

Grothendieck bound in a single quantum system

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Grothendieck's bound is used in the context of a single quantum system, in contrast to previous work which used it for multipartite entangled systems and the violation of Bell-like inequalities. Roughly speaking the Grothendieck theorem considers a 'classical' quadratic form \mathcal{C} that uses complex numbers in the unit disc, and takes values less than 1. It then proves that if the complex numbers are replaced with vectors in the unit ball of the Hilbert space, then the 'quantum' quadratic form \mathcal{Q} might take values greater than 1, up to the complex Grothendieck constant k_G . The Grothendieck theorem is reformulated here in terms of arbitrary matrices (which are multiplied with appropriate normalisation prefactors), so that it is directly applicable to quantum quantities. The emphasis in the paper is in the 'Grothendieck region' $(1, k_G)$, which is a classically forbidden region in the sense that \mathcal{C} cannot take values in it. Necessary (but not sufficient) conditions for \mathcal{Q} taking values in the Grothendieck region are given. Two examples that involve physical quantities in systems with 6 and 12-dimensional Hilbert space, are shown to lead to \mathcal{Q} in the Grothendieck region $(1, k_G)$. They involve projectors of the overlaps of novel generalised coherent states that resolve the identity and have a discrete isotropy.

I. INTRODUCTION

Various inequalities play an important role in a quantum context. Uncertainty relations, entropic inequalities [1–3], Bell inequalities in multipartite entangled systems (e.g., [4–6]), etc. An important inequality in a pure mathematics context is the Grothendieck theorem [7–10], which has been applied in many areas. Work on examples that take values near the real and complex Grothendieck constants, is discussed in [11–13]. Applications to graph theory and computer science are discussed in [14].

The Grothendieck theorem has been used in a quantum context, for multipartite entangled systems [15–22]. Roughly speaking violation of Bell-like inequalities (e.g., the Clauser, Horne, Shimony, and Holt inequality [5]), corresponds to the fact that in the Hilbert space formalism some quantities can take values greater than one and up to the Grothendieck constant k_G . We note that in a quantum context, all previous work on the Grothendieck theorem is for entangled multipartite systems. In this paper we discuss a different application of the Grothendieck theorem which involves a single quantum system (and is not related to entanglement).

The original formulation of the Grothendieck theorem [7] was in the context of tensor product of Banach spaces, and this leads to the impression that applications in a quantum context should be for multipartite systems described by tensor products of Hilbert spaces. But all later mathematical work on Grothendieck's theorem [8–10] emphasised that the theory can also be formulated and is interesting, outside the framework of tensor product theory. And this motivated our work that uses a single quantum system (and is totally unrelated to tensor products, multipartite systems and entanglement).

The Grothendieck theorem considers a quadratic form \mathcal{C} that uses complex numbers in the unit disc, and takes values in $[0, 1]$. It then proves that if the complex numbers are replaced with vectors in the unit ball of the Hilbert space, the corresponding quantity \mathcal{Q} takes values in $[0, k_G)$, where k_G is the complex Grothendieck constant (for which it is known that $1 < k_G \leq 1.4049$). The complex numbers in the unit disc can be interpreted as classical quantities, and the vectors as quantum quantities (which embody the superposition principle through addition of vectors). In this sense going from \mathcal{C} to \mathcal{Q} is a passage from classical to quantum mechanics.

The Grothendieck bound is a 'mathematical ceiling' of the Hilbert formalism, and in turn of the quantum formalism which is intimately related to it. The 'classical ceiling' for \mathcal{C} is 1, while the 'quantum ceiling' for \mathcal{Q} is k_G . When \mathcal{Q} crosses from $[0, 1]$ to the 'Grothendieck region' $(1, k_G)$, it enters a classically forbidden region, and the study of this is the objective of this paper because it is 'quantum mechanics on the edge'. There are

large families of examples which show quantum behaviour (e.g., the Wigner and Weyl functions show clearly quantum interference), and yet the corresponding $\mathcal{Q} \in [0, 1]$ (section VI). In this sense the Grothendieck region is new territory of quantum mechanics with rare examples, e.g., the examples in sections 7, 8 (in Mathematics sometimes the interesting features are found in rare examples). Future work with random sampling of matrices, could quantify how rare the examples with $\mathcal{Q} \in (1, k_G)$ are.

We reformulate the Grothendieck theorem in terms of arbitrary $d \times d$ complex matrices, which are normalised. In this form the Grothendieck theorem is directly applicable to quantum mechanical quantities which are usually products of matrices. In order to do this we need two different types of normalisation which are introduced in sections 3,4. We then reformulate the Grothendieck theorem in terms of arbitrary matrices, which are normalised with these factors (proposition V.1), in section 5.

In section 6 we show that there are large families of examples with \mathcal{Q} which cannot take values in the Grothendieck region $(1, k_G)$. This leads to necessary (but not sufficient) conditions for \mathcal{Q} taking values in the Grothendieck region (corollary V.2 and proposition VI.1).

In section 7 we give a physical example that leads to $\mathcal{Q} \in (1, k_G)$. This example involves a projector in a quantum system with 6-dimensional Hilbert space. This projector contains the overlaps of novel generalised coherent states in a 3-dimensional Hilbert space, that resolve the identity and have a discrete isotropy. An analytical method shows that \mathcal{Q} enters the Grothendieck region $(1, k_G)$, and a numerical maximisation method shows that in this example, \mathcal{Q} can take the maximum value $\frac{6}{5}$.

In section 8 we generalise this example. Starting from novel generalised coherent states in a 4-dimensional Hilbert space that resolve the identity and have a discrete isotropy, we define (through their overlaps) a projector in a 12-dimensional Hilbert space, which leads to $\mathcal{Q} \in (1, k_G)$.

We conclude in section 9 with a discussion of our results.

II. PRELIMINARIES AND NOTATION

We consider a quantum system with variables in \mathbb{Z}_d (the integers modulo d), described by a d -dimensional Hilbert space $H(d)$. For a vector \mathbf{x} in $H(d)$, the scalar product and the norm are given by

$$(\mathbf{x}, \mathbf{y}) = \sum_i x_i^* y_i; \quad \|\mathbf{x}\| = \sqrt{(\mathbf{x}, \mathbf{x})}. \quad (1)$$

We will also use the usual bra and ket notation for normalised vectors in $H(d)$.

Let M be a complex $d \times d$ matrix with singular values s_i . We define the matrix norms

$$\|M\|_1 = \sum_{i,j} |M_{ij}|; \quad \|M\|_2 = \sqrt{\sum_{i,j} |M_{ij}|^2} = \sqrt{\text{Tr}(MM^\dagger)} = \sqrt{\sum_i s_i^2} \quad (2)$$

$\|M\|_2$ is the Frobenius norm, and it is invariant under unitary transformations. If e_i are the eigenvalues of M , its spectral radius is

$$e_{\max} = \max\{|e_i|\}; \quad e_{\max} \leq \|M\|_1; \quad e_{\max} \leq \|M\|_2. \quad (3)$$

We also define the spectral norm:

$$\|M\|_{\text{spe}} = \max_{\mathbf{x}} \frac{\|M\mathbf{x}\|}{\|\mathbf{x}\|} = \mathfrak{s}_{\max}. \quad (4)$$

Here \mathfrak{s}_{\max} is the largest singular value of M (for normal matrices $\mathfrak{s}_{\max} = e_{\max}$).

Example II.1. We consider the Fourier matrix

$$F_{ij} = \frac{1}{\sqrt{d}} \omega^{ij}; \quad \omega = \exp\left(\frac{i2\pi}{d}\right); \quad F^4 = \mathbf{1}. \quad (5)$$

In this case

$$\|F\|_1 = d\sqrt{d}; \quad \|F\|_2 = \sqrt{d}; \quad e_{\max} = 1. \quad (6)$$

Example II.2. We consider a density matrix ρ . In this case

$$\|\rho\|_1 \geq 1; \quad 1 \geq e_{\max} \geq \frac{1}{d}. \quad (7)$$

Indeed $\rho = UDU^\dagger$, where U is a unitary matrix and D is a diagonal matrix with its eigenvalues e_i . Then

$$\|\rho\|_1 \geq \sum_i |\rho_{ii}| = \sum_i \left| \sum_k U_{ik} e_k U_{ik}^* \right| \geq \left| \sum_k e_k \left(\sum_i U_{ik} U_{ik}^* \right) \right| = 1. \quad (8)$$

Also for non-negative numbers the maximum value is greater than the average value which for the eigenvalues of a density matrix is $\frac{1}{d}$.

