

## Chapter 7

# Quantumness according to Grothendieck quantities in a single finite quantum system

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### 7.1 Introduction

The Grothendieck inequality [1–7] in pure mathematics, provides a ‘ceiling’ for the Hilbert space formalism. The original formulation of the Grothendieck theorem [1] was in the context of a tensor product of Banach spaces, and this might give the wrong impression that applications in a quantum context should be only for multipartite systems described by tensor products of Hilbert spaces. Indeed the Grothendieck formalism has been used with multipartite entangled systems in refs [8–15] and has been linked to Bell-like inequalities.

Later mathematical work [2–4] emphasised that the Grothendieck theorem can be formulated outside tensor product theory. This motivated our work in refs[16, 17] that uses the Grothendieck bound in a single quantum system, and is totally unrelated to multipartite entangled systems.

The Grothendieck formalism considers a ‘classical’ quadratic form  $\mathcal{C}$  that uses complex numbers in the unit disc (scalars). It also considers a ‘quantum’ quadratic form  $\mathcal{Q}$  that replaces the scalars with vectors in the unit ball of a Hilbert space. Going from  $\mathcal{C}$  to  $\mathcal{Q}$ , can be viewed as a passage from classical physics to quantum physics. The Grothendieck theorem shows that if the classical  $\mathcal{C} \leq 1$ , the corresponding quantum  $\mathcal{Q}$  might take values greater than 1, up to the complex Grothendieck constant  $k_G$ . The region  $(1, k_G)$  is classically forbidden in the sense that  $\mathcal{C}$  does not take values in it, and for this reason

examples with  $\mathcal{Q} \in (1, k_G)$  can be viewed as ‘ultra-quantum’. Such examples have been presented in refs[16, 17], and are not discussed here.

Quantumness in a single quantum system with finite-dimensional Hilbert space (we do not consider here multipartite systems and entanglement) can be linked with various attributes as follows:

- Q1. **The Grothendieck quantity  $\mathcal{Q}$  takes values in the region  $(1, k_G)$ .** We have explored this approach for a single quantum system in refs[16, 17], and gave several examples. Here we study its relationship with other approaches to quantumness. We also give transformations that leave  $\mathcal{Q}$  invariant (proposition 7.4.1).
- Q2. **Fourier duality and uncertainty relations:** Fourier duality underpins Harmonic Analysis and Quantum Mechanics which is based on it. One aspect of this is the uncertainty relations, which are studied by comparing the uncertainty (quantified in various ways) for a density matrix  $\theta$  with the uncertainty for its ‘Fourier dual density matrix’  $\hat{\theta} = F\theta F^\dagger$  (where  $F$  is the Fourier transform given below in Eq.(7.19)). If the uncertainty for  $\theta$  is small, then the uncertainty for  $\hat{\theta}$  is large. Motivated by this we explored whether for a density matrix  $\theta$  with Grothendieck quantity  $\mathcal{Q}(\theta) \leq 1$ , its Fourier dual density matrix  $\hat{\theta}$  has  $\mathcal{Q}(\hat{\theta}) \geq 1$ . We show that this is **not** true in general. In proposition 7.4.1 we show that for a diagonal density matrix  $\theta$ , we get  $\mathcal{Q} \leq 1$  for both  $\theta$  and  $\hat{\theta}$ . Although this is proved only for diagonal  $\theta$ , it does show that the Fourier transform **cannot** (in general) change a state with  $\mathcal{Q} \leq 1$  into a state with  $\mathcal{Q} > 1$ . Fourier duality does not play as important role for quantumness according to Grothendieck quantities, as for uncertainty relations. Quantumness according to Grothendieck quantities is different from quantumness according to uncertainty relations.
- Q3. **Quantum interference:** this is best shown as oscillations in quantities  $\langle f|U|g\rangle$  where  $U$  is a unitary operator (e.g., refs[18, 19] for systems with large dimension). We show that for **any** unitary operator, the corresponding Grothendieck quantity  $\mathcal{Q} \leq 1$  (proposition 7.5.1). Therefore quantumness according to Grothendieck quantities is different from quantumness according to quantum interference.
- Q4. **Violation of various probabilistic inequalities:** Bell-like formalisms. A link of quantumness according to Q1 with Q4 has been discussed in the literature (in refs[8–15] for multipartite systems, and in ref[17] for a single quantum system), and is not discussed here.

These attributes are complementary to each other, but they are not the same. Each of them approaches quantumness from a different angle. In this paper we compare quantumness according to Q1 and Q2, and also quantumness according to Q1 and Q3, in a single quantum system.

## 7.2 Preliminaries

Let  $\pi$  be a permutation

$$(0, 1, \dots, d-1) \xrightarrow{\pi} (\pi(0), \pi(1), \dots, \pi(d-1)). \quad (7.1)$$

$\pi$  is an element of the symmetric group  $\mathcal{S}_d$  [20] which has  $d!$  elements. Multiplication in this group is the composition:

$$(0, 1, \dots, d-1) \xrightarrow{\pi} (\pi(0), \pi(1), \dots, \pi(d-1)) \xrightarrow{\varpi} (\varpi[\pi(0)], \varpi[\pi(1)], \dots, \varpi[\pi(d-1)]). \quad (7.2)$$

We will use the notation  $(\varpi\pi)(i) = \varpi[\pi(i)]$ . The unity is

$$(0, 1, \dots, d-1) \xrightarrow{1} (0, 1, \dots, d-1). \quad (7.3)$$

A permutation matrix  $M(\pi)$  is a  $d \times d$  matrix with elements

$$[M(\pi)]_{ij} = \delta(i, \pi(j)) \quad (7.4)$$

where  $\delta$  is the Kronecker delta. Clearly

$$\begin{aligned} M(\varpi)M(\pi) &= M(\varpi\pi); & M(\mathbf{1}) &= \mathbf{1}; & M(\pi^{-1}) &= [M(\pi)]^{-1} = [M(\pi)]^\dagger; \\ & & [M(\pi)]^\dagger M(\pi) &= \mathbf{1} \end{aligned} \quad (7.5)$$

The matrices  $M(\pi)$  form a representation of the group  $\mathcal{S}_d$ .

If  $\theta$  is a  $d \times d$  matrix, then

$$\{[M(\pi)]^\dagger \theta [M(\pi)]\}_{ij} = \theta_{\pi(i), \pi(j)} \quad (7.6)$$

is another matrix whose elements are a permutation of the elements of  $\theta$ . The diagonal elements in  $\theta$ , remain diagonal elements after the transformation.

### 7.3 Grothendieck bound

The Grothendieck theorem considers quadratic form

$$\mathcal{C}(\theta) = \left| \sum_{r,s=1}^d \theta_{rs} a_r b_s \right|; \quad |a_r| \leq 1; \quad |b_s| \leq 1. \quad (7.7)$$

Here  $\theta$  is a  $d \times d$  complex matrix.  $\mathcal{C}(\theta)$  is a ‘classical quantity’ in the sense that the  $a_r, b_s$  are scalars in the unit disc  $D = \{|z| \leq 1\}$ .

It also considers the corresponding quadratic forms where the scalars are replaced with vectors in the unit ball in a  $d$ -dimensional Hilbert space  $H(d)$ :

$$\mathcal{Q}(\theta) = \left| \sum_{r,s} \theta_{rs} \lambda_r \mu_s \langle u_r | v_s \rangle \right|; \quad |u_r\rangle, |v_r\rangle \in H(d); \quad \lambda_r, \mu_r \leq 1. \quad (7.8)$$

Using the bra-ket notation for normalised vectors, the  $\lambda_r |u_r\rangle, \mu_s |v_s\rangle$  are vectors in the unit ball in  $H(d)$ .  $\mathcal{Q}(\theta)$  is a ‘quantum quantity’ in the sense that the scalars have been replaced with vectors. The Grothendieck theorem states that if  $\mathcal{C}(\theta) \leq 1$ , the  $\mathcal{Q}(\theta)$  is smaller than a constant  $k_G$ :

$$\mathcal{C}(\theta) \leq 1 \rightarrow \mathcal{Q}(\theta) \leq k_G. \quad (7.9)$$

$k_G$  is the complex Grothendieck constant which does not depend on the dimension  $d$ , and for which it is known that  $k_G \leq 1.4049$ . Its exact value is not known and bounds for its exact value are discussed in [5–7].  $k_G$  is a kind of ‘ceiling’ of the Hilbert space (and quantum) formalism.

Values of  $\mathcal{Q}(\theta)$  in the region  $(1, k_G)$  are of special importance, because this is a classically forbidden region (the  $\mathcal{C}(\theta)$  cannot take values in it). Families of examples that take values in the  $(1, k_G)$  region have been given in refs[16, 17], and are not presented here. These examples are ‘ultra quantum’ in the sense that the corresponding  $\mathcal{Q}(\theta)$  is near the ‘ceiling’  $k_G$  of the Hilbert space and quantum formalisms.

### 7.3.1 Grothendieck bound as the trace of a product of matrices

Many physical quantities are usually expressed as the trace of some product of matrices. For this reason we rewrite  $\mathcal{Q}(\theta)$  in Eq.(7.8), as the trace of a product of matrices.

**Definition 7.3.1.** For any  $d \times d$  matrix  $\theta$ ,

$$g(\theta) = \sup \left\{ \mathcal{C}(\theta) = \left| \sum_{r,s=1}^d \theta_{rs} a_r b_s \right|; \quad |a_r| \leq 1; \quad |b_s| \leq 1 \right\} \quad (7.10)$$

$G_d$  is the set of  $d \times d$  complex matrices with  $g(\theta) \leq 1$ .

If  $\theta$  is an arbitrary matrix, then  $\frac{\theta}{g(\theta)} \in G_d$ . By definition, matrices in  $G_d$  have  $\mathcal{C}(\theta) \leq 1$ . For normal matrices it is known that  $g(\theta) \leq de_{\max}$ [16, 17], where  $e_{\max}$  is the maximum of the absolute values of the eigenvalues of the matrix  $\theta$ .

**Definition 7.3.2.** For any  $d \times d$  matrix  $M$ ,

$$\mathcal{N}(M) = \max_i \sqrt{\sum_j |M_{ij}|^2} = \max_i \sqrt{(MM^\dagger)_{ii}} \quad (7.11)$$

$\mathcal{S}_d$  is the set of matrices  $M$  with  $\mathcal{N}(M) \leq 1$ .

All unitary matrices belong in  $\mathcal{S}_d$ . If  $M$  is an arbitrary matrix, then  $\frac{M}{\mathcal{N}(M)} \in \mathcal{S}_d$ .

The Grothendieck theorem can be expressed in terms of the trace of a product of three matrices as follows[16]. If  $\theta \in G_d$  and  $V, W \in \mathcal{S}_d$  then

$$\mathcal{Q}(\theta) = |\text{Tr}(\theta VW^\dagger)| \leq k_G. \quad (7.12)$$

The relationship of this expression to Eq.(7.8) is seen if we take  $V$  to be a  $d \times d$  matrix that has the components of  $\mu_s |v_s\rangle$  in the  $s$ -row (then  $V \in \mathcal{S}_d$ ), and  $W$  to be a matrix that has the components of  $\lambda_r |u_r\rangle$  in the  $r$ -row (then  $V \in \mathcal{S}_d$ ). In this case  $W^\dagger$  has the complex conjugates of the components of  $\lambda_r |u_r\rangle$  in the  $r$ -column.

For arbitrary matrices we can write this as

$$\mathcal{Q}(\theta) = \left| \text{Tr} \left( \frac{\theta}{g(\theta)} \frac{V}{\mathcal{N}(V)} \frac{W^\dagger}{\mathcal{N}(W^\dagger)} \right) \right| \leq k_G. \quad (7.13)$$

Values of  $\mathcal{Q}(\theta)$  in the region  $(1, k_G)$  are of special importance. The region  $(1, k_G)$  is a classically forbidden region (the  $\mathcal{C}(\theta)$  cannot take values in it). Families of examples

that take values in  $(1, k_G)$  have been given in refs[16, 17]. These examples are ‘ultra quantum’ in the sense that they are near the ‘ceiling’  $k_G$  of the Hilbert space and quantum formalisms.

**Proposition 7.3.3.**

(1) Let  $M(\pi)$  be a permutation matrix (Eq.(7.4)).  $\mathcal{Q}(\theta)$  (in Eqs.(7.12), (7.13)) is invariant under the transformations:

$$\theta \rightarrow M(\pi)\theta[M(\pi)]^\dagger; \quad V \rightarrow M(\pi)V[M(\pi)]^\dagger; \quad W^\dagger \rightarrow M(\pi)W^\dagger[M(\pi)]^\dagger \quad (7.14)$$

(2)  $\mathcal{Q}(\theta)$  is **not** invariant under general unitary transformations  $U$ :

$$\theta \rightarrow U\theta U^\dagger; \quad V \rightarrow UVU^\dagger; \quad W^\dagger \rightarrow UW^\dagger U^\dagger. \quad (7.15)$$

*Proof.*

(1) We use the expression in Eq.(7.13) for  $\mathcal{Q}(\theta)$ . It is easily seen that

$$\begin{aligned} g(M(\pi)\theta[M(\pi)]^\dagger) &= g(\theta); \quad \mathcal{N}(M(\pi)V[M(\pi)]^\dagger) = \mathcal{N}(V); \\ \mathcal{N}(M(\pi)W^\dagger[M(\pi)]^\dagger) &= \mathcal{N}(W^\dagger). \end{aligned} \quad (7.16)$$

Therefore  $\mathcal{Q}(\theta)$  is invariant under permutations.

(2) For more general unitary transformations

$$g(U\theta U^\dagger) \neq g(\theta); \quad \mathcal{N}(UVU^\dagger) \neq \mathcal{N}(V); \quad \mathcal{N}(UW^\dagger U^\dagger) \neq \mathcal{N}(W^\dagger). \quad (7.17)$$

Therefore  $\mathcal{Q}(\theta)$  is **not** invariant under general unitary transformations. The same argument in terms of the expression in Eq.(7.12) is that if  $\theta \in G_d$  and  $V, W \in \mathcal{S}_d$ , the transformed matrices after a unitary transformation might not belong to  $G_d$  and  $\mathcal{S}_d$ . □

**Remark 7.3.4.** We will see below that for the diagonal matrices in Eq.(7.22) (which includes diagonal density matrices),  $\mathcal{Q}(\theta)$  cannot take values greater than one. This is not surprising because a diagonal density matrix is simply a probabilistic mixture of states. In order to get  $\mathcal{Q}(\theta) > 1$  we need off-diagonal elements in the matrix  $\theta$ . Quantumness is in the off-diagonal elements of a density matrix, which are intimately connected to the superposition principle. Proposition 7.3.3 (second part) shows that this argument is **not** invalidated by the fact that we can diagonalise matrices with a unitary transformation. Superposition is a basis-dependent concept. In a two dimensional space we consider two orthonormal bases  $\{\vec{v}_1, \vec{v}_2\}$  and  $\{\frac{\vec{v}_1 + \vec{v}_2}{\sqrt{2}}, \frac{\vec{v}_1 - \vec{v}_2}{\sqrt{2}}\}$ . Then the vector  $\vec{v}_1 + \vec{v}_2$  is a superposition with respect to the first basis, but it is not a superposition with respect to the second basis.

**Remark 7.3.5.** If  $\text{rank}(\theta) < d$ , let  $\mathfrak{N}_r, \mathfrak{N}'_r$  be vectors in the right and left null space of  $\theta$ ,  $R_s, R'_s$  arbitrary vectors in  $H(d)$ , and  $M_{rs} = \mathfrak{N}_r R_s$  and  $M'_{rs} = R'_s \mathfrak{N}'_r$ . It is easily seen that

$$\mathcal{Q}(\theta) = \left| \text{Tr} \left( \frac{\theta}{g(\theta)} \frac{V}{\mathcal{N}(V)} \frac{W^\dagger}{\mathcal{N}(W^\dagger)} \right) \right| = \left| \text{Tr} \left[ \left( \frac{W^\dagger}{\mathcal{N}(W^\dagger)} + M' \right) \frac{\theta}{g(\theta)} \left( \frac{V}{\mathcal{N}(V)} + M \right) \right] \right| \quad (7.18)$$

## 7.4 Quantumness according to Grothendieck bound is different from quantumness according to uncertainty relations

We consider the Fourier matrix

$$F_{rs} = \frac{1}{\sqrt{d}} \omega^{rs}; \quad \omega = \exp\left(\frac{i2\pi}{d}\right); \quad r, s \in \mathbb{Z}_d. \quad (7.19)$$

Here  $\mathbb{Z}_d$  is the ring of integers modulo  $d$ .

Uncertainty relations are studied by comparing uncertainties (quantified in various ways) for a density matrix  $\theta$ , and for its Fourier dual density matrix  $\hat{\theta} = F\theta F^\dagger$ . For systems with finite-dimensional Hilbert space considered here, usually entropic quantities related to  $\theta, \hat{\theta}$  are used to quantify uncertainty[21–23]. If  $|n\rangle$  is an orthonormal basis, let

$$\begin{aligned} E(\theta) &= -\sum p_n \log p_n; \quad p_n = \langle n | \theta | n \rangle \\ E(\hat{\theta}) &= -\sum q_n \log q_n; \quad q_n = \langle n | \hat{\theta} | n \rangle. \end{aligned} \quad (7.20)$$

Then

$$E(\theta) + E(\hat{\theta}) \geq \log d. \quad (7.21)$$

Therefore if the entropic uncertainty of  $\theta$  is small ( $E(\theta) \leq \frac{1}{2} \log d$ ) then the entropic uncertainty of  $\hat{\theta}$  is large ( $E(\hat{\theta}) \geq \frac{1}{2} \log d$ ).

Motivated by this we explore the role of Fourier duality for quantumness according to Grothendieck quantities. We calculated the Grothendieck quantity  $\mathcal{Q}$  for a diagonal density matrix  $\theta$ , and its Fourier dual density matrix  $\hat{\theta} = F\theta F^\dagger$  (the proposition below is for a wide class of diagonal matrices that includes all diagonal density matrices).

**Proposition 7.4.1.** *Let  $\theta$  be the diagonal matrix*

$$\theta = \text{diag}(z_0, \dots, z_{d-1}); \quad \sum_r |z_r| = 1; \quad z_r \in \mathbb{C}; \quad r \in \mathbb{Z}_d. \quad (7.22)$$

Also let  $\hat{\theta} = F\theta F^\dagger$ . Then:

$$\mathcal{Q}\left(\frac{\theta}{g(\theta)}\right) \leq 1; \quad \mathcal{Q}\left(\frac{\hat{\theta}}{g(\hat{\theta})}\right) \leq 1. \quad (7.23)$$

*Proof.* (1) We prove that  $g(\theta) = 1$ . We first prove that  $\mathcal{C}(\theta) \leq 1$ :

$$\mathcal{C}(\theta) = \left| \sum_r z_r a_r b_r \right| \leq \sum_r |z_r| \cdot |a_r b_r| \leq 1; \quad |a_r| \leq 1; \quad |b_s| \leq 1. \quad (7.24)$$

If  $z_r = |z_r| \exp(i\phi_r)$ , we chose  $a_r b_r = \exp(-i\phi_r)$  and we get  $\mathcal{C}(\theta) = 1$ . Therefore  $g(\theta) = 1$ , and  $\theta \in G_d$ .

Also

$$\mathcal{Q}\left(\frac{\theta}{g(\theta)}\right) = \mathcal{Q}(\theta) = \left| \sum_r z_r \lambda_r \mu_r \langle u_r | v_r \rangle \right| \leq \sum_r |z_r| \lambda_r \mu_r |\langle u_r | v_r \rangle| \leq 1$$

$$|u_r\rangle, |v_r\rangle \in H(d); \quad \lambda_r, \mu_r \leq 1. \quad (7.25)$$

If  $z_r = |z_r| \exp(i\phi_r)$ , we chose  $|v_r\rangle = \exp(-i\phi_r) |u_r\rangle$  and  $\lambda_r = \mu_r = 1$ , and we get the maximum value one. This proves the first inequality in Eq.(7.23).

(2) We consider the matrix  $\hat{\theta} = F\theta F^\dagger$  where  $\theta$  is the diagonal matrix in Eq.(7.22):

$$\hat{\theta}_{rs} = \frac{1}{d} \sum_t \omega^{(r-s)t} z_t. \quad (7.26)$$

This is a circulant matrix:

$$\hat{\theta}_{r,r+\nu} = \tilde{\theta}_\nu = \frac{1}{d} \sum_t \omega^{-\nu t} z_t; \quad \nu, t \in \mathbb{Z}_d. \quad (7.27)$$

In this case

$$\mathcal{C}(\hat{\theta}) = \left| \sum_{r,s} \hat{\theta}_{rs} a_r b_s \right| = \left| \sum_\nu \tilde{\theta}_\nu \left( \sum_r a_r b_{r+\nu} \right) \right|. \quad (7.28)$$

Here we changed variables from  $r, s$  in  $\mathbb{Z}_d$ , to  $r, \nu = s - r$  in  $\mathbb{Z}_d$ . We choose  $a_r = \omega^{-\kappa r}$  and  $b_{r+\nu} = \omega^{\kappa(r+\nu)}$  (where  $r, \kappa, \nu \in \mathbb{Z}_d$ ) and we show that in this case

$$\begin{aligned} \mathcal{C}(\hat{\theta}) &= \left| \sum_\nu \tilde{\theta}_\nu \left( \sum_r a_r b_{r+\nu} \right) \right| = d \left| \sum_\nu \tilde{\theta}_\nu \omega^{\kappa\nu} \right| = \left| \sum_\nu \sum_t z_t \omega^{(\kappa-t)\nu} \right| \\ &= d \left| \sum_t z_t \delta(\kappa, t) \right| = d |z_\kappa|. \end{aligned} \quad (7.29)$$

Since  $g(\hat{\theta})$  is the supremum of all  $\mathcal{C}(\hat{\theta})$  (for any value of  $\kappa$ ), it follows that

$$g(\hat{\theta}) \geq d \max\{|z_\kappa|\} \geq 1. \quad (7.30)$$

The  $\frac{\hat{\theta}}{g(\hat{\theta})} \in G_d$ . We next show that

$$\begin{aligned} \mathcal{Q}\left(\frac{\hat{\theta}}{g(\hat{\theta})}\right) &= \frac{1}{g(\hat{\theta})} \left| \sum_\nu \tilde{\theta}_\nu \left( \sum_r \lambda_r \mu_{r+\nu} \langle u_r | v_{r+\nu} \rangle \right) \right| \\ &\leq \frac{1}{g(\hat{\theta})} \sum_\nu \left[ |\tilde{\theta}_\nu| \left| \sum_r \lambda_r \mu_{r+\nu} \langle u_r | v_{r+\nu} \rangle \right| \right] \end{aligned} \quad (7.31)$$

Since

$$\left| \sum_r \lambda_r \mu_{r+\nu} \langle u_r | v_{r+\nu} \rangle \right| \leq \sum_r |\lambda_r \mu_{r+\nu} \langle u_r | v_{r+\nu} \rangle| \leq d \quad (7.32)$$

we get

$$\mathcal{Q} \left( \frac{\widehat{\theta}}{g(\widehat{\theta})} \right) = \frac{1}{g(\widehat{\theta})} d \sum_{\nu} |\widetilde{\theta}_{\nu}|. \quad (7.33)$$

From Eq.(7.27) we get

$$d|\widetilde{\theta}_{\nu}| \leq \sum_t |\omega^{-\nu t} z_t| = 1, \quad (7.34)$$

and taking into account Eq.(7.30) we conclude that

$$\mathcal{Q} \left( \frac{\widehat{\theta}}{g(\widehat{\theta})} \right) \leq 1. \quad (7.35)$$

This proves the second inequality in Eq.(7.23). □

We found that for diagonal  $\theta$  the  $\mathcal{Q} \leq 1$  for both  $\theta$  and  $\widehat{\theta}$ . The Fourier transform cannot (in general) change a state with  $\mathcal{Q} \leq 1$  into a state with  $\mathcal{Q} > 1$ . Fourier duality does not play an important role for quantumness according to Grothendieck quantities. Fourier duality is central for uncertainty relations, and therefore quantumness according to Grothendieck quantities is different from quantumness according to uncertainty relations.

## 7.5 Quantumness according to Grothendieck bound is different from quantumness according to quantum interference

Let  $\theta = |f\rangle\langle g|$ . We consider the corresponding matrix

$$\theta_{rs} = f_r g_s^*; \quad \sum_r |f_r|^2 = \sum_r |g_r|^2 = 1. \quad (7.36)$$

Also let  $U$  be a unitary matrix. The  $\text{Tr}(\theta U)$  is a wide class of quantum quantities.

We next calculate  $\mathcal{Q}$  using Eq.(7.13) for the matrix  $\frac{\theta}{g(\theta)} \in G_d$ , and  $V = U$  where  $U$  is a unitary matrix (and therefore  $U \in \mathcal{S}_d$ ), and  $W = \mathbf{1}_d$ :

$$\mathcal{Q} \left( \frac{\theta}{g(\theta)} \right) = \frac{\text{Tr}(\theta U)}{g(\theta)}. \quad (7.37)$$

**Proposition 7.5.1.**

$$\mathcal{Q} \left( \frac{\theta}{g(\theta)} \right) = \frac{\text{Tr}(\theta U)}{g(\theta)} \leq 1. \quad (7.38)$$

*Proof.* Since  $\text{Tr}(\theta U) \leq 1$  it is sufficient to prove that  $g(\theta) > 1$ . Indeed

$$\mathcal{C}(\theta) = \left| \sum_{r,s} f_r g_s^* a_r b_s \right|; \quad |a_r| \leq 1; \quad |b_s| \leq 1. \quad (7.39)$$

We choose  $a_r, b_s$  such that  $f_r a_r = |f_r|$  and  $g_s^* b_s = |f_s|$ . Then

$$g(\theta) \geq \mathcal{C}(\theta) = \sum_r |f_r| \sum_s |g_s| \geq 1. \quad (7.40)$$

This completes the proof.  $\square$

Oscillatory behaviour in quantities  $\langle g|U|f \rangle$  (e.g., [18, 19] in systems with large dimension), shows the quantum interference aspect of the quantumness of various states. But we have shown that the Grothendieck bound does not exceed one. So quantum interference described through oscillatory behaviour in quantities  $\langle g|U|f \rangle$ , and the Grothendieck bound describe different and complementary aspects of quantumness.

## 7.6 Discussion

The Grothendieck formalism provides a different approach to quantumness. It can be interpreted as a passage from classical to quantum mechanics, because it replaces a classical quadratic form  $\mathcal{C}$  that uses complex numbers in the unit disc, with a quantum quadratic form  $\mathcal{Q}$  that involves vectors in the unit ball of a Hilbert space. The Grothendieck theorem shows that if  $\mathcal{C} \leq 1$ , the corresponding quantum  $\mathcal{Q}$  might take values greater than 1, up to the complex Grothendieck constant  $k_G$ . Examples with  $\mathcal{Q} \in (1, k_G)$  (and in particular with  $\mathcal{Q}$  close to the upper bound  $k_G$ ) are ‘ultra-quantum’.

In this paper we consider the Grothendieck formalism in the context of a single quantum system with finite-dimensional Hilbert space. We compared and contrasted quantumness in the sense of the Grothendieck formalism with quantumness expressed through Fourier duality and uncertainty relations. If the uncertainty of a density matrix  $\theta$  is small, the uncertainty of its Fourier dual matrix  $\hat{\theta}$  is large. We explored whether a matrix  $\theta$  with  $\mathcal{Q}(\theta) \leq 1$ , has Fourier dual matrix  $\hat{\theta}$  with  $\mathcal{Q}(\hat{\theta})$  greater than one. Through an example (proposition 7.4.1), we have shown that this not true. Quantumness according to Grothendieck quantities is different from quantumness according to uncertainty relations.

We also compared and contrasted quantumness in the sense of the Grothendieck formalism with quantumness in the sense of quantum interference as shown with oscillations in quantities  $\langle g|U|f \rangle$  (where  $U$  is a unitary operator). We have shown that for all matrices  $\langle f|U|f \rangle$  (where  $U$  is **any** unitary operator) the corresponding Grothendieck quantity  $\mathcal{Q} \leq 1$  (proposition 7.5.1). Quantumness according to Grothendieck quantities is different from quantumness according to quantum interference.

We conclude that various approaches to quantumness are different from each other, and play complementary role to each other.

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