in the last line follow from Proposition 6.16 (applied to $k = 2$). An application of Corollary 7.4 (or the original proof of [57, Theorem 3.1]) therefore implies

$$\text{sign}(\overline{\zeta}) h_{b,b}(\zeta) = H_{r(b),s(b)}(\rho) = \frac{\pi}{4} \rho \, {}_2F_1\Big(\frac{1}{2}, \frac{1}{2}, 2; \rho^2\Big) = h_{f_2,f_2}(\rho).$$

Hence,

$$h_{b,b}(\zeta) = \text{sign}(\zeta) \, \mathbb{E}\Big[\Big\langle \frac{\mathbf{X}}{\|\mathbf{X}\|_2}, \frac{\mathbf{Y}}{\|\mathbf{X}\|_2} \Big\rangle\Big] = \frac{\pi}{4} \zeta \, {}_2F_1\Big(\frac{1}{2}, \frac{1}{2}, 2; |\zeta|^2\Big) = \text{sign}(\zeta) \, h_{f_2,f_2}(|\zeta|) \, .$$

A highly non-trivial part in [57] consists of a multi-page proof of the fact that $h_{f_2,f_2}^{-1} = H_{r(b),s(b)}^{-1} \in W_+^\omega((-1, 1))$, implying that $\big(h_{f_2,f_2}^{-1}\big)_{\text{abs}}$ is well-defined (cf. [57, Lemma 2.6]). The Maclaurin series of $\big(h_{f_2,f_2}^{-1}\big)_{\text{abs}}$ can e.g. be approximated by the Taylor polynomial of degree 7 as:

$$\big(h_{f_2,f_2}^{-1}\big)_{\text{abs}}(s) = \frac{4}{\pi} s + \frac{8}{\pi^3} s^3 + 0 \cdot s^5 + \frac{16}{\pi^7} s^7 + o(|s|^7). \tag{7.231}$$

Hence (cf. Proposition 6.16 and (7.230)),

$$\frac{K_G^{\mathbb{R}}}{\sqrt{2}} \overset{(1.1)}{\leq} K_G^{\mathbb{C}} \overset{(7.230)}{\leq} \min\Big\{\frac{1}{h_{f_2,f_2}^{\text{hyp}}(1)}, \big(h_{f_2,f_2}^{-1}\big)_{\text{abs}}(1)\Big\} \tag{7.232}$$

$$\leq \big(h_{f_2,f_2}^{-1}\big)_{\text{abs}}(1) = \frac{4}{\pi} + \frac{8}{\pi^3} + \frac{16}{\pi^7} + o(1) \approx 1{,}53655 + o(1). \tag{7.233}$$

These facts follow from [57], respectively (6.159) and (9.241), where the latter is applied to

$$\alpha_\nu := \begin{cases} 0 & \text{if } \nu \text{ is even} \\ \frac{\pi}{2} \frac{((\nu-2)!!)^2}{((\nu-1)!!)^2 \, (\nu+1)} & \text{if } \nu \text{ is odd} \end{cases} \text{ and } \alpha_\nu^\times := \frac{\alpha_\nu}{\alpha_1} = \frac{\alpha_\nu}{c_2^2} = \frac{4}{\pi} \alpha_\nu \, .$$

Already a numerical calculation of the single root $0 < c^* < \frac{\pi}{4}$ of the polynomial $s \mapsto \frac{4}{\pi} s + \frac{8}{\pi^3} s^3 + \frac{16}{\pi^7} s^7 - 1$ leads to the number $\frac{1}{c^*} \approx 1.40449$. The latter outcome should now be compared with the result of Haagerup in [57] .

8. A summary scheme of the main result

To highlight and summarise our approach, it completely suffices to list in detail the single steps and assumptions in the form of a "flowchart", possibly leading to a computer-aided approach regarding the implementation of an approximation to the lowest upper bound of the Grothendieck constant $K_G^{\mathbb{F}}$ as a next step. *Very likely, high-performance computers are required to perform these approximations. That (technical) implementation would go however far beyond the scope of our groundwork; especially since we have no access to equipment of this type.*

Fix $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$ and $k \in \mathbb{N}$.

(SIGN) Choose a function $0 \neq b : \mathbb{F}^k \longrightarrow \mathbb{F}$, which satisfies the following conditions:

(a) b is circularly symmetric (*cf.* *Definition 7.3*);

(b) $b \in L^\infty(\mathbb{F}^k)$.

(CCP) Consider the function $b_{\mathbb{F}}^\circ : \mathbb{C}^k \longrightarrow \mathbb{C}$, defined as

$$b^\circ \equiv b_{\mathbb{F}}^\circ := \begin{cases} \left(\frac{b}{\|b\|_{\gamma_k}}\right)^{\mathbb{C}} & \text{if } \mathbb{F} = \mathbb{R} \\ \frac{b}{\|b\|_{\gamma_k^{\mathbb{C}}}} & \text{if } \mathbb{F} = \mathbb{C}\,. \end{cases}$$

Then $\|b^\circ\|_{\gamma_k^{\mathbb{C}}} = 1$ and $1 \leq \|b^\circ\|_\infty = \frac{\|b\|_\infty^{\mathbb{F}}}{\|b\|_{\gamma_k^{\mathbb{F}}}}$ (*cf.* (2.29)). Construct its allocated homeomorphic real CCP function $H_{r(b^\circ),s(b^\circ)} = h_{r(b^\circ),r(b^\circ)} + h_{s(b^\circ),s(b^\circ)}$ (*cf.* *Corollary 7.4*-(iii) *and* *Remark 7.6*).

(CRA) Assume that $\psi_b := H^{-1}_{r(b^\circ),s(b^\circ)}\big|_{(-1,1)} \in W_+^\omega((-1,1))$ (*cf.* *Definition 5.11*).

An application of Lemma 6.11, Corollary 6.46 and Theorem 7.14 consequently leads to the following result which holds for both, $\mathbb{R}$ and $\mathbb{C}$ simultaneously:

Assume that (SIGN), (CCP) and (CRA) are satisfied. Then $\Big(H^{-1}_{r(b^\circ),s(b^\circ)}\Big|_{(-1,1)}\Big)_{\text{abs}}(1) > 1$. Put $c^*_{\mathbb{F}} := H^{\text{hyp}}_{r(b^\circ),s(b^\circ)}(1)$. Then $0 < c^*_{\mathbb{F}} < 1$, and the following two statements hold:

(i)

$$K^{\mathbb{F}}_G \leq \frac{1}{c^*_{\mathbb{F}}} \, \|b^\circ\|^2_\infty \, .$$

(ii) Let $1 \leq \kappa_* < K^{\mathbb{F}}_G$. If $\|b\|^{\mathbb{F}}_\infty = \|b\|_{\gamma^{\mathbb{F}}_k}$, then $0 < H^{\text{hyp}}_{r(b^\circ),s(b^\circ)}(\kappa_*) < 1$ and there is exactly one number $\gamma^*_{\mathbb{F}} \equiv \gamma^*_{\mathbb{F}}(b) \in (H^{\text{hyp}}_{r(b^\circ),s(b^\circ)}(\kappa_*), 1]$, such that

$$K^{\mathbb{F}}_G = \Big(H^{-1}_{r(b^\circ),s(b^\circ)}\Big|_{(-1,1)}\Big)_{\text{abs}}(\gamma^*_{\mathbb{F}}) \leq \min\left\{\frac{1}{c^*_{\mathbb{F}}}, \, \Big(H^{-1}_{r(b^\circ),s(b^\circ)}\Big|_{(-1,1)}\Big)_{\text{abs}}(1)\right\}.$$

Again, we recognise that Maclaurin series representation (or at least its approximation by the Taylor polynomial of a given degree) and Maclaurin series inversion of CCP functions play the key role regarding the search for the lowest upper bound of the Grothendieck constant $K^{\mathbb{F}}_G$. Unfortunately, a closed form representation of the coefficients of the inverse of a Taylor series runs against a well-known combinatorial complexity issue (due to the presence of ordinary partial Bell polynomials as building blocks of these coefficients - cf. Subsection 9.1 below for details), which in general does not allow a closed form representation of these coefficients. The inverse of the real function factor of the Haagerup function is one such example. It is given by

$$[-1,1] \ni \tau \mapsto H_{r(\text{sign}),s(\text{sign})}(\tau) = h_{f_2,f_2}(\tau) = \frac{\pi}{4}\,\tau\,{}_2F_1\Big(\frac{1}{2},\frac{1}{2},2;\tau^2\Big)$$

in the complex case (cf. [57], Remark on page 216 and Example 7.15), as opposed to the Grothendieck function

$$[-1,1] \ni \rho \mapsto H_{r(\text{sign}^{\mathbb{C}}),s(\text{sign}^{\mathbb{C}})}(\rho) = h_{\text{sign},\text{sign}}(\rho) = \frac{2}{\pi}\arcsin(\rho)$$

in the real case.

9. Concluding remarks and open problems

Not very surprisingly, the long-standing, intensive and technically quite demanding attempts to compute the - still not available - value of the real and complex Grothendieck constants (an open problem since 1953) leads to further projects and open problems, such as the following ones; addressed in particular to researchers who also wish to get a better understanding of the reasons underlying these topics.

9.1. Open problem 1: Grothendieck constant versus Taylor series inversion

Only between 2011 and 2013 it was shown that $K_G^{\mathbb{R}}$ is strictly smaller than Krivine's upper bound, stating that $K_G^{\mathbb{R}} < \frac{\pi}{2\ln(1+\sqrt{2})}$ (cf. [22] and Example 6.51). Consequently, in the real case sign is not the "optimal" function to choose (answering a question of H. König to the negative - cf. [86]). So, if we wish to reduce the value of the upper bound of the real Grothendieck constant we have to look for functions $b : \mathbb{R}^k \longrightarrow \mathbb{R}$ which are different from $\text{sign} : \mathbb{R} \longrightarrow \{-1, 1\}$. However, these functions are required to satisfy any of the conditions in the workflow, listed in Section 8. In particular, we have to look for both, the Fourier-Hermite coefficients of the Taylor series (respectively the approximating Taylor polynomial) of $H_{r(b),s(b)} = h_{r(b),r(b)} + h_{s(b),s(b)}$ and the coefficients of the Taylor series of both, the *inverse* function $H_{r(b),s(b)}^{-1}$ and $\big(H_{r(b),s(b)}^{-1}\big)_{\text{abs}}$. It is well-known that the latter task increases rapidly in computational complexity if we want to calculate such Taylor coefficients of a higher degree, leading to the involvement of highly non-trivial combinatorial facts, reflected in the use of partitions of positive integers and partial exponential Bell polynomials as part of the Taylor coefficients of the inverse Taylor series (a thorough introduction to this framework including the related Lagrange-Bürmann inversion formula is given in [28, 84]).

To reveal the origin of these difficulties let us focus on the one-dimensional real case. Let $b \in L^2(\mathbb{R}, \gamma_1)$ be given. Assume that $\alpha_0 := h_{b,b}(0) = 0$ (which is the case if b were odd). First recall from (6.134) that

$$h_{b,b}(\rho) = \sum_{n=1}^{\infty} \langle b, H_n \rangle_{\gamma_1}^2 \, \rho^n$$

for all $\rho \in [-1, 1]$, where for $n \in \mathbb{N}$ and $x \in \mathbb{R}$

$$H_n(x) := \frac{1}{\sqrt{n!}} (-1)^n \exp\Big(\frac{x^2}{2}\Big) \frac{\mathrm{d}^n}{\mathrm{d}x^n} \exp\Big(-\frac{x^2}{2}\Big)$$

denotes the (probabilistic version of the) n-th Hermite polynomial. Put $\alpha_n := \langle b, H_n \rangle_{\gamma_1}^2$. If $h_{b,b}'(0) = \alpha_1 > 0$, we know that the real analytic function $h_{b,b}\big|_{(-1,1)}$ is invertible around $0 = h_{b,b}(0)$. Its inverse is also expressible as a power series there; i.e., around 0, $\Big(h_{b,b}\big|_{(-1,1)}\Big)^{-1}$ is real analytic, too. Hence, given the assumption (CRA), listed in Section 8, it follows that $g_b(y) := h_{b,b}^{-1}(y) = \sum_{n=1}^{\infty} \beta_n \, y^n$ for all $y \in [-1, 1]$, where $\beta_1 = \frac{1}{\alpha_1}$ and

$$\begin{aligned} \beta_n &= \frac{1}{n} \sum_{k=1}^{n-1} \frac{1}{\alpha_1^{n+k}} (-1)^k \binom{n-1+k}{k} B_{n-1,k}^{\circ}(\alpha_2, \alpha_3, \ldots, \alpha_{n-k+1}) \\ &= \frac{1}{n\alpha_1^n} \sum_{k=1}^{n-1} (-1)^k \binom{n-1+k}{k} B_{n-1,k}^{\circ}\Big(\frac{\alpha_2}{\alpha_1}, \frac{\alpha_3}{\alpha_1}, \ldots, \frac{\alpha_{n-k+1}}{\alpha_1}\Big) \end{aligned} \tag{9.234}$$

for all $n \in \mathbb{N}_2$. In this context,

$$B_{n,k}^{\circ}(x_1, x_2, \ldots, x_{n-k+1}) := \sum_{\nu \in P(n,k)} \binom{k}{\nu_1, \nu_2, \ldots, \nu_{n-k+1}} \prod_{i=1}^{n-k+1} x_i^{\nu_i} = \sum_{\nu \in P(n,k)} k! \frac{x^{\nu}}{\nu!}$$

denotes the ordinary partial Bell polynomial, where the multinomial coefficient $\binom{\sum_{i=1}^{n-k+1}\nu_i}{\nu_1,\nu_2,\ldots,\nu_{n-k+1}} := \frac{\left(\sum_{i=1}^{n-k+1}\nu_i\right)!}{\prod_{i=1}^{n+1-k}\nu_i!}$ represents the number of ways of depositing $\sum_{i=1}^{n-k+1}\nu_i$ distinct objects into $n-k+1$ distinct bins, with ν_i objects in the i'th bin and $P(n,k)$ indicates the set of all multi-indices $\nu \equiv (\nu_1,\nu_2,\ldots,\nu_{n+1-k}) \in \mathbb{N}_0^{n-k+1}$ $(k \leq n)$ which satisfy the Diophantine equations

$$\sum_{i=1}^{n+1-k}\nu_i = k \text{ and } \sum_{i=1}^{n+1-k} i\,\nu_i = n\,;$$

i.e., summation is extended over all partitions of the number n into k positive (non-zero) integers (cf. e.g. [28, 30, 102, 139]). Observe that (dependent on the choice on n and k, of course) these Diophantine equations may have an extremely large, if not even an unmanageable set of solutions! Already that definition implies the well-known and important fact that

$$B^\circ_{n,k}(abx_1, ab^2x_2, \ldots, ab^{n-k+1}x_{n-k+1}) = a^k\,b^n B^\circ_{n,k}(x_1,x_2,\ldots,x_{n-k+1}), \tag{9.235}$$

for all $a,b,x_1,\ldots,x_{n-k+1} \in \mathbb{C}$. If the element $(x_1,\ldots,x_{n-k+1}) \in \mathbb{N}_0^{n-k+1}$ consists of at most 2 non-zero elements, x_{i_1} and x_{i_2}, say $(i_1 < i_2)$, we only have to sum over the set of all $\nu \in P(n,k)$, such that $\nu_i = 0$ for all $i \notin \{i_1,i_2\}$ (since $0^0 = 1$). In this case, the Diophantine equations reduce to a simple 2-dimensional linear equation system. The latter has a solution $(\nu_{i_1},\nu_{i_2}) \in \mathbb{N}_0^2$ if and only if

$$i_1 \leq \frac{n}{k} \leq i_2 \text{ and } i_2 - i_1 \text{ divides both, } ki_2 - n \in \mathbb{N}_0 \text{ and } n - ki_1 \in \mathbb{N}_0\,. \tag{9.236}$$

The solution $(\nu_{i_1},\nu_{i_2}) \in \mathbb{N}_0^2$ is then unique and given as

$$\nu_{i_1} = \frac{ki_2 - n}{i_2 - i_1} \text{ and } \nu_{i_2} = \frac{n - ki_1}{i_2 - i_1}\,.$$

Hence, if (9.236) is satisfied, we immediately recognise that

$$B^\circ_{n,k}(0,0,\ldots,0,x_{i_1},0,0,\ldots,0,x_{i_2},0,0,\ldots,0) = \binom{k}{\nu_{i_1}} x_{i_1}^{\nu_{i_1}} x_{i_2}^{\nu_{i_2}}\,.$$

In particular, if $k \leq n \leq 2k$, we reobtain the well-known special case

$$B^\circ_{n,k}(x,y,0,\ldots 0) = \binom{k}{2k-n} x^{2k-n} y^{n-k} \text{ for all } x,y \in \mathbb{C}\,.$$

In the literature, one frequently finds the so-called *exponential partial Bell polynomials* $B_{n,k}$, characterised as (cf. e.g. [28, Remark on page 136])

$$B_{n,k}(x_1,\ldots,x_{n-k+1}) := \frac{n!}{k!} B^\circ_{n,k}\Big(\frac{x_1}{1!}, \frac{x_2}{2!}, \ldots, \frac{x_{n-k+1}}{(n-k+1)!}\Big), \tag{9.237}$$

implying that any result about $B_{n,k}$ can be directly converted into a result about $B^{\circ}_{n,k}$ and conversely. For example, if $n > k$, then [28, formula (3l)] transforms very pleasantly and reiteratively into

$$\begin{aligned} B^{\circ}_{n,k}(x_1, x_2, \dots x_{n-k+1}) &= \sum_{l=k-\alpha(n,k)}^{k-1} \binom{k}{l} x_1^l \, B^{\circ}_{n-k,k-l}(x_2, \dots, x_{n-2k+l+1}) \\ &= x_1^{k-\alpha(n,k)} \sum_{l=0}^{\alpha(n,k)-1} \binom{k}{\alpha(n,k)-l} x_1^l \, B^{\circ}_{n-k,\alpha(n,k)-l}(x_2, \dots, x_{(n-2k)^+ + l+2}) \end{aligned}$$

for all $x_1, x_2, \dots, x_{n-k+1} \in \mathbb{C}$, where $\alpha(n,k) := \min\{n-k, k\}$. Another application of (9.237) implies the well-known fact that (9.234) is equivalent to

$$\left(h^{-1}_{b,b}\right)^{(n)}(0) = \sum_{k=1}^{n-1} \frac{1}{\delta_1^{n+k}} (-1)^k \frac{(n-1+k)!}{(n-1)!} B_{n-1,k}(\delta_2, \delta_3, \dots, \delta_{n-k+1}), \tag{9.238}$$

where $\delta_l := \frac{h^{(l)}_{b,b}(0)}{l}, l \in [n-k+1]$ (cf. [28, Theorem E on p. 150]).

Regarding an explicit recursive construction of these polynomials in full generality, yet without having to know the sets $P(n,k)$ beforehand, we recall the important fact that any ordinary partial Bell polynomial $B^{\circ}_{n,k}$ actually arises as a (kind of) discrete convolution of two ordinary partial Bell polynomial series. More precisely, we have:

Lemma 9.1. *Let $m \in \mathbb{N}_0$, $k \in \mathbb{N}$, $n \in \mathbb{N}_k$ and $x_1, \dots, x_{n-k+1} \in \mathbb{C}$. Then the following equalities are satisfied:*

(i) $B^{\circ}_{m,0}(x_1, \dots, x_{m+1}) = \delta_{m0}$ *and*

$$B^{\circ}_{n,k}(x_1, \dots, x_{n-k+1}) = \sum_{i=k-1}^{n-1} x_{n-i} \, B^{\circ}_{i,k-1}(x_1, \dots, x_{i-k+2}) = \sum_{i=1}^{n-k+1} x_i \, B^{\circ}_{n-i,k-1}(x_1, \dots, x_{n-k+2-i}).$$

(ii)

$$\begin{aligned} nB^{\circ}_{n,k}(x_1, \dots, x_{n-k+1}) &= k \sum_{i=k-1}^{n-1} (n-i) x_{n-i} \, B^{\circ}_{i,k-1}(x_1, x_2, \dots, x_{i-k+2}) \\ &= k \sum_{i=1}^{n-k+1} i x_i \, B^{\circ}_{n-i,k-1}(x_1, x_2, \dots, x_{n-k+2-i}). \end{aligned}$$

Proof. (i) Follows from [28, page 136, formula (3k)], respectively [112, page 366, formula (13)].
(ii) See [30, formula (2.3) and its equivalent (unnumbered) representation on page 1546 (line 3)]. □

Lemma 9.1 obviously implies the following multiple-sum representation of the ordinary partial Bell polynomials:

$$B^{\circ}_{n,k+1}(x_1, x_2, \dots, x_{n-k}) = \sum_{i_1=k}^{n-1} \sum_{i_2=k-1}^{i_1-1} \dots \sum_{i_k=1}^{i_{k-1}-1} x_{n-i_1} \prod_{\nu=2}^{k} x_{i_{\nu-1}-i_\nu} \, x_{i_k} \tag{9.239}$$

for all $k \in \mathbb{N}$, $n \in \mathbb{N}_{k+1}$ and $x_1, x_2, \ldots, x_{n-k} \in \mathbb{C}$. For the convenience of the readers, we list a few examples of ordinary partial Bell polynomials that can be displayed in closed form. For review, we refer to the widely comprehensive table of these polynomials on page 309 of [28] (enumerating all polynomials $B^{\circ}_{n,m}$ for which $10 \geq n \geq m \geq 1$). To this end, fix $k \in \mathbb{N}$ and $x_1, \ldots, x_{k+1} \in \mathbb{C}$. Then

(i) $B_{0,0}(x_1) = 1$ and $B^{\circ}_{k,0}(x_1, \ldots, x_{k+1}) = 0$.

(ii) $B^{\circ}_{k,1}(x_1, \ldots, x_k) = x_k$ and $B_{k,k}(x_1) = x_1^k$.

(iii) $B^{\circ}_{k+1,k}(x_1, x_2) = k\, x_1^{k-1}\, x_2$.

(iv) $B^{\circ}_{k+2,k}(x_1, x_2, x_3) = \binom{k}{2}\, x_1^{k-2}\, x_2^2 + k\, x_1^{k-1}\, x_3$ if $k \geq 2$.

(v) $B^{\circ}_{k+3,k}(x_1, x_2, x_3, x_4) = \binom{k}{3}\, x_1^{k-3}\, x_2^3 + k(k-1)\, x_1^{k-2}\, x_2\, x_3 + k\, x_1^{k-1}\, x_4$ if $k \geq 3$.

(vi) $B^{\circ}_{k+4,k}(x_1, \ldots, x_5) = \binom{k}{4}\, x_1^{k-4}\, x_2^4 + \binom{k}{3}\, x_1^{k-3}(3\, x_2^2\, x_3) + \binom{k}{2}\, x_1^{k-2}(x_3^2 + 2\, x_2\, x_4) + k\, x_1^{k-1}\, x_5$ if $k \geq 4$.

Moreover, we have

$$B^{\circ}_{k,2}(x_1, \ldots, x_{k-1}) = \sum_{i=1}^{k-1} x_i\, x_{k-i} \text{ if } k \geq 2\,.$$

Since the Taylor series of the inverse of the "standardised" Taylor series $\sum_{n=1}^{\infty} \alpha_n^{\times}\, \rho^n = \frac{1}{\alpha_1}\, h_{b,b}(\rho)$ of the function $h_{b,b}$ obviously is given by $\left(\frac{1}{\alpha_1}\, h_{b,b}\right)^{-1}(y) = h_{b,b}^{-1}(\alpha_1\, y) = \sum_{n=1}^{\infty}(\beta_n\, \alpha_1^n) y^n$ for all $y \in [-1, 1]$, where $\alpha_n^{\times} := \frac{\alpha_n}{\alpha_1}$ $(n \in \mathbb{N})$, it follows that the n-th Taylor series coefficient $\beta_n^{\times}$ of the Taylor series of $\left(\frac{1}{\alpha_1}\, h_{b,b}\right)^{-1}$ is given by $\beta_n^{\times} = \beta_n\, \alpha_1^n$. Consequently,

$$\beta_n\, \alpha_1^n = \beta_n^{\times} = \frac{1}{n} \sum_{k=1}^{n-1} (-1)^k \binom{n-1+k}{k}\, B^{\circ}_{n-1,k}(\alpha_2^{\times}, \alpha_3^{\times}, \ldots, \alpha_{n-k+1}^{\times}) \tag{9.240}$$

(due to (9.234)). In the odd case, i.e., if in addition $\alpha_{2n} = 0$ for all $n \in \mathbb{N}$, the intrinsic combinatorical complexity of (9.234) can be even further reduced, possibly allowing a non-negligible saving of computing time (see Corollary 9.6).

We explicitly list $\beta_1, \beta_2, \beta_3, \beta_4, \beta_5, \beta_6$ and β_7 in full generality. To this end, as discussed above, if $\alpha_1 \neq 0$, we have to consider the Taylor coefficents $\alpha_n^{\times} := \frac{\alpha_n}{\alpha_1}, n \in \mathbb{N}$ of the "standardised" Taylor series $\frac{1}{\alpha_1} h_{b,b}$. Note again that $\alpha_1^\times = 1$. (9.234) therefore implies that

$$
\begin{aligned}
&\beta_1\,\alpha_1 = 1 = \alpha_1^\times\\
&\beta_2\,\alpha_1^2 = -\alpha_2^\times\\
&\beta_3\,\alpha_1^3 = -\alpha_3^\times + 2(\alpha_2^\times)^2\\
&\beta_4\,\alpha_1^4 = -\alpha_4^\times + 5\alpha_2^\times\alpha_3^\times - 5(\alpha_2^\times)^3\\
&\beta_5\,\alpha_1^5 = -\alpha_5^\times + 6\alpha_2^\times\alpha_4^\times + 3(\alpha_3^\times)^2 - 21(\alpha_2^\times)^2\alpha_3^\times + 14(\alpha_2^\times)^4\\
&\beta_6\,\alpha_1^6 = -\alpha_6^\times + 7\alpha_2^\times\alpha_5^\times + 7\alpha_3^\times\alpha_4^\times - 28\alpha_2^\times(\alpha_3^\times)^2 - 28(\alpha_2^\times)^2\alpha_4^\times + 84(\alpha_2^\times)^3\alpha_3^\times - 42(\alpha_2^\times)^5\\
&\beta_7\,\alpha_1^7 = -\alpha_7^\times + 8\alpha_2^\times\alpha_6^\times + 8\alpha_3^\times\alpha_5^\times + 4(\alpha_4^\times)^2 - 36(\alpha_2^\times)^2\alpha_5^\times - 72\alpha_2^\times\alpha_3^\times\alpha_4^\times - 12(\alpha_3^\times)^3 + 120(\alpha_2^\times)^3\alpha_4^\times\\
&\qquad\qquad + 180(\alpha_2^\times)^2(\alpha_3^\times)^2 - 330(\alpha_2^\times)^4\alpha_3^\times + 132(\alpha_2^\times)^6\,.
\end{aligned}
\tag{9.241}
$$

In fact, if we make use of the key result, listed in [148], paired with the general Theorem [26, p. 222], we are able to present a (purely linear algebraic and algorithmic) representation of each coefficient β_n, which avoids an explicit use of ordinary partial Bell polynomials (where no closed form seems to be available). To the best of our knowledge, in this context, that representation had not been published before. Instead of ordinary partial Bell polynomials, we have to calculate determinants of leading principal submatrices. Of course, the computational combinatoric complexity induced by the increasing size of partial Bell polynomials transforms into the rapidly increasing computing time, induced by the increasing size of the determinants including the need to sum proper parts of determinants of different size. However, that summation is a recurrence relation (see (9.244) and the instructive Example 9.3).

Firstly, if $\alpha_1 \neq 0$, an enhancement of [148] reveals the following explicit representation of each coefficient β_n $(n \in \mathbb{N}_2)$:

$$
\begin{aligned}
\beta_n &= \frac{(-1)^{n-1}}{n!\,\alpha_1^n}\,\det(A_n * T_n(1, \alpha_2^\times, \alpha_3^\times, \dots, \alpha_n^\times))\\
&= \frac{(-1)^{n-1}}{n!\,\alpha_1^{2n-1}}\,\det(A_n * T_n(\alpha_1, \alpha_2, \dots, \alpha_n))\\
&= \frac{1}{n!\,\alpha_1^{2n-1}}\,\det(-(A_n * T_n(\alpha_1, \alpha_2, \dots, \alpha_n))),
\end{aligned}
\tag{9.242}
$$

where $*$ again denotes the Hadamard product and the matrices $A_n \in \mathbb{M}_{n-1}(\mathbb{R})$ and $T_n \equiv T_n(x_1, x_2, \dots, x_n) \in \mathbb{M}_{n-1}(\mathbb{R})$ $(x_1, \dots, x_n \in \mathbb{C})$ are respectively defined as

$$
A_n := \begin{pmatrix}
n & 1 & 0 & 0 & 0 & \cdots & 0 & 0\\
2n & n+1 & 2 & 0 & 0 & \cdots & 0 & 0\\
3n & 2n+1 & n+2 & 3 & 0 & \cdots & 0 & 0\\
4n & 3n+1 & 2n+2 & n+3 & 4 & \cdots & 0 & 0\\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots\\
(n-3)n & (n-4)n+1 & (n-5)n+2 & \cdots & \cdots & \cdots & n-3 & 0\\
(n-2)n & (n-3)n+1 & (n-4)n+2 & \cdots & \cdots & \cdots & n+(n-3) & n-2\\
(n-1)n & (n-2)n+1 & (n-3)n+2 & \cdots & \cdots & \cdots & 2n+(n-3) & n+(n-2)
\end{pmatrix}
$$

and

$$T_n \equiv T_n(x_1, x_2, \dots, x_n) := \begin{pmatrix} x_2 & x_1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ x_3 & x_2 & x_1 & 0 & 0 & \cdots & 0 & 0 \\ x_4 & x_3 & x_2 & x_1 & 0 & \cdots & 0 & 0 \\ x_5 & x_4 & x_3 & x_2 & x_1 & \cdots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ x_{n-2} & x_{n-3} & \cdots & \cdots & x_3 & x_2 & x_1 & 0 \\ x_{n-1} & x_{n-2} & \cdots & \cdots & \cdots & x_3 & x_2 & x_1 \\ x_n & x_{n-1} & x_{n-2} & \cdots & \cdots & x_4 & x_3 & x_2 \end{pmatrix}.$$

Obviously, the Toeplitz matrix $T_n(x_1, x_2, \dots, x_n)$ is well-defined for any $x_1, \dots, x_n \in \mathbb{C}$. Observe that the appearance of the rather uncommon factor $\frac{1}{\alpha_1^{2n-1}} = \frac{1}{\alpha_1^n} \cdot \frac{1}{\alpha_1^{n-1}}$ in (9.242) actually originates from the simple, yet important, transformation

$$T_n \equiv T_n(\alpha_1, \alpha_2, \dots, \alpha_n) = \alpha_1 \, T_n(1, \alpha_2^{\times}, \alpha_3^{\times}, \dots, \alpha_n^{\times}). \tag{9.243}$$

More precisely, if $n \in \mathbb{N}$ and $(i,j) \in [n-1] \times [n-1]$, we have:

$$(A_n)_{ij} := \begin{cases} 0 & \text{if } j \geq i+2 \\ i & \text{if } j = i+1 \\ (i-j+1)n + j - 1 & \text{if } j \leq i \end{cases} \text{ and } (T_n)_{ij} := \begin{cases} 0 & \text{if } j \geq i+2 \\ \alpha_1 & \text{if } j = i+1 \\ x_{i-j+2} & \text{if } j \leq i \end{cases}.$$

Comparing (9.234) and (9.242), it follows that for all $\alpha_1 \in \mathbb{C}^*$ and $\alpha_2, \dots, \alpha_n \in \mathbb{C}$

$$\det((A_n * T_n(\alpha_1, \dots, \alpha_n))) = \alpha_1^{n-1} \sum_{k=1}^{n-1} (-1)^{n-1+k} \frac{(n-1+k)!}{k!} B^{\circ}_{n-1,k}(\alpha_2^{\times}, \alpha_3^{\times}, \dots, \alpha_{n-k+1}^{\times}).$$

Hence,

$$\det((A_n * T_n(1, \alpha_2^{\times}, \alpha_3^{\times}, \dots, \alpha_n^{\times}))) = \sum_{k=1}^{n-1} (-1)^{n-1+k} \frac{(n-1+k)!}{k!} B^{\circ}_{n-1,k}(\alpha_2^{\times}, \alpha_3^{\times}, \dots, \alpha_{n-k+1}^{\times}).$$

Remark 9.2 (Connection to Apostol's approach in [7]). In fact, it can be shown that

$$\det\Big(- \Big(A_n * T_n\Big(x_1, \frac{x_2}{2!}, \frac{x_3}{3!}, \dots, \frac{x_n}{n!}\Big)\Big)\Big) = P_n(x_1, \dots, x_n) \text{ for all } x_1, \dots, x_n \in \mathbb{C}$$

precisely coincides with the function P_n, introduced in [7] (due to the convolution representation and the partial derivative structure of ordinary partial Bell polynomials)! In particular,

$$\begin{aligned} P_n(1, x_2, \dots, x_n) &= \sum_{k=1}^{n-1} (-1)^k \frac{(n-1+k)!}{k!} B^{\circ}_{n-1,k}\Big(\frac{x_2}{2!}, \frac{x_3}{3!}, \dots, \frac{x_{n-k+1}}{(n-k+1)!}\Big) \\ &= \det\Big(- \Big(A_n * T_n\Big(1, \frac{x_2}{2!}, \frac{x_3}{3!}, \dots, \frac{x_n}{n!}\Big)\Big)\Big). \end{aligned}$$

Due to (9.243), it follows that

$$A_n * T_n(\alpha_1, \dots, \alpha_n) = \alpha_1 (A_n * T_n(1, \alpha_2^{\times}, \dots, \alpha_n^{\times})) = \alpha_1 B_n[n-1](\alpha_2^{\times}, \dots, \alpha_n^{\times}),$$

where for any $p \in [n-1]$ and $x_1, \ldots, x_p \in \mathbb{C}$, the matrix $B_n[p] \equiv B_n[p](x_1, \ldots, x_p) \in \mathbb{M}_p(\mathbb{C})$ is defined as

$$B_n[p] := \begin{pmatrix} nx_1 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 2nx_2 & (n+1)x_1 & 2 & 0 & 0 & \cdots & 0 & 0 \\ 3nx_3 & (2n+1)x_2 & (n+2)x_1 & 3 & 0 & \cdots & 0 & 0 \\ 4nx_4 & (3n+1)x_3 & (2n+2)x_2 & (n+3)x_1 & 4 & \cdots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ (p-2)nx_{p-2} & ((p-3)n+1)x_{p-3} & ((p-4)n+2)x_{p-4} & \cdots & \cdots & \cdots & p-2 & 0 \\ (p-1)nx_{p-1} & ((p-2)n+1)x_{p-2} & ((p-3)n+2)x_{p-3} & \cdots & \cdots & \cdots & (n+(p-2))x_1 & p-1 \\ pnx_p & ((p-1)n+1)x_{p-1} & ((p-2)n+2)x_{p-2} & \cdots & \cdots & \cdots & (2n+(p-2))x_2 & (n+(p-1)x_1) \end{pmatrix}$$

$B_n[p]$ therefore denotes the p-th leading principal submatrix of the matrix $B_n[n-1]$ if $p \in [n-1]$ (cf. e.g. [68, 0.7.1]). More precisely, if $p \in [n-1]$ and $i, j \in [p]$, then:

$$B_n[p](x_1, x_2, \ldots, x_p)_{ij} := \begin{cases} 0 & \text{if } j \geq i+2 \\ i & \text{if } j = i+1 \\ ((i-j+1)n + j - 1)x_{i-j+1} & \text{if } j \leq i\,. \end{cases}$$

Equipped with all p leading principal submatrices $B_n[1], B_n[2], \ldots, B_n[p-1]$ of $B_n[p]$ and the "incipient matrix" $B_n[0] := (1)$, we may apply the main (unnumbered) theorem on page 222 of [26] to the matrix $B_n[p](x_1, \ldots, x_p)$, and it follows that

$$\det(B_n[p](x_1, \ldots, x_p)) = (p-1)! \sum_{k=1}^{p} (-1)^{p-k} \frac{pn - (k-1)(n-1)}{(k-1)!} x_{p-k+1} \det(B_n[k-1]). \tag{9.244}$$

Consequently, if $p = n-1$, it follows that

$$\begin{aligned} \det(A_n * T_n(\alpha_1, \ldots, \alpha_n)) &= \alpha_1^{n-1} \det(B_n[n-1](\alpha_2^\times, \ldots, \alpha_n^\times)) \\ &= \alpha_1^{n-1} (n-2)! \sum_{k=1}^{n-1} (-1)^{n-1-k} \frac{(n-1)(n-k+1)}{(k-1)!} \alpha_{n-k+1}^\times \det(B_n[k-1](\alpha_2^\times, \ldots, \alpha_k^\times)) \\ &= \alpha_1^{n-1} (n-1)! \sum_{k=1}^{n-1} (-1)^{n-k-1} \frac{n-k+1}{(k-1)!} \alpha_{n-k+1}^\times \det(B_n[k-1](\alpha_2^\times, \ldots, \alpha_k^\times)). \end{aligned} \tag{9.245}$$

Thus,

$$\beta_n \, \alpha_1^n \overset{(9.242)}{=} \frac{1}{n} \sum_{k=1}^{n-1} (-1)^k \frac{n-k+1}{(k-1)!} \alpha_{n-k+1}^\times \det(B_n[k-1](\alpha_2^\times, \ldots, \alpha_k^\times))\,.$$

In particular, if $n = 2m+1 \in \mathbb{N}_3$ is odd ($m \in \mathbb{N}$) and $\alpha_{2l} := 0$ for all $l \in \mathbb{N}$, then

$$\begin{aligned} \beta_n \, \alpha_1^n &= \frac{1}{n} \sum_{\substack{k=1 \\ k \text{ odd}}}^{n-1} (-1)^k \frac{n-k+1}{(k-1)!} \alpha_{n-k+1}^\times \det(B_n[k-1](0, \alpha_3^\times, 0 \ldots, 0, \alpha_k^\times)) \\ &= -\alpha_{2m+1}^\times - \frac{1}{2m+1} \sum_{r=1}^{m-1} \frac{2(m-r)+1}{(2r)!} \alpha_{2(m-r)+1}^\times \det(B_{2m+1}[2r](0, \alpha_3^\times, 0 \ldots, 0, \alpha_{2r+1}^\times)). \end{aligned}$$

Note also that (9.244) implies that

$$\det(B_{2m+1}[2r](0,x_1,0,x_2,0,\ldots,0,x_r)) = -2(2r-1)!\Big((2m+1)r\,x_r + \sum_{k=1}^{r-1} p_k(r,m)\,x_{r-k}\Big) \tag{9.246}$$

for all $m \in \mathbb{N}$, $r \in [m]$ and $x_1,\ldots,x_r \in \mathbb{C}$, where

$$p_k(r,m) := \frac{2m(r-k)+r}{(2k)!}\det(B_{2m+1}[2k](0,x_1,0\ldots,0,x_k) \quad (k \in [r-1]).$$

Example 9.3. Fix $m \in \mathbb{N}$. Assume for simplification that $\alpha_1 = 1$ $\alpha_{2l} = 0$ for all $l \in \mathbb{N}$. Then $\alpha_n^\times = \alpha_n$ for all $n \in \mathbb{N}$. If $r \in \{1,2\}$, the calculation of $\det(B_{2m+1}[2r])$ is very straightforward:

$$\det(B_{2m+1}[2](0,\alpha_3)) = -2(2m+1)\alpha_3 = 2!(-1)^1\binom{2m+1}{1}\alpha_3 = 2!(-1)^1\binom{2m+1}{1}B^\circ_{1,1}(\alpha_3),$$

and

$$\begin{aligned}\det(B_{2m+1}[4](0,\alpha_3,0,\alpha_5)) &\overset{(9.246)}{=} -12\left(2(2m+1)\alpha_5 + \frac{2m+2}{2}\det(B_{2m+1}[2])\alpha_3\right)\\ &= -12\left(2(2m+1)\alpha_5 + \frac{2m+2}{2}\big(-2(2m+1)\alpha_3\big)\alpha_3\right)\\ &= 4!\Big(-\binom{2m+1}{1}\alpha_5 + \binom{2m+2}{2}\alpha_3^2\Big)\\ &= 4!\Big((-1)^1\binom{2m+1}{1}B^\circ_{2,1}(\alpha_3,\alpha_5) + (-1)^2\binom{2m+2}{2}B^\circ_{2,2}(\alpha_3)\Big).\end{aligned}$$

If $r = 3$, a little more calculation effort is required, also triggered by a significant transformation step:

$$\begin{aligned}\det(B_{2m+1}[6](0,\alpha_3,0,\alpha_5,0,\alpha_7)) &\overset{(9.246)}{=} -240\left(3(2m+1)\alpha_7 + \frac{4m+3}{2}\det(B_{2m+1}[2])\alpha_5 + \frac{2m+3}{4!}\det(B_{2m+1}[4])\alpha_3\right)\\ &= -240\Big(3\binom{2m+1}{1}\alpha_7 - (4m+3)\binom{2m+1}{1}\alpha_3\alpha_5\\ &\quad + (2m+3)\Big(-\binom{2m+1}{1}\alpha_5 + \binom{2m+2}{2}\alpha_3^2\Big)\alpha_3\Big)\\ &= -240\Big(3\binom{2m+1}{1}\alpha_7 - 3\binom{2m+2}{2}(2\alpha_3\alpha_5) + (2m+3)\binom{2m+2}{2}\alpha_3^3\Big)\\ &= 6!\Big(-\binom{2m+1}{1}\alpha_7 + \binom{2m+2}{2}(2\alpha_3\alpha_5) - \binom{2m+3}{3}\alpha_3^3\Big)\\ &= 6!\Big((-1)^1\binom{2m+1}{1}B^\circ_{3,1}(\alpha_3,\alpha_5,\alpha_7) + (-1)^2\binom{2m+2}{2}B^\circ_{3,2}(\alpha_3,\alpha_5)\\ &\quad + (-1)^3\binom{2m+3}{3}B^\circ_{3,3}(\alpha_3)\Big).\end{aligned}$$

In fact, the emerging structure can be kept in the case of $r = 4$, since

$$\begin{aligned}\det(B_{2m+1}[8])(0,\alpha_3,0,\alpha_5,0,\alpha_7,0,\alpha_9) &\overset{(9.246)}{=} -2\cdot 7!\Big(4(2m+1)\alpha_9 + \frac{6m+4}{2}\det(B_{2m+1}[2])\alpha_7 \\ &\quad + \frac{4m+4}{4!}\det(B_{2m+1}[4])\alpha_5 + \frac{2m+4}{6!}\det(B_{2m+1}[6])\alpha_3\Big) \\ &= 8!\Big(-\binom{2m+1}{1}\alpha_9 + \binom{2m+2}{2}(2\alpha_3\alpha_7+\alpha_5^2) - \binom{2m+3}{3}(3\alpha_3^2\alpha_5) \\ &\quad + \binom{2m+4}{4}\alpha_3^4\Big) \\ &= 8!\Big((-1)^1\binom{2m+1}{1}B^\circ_{4,1}(\alpha_3,\alpha_5,\alpha_7,\alpha_9) + (-1)^2\binom{2m+2}{2}B^\circ_{4,2}(\alpha_3,\alpha_5,\alpha_7) \\ &\quad + (-1)^3\binom{2m+3}{3}B^\circ_{4,3}(\alpha_3,\alpha_5) + (-1)^4\binom{2m+4}{4}B^\circ_{4,4}(\alpha_3)\Big).\end{aligned}$$

A relentless focus on Example 9.3 therefore leads to a non-obvious simplification of (9.240) which reduces the analysis of complex partition sets $P(2m,k)$ and related non-trivial ordinary partial Bell polynomials $B^\circ_{2m,k}(0,\alpha_3,0,\alpha_5,0,\alpha_7,0,\ldots)$ to that one of partition sets $P(m,l)$ and related "fully occupied" ordinary partial Bell polynomials $B^\circ_{m,l}(\alpha_3,\alpha_5,\alpha_7,\ldots)$. In fact, the following result holds:

Proposition 9.4. *Let $(x_n)_{n\in\mathbb{N}}$ be an arbitrary sequence of complex numbers. Let $m\in\mathbb{N}$ and $r\in[m]$. Then*

$$\det(B_{2m+1}[2r](0,x_1,0,x_2,\ldots,0,x_r)) = (2r)!\sum_{l=1}^{r}(-1)^l\binom{2m+l}{l}B^\circ_{r,l}(x_1,x_2,\ldots,x_{r-l+1}).$$

Proof. If $m\in\mathbb{N}$ and $r\in[m]$, put $\alpha_{2i+1}:=x_i$, where $i\in[r]$. We make use of a version of the principle of transfinite induction (which generalises induction over natural numbers), known as the principle of Noetherian induction. To this end, we consider the set

$$\mathcal{M} := \{(n,\nu)\in\mathbb{N}\times\mathbb{N} : n+1>\nu\} = \{(n,\nu)\in\mathbb{N}\times\mathbb{N} : n\geq\nu\}\,.$$

Then $(\mathcal{M},<_{\text{lex}})$ is a well-founded totally ordered set, where $<_{\text{lex}}$ denotes the lexicographic order on $(\mathbb{N},<)\times(\mathbb{N},<)$; i.e., $(l,\kappa)<_{\text{lex}}(m,\mu)$ if and only if $l<m$ or ($l=m$ and $\kappa<\mu$) (cf. [41, Chapter 6.3 including the table on p. 87]). Obviously, $(1,1)$ is the minimal element of $\mathcal{M}$ which satisfies the claim, so that the induction basis is fulfilled. Let $(m,r)\in\mathcal{M}$ be non-minimal. Then $m\geq 2$. Clearly, if $r=1$, then $(m,r)=(m,1)\in\mathcal{M}$ satisfies the claim. So, we have to consider the case $r\geq 2$. Let $k\in[r-1]$. Then $(m,k)<_{\text{lex}}(m,r)$. Hence, because of the induction assumption, it follows that

$$\det(B_{2m+1}[2k]) = (2k)!\sum_{i=1}^{k}(-1)^l\binom{2m+i}{i}B^\circ_{k,i}(\alpha_3,\alpha_5,\ldots,\alpha_{2(k-i)+3}). \tag{9.247}$$

If we insert (9.247) into (9.246), we obtain

$$\det(B_{2m+1}[2r]) = -2(2r-1)!\Big((2m+1)r\,\alpha_{2r+1} + \sum_{k=1}^{r-1}p_k(r,m)\,\alpha_{2(r-k)+1}\Big),$$

where

$$p_k(r,m) = \frac{2m(r-k)+r}{(2k)!}\,\det(B_{2m+1}[2k])$$
$$= \big((2m+1)r - 2mk\big)\sum_{i=1}^{k}(-1)^i\binom{2m+i}{i}B^{\circ}_{k,i}(\alpha_3,\alpha_5,\ldots,\alpha_{2k+3-2i}).$$

Consequently,

$$-\frac{\det(B_{2m+1}[2r])}{2(2r-1)!} - (2m+1)r\,\alpha_{2r+1}$$
$$= \sum_{k=1}^{r-1}\sum_{i=1}^{k}\big(2m(r-k)+r\big)\,(-1)^i\binom{2m+i}{i}\,\alpha_{2(r-k)+1}\,B^{\circ}_{k,i}(\alpha_3,\alpha_5,\ldots,\alpha_{2k+3-2i})$$
$$= \sum_{l=1}^{r-1}(-1)^l\binom{2m+l}{l}\sum_{j=l}^{r-1}\big(2m(r-j)+r\big)\,\alpha_{2(r-j)+1}\,B^{\circ}_{j,l}(\alpha_3,\alpha_5,\ldots,\alpha_{2(j-l+1)+1}).$$

Thereby, the last equality is a special case of the double sum representation

$$\sum_{k=1}^{r-1}\sum_{i=1}^{k} b_{ki}\,c_{ik} = \sum_{k=1}^{r-1}\sum_{i=k}^{r-1} b_{ik}\,c_{ki} = \sum_{l=1}^{r-1}\sum_{j=l}^{r-1} b_{jl}\,c_{lj}, \tag{9.248}$$

which originates from the calculation of the trace of the matrix product of the lower triangular matrix $(b_{ki}\,\mathbb{1}_{\{(\mu,\nu):\mu\geq\nu\}}(k,i))$ and the upper triangular matrix $(c_{lj}\,\mathbb{1}_{\{(\mu,\nu):\mu\leq\nu\}}(l,j))$ and the trace of its transpose, which both are equal. Finally, since

$$\sum_{j=l}^{r-1}(2m(r-j)+r)\,\alpha_{2(r-j)+1}\,B^{\circ}_{j,l}(\alpha_3,\alpha_5,\ldots,\alpha_{2(j-l)+3}) = \frac{r(2m+l+1)}{l+1}\,B^{\circ}_{r,l+1}(\alpha_3,\ldots,\alpha_{2(r-l)+1})$$

(due to Lemma 9.1, applied to $n := r$, $k := l+1$, $\zeta := 2m$ and $i := j$), it follows that

$$r\left(\frac{\det(B_{2m+1}[2r])}{(2r)!} + (2m+1)\,\alpha_{2r+1}\right) = \frac{\det(B_{2m+1}[2r])}{2(2r-1)!} + (2m+1)r\,\alpha_{2r+1}$$
$$= -r\sum_{l=1}^{r-1}(-1)^l\binom{2m+l+1}{l+1}B^{\circ}_{r,l+1}(\alpha_3,\ldots,\alpha_{2(r-l)+1})$$
$$= r\sum_{l=2}^{r}(-1)^l\binom{2m+l}{l}B^{\circ}_{r,l}(\alpha_3,\ldots,\alpha_{2(r-l)+3}),$$

which concludes the Noetherian induction step, and the claim follows. □

Altogether, Lemma 9.1, Proposition 9.4 and (9.248), together with our previously mentioned analysis of the structure of β_{2m+1}, imply the following two fundamental results:

Theorem 9.5. *Let $m \in \mathbb{N}_2$ and $x_1,\ldots,x_{m-1} \in \mathbb{C}$. Then*

$$\sum_{r=1}^{m-1}\frac{2(m-r)+1}{(2r)!}\,x_{m-r}\,\det\Big(B_{2m+1}[2r](0,x_1,0,x_2,\ldots,0,x_r)\Big)$$
$$= \frac{1}{(2m)!}\sum_{r=2}^{m}(-1)^{r-1}\frac{(2m+r)!}{r!}\,B^{\circ}_{m,r}(x_1,x_2,\ldots,x_{m-r+1}).$$

Proof. By consecutive application of Proposition 9.4 and (9.248), it follows that

$$\begin{aligned}
&\sum_{r=1}^{m-1} \frac{2(m-r)+1}{(2r)!}\, x_{m-r}\, \det\Big(B_{2m+1}[2r](0,x_1,0,x_2,\ldots,0,x_r)\Big)\\
&= \sum_{r=1}^{m-1}\sum_{l=1}^{r} (-1)^l\,(2(m-r)+1)\binom{2m+l}{l}\, x_{m-r}\, B^\circ_{r,l}(x_1,x_2,\ldots,x_{r-l+1})\\
&= \sum_{r=1}^{m-1} (-1)^r \binom{2m+r}{r} \sum_{l=r}^{m-1} (2(m-l)+1)\, x_{m-l}\, B^\circ_{l,r}(x_1,x_2,\ldots,x_{l-r+1}).
\end{aligned}$$

However, the latter expression equals

$$\begin{aligned}
&\sum_{r=1}^{m-1} (-1)^r\, 2\binom{2m+r}{r} \sum_{l=r}^{m-1} (m-l)\, x_{m-l}\, B^\circ_{l,r}(x_1,x_2,\ldots,x_{l-r+1})\\
&+ \sum_{r=1}^{m-1} (-1)^r \binom{2m+r}{r} \sum_{l=r}^{m-1} x_{m-l}\, B^\circ_{l,r}(x_1,x_2,\ldots,x_{l-r+1}).
\end{aligned}$$

Thus, we can now apply Lemma 9.1 to both summands, and a final shift of the index r in the single remaining sum $(\sum_{r=1}^{m-1} a_{r+1} = \sum_{r=2}^{m} a_r)$ clearly finishes the proof. □

Corollary 9.6. *Let $f(\rho) = \sum_{n=0}^{\infty} \alpha_{2n+1}\,\rho^{2n+1}$ be an odd real analytic function, convergent on $(-r,r) \subseteq \mathbb{R}$, where $r > 0$ denotes the radius of convergence of f. Assume that $f'(0) = \alpha_1 \neq 0$, implying that f is invertible around 0. Consider the real analytic odd inverse function $f^{-1} : V \longrightarrow \mathbb{R}$, where V is an open neighbourhood of $f(0) = 0$. If $f^{-1}(y) = \sum_{m=0}^{\infty} \beta_{2m+1}\, y^{2m+1}$ for all $y \in V$, then $\beta_1 = \frac{1}{\alpha_1}$ and*

$$\begin{aligned}
\beta_{2m+1} &= -\frac{1}{\alpha_1^{2m+1}}\Big(\alpha^\times_{2m+1} + \frac{1}{2m+1}\sum_{r=1}^{m-1}\frac{2(m-r)+1}{(2r)!}\,\alpha^\times_{2(m-r)+1}\,\det\Big(B_{2m+1}[2r](0,\alpha^\times_3,0,\alpha^\times_5,\ldots,0,\alpha^\times_{2r+1})\Big)\Big)\\
&= \frac{1}{(2m+1)!\,\alpha_1^{2m+1}}\sum_{r=1}^{m}(-1)^r\frac{(2m+r)!}{r!}\,B^\circ_{m,r}(\alpha^\times_3,\alpha^\times_5,\ldots,\alpha^\times_{2(m-r+1)+1})
\end{aligned}$$

for all $m \in \mathbb{N}$, where $\alpha^\times_{2\nu+1} := \frac{\alpha_{2\nu+1}}{\alpha_1}$ $(\nu \in \mathbb{N})$.

As a little, yet illuminating exercise, we recommend the readers to perform the rather quick calculation of the first 3 Taylor coefficents of the inverse of the odd function $f := 3\sinh$, say, by applying Corollary 9.6! The outcome could be double-checked by means of `https://en.wikipedia.org/wiki/Inverse_hyperbolic_functions#Series_expansions`. Moreover, because of [139, Theorem 2] the coefficients β_{2m+1} satisfy the following, interesting recurrence relation:

$$\begin{aligned}
\beta_{2m+1}\alpha_1^{2m+1} &= -\sum_{r=0}^{m-1}(\beta_{2r+1}\alpha_1^{2r+1})\,B^\circ_{2m+1,2r+1}(\alpha^\times_1,0,\alpha^\times_3,0,\alpha^\times_5,\ldots,0,\alpha^\times_{2(m-r)+1})\\
&= -\sum_{r=0}^{m-1}\beta_{2r+1}\,B^\circ_{2m+1,2r+1}(\alpha_1,0,\alpha_3,0,\alpha_5,\ldots,0,\alpha_{2(m-r)+1})
\end{aligned}$$

for all $m \in \mathbb{N}$.

In a nutshell, we recognise that already in the one-dimensional case, at least two hard open problems appear. On the one hand we need to know the explicit value of the Fourier-Hermite coefficients (cf. Proposition 6.3)

$$\sqrt{n!}\,\langle b, H_n\rangle_{\gamma_1} = \sqrt{n!}\,\mathbb{E}[b(X)H_n(X)] = \frac{\mathrm{d}^n}{\mathrm{d}t^n}\mathbb{E}[b(X+t)]\Big|_{t=0},$$

where $X \sim N_1(0,1)$. On the other hand, we have to look for a closed form expression of the coefficients β_n (if it were available at all), where the latter involves the complex recursive structure of ordinary partial Bell polynomials or related determinants. For example (keeping the Haagerup function in mind - cf. Example 7.15 and Remark 4.1), our question of the value of

$$\frac{\pi^k}{4^k}\,B^{\circ}_{n,k}\Big(\frac{1}{8}, \frac{3}{64}, \frac{25}{1024}, \ldots, \frac{((2(n-k)+1)!!)^2}{((2(n-k+1))!!)^2\,(n-k+2)}\Big)$$

very recently lead to an in depth-analysis, published in [38]. It appears to us that in general one cannot use proofs by standard induction on $n \in \mathbb{N}$ to verify statements about Bell polynomials. The Noetherian Induction Principle seems to be more appropriate here (as we have seen for example, in the proof of Proposition 9.4). In this context, we would like to draw attention to another recently published paper, where the authors point to similar difficulties including the formulation of related - open - problems (cf. [96]). Moreover, the solved examples in [96] show the large combinatorial barriers which we have to resolve while working with (partial) Bell polynomials.

Keeping these problems and barriers in mind, the following research topics and problems - which actually do not require any knowledge of the Grothendieck inequality - arise naturally:

(RP1) Continue to investigate the structure of partial Bell polynomials; possibly under inclusion of the use of high-performance computers and related (algebraic) software tools.

(RP2) Develop a software package which puts Corollary 9.6 into practice.

(RP3) Look for an explicit analytic expression for the *inverse* function of the main building block of the Haagerup function; i.e., the inverse of the strictly increasing odd function

$$[-1,1] \ni x \mapsto x\,{}_2F_1\Big(\frac{1}{2}, \frac{1}{2}, 2; x^2\Big)$$

(if available!), where as usual ${}_2F_1(a,b,c;\cdot)$ denotes the classic Gaussian hypergeometric function (cf. Example 7.15). Obviously, the inverse of $[-1,1] \ni x \mapsto x\cdot{}_2F_1(\frac{1}{2}, \frac{1}{2}, \frac{3}{2}; x^2) = \arcsin(x) = \sin^{-1}(x)$ is the function sin. However, what about the inverses of (invertible) functions ${}_2F_1(a,b,c;\cdot)$ in general? Do we have to work with elliptic integrals here? What part does the Jacobi elliptic function play in this? A complex-analytic approach to a part of this problem using contour integration is given in [17, Chapter 5, including Theorem 5.6.18].

9.2. Open problem 2: Interrelation between the Grothendieck inequality and copulas

If we thouroughly overhaul the CCP function $[-1,1] \ni \rho \mapsto \frac{2}{\pi}\arcsin(\rho)$ we recognise that some knowledge of Gaussian copulas (i.e., finite-dimensional multivariate distribution functions of univariate marginals generated by the distribution function of Gaussian random vectors - cf., e.g., [105, 111, 133, 143]) and (the probabilistic version) of the Hermite polynomials might become very fruitful regarding our indicated search for different " suitable" CCP functions. $[-1,1] \ni \rho \mapsto \psi(\frac{1}{2}, \frac{1}{2}; t) = \frac{2}{\pi}\arcsin(\rho)$ namely reveals as a special case of the CCP function

$$[-1,1] \ni \rho \mapsto \psi(p,p;\rho) = \frac{1}{c(p)}\sum_{n=1}^{\infty}\frac{1}{n}\,H_{n-1}^2(\Phi^{-1}(p))\,\rho^n = \frac{1}{2\pi\,p(1-p)}\,\exp(-(\Phi^{-1}(p))^2)\,\rho\sum_{n=0}^{\infty}\frac{1}{n+1}\,H_n^2(\Phi^{-1}(p))\,\rho^n\,,$$

where $0 < p < 1$ and

$$c(p) := \frac{p(1-p)}{\varphi^2(\Phi^{-1}(p))} = 2\pi\,p(1-p)\exp((\Phi^{-1}(p))^2) = \sum_{n=0}^{\infty}\frac{1}{n+1}\,H_n^2(\Phi^{-1}(p))\,.$$

If we put

$$b_p(x) := \operatorname{sign}(x - \Phi^{-1}(p)) = 2\mathbb{1}_{[\Phi^{-1}(p),\infty)}(x) - 1 = 1 - 2\mathbb{1}_{(-\infty,\Phi^{-1}(p))}(x) \in \{-1,1\}\,,$$

where $x \in \mathbb{R}$, then the tetrachoric series expansion of the bivariate Gaussian copula (cf. [8, 55, 101]) implies the following generalisation of the Grothendieck equality:

$$\begin{aligned} h_p(\rho) := h_{b_p}(\rho) : &= \mathbb{E}[b_p(X)\,b_p(Y)] = (2p-1)^2 + \frac{2}{\pi}\exp(-(\Phi^{-1}(p))^2)\sum_{n=1}^{\infty}\frac{1}{n}H_{n-1}^2(\Phi^{-1}(p))\rho^n \\ &= (2p-1)^2 + 4p(1-p)\psi(p,p;\rho)\,. \end{aligned}$$

Due to our construction of $\psi(p,p;\cdot)$ the latter is clearly equivalent to

$$\rho(b_p(X), b_p(Y)) = \psi(p,p;\rho)$$

for all $p \in (0,1)$, $\rho \in [-1,1]$ and $(X,Y) \sim N_2(0,\Sigma_2(\rho))$, where $\rho(b_p(X), b_p(Y))$ denotes Pearson's correlation coefficient between the random variables $b_p(X)$ and $b_p(Y)$. Unfortunately,

$$h_p(\rho) = \psi(p,p;\rho) \text{ for all } \rho \in [-1,1] \text{ if and only if } p = \frac{1}{2}\,.$$

These facts clearly lead to further research problems; namely:

(RP4) Prove whether there are $p \in (-1,1) \setminus \{\frac{1}{2}\}$ and functions $\chi_p : \mathbb{R} \longrightarrow \{-1,1\}$ such that $\psi(p,p;\rho) = h_{\chi_p}(\rho) = \mathbb{E}[\chi_p(X)\,\chi_p(Y)]$ for all $\rho \in [-1,1]$ and $(X,Y) \sim N_2(0,\Sigma_2(\rho))$, so that the condition (SIGN) of our workflow is satisfied for h_{χ_p}.

(RP5) Generalise the above approach (which is built on the tetrachoric series of the bivariate Gaussian copula) to the n-variate case, where $n \in \mathbb{N}_3$.

(RP6) Verify whether the above approach can be transferred to the complex case. Could we then similarly generalise the Haagerup equality?

(RP7) If (RP4), respectively (RP5) holds, prove whether the condition (CRA) of the scheme holds. If this were the case, calculate (respectively approximate numerically) the related upper bound of $K_G^{\mathbb{R}}$. Include high-performance computers and computer algebra systems if necessary.

9.3. Open problem 3: Non-commutative dependence structures in quantum mechanics and the Grothendieck inequality

Even a mathematical modelling of *non-commutative dependence* in quantum theory and its applications to quantum information and quantum computation is strongly linked with the existence of the real Grothendieck constant $K_G^{\mathbb{R}}$.

The latter can be very roughly adumbrated as follows: the experimentally proven non-Kolmogorovian (non-commutative) nature of the underlying probability theory of quantum physics leads to the well-known fact that in general a normal state of a composite quantum system cannot be represented as a convex combination of a product of normal states of the subsystems. This phenomenon is known as *entanglement* or *quantum correlation*. The Einstein-Podolsky-Rosen paradox, the violation of Bell's inequalities (limiting *spatial* correlation) and the Leggett-Garg inequalities (limiting *temporal* correlation) in quantum mechanics and related theoretical and experimental research implied a particular focus on a deeper understanding of this type of correlation - and hence to the *modelling of a specific type of dependence* of two (ore more) quantum observables in a composite quantum system, measured by two (or more) space-like separated instruments, each one having a classical parameter (such as the orientation of an instrument which measures the spin of a particle). In this context, a Leggett-Garg inequality (LGI) could be viewed as a "Bell inequality in time". The transition probability function, i. e., the *joint* probability distribution of observables in some fixed state of the system (considered as a function of the aforementioned parameters) may violate Bell's inequalities and is therefore not realisable in "classical" (commutative) physics. The surprising fact, firstly recognised by B. S. Tsirel'son (cf. [9, Ch. 11.2] and [113, 140, 142]), is that also this - experimentally verified - gap is an implication of the existence of the real Grothendieck constant $K_G^{\mathbb{R}} > 1$ (also known as *Tsirel'son bound*)! In other words, $K_G^{\mathbb{R}}$ indicates "how non-local quantum mechanics can be at most".

Already in the classical Kolmogorovian model, i. e., in the framework of probability space triples $(\Omega, \mathcal{F}, \mathbb{P})$, a rigorous description of tail dependence - which *exceeds* the standard dependence measure, given by Pearson's correlation coefficient, is a challenging task. To disclose (and simulate) the geometry of dependence one has to determine finite-dimensional multivariate distribution functions of univariate marginals, hence *copulas*. In the description of research problem 2 we have seen that Gaussian copulas are lurking in the Grothendieck equality. More precisely, we have (cf. [137]):

Example (Stieltjes, 1889). Let $\rho \in [-1, 1]$. Let $X, Y \sim N_1(0, 1)$ such that $\mathbb{E}[XY] = \rho$. Then

$$\mathbb{E}[\text{sign}(X)\text{sign}(Y)] = 4\, C^{\text{Ga}}(\tfrac{1}{2}, \tfrac{1}{2}; \rho) - 1 = \frac{2}{\pi}\arcsin(\rho) = \frac{2}{\pi}\arcsin(\mathbb{E}[XY]),$$

where $[-1, 1] \ni \rho \mapsto C^{\text{Ga}}(\frac{1}{2}, \frac{1}{2}; \rho)$ denotes the bivariate Gaussian copula with Pearson's correlation coefficient ρ as parameter, evaluated at $(\frac{1}{2}, \frac{1}{2})$.

Keeping a *non-commutative* version of the Grothendieck inequality at the back of our mind (cf. [119, 140, 142]), our conjecture is that copulas in function spaces play a non-negligible role here. Unfortunately, compared to the finite-dimensional setting, the advent of the latter confronts us with non-trivial difficulties. For example, by no means it is clear how marginals can be defined in an infinite-dimensional measurable vector space. If X is a random variable in a separable Hilbert space H, projections onto an orthonormal basis $(\langle X, e_n \rangle)_{n\in\mathbb{N}}$ are reasonable candidates. This case was treated in [59]. If in addition the space considered is a reproducing kernel Hilbert space of functions, over $[0, 1]$ say, an equally natural option for marginals would be function evaluations $\{X(t) : t \in [0, 1]\}$. Here, a new framework is required, including the preparation of a general concept of marginals for measurable vector spaces (cf. [13]). Consequently, we arrive at problems of the following type:

(RP8) Look for objects like "non-commutative copulas", leading to a search for "non-commutative distribution functions in measurable vector spaces", including a non-commutative version of the famous result of Sklar (cf. [111] and the references cited therein).

(RP9) Create a "multivariate" spectral theory of *non-commuting* normal operator tuples and introduce non-commutative tail dependency measures in non-commutative C^*-algebras and operator spaces.

Let us close Section 9 briefly with the following "blue-sky" research questions, which appear quite naturally and are completely unanswered. Can we improve the approximation results in the commutative case if we remove the underlying Gaussian structure in the Grothendieck inequality (for both fields, $\mathbb{R}$ and $\mathbb{C}$) and implement tail dependent distribution functions instead (such as the generalised extreme value (GEV) distribution)? What about infinitely divisible probability distributions in general? It is very likely that the use of correlation matrices and CCP functions, including linked *Gaussian* copula approaches, would not be enough any more (just as it is with Brownian motion which is a special case of a Lévy process, yet without jumps). So, could even general semimartingale techniques help to improve the approximations (cf., e.g., [42, 87])?

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