A. The symmetric group Σ_ν

Let π be a permutation of elements of \mathbb{Z}_ν :

$$(0, 1, \dots, \nu - 1) \xrightarrow{\pi} (\pi(0), \pi(1), \dots, \pi(\nu - 1)). \quad (9)$$

π with the composition

$$(0, 1, \dots, \nu - 1) \xrightarrow{\pi} (\pi(0), \pi(1), \dots, \pi(\nu - 1)) \xrightarrow{\varpi} (\varpi[\pi(0)], \varpi[\pi(1)], \dots, \varpi[\pi(\nu - 1)]). \quad (10)$$

is an element of the symmetric group Σ_ν [23] which has $\nu!$ elements.

A permutation matrix τ_π is a $\nu \times \nu$ matrix with elements

$$\tau_\pi(i, j) = \delta(\pi(i), j), \quad (11)$$

Each row and each column have one element equal to 1 and the other $\nu - 1$ elements equal to 0.

III. THE SET \mathcal{S}_d OF $d \times d$ MATRICES

In this section we introduce the first normalisation of $d \times d$ complex matrices. We regard a matrix M as a set of d row vectors which we denote as \widehat{M}_i , with norms

$$\|\widehat{M}_i\| = \sqrt{\sum_j |M_{ij}|^2} = \sqrt{(MM^\dagger)_{ii}}; \quad \sum_i \|\widehat{M}_i\|^2 = (\|M\|_2)^2. \quad (12)$$

We define the normalisation factor for the matrix M

$$\mathcal{N}(M) = \max_i \|\widehat{M}_i\| = \max_i \sqrt{\sum_j |M_{ij}|^2} = \max_i \sqrt{(MM^\dagger)_{ii}}. \quad (13)$$

If z is a complex number, then

$$\mathcal{N}(zM) = |z| \mathcal{N}(M). \quad (14)$$

In general

$$\mathcal{N}(UMU^\dagger) \neq \mathcal{N}(M) \quad (15)$$

where U is a unitary transformation. Therefore in the calculation of the normalisation factor of an operator θ , it is important to specify an orthonormal basis $|u_i\rangle$ with respect to which we first find the matrix $\langle u_i|\theta|u_j\rangle$ and then the corresponding $\mathcal{N}(\theta; |u_i\rangle)$. In a different basis the \mathcal{N} will be different (in general). For operators, the notation will indicate clearly the basis.

In general $\mathcal{N}(M) \neq \mathcal{N}(M^\dagger)$. But for normal matrices $\mathcal{N}(M) = \mathcal{N}(M^\dagger)$, as shown in the following proposition.

Proposition III.1.

(1) If M is a matrix with singular values \mathfrak{s}_i

$$\frac{1}{\sqrt{d}}\|M\|_2 = \sqrt{\frac{\sum_i \mathfrak{s}_i^2}{d}} \leq \mathcal{N}(M) \leq \|M\|_2 \quad (16)$$

Under unitary transformations the two bounds are invariant, and the $\mathcal{N}(M)$ varies between them. If all $\|\widehat{M}_i\|$ are equal to each other, then the left inequality becomes equality. If all $\|\widehat{M}_i\|$ except one are zero (i.e., if all rows except one are zero), then the right inequality becomes equality.

(2) If M is a normal matrix and e_{\max} its spectral radius, then

$$\frac{1}{\sqrt{d}}\|M\|_2 = \sqrt{\frac{\sum_i |e_i|^2}{d}} \leq \mathcal{N}(M) = \mathcal{N}(M^\dagger) \leq e_{\max}. \quad (17)$$

Under unitary transformations the two bounds are invariant, and the $\mathcal{N}(M)$ varies between them. If all $\|\widehat{M}_i\|$ are equal to each other, then the left inequality becomes equality. If M is diagonal, then the right inequality becomes equality.

In the special case that M is a density matrix ρ , Eq.(17) becomes

$$\sqrt{\frac{\text{Tr}(\rho^2)}{d}} \leq \mathcal{N}(\rho) \leq e_{\max} \leq 1. \quad (18)$$

(3) For a unitary matrix U , we get $\mathcal{N}(U) = 1$ and $\|U\|_2 = \sqrt{d}$.

Proof.

(1) Since $\sum_i \|\widehat{M}_i\|^2 = (\|M\|_2)^2$, it follows that the maximum value of $\|\widehat{M}_i\|$ is $\|M\|_2$. If all $\|\widehat{M}_i\|$ except one are zero, then clearly the maximum value of $\|\widehat{M}_i\|$ is equal to $\|M\|_2$.

The $\sum_i \|\widehat{M}_i\|^2 = (\|M\|_2)^2$ also implies that the average value of $\|\widehat{M}_i\|$ is $\frac{1}{\sqrt{d}}\|M\|_2$. For positive numbers, the maximum value is greater than the average value and this proves the left inequality in Eq.(16). If all $\|\widehat{M}_i\|$ are equal to each other, then the maximum value of $\|\widehat{M}_i\|$ is equal to their average. In this case the left inequality becomes equality.

(2) We have

$$\mathcal{N}(M) = \max_i \sqrt{(MM^\dagger)_{ii}}; \quad \mathcal{N}(M^\dagger) = \max_i \sqrt{(M^\dagger M)_{ii}} \quad (19)$$

For normal matrices $M^\dagger M = MM^\dagger$ and therefore $\mathcal{N}(M) = \mathcal{N}(M^\dagger)$.

A normal matrix can be diagonalised with a unitary transformation as $M = UDU^\dagger$, where U is a unitary matrix, and $D = \text{diag}(e_0, \dots, e_{d-1})$. Then

$$\begin{aligned} \sum_j |M_{ij}|^2 &= \sum_j \left| \sum_k U_{ik} e_k U_{jk}^* \right|^2 = \sum_j \left(\sum_{k_1, k_2} U_{ik_1} e_{k_1} U_{jk_1}^* U_{ik_2}^* e_{k_2} U_{jk_2} \right) \\ &= \sum_{k_1, k_2} U_{ik_1} e_{k_1} U_{ik_2}^* e_{k_2} \left(\sum_j U_{jk_1}^* U_{jk_2} \right) = \sum_{k_1, k_2} U_{ik_1} e_{k_1} U_{ik_2}^* e_{k_2} \delta_{k_1 k_2} \\ &= \sum_{k_1} |U_{ik_1} e_{k_1}|^2 \leq (e_{\max})^2 \sum_{k_1} |U_{ik_1}|^2 = (e_{\max})^2 \end{aligned} \quad (20)$$

This proves the right inequality in Eq.(17). Clearly if M is diagonal, this inequality becomes equality.

The left inequality in Eq.(17) is the same as in Eq.(16). We note here that for normal matrices $\|M\|_2 = \sqrt{\sum_i |e_i|^2}$.

For a density matrix, $\|\rho\|_2 = \sqrt{\text{Tr}(\rho^2)} = \sqrt{\sum_i e_i^2}$.

(3) From Eq.(13) follows that $\mathcal{N}(U) = 1$ and then $\|U\|_2 = \sqrt{d}$.

□

Definition III.2. \mathcal{S}_d is the set of all matrices M with $\mathcal{N}(M) \leq 1$.

If V belongs to \mathcal{S}_d , then the matrix zV with $|z| \leq 1$ also belongs to \mathcal{S}_d .

Proposition III.3.

(1) For any $d \times d$ complex matrix \mathcal{V} , the matrix

$$V = \frac{1}{\mathcal{N}(\mathcal{V})} \mathcal{V}, \quad (21)$$

belongs to \mathcal{S}_d .

(2) All unitary matrices belong to \mathcal{S}_d . In particular the matrix $\mathbf{1}$ belongs to \mathcal{S}_d .

(3) If V belongs to \mathcal{S}_d , the V^\dagger might not belong to \mathcal{S}_d .

Proof.

(1) The normalisation factor ensures that the d rows of V , are vectors with norm less or equal to 1. In fact the maximum of these d norms is one.

(2) The normalisation factor for unitary matrices is one.

(3) We have explained earlier that in general $\mathcal{N}(V) \neq \mathcal{N}(V^\dagger)$, and therefore the $\mathcal{N}(V) \leq 1$ does not imply $\mathcal{N}(V^\dagger) \leq 1$.

□

IV. THE SET G_d OF $d \times d$ MATRICES

In this section we introduce the second normalisation of $d \times d$ complex matrices. Let $\mathcal{D} = \{|z| \leq 1\}$ be the unit disc in the complex plane, and \mathcal{D}^d the set of all d -tuples (s_0, \dots, s_{d-1}) where $s_i \in \mathcal{D}$.

Definition IV.1. G_d is the set of all $d \times d$ complex matrices θ , such that for all d -tuples (s_0, \dots, s_{d-1}) and (t_0, \dots, t_{d-1}) in \mathcal{D}^d , we get

$$C = \left| \sum_{i,j} \theta_{ij} s_i t_j \right| \leq 1; \quad |s_i| \leq 1; \quad |t_j| \leq 1. \quad (22)$$

If θ belongs in G_d , then the matrix $z\theta$ with $|z| \leq 1$ also belongs to G_d .

Definition IV.2. G'_d is the set of all $d \times d$ complex matrices θ , such that for all d -tuples (s_0, \dots, s_{d-1}) and (t_0, \dots, t_{d-1}) where $\sum_i |s_i|^2 \leq d$, $\sum_j |t_j|^2 \leq d$, we get

$$\left| \sum_{i,j} \theta_{ij} s_i t_j \right| \leq 1; \quad \sum_i |s_i|^2 \leq d; \quad \sum_j |t_j|^2 \leq d. \quad (23)$$

Here we use d -tuples which belong to a superset of \mathcal{D}^d , and therefore $G'_d \subset G_d$. The physical importance of G'_d is seen in proposition VI.1 below. For normal matrices $\theta \in G'_d$ the quantity \mathcal{Q} (defined later) cannot take values in the Grothendieck region $(1, k_G)$. A necessary (but not sufficient) condition for $\mathcal{Q} \in (1, k_G)$ is that $\theta \in G_d \setminus G'_d$.

Definition IV.3. For any $d \times d$ complex matrix θ ,

$$g(\theta) = \sup \left\{ \left| \sum_{i,j} \theta_{ij} s_i t_j \right|; \quad |s_i| \leq 1; \quad |t_j| \leq 1 \right\}, \quad (24)$$

and

$$g'(\theta) = \sup \left\{ \left| \sum_{i,j} \theta_{ij} s_i t_j \right|; \quad \sum_i |s_i|^2 \leq d; \quad \sum_j |t_j|^2 \leq d \right\}. \quad (25)$$

Proposition IV.4. $g'(\theta) = d\mathfrak{s}_{\max}$ where \mathfrak{s}_{\max} is the largest singular value of θ . For normal matrices $g'(\theta) = d\epsilon_{\max}$, and for unitary matrices $g'(\theta) = d$.

Proof. We consider the vectors

$$\mathbf{s} = \left(\frac{s_i}{\sqrt{d}} \right); \quad \theta\mathbf{t} = \left(\sum_j \theta_{ij} \frac{t_j}{\sqrt{d}} \right). \quad (26)$$

In Eq.(25) we have $\sum_i |s_i|^2 \leq d$ and $\sum_j |t_j|^2 \leq d$, but since we are interested in the supremum we take $\|\mathbf{s}\| = \|\mathbf{t}\| = 1$. Then

$$\|\theta\|_{\text{spe}} = \max_{\|\mathbf{t}\|=1} \|\theta\mathbf{t}\| = \mathfrak{s}_{\max}. \quad (27)$$

We use the Cauchy-Schwartz inequality and we get

$$\left| \sum_{i,j} \theta_{ij} s_i t_j \right| = d|(\mathbf{s}, \theta\mathbf{t})| \leq d\|\mathbf{s}\| \cdot \|\theta\mathbf{t}\| \leq d\mathfrak{s}_{\max}. \quad (28)$$

We note that we get equality only if the two vectors are proportional to each other, i.e., if we choose

$$\mathbf{s} = \frac{\theta \mathbf{t}}{\|\theta \mathbf{t}\|}. \quad (29)$$

This proves that $g'(\theta) = d\mathfrak{s}_{\max}$.

For normal matrices $\mathfrak{s}_{\max} = e_{\max}$, and for unitary matrices $e_{\max} = 1$. □

It is easily seen that

- By definition if $\theta \in G_d$ then $g(\theta) \leq 1$, and if $\theta \in G'_d$ then $g'(\theta) \leq 1$.
- The following inequalities hold:

$$g(\theta) \leq g'(\theta) = d\mathfrak{s}_{\max}; \quad g(\theta) \leq \|\theta\|_1. \quad (30)$$

- For any $d \times d$ complex matrix θ , we get

$$\begin{aligned} \lambda \leq \frac{1}{d\mathfrak{s}_{\max}} &\rightarrow \lambda\theta \in G'_d \\ \frac{1}{d\mathfrak{s}_{\max}} \leq \lambda \leq \frac{1}{g(\theta)} &\rightarrow \lambda\theta \in G_d \setminus G'_d. \end{aligned} \quad (31)$$

- Necessary (but not sufficient) conditions for $\theta \in G'_d$, are:

$$|\theta_{ij}| \leq \frac{1}{d}; \quad \|\theta\|_1 \leq d; \quad \|\theta\|_2 \leq 1. \quad (32)$$

We prove this if we take $s_i = t_j = \sqrt{d}$ and the rest of them zero.

- Necessary (but not sufficient) conditions for $\theta \in G_d$, are

$$|\theta_{ij}| \leq 1; \quad \|\theta\|_1 \leq d^2; \quad \|\theta\|_2 \leq d. \quad (33)$$

We prove this if we take $s_i = t_j = 1$ and the rest of them zero.

- If U is a unitary matrix then in general

$$g(U\theta U^\dagger) \neq g(\theta) \quad (34)$$

Example IV.5. We consider the matrix

$$\begin{aligned} \theta_{ij} &= 1 \text{ if } i = a \text{ and } j = b \\ \theta_{ij} &= 0 \text{ otherwise} \end{aligned} \quad (35)$$

Then:

- For $\frac{1}{d} < \lambda \leq 1$, the matrix $\lambda\theta$ belongs in G_d but does not belong in G'_d .
- For $\lambda \leq \frac{1}{d}$ the matrix $\lambda\theta$ belongs in G'_d (and therefore in G_d).

Indeed, if $|s_i| \leq 1$, $|t_j| \leq 1$ and $\lambda \leq 1$ the matrix $\lambda\theta$ gives

$$\lambda \left| \sum_{i,j} \theta_{ij} s_i t_j \right| = \lambda |s_a t_b| \leq 1. \quad (36)$$

But if $s_i = t_j = \sqrt{d}$ and the other s_k, t_k are zero (in which case $\sum_i |s_i|^2 \leq d$ and $\sum_j |t_j|^2 \leq d$), we get

$$\lambda \left| \sum_{i,j} \theta_{ij} s_i t_j \right| = \lambda d. \quad (37)$$

Therefore only for $\lambda \leq \frac{1}{d}$ the matrix $\lambda\theta \in G'_d$. And for $\frac{1}{d} < \lambda \leq 1$, the matrix $\lambda\theta$ belongs in $G_d \setminus G'_d$.

Example IV.6. Let π be a permutation as in Eq.(9). We consider the $d \times d$ matrix with elements

$$\theta_{ij} = a_i \delta(i, \pi(j)); \quad \|\theta\|_1 = \sum_i |a_i| \leq 1, \quad (38)$$

They are related to the permutation matrices in Eq(11), but here the ones are replaced with a_i (with $\sum_i |a_i| \leq 1$). Each row and each column have one of the elements a_i , and the other $d - 1$ elements equal to 0. Then $g(\theta) = \|\theta\|_1 \leq 1$ and θ belongs to G_d .

Examples are the ‘backslash’ matrices

$$\theta_{ij} = a_i \delta_{i,j+k}; \quad \|\theta\|_1 = \sum_i |a_i| \leq 1, \quad (39)$$

and also the ‘forward slash’ matrices

$$\theta_{ij} = a_i \delta_{i,-j+k}; \quad \|\theta\|_1 = \sum_i |a_i| \leq 1. \quad (40)$$

We have seen that $g(\theta) \leq \|\theta\|_1$, and we now explore when this is equality and when it is a strict inequality. We consider the expression $\sum_{i,j} \theta_{ij} s_i t_j$ and express the non-zero elements of θ_{ij} and the s_i, t_j as

$$\theta_{ij} = |\theta_{ij}| \exp(i\phi_{ij}); \quad s_i = |s_i| \exp(-i\chi_i); \quad t_j = |t_j| \exp(-i\psi_j). \quad (41)$$

Then

$$\left| \sum_{i,j} \theta_{ij} s_i t_j \right| = \left| \sum_{i,j} |\theta_{ij} s_i t_j| \exp[i(\phi_{ij} - \chi_i - \psi_j)] \right| \quad (42)$$

Therefore if for all $\theta_{ij} \neq 0$ we have

$$\phi_{ij} - \chi_i - \psi_j = 0, \quad (43)$$

then $g(\theta)$ takes its maximum possible value $\|\theta\|_1$ (we take $|s_i| = |t_j| = 1$, and choose the solutions of the system as their phases χ_i, ψ_j). If N elements θ_{ij} are non-zero, this is a system of N equations with $2d$ unknowns (χ_i, ψ_j). If this system has a solution then $g(\theta) = \|\theta\|_1$, otherwise $g(\theta) < \|\theta\|_1$.

Roughly speaking the system will have a solution when $N \leq 2d$, and it will have no solution when $N > 2d$. But this is not always true (see example IV.9 below).

Lemma IV.7. We express the system in Eq.(43) as $AB = C$ where A is a $N \times (2d)$ matrix, and B, C are columns with $2d$ and N elements, correspondingly. We also consider the $N \times (2d + 1)$ ‘augmented matrix’ D , which is the matrix A with the matrix C as an extra column. Then

- if $\text{rank}(D) > \text{rank}(A)$, then the system has no solution and $g(\theta) < \|\theta\|_1$.
- if $\text{rank}(D) = \text{rank}(A)$, then the system has a solution and $g(\theta) = \|\theta\|_1$.

Proof. This is based on the Rouché-Capelli theorem. \square

In the proposition below we give general examples of matrices in G_d . We also give stronger results (i.e., with larger prefactor) for normal matrices.

Proposition IV.8. (1) For any $d \times d$ complex matrix M , the matrix λM with

$$\lambda \leq \frac{1}{\|M\|_1} \quad (44)$$

belongs to G_d .

(2) Let M be a $d \times d$ normal matrix with spectral radius e_{\max} . Then

$$\begin{aligned} \lambda M \in G'_d; \quad & \text{for } \lambda \leq \frac{1}{de_{\max}} \\ \lambda M \in G_d \setminus G'_d; \quad & \text{for } \frac{1}{de_{\max}} \leq \lambda \leq \frac{1}{g(M)}. \end{aligned} \quad (45)$$

Proof. (1) This follows from the fact that $g(M) \leq \|M\|_1$.

(2) We use Eq.(31) with $\mathfrak{s}_{\max} = e_{\max}$ for normal matrices. \square

Example IV.9. We consider the Hermitian matrix

$$M = \begin{pmatrix} a & b \\ b^* & -c \end{pmatrix}; \quad a \geq c > 0; \quad b \in \mathbb{C}; \quad b \neq 0. \quad (46)$$

In this case the system of Eq.(43) has 4 equations with 4 unknowns:

$$\begin{aligned} \chi_0 + \psi_0 &= 0 \\ \chi_1 + \psi_1 &= -\pi \\ \chi_0 + \psi_1 &= \arg(b) \\ \chi_1 + \psi_0 &= -\arg(b), \end{aligned} \quad (47)$$

It is easily seen that this system has no solution, and therefore $g(M) < \|M\|_1 = a+c+2|b|$ (for more complicated examples we can use lemma IV.7).

For the matrix M we find

$$e_{\max} = \frac{1}{2} \left[a - c + \sqrt{(a+c)^2 + 4|b|^2} \right]. \quad (48)$$

Then

$$\begin{aligned} \lambda M \in G'_2 \quad & \text{for } \lambda \leq \frac{1}{\left[a - c + \sqrt{(a+c)^2 + 4|b|^2} \right]} \\ \lambda M \in G_2 \setminus G'_2 \quad & \text{for } \frac{1}{\left[a - c + \sqrt{(a+c)^2 + 4|b|^2} \right]} \leq \lambda \leq \frac{1}{a+c+2|b|} \end{aligned} \quad (49)$$

Here we do not know the exact value of $\frac{1}{g(M)}$, and we used the $\frac{1}{a+c+2|b|}$ which is a lower bound to it. But clearly there are some values of λ greater than $\frac{1}{a+c+2|b|}$ for which $\lambda M \in G_2 \setminus G'_2$.

V. THE GROTHENDIECK THEOREM IN TERMS OF MATRICES IN \mathcal{S}_d AND G_d

Let \mathcal{B}_d the unit ball in the Hilbert space $H(d)$ (it contains vectors $\lambda|u\rangle$ with $\lambda \leq 1$). The Grothendieck theorem proves that if Eq.(22) holds (i.e., if $\theta \in G_d$), then for all $(\lambda_0|u_0\rangle, \dots, \lambda_{d-1}|u_{d-1}\rangle)$ and $(\mu_0|v_0\rangle, \dots, \mu_{d-1}|v_{d-1}\rangle)$ where $\lambda_i|u_i\rangle, \mu_j|v_j\rangle \in \mathcal{B}_d$, we get

$$\mathcal{Q} = \left| \sum_{i,j} \theta_{ij} \lambda_i \mu_j \langle u_i | v_j \rangle \right| \leq k(d) \leq k_G; \quad \lambda_i, \mu_j \leq 1. \quad (50)$$

Here $k(d)$ is a constant that depends on the dimension d . $k(d)$ is a non-decreasing function of d (because every matrix can be written as a larger matrix with extra zeros). Then

$$\lim_{d \rightarrow \infty} k(d) = k_G. \quad (51)$$

k_G is the complex Grothendieck constant, which does not depend on the dimension d . Its exact value is not known, but it is known that $1 < k_G \leq 1.4049$.

An obvious upper bound for the left hand side in Eq.(50) is $\|\theta\|_1$. Therefore we rewrite Eq.(50) as

$$\mathcal{Q} = \left| \sum_{i,j} \theta_{ij} \lambda_i \mu_j \langle u_i | v_j \rangle \right| \leq \min(k_G, \|\theta\|_1); \quad \lambda_i, \mu_j \leq 1. \quad (52)$$

Proposition V.1. *Let θ, V, W be $d \times d$ matrices such that $\theta \in G_d$ and $W, V \in \mathcal{S}_d$. Then*

$$\mathcal{Q} = |\text{Tr}(\theta V W^\dagger)| \leq \min(k_G, \|\theta\|_1). \quad (53)$$

For arbitrary matrices, appropriate normalisation (as in propositions III.3, IV.8) leads to matrices that satisfy the requirement $\theta \in G_d$ and $W, V \in \mathcal{S}_d$.

Proof. We consider the $d \times d$ matrix A with elements

$$A_{ji} = \lambda_i \mu_j \langle u_i | v_j \rangle; \quad \lambda_i, \mu_j \leq 1. \quad (54)$$

The matrix A can be written as $A = V W^\dagger$ where V is a $d \times d$ matrix that has the components of $\mu_j|v_j\rangle$ in the j -row, and W is a matrix that has the components of $\lambda_i|u_i\rangle$ in the i -row (therefore W^\dagger has the complex conjugates of the components of $\lambda_i|u_i\rangle$ in the i -column). Consequently W, V are matrices with d row vectors that have norm less or equal to 1:

$$\sum_j |W_{ij}|^2 \leq 1; \quad \sum_j |V_{ij}|^2 \leq 1. \quad (55)$$

Therefore W, V belong to \mathcal{S}_d . So Eq.(52) leads to Eq.(53).

If we take $\lambda_i = 1$ and $|u_i\rangle$ to be the orthonormal basis

$$|u_i\rangle = (0, \dots, 0, 1_i, 0, \dots, 0)^\dagger \quad (56)$$

then $W = \mathbf{1}$. □

From this proposition follows immediately the following:

Corollary V.2. *Let θ, V, W be $d \times d$ matrices such that $\theta \in G_d$ (and therefore by definition $g(\theta) \leq 1$) and $W, V \in \mathcal{S}_d$. A necessary (but not sufficient) condition for $\mathcal{Q} = |\text{Tr}(\theta V W^\dagger)| \in (1, k_G)$ is that*

$$g(\theta) \leq 1 < \|\theta\|_1. \quad (57)$$

A. Non-diagonal elements are important for $\mathcal{Q} \in (1, k_G)$

Proposition V.3. *Let $W, V \in \mathcal{S}_d$ and θ be a diagonal matrix with $\sum_i |\theta_{ii}| \leq 1$, in which case $\theta \in G_d$ (see example IV.6). Then $\mathcal{Q} = |\text{Tr}(\theta VW^\dagger)| \leq 1$ (it cannot take values in the region $(1, k_G)$).*

Proof. A direct and easy way to prove this is from the following inequalities (for diagonal matrix θ):

$$\begin{aligned} \mathcal{C} &= \left| \sum_{i,j} \theta_{ij} s_i t_j \right| \leq \sum_i |\theta_{ii}| \leq 1; \quad |s_i| \leq 1; \quad |t_j| \leq 1 \\ \mathcal{Q} &= \left| \sum_{i,j} \theta_{ij} \lambda_i \mu_j \langle u_i | v_j \rangle \right| \leq \sum_i |\theta_{ii}| \leq 1; \quad \lambda_i, \mu_j \leq 1. \end{aligned} \quad (58)$$

□

It follows that if $\mathcal{Q} = |\text{Tr}(\theta VW^\dagger)| \in (1, k_G)$, then the matrix θ has non-zero off-diagonal elements, **in a basis such that the assumptions $W, V \in \mathcal{S}_d$ and $\theta \in G_d$ hold**. If the matrix θ is diagonalisable with a unitary transformation U as $\theta = U \theta_{\text{diag}} U^\dagger$ (where θ_{diag} is a diagonal matrix with its eigenvalues), then

$$\mathcal{Q} = |\text{Tr}(\theta VW^\dagger)| = |\text{Tr}[\theta_{\text{diag}}(U^\dagger V U)(U^\dagger W^\dagger U)]| \in (1, k_G). \quad (59)$$

There is no contradiction between the right hand side of this equation and our statement that if $\mathcal{Q} \in (1, k_G)$ then θ has non-zero off-diagonal elements. If $V, W \in \mathcal{S}_d$, the $U^\dagger V U$ and $U^\dagger W^\dagger U$ might not belong to \mathcal{S}_d (related to this is Eq.(15)) and then proposition V.1 does not apply to the right hand side of this expression.

In the ‘Grothendieck formalism’, the assumption $\mathcal{C} \leq 1$ in Eq.(22) might not hold after unitary transformations of the matrix θ (related is Eq.(34)). In the formulation in proposition V.1, the assumptions $V, W \in \mathcal{S}_d$ might not hold after unitary transformations.

If θ is a density matrix, the non-diagonal elements are physically important because they are related to the superposition principle. A diagonal density matrix simply represents a probabilistic mixture of states. ‘Quantumness’ is in the non-diagonal elements. In this sense quantumness (non-diagonal elements in the density matrix) are needed for $\mathcal{Q} \in (1, k_G)$.

B. Examples and physical importance

Many physical quantities can be written as $\text{Tr}(\theta VW^\dagger)$. The requirement in proposition V.1 that $\theta \in G_d$ and $W, V \in \mathcal{S}_d$, is not a restriction, because we have shown that arbitrary matrices with appropriate normalisation will satisfy this requirement (propositions III.3, IV.8).

Examples:

- If θ is a density matrix and VW^\dagger is an observable (Hermitian operator) then $|\text{Tr}(\theta VW^\dagger)|$ is the expectation value $|\langle VW^\dagger \rangle|$. Alternatively, if θ is a Hermitian operator and VW^\dagger is a density matrix, then $|\text{Tr}(\theta VW^\dagger)|$ is the expectation value $|\langle \theta \rangle|$.
- If θ is a density matrix and VW^\dagger is a displacement operator or displaced parity operator (defined for example in [24, 25] and in the references therein), then $|\text{Tr}(\theta VW^\dagger)|$ is the absolute value of the Weyl or the Wigner function correspondingly.

From a physical point of view, the Grothendieck theorem replaces the complex numbers $s_i, t_j \in \mathcal{D}$ in \mathcal{C} , with the vectors $\lambda_i |u_i\rangle, \mu_j |v_j\rangle \in \mathcal{B}_d$ in \mathcal{Q} . We regard the s_i, t_j as classical quantities, and the $\lambda_i |u_i\rangle, \mu_j |v_j\rangle$ as the corresponding quantum quantities (which are vectors so that we can have superpositions). Roughly speaking the Grothendieck theorem says that when a classical quadratic form \mathcal{C} takes values less than 1, the

corresponding quantum quantity \mathcal{Q} might take values greater than 1, up to the Grothendieck constant k_G . Quantum Mechanics is described with Hilbert spaces, and should agree with all predictions of the Hilbert space formalism, like the Grothendieck bounds.

In this paper we are particularly interested in the Grothendieck region $(1, k_G)$ which cannot be reached by the corresponding classical models, and which (as we explain below) is related to non-diagonal elements in the density matrix, that in turn are related to the superposition principle. Quantities for which \mathcal{Q} takes values in the Grothendieck region $(1, k_G)$, are in the ‘mathematical ceiling’ of the Hilbert space formalism and therefore of the quantum formalism that is based on it. They are quantum mechanics ‘on the edge’.

We explain below in section VI that important quantities like the Wigner and Weyl functions which show clearly quantum phenomena (like quantum interference), do not take values in the Grothendieck region. In this sense the Grothendieck region is a ‘new territory’ with rare examples of quantum mechanics. The term ‘rare’ needs further work to be quantified, but a result in this direction is in the next section, where we show that there are large families of examples which cannot take values in $(1, k_G)$.

Later in sections VII, VIII we give physical examples which take values in $(1, k_G)$.

VI. FAMILIES OF EXAMPLES WHICH CANNOT TAKE VALUES IN $(1, k_G)$

In the rest of the paper we are interested in the case where $\mathcal{Q} = |\text{Tr}(\theta VW^\dagger)|$ with $\theta \in G_d$ and $W, V \in \mathcal{S}_d$, takes values in the Grothendieck region $(1, k_G)$. In this section we show that there are large families of examples where \mathcal{Q} cannot take values in the Grothendieck region $(1, k_G)$. They include physical quantities like the Wigner and Weyl functions that show clearly quantum interference.

This implies that examples that take values in the Grothendieck region are infrequent. Especially if we want to get close to k_G we need large matrices [11]. How infrequent examples with values in the Grothendieck region are, could be quantified in future work by producing randomly a triplet of matrices (normalise them appropriately so that the first belongs in G_d and the other two in \mathcal{S}_d) and then find the percentage for which $\mathcal{Q} \in (1, k_G)$.

The following proposition shows that for normal matrices in G'_d (which can be written as $\frac{K}{de_{\max}}$ where K is any normal matrix), we get $\mathcal{Q} \leq 1$.

Proposition VI.1. *Let K be a $d \times d$ normal matrix, M any $d \times d$ complex matrix, and*

$$\theta = \frac{K}{de_{\max}} \in G'_d; \quad V = \frac{M}{\mathcal{N}(M)} \in \mathcal{S}_d; \quad W = \mathbf{1} \in \mathcal{S}_d. \quad (60)$$

Then

$$\mathcal{Q} = |\text{Tr}(\theta VW^\dagger)| = \frac{1}{de_{\max}\mathcal{N}(M)} |\text{Tr}(KM)| \leq 1. \quad (61)$$

We get $\mathcal{Q} = 1$ when $K_{ij} = aM_{ij}$ with $a \leq 1$, and also $\|K\|_2 = \sqrt{de_{\max}}$ and $\|M\|_2 = \sqrt{d}\mathcal{N}(M)$.

Proof. $\text{Tr}(KM)$ can be viewed as inner product of a vector with d^2 elements K_{ij} with a vector with d^2 elements M_{ji} . We apply the Cauchy-Schwartz inequality and we get:

$$|\text{Tr}(KM)| = \left| \sum_{i,j} K_{ij}M_{ji} \right| \leq \sqrt{\sum_{i,j} |K_{ij}|^2} \sqrt{\sum_{i,j} |M_{ji}|^2} = \|K\|_2 \|M\|_2. \quad (62)$$

But for normal matrices, $\|K\|_2 \leq \sqrt{de_{\max}}$ (Eq.(17)). Also $\|M\|_2 \leq \sqrt{d}\mathcal{N}(M)$ (Eq.(16)). Therefore $\|K\|_2 \|M\|_2 \leq de_{\max}\mathcal{N}(M)$. This proves the statement.

In order to get equality in Eq.(61), we need K_{ij} to be proportional to M_{ij} and also $\|K\|_2 = \sqrt{de_{\max}}$ and $\|M\|_2 = \sqrt{d}\mathcal{N}(M)$. We have seen in Eq.(17) that for normal matrices $\mathcal{N}(M) \leq e_{\max}$ and this gives $a \leq 1$. \square

Corollary VI.2. For a normal matrix θ , a necessary (but not sufficient) condition for $\mathcal{Q} \in (1, k_G)$ is that $\theta \in G_d \setminus G'_d$.

Example VI.3. For unitary matrices $e_{\max} = 1$ and $\mathcal{N} = 1$. We take

$$\theta = \frac{1}{d}F^2 \in G'_d; \quad V = F^2 \in \mathcal{S}_d; \quad W = \mathbf{1} \in \mathcal{S}_d \quad (63)$$

where F is the Fourier transform in Eq.(5), and we get

$$\mathcal{Q} = |\text{Tr}(\theta V W^\dagger)| = \frac{1}{d} \text{Tr}(\mathbf{1}) = 1. \quad (64)$$

Below are more cases which cannot take values in the Grothendieck region.

Example VI.4. For a density matrix ρ and a unitary matrix U ,

$$|\text{Tr}(\rho U)| \leq 1. \quad (65)$$

Indeed if e_i and $|e_i\rangle$ are the eigenvalues and eigenvectors of ρ , we get

$$|\text{Tr}(\rho U)| = \left| \sum_i e_i \langle e_i | U | e_i \rangle \right| \leq \sum_i e_i |\langle e_i | U | e_i \rangle| \leq \sum_i e_i = 1. \quad (66)$$

Application of the Grothendieck theorem would be to use proposition V.1 with

$$\theta = \frac{\rho}{de_{\max}} \in G'_d; \quad V = U \in \mathcal{S}_d; \quad W = \mathbf{1} \in \mathcal{S}_d, \quad (67)$$

where e_{\max} is the spectral radius of ρ . This gives the upper bound

$$\frac{1}{de_{\max}} |\text{Tr}(\rho U)| \leq \min \left(k_G, \frac{\|\rho\|_1}{de_{\max}} \right) \rightarrow |\text{Tr}(\rho U)| \leq \min (de_{\max} k_G, \|\rho\|_1) \quad (68)$$

We have seen in example II.2 that $\|\rho\|_1 \geq 1$ and $de_{\max} \geq 1$. Therefore for $|\text{Tr}(\rho U)|$, the upper bound 1 in Eq.(66) is better (lower) than the bound in Eq.(68). It is seen that $|\text{Tr}(\rho U)|$ cannot take values in the Grothendieck region which in this case is $de_{\max} \times (1, k_G)$.

Physical examples of $\text{Tr}(\rho U)$ are the Weyl and Wigner functions. If U is one of the displacement operators $D(a, b)$ (defined for example in [24, 25] and in the references therein), then

$$\mathcal{Q}(a, b) = |\text{Tr}[\rho D(a, b)]| \quad (69)$$

is the absolute value of the Weyl function. Also if U is one of the displaced parity operators $P(a, b)$ (defined for example in [24, 25] and in the references therein) we get the absolute value of the Wigner function

$$\mathcal{Q}(a, b) = |\text{Tr}[\rho P(a, b)]|. \quad (70)$$

These functions show quantum behaviour, and yet they cannot take values in the Grothendieck region.

VII. EXAMPLE IN $H(6)$ WITH VALUES IN THE GROTHENDIECK REGION $(1, k_G)$

We give an example that involves physical quantities in a quantum system with 6-dimensional Hilbert space. We start with novel generalised coherent states in $H(3)$ with a discrete isotropy. Their overlaps lead to a 6×6 projector Π . In section VIII A we show that the discrete isotropy of the coherent states leads to the strict inequality $g(\Pi) < 6$. Consequently, \mathcal{Q} that involves $\lambda \Pi$ with $\lambda \in (\frac{1}{6}, \frac{1}{g(\Pi)})$ takes values in the Grothendieck region $(1, k_G)$.

In section VIII D, we perform a numerical maximisation which proves that $g(\Pi) = 5$ and then \mathcal{Q} can reach the value $\frac{6}{5}$. If go to large matrices, numerical maximisation with large number of variables can be difficult, and there is merit in analytical methods like the one in section VIII A.

A. Generalised coherent states in $H(3)$ with discrete isotropy

In $H(3)$, we introduce the following 6 quantum states

$$\begin{aligned} |a_0\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}; & |a_1\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}; & |a_2\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \\ |a_3\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}; & |a_4\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}; & |a_5\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} \end{aligned} \quad (71)$$

They have been used in ref[11] in a real Hilbert space in connection with the real Grothendieck constant. Here, firstly we interpret them as generalised coherent states in $H(3)$, and we use them in a complex Hilbert space in connection with the complex Grothendieck constant. We note a discrete isotropy in these states, in the sense that the relationship of a state $|a_i\rangle$ to the rest of them, is the same for all i . This intuitive and qualitative statement is quantified below.

The states $\{|a_i\rangle\}$ are generalised coherent states in the sense of the following proposition:

Proposition VII.1. (1) *The states $\{|a_i\rangle\}$ resolve the identity:*

$$\frac{1}{2} \sum_{i=0}^5 |a_i\rangle\langle a_i| = \mathbf{1}. \quad (72)$$

(2) *The set $\{|a_0\rangle, \dots, |a_5\rangle\}$ is invariant under transformations in the symmetric group Σ_3 , in the sense that for any $\tau_\pi \in \Sigma_3$ (defined in Eq.(11)) and any i the state $\tau_\pi|a_i\rangle$ is one of the states $|a_j\rangle$ (possibly with a physically insignificant phase factor).*

(3) *There is a ‘discrete isotropy’ between the states $|a_i\rangle$, in the sense that the set of 6 non-independent probabilities*

$$A_i = \{|\langle a_i|a_j\rangle|^2 \mid j = 0, \dots, 5\}, \quad (73)$$

is the same for all i . Therefore the following sum does not depend on i :

$$\sum_{j=0}^5 |\langle a_i|a_j\rangle|^r = 1 + \frac{1}{2^{r-2}}; \quad r = 1, 2, 3, \dots \quad (74)$$

For $r = 1$ this sum involves square roots of the probabilities $|\langle a_i|a_j\rangle|^2$. For $r = 2$ this result follows immediately from the resolution of the identity in Eq.(72).

Proof. (1) This is proved with direct calculation using the vectors in Eq.(71).

(2) This is also proved with direct calculation using the vectors in Eq.(71).

(3) We see this through the projector Π in Eq.(80) below (which contains the overlaps of the coherent states). Each row or each column has one $|\Pi_{ij}| = \frac{2}{4}$, four $|\Pi_{ij}| = \frac{1}{4}$, and one $|\Pi_{ij}| = 0$. From this follows immediately Eq.(74). □

Coherent states resolve the identity and their set is invariant under some group of transformations. Many of the coherent states studied in the literature, are non-orthogonal to each other. In the present case the state $|a_i\rangle$ is orthogonal to the state $|a_{i+3}\rangle$ (the indices are defined modulo 6).

For any state $|f\rangle$ the $\{|\langle f|a_i\rangle|^2\}$ is a set of 6 non-independent probabilities with

$$\frac{1}{2} \sum_{i=0}^5 |\langle f|a_i\rangle|^2 = 1. \quad (75)$$

The $|a_i\rangle\langle a_i|$ and $|a_j\rangle\langle a_j|$ do not commute, and therefore these probabilities are not simultaneously measurable. They can be measured using different ensembles of the state $|f\rangle$ for each measurement.

An arbitrary state in $H(3)$

$$|f\rangle = \begin{pmatrix} f_0 \\ f_1 \\ f_2 \end{pmatrix}; \quad |f_0|^2 + |f_1|^2 + |f_2|^2 = 1, \quad (76)$$

can be expanded in terms of them as

$$|f\rangle = \sum_{i=0}^5 f_i |a_i\rangle; \quad f_i = \frac{1}{2} \langle a_i|f\rangle; \quad \langle g|f\rangle = \sum_{i=0}^2 g_i^* f_i = 2 \sum_{i=0}^5 g_i^* f_i. \quad (77)$$

It is easily seen that

$$\begin{aligned} f_0 &= \frac{1}{2\sqrt{2}}(f_0 + f_1); & f_1 &= \frac{1}{2\sqrt{2}}(f_0 + f_2); & f_2 &= \frac{1}{2\sqrt{2}}(f_1 + f_2) \\ f_3 &= \frac{1}{2\sqrt{2}}(f_0 - f_1); & f_4 &= \frac{1}{2\sqrt{2}}(f_0 - f_2); & f_5 &= \frac{1}{2\sqrt{2}}(f_1 - f_2). \end{aligned} \quad (78)$$

and therefore

$$\sum_{i=0}^2 |f_i|^2 = 2 \sum_{i=0}^5 |f_i|^2. \quad (79)$$

Since the $\{|a_i\rangle\}$ form an over-complete basis, this expansion is not unique. It is seen that a quantum state $|f\rangle$ in $H(3)$ can be represented with a 6-tuple, but not every 6-tuple represents a quantum state in $H(3)$.

B. The projector Π of overlaps between the coherent states

We now consider the 6×6 projector

$$\Pi_{ij} = \frac{1}{2} \langle a_i|a_j\rangle = \frac{1}{4} \begin{pmatrix} 2 & 1 & 1 & 0 & 1 & 1 \\ 1 & 2 & 1 & 1 & 0 & -1 \\ 1 & 1 & 2 & -1 & -1 & 0 \\ 0 & 1 & -1 & 2 & 1 & -1 \\ 1 & 0 & -1 & 1 & 2 & 1 \\ 1 & -1 & 0 & -1 & 1 & 2 \end{pmatrix}; \quad \Pi^2 = \Pi; \quad \text{rank}(\Pi) = 3. \quad (80)$$

Π has the eigenvalues 1 (with multiplicity 3) and 0 (with multiplicity 3).

All columns (and rows) of Π are 6-tuples that span a 3-dimensional space isomorphic to $H(3)$. But we also have the 3-dimensional null space of Π which we denote as $H(3)_{\text{null}}$. The projector $\mathbf{1} - \Pi$ projects into $H(3)_{\text{null}}$. We also define the space

$$H(6) = H(3) \oplus H(3)_{\text{null}}. \quad (81)$$

For Π we get $de_{\text{max}} = 6$, and from Eq.(27) it follows that $g(\Pi) \leq 6$. We recall here that the proof of this is based on the Cauchy-Schwartz inequality. We show below that due to the discrete isotropy of the coherent states, the Cauchy-Schwartz inequality cannot become equality in the present context.

Lemma VII.2. *The strict inequality $g(\Pi) < 6$ holds.*

Proof. We get equality in Eq.(28) only if Eq.(29) holds (in which case the Cauchy-Schwartz inequality becomes equality). We assume that the 6-tuples

$$\begin{aligned} \mathbf{s} &= (s_0, \dots, s_5); \quad |s_i| \leq 1 \\ \mathbf{t} &= (t_0, \dots, t_5); \quad |t_i| \leq 1, \end{aligned} \quad (82)$$

give $g(\Pi) = 6$. Then \mathbf{s} and $\mathbf{t}' = \Pi\mathbf{t}$ are proportional to each other, and therefore they both belong in $H(3)$. Since

$$\left| \sum_{i,j} \Pi_{ij} s_i t_j \right| = \left| \sum_{i=0}^5 s_i t'_i \right| \leq \max \left(\sum_{i=0}^5 |s_i|^2 \right), \quad (83)$$

it follows that a necessary condition for $g(\Pi) = 6$ is that all $|s_i| = 1$.

Since \mathbf{s} is in $H(3)$, it can be represented with a vector $(\sigma_0, \sigma_1, \sigma_2)$ (which is not normalised) such that the analogue of Eq.(78) gives

$$\begin{aligned} |\sigma_0 + \sigma_1| &= 2\sqrt{2}|s_0| = 2\sqrt{2}; & |\sigma_0 + \sigma_2| &= 2\sqrt{2}|s_1| = 2\sqrt{2}; & |\sigma_1 + \sigma_2| &= 2\sqrt{2}|s_2| = 2\sqrt{2} \\ |\sigma_0 - \sigma_1| &= 2\sqrt{2}|s_3| = 2\sqrt{2}; & |\sigma_0 - \sigma_2| &= 2\sqrt{2}|s_4| = 2\sqrt{2}; & |\sigma_1 - \sigma_2| &= 2\sqrt{2}|s_5| = 2\sqrt{2} \end{aligned} \quad (84)$$

From this follows easily that

$$|\sigma_0|^2 + |\sigma_1|^2 = 8; \quad |\sigma_0|^2 + |\sigma_2|^2 = 8; \quad |\sigma_1|^2 + |\sigma_2|^2 = 8. \quad (85)$$

We cannot have equality in all three of these relations, because this would require

$$|\sigma_0| = |\sigma_1| = |\sigma_2| = 2, \quad (86)$$

and this cannot satisfy all relations in Eq.(84).

We note that the sets of equations (84), (85), (86) are invariant under permutations of the $(\sigma_0, \sigma_1, \sigma_2)$. This is related to the discrete isotropy of the coherent states that underpin the projector Π and the present proof.

We conclude that we cannot have all $|s_i| = 1$ and therefore we cannot have $g(\Pi) = 6$. □

C. Example in $H(6)$ that involves the projector Π and takes values in the Grothendieck region $(1, k_G)$

We consider a quantum system with Hilbert space $H(6)$, and the matrices

$$\theta = \lambda\Pi; \quad V = W = \sqrt{2}\Pi \in \mathcal{S}_6 \quad (87)$$

Here $\mathcal{N}(\Pi) = \frac{1}{\sqrt{2}}$ and therefore $\sqrt{2}\Pi \in \mathcal{S}_6$. Since $g(\Pi) < 6$, we define

$$\epsilon = \frac{1}{g(\Pi)} - \frac{1}{6} > 0. \quad (88)$$

Therefore Eq(45) gives

$$\begin{aligned} \lambda\Pi &\in G_6 \setminus G'_6 \quad \text{for } \frac{1}{6} \leq \lambda \leq \frac{1}{6} + \epsilon \\ \lambda\Pi &\in G'_6 \quad \text{for } \lambda \leq \frac{1}{6}. \end{aligned} \quad (89)$$

For the matrices in Eq.(87) we get

$$|\text{Tr}(\theta VW^\dagger)| = 2\lambda\text{Tr}(\Pi) = 6\lambda. \quad (90)$$

For $\lambda \leq \frac{1}{6}$ (in which case $\theta = \lambda\Pi \in G'_6$), the $|\text{Tr}(\theta VW^\dagger)|$ takes values in the region $(0, 1)$. For $\frac{1}{6} \leq \lambda \leq \frac{1}{6} + \epsilon$ (in which case $\theta = \lambda\Pi \in G_6 \setminus G'_6$) the $|\text{Tr}(\theta VW^\dagger)|$ takes values in $[1, 1 + 6\epsilon]$ within the Grothendieck region.

We note that $\rho = \frac{1}{6}VW^\dagger = \frac{1}{3}\Pi$ is a density matrix in quantum systems with Hilbert space $H(6)$, and that

$$\text{Tr}(\rho^2) = \frac{1}{3}; \quad E = -\text{Tr}\rho \log \rho = \log 3. \quad (91)$$

Also $\Theta = 6\theta = 6\lambda\Pi$ is an observable in quantum systems with Hilbert space $H(6)$. Therefore Eq.(90) can be written as

$$|\langle \Theta \rangle| = |\text{Tr}(\rho\Theta)| = 6\lambda. \quad (92)$$

This is an experimentally measurable quantity.

The above analytical method is based on the inequality $g(\Pi) < 6$, and it shows that \mathcal{Q} exceeds 1. In the next subsection we perform a numerical maximisation and show that $g(\Pi) = 5$. This gives a maximum value of \mathcal{Q} equal to $\frac{6}{5}$.

D. Numerical evaluation of $g(\Pi)$

In this section we perform numerically the maximisation and find $g(\Pi) = 5$. We then use the $\theta = \frac{1}{5}\Pi$ in the Grothendieck theorem.

Since

$$\left| \sum_{i,j} \Pi_{ij} s_i t_j \right| \leq \frac{1}{2} \max_{\{t_j\}} \left\| \sum_j t_j |a_j\rangle \right\|^2 \quad |s_i| \leq 1; \quad |t_j| \leq 1, \quad (93)$$

we have to prove that

$$\begin{aligned} \max_{\{t_j\}} \left\| \sum_j t_j |a_j\rangle \right\|^2 &= \frac{1}{2}(A^2 + B^2 + C^2) = 10; \quad |t_j| \leq 1 \\ A &= |t_0 + t_1 + t_3 + t_4| \leq 4; \quad B = |t_0 + t_2 - t_3 + t_5| \leq 4; \quad C = |t_1 + t_2 - t_4 - t_5| \leq 4 \end{aligned} \quad (94)$$

We note that the t_3, t_4, t_5 appear with both signs plus and minus in these expressions. Consequently, for

$$\begin{aligned} t_0 = t_1 = t_2 = t_3 = t_4 = t_5 &= 1, \\ t_0 = t_1 = t_2 = -t_3 = t_4 = t_5 &= 1, \\ t_0 = t_1 = t_2 = t_3 = t_4 = -t_5 &= 1, \end{aligned} \quad (95)$$

etc., we get $\{A, B, C\} = \{4, 2, 0\}$ and $\left\| \sum_j t_j |a_j\rangle \right\|^2 = 10$. In order to show that this is the maximum, we take $t_i = R_i \exp(i\chi_i)$ and we find

$$\begin{aligned} A &= |R_0 \exp(i\chi_0) + R_1 \exp(i\chi_1) + R_3 \exp(i\chi_3) + R_4 \exp(i\chi_4)| \\ B &= |R_0 \exp(i\chi_0) + R_2 \exp(i\chi_2) - R_3 \exp(i\chi_3) + R_5 \exp(i\chi_5)| \\ C &= |R_1 \exp(i\chi_1) + R_2 \exp(i\chi_2) - R_4 \exp(i\chi_4) - R_5 \exp(i\chi_5)|. \end{aligned} \quad (96)$$

We used the MATLAB algorithm 'fmincon' to minimise $-(A^2 + B^2 + C^2)$ which is a function of the 12 variables (R_i, χ_i) with the constraints

$$R_i \in [0, 1]; \quad \chi_i \in [-\pi, \pi]. \quad (97)$$

This is a gradient based algorithm, which starts from an initial value of the 12 parameters and moves towards the minimum. We used many initial values of the parameters in the neighbourhood of $t_0 = t_1 = t_2 = t_3 = t_4 = t_5 = 1$ (e.g., $R_i = 0.5, \chi_i = 0.5$) and they all showed that the minimum is at $R_i = 1$ and $\chi_i = 0$. This shows that $\max_{\{t_j\}} \|\sum_j t_j |a_j\rangle\|^2 = 10$ and therefore $g(\Pi) = 5$.

Using this with the example in section VII C, we get a maximum value of \mathcal{Q} equal to $\frac{6}{5}$.

VIII. EXAMPLE IN $H(12)$ WITH VALUES IN THE GROTHENDIECK REGION $(1, k_G)$

This example is a generalisation of the previous one. We use the same notation, so that we can avoid repetition as much as possible.

We first note that the vectors in Eq.(71) can be viewed as the columns of the Fourier matrix (with $d = 2$),

$$F = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad (98)$$

‘diluted’ with zeros. Inspired by this observation, we do below something similar with the Fourier matrix for $d = 3$:

$$F = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega \end{pmatrix}; \quad \omega = \exp\left(i\frac{2\pi}{3}\right). \quad (99)$$

A. Generalised coherent states in $H(4)$ with discrete isotropy

In a $H(4)$ we consider the 12 normalised vectors $|a_i\rangle$ in table I (the components of $\sqrt{3}|a_i\rangle$ are shown). Here $\omega = \exp(i\frac{2\pi}{3})$. The states $\{|a_i\rangle\}$ are generalised coherent states in the sense of the following proposition:

Proposition VIII.1. (1) *The states $\{|a_i\rangle\}$ resolve the identity:*

$$\frac{1}{3} \sum_{i=0}^{11} |a_i\rangle\langle a_i| = \mathbf{1}. \quad (100)$$

(2) *The set $\{|a_0\rangle, \dots, |a_{11}\rangle\}$ is invariant under transformations in the symmetric group Σ_4 , in the sense that for any $\tau_\pi \in \Sigma_4$ (defined in Eq.(11)) and any i the state $\tau_\pi|a_i\rangle$ is one of the states $|a_j\rangle$ (possibly with a physically insignificant phase factor).*

(3) *There is a ‘discrete isotropy’ between the states $|a_i\rangle$, in the sense that the set of 12 non-independent probabilities*

$$A_i = \{|\langle a_i|a_j\rangle|^2 \mid j = 0, \dots, 11\}, \quad (101)$$

is the same for all i . Therefore the following sum does not depend on i :

$$\sum_{j=0}^{11} |\langle a_i|a_j\rangle|^r = 1 + \frac{2^r + 2}{3^{r-1}}; \quad r = 1, 2, 3, \dots \quad (102)$$

For $r = 1$ this sum involves square roots of the probabilities $|\langle a_i|a_j\rangle|^2$. For $r = 2$ this result follows immediately from the resolution of the identity in Eq.(100).

Proof. (1) This is proved with direct calculation using the vectors in table I.

- (2) This is also proved with direct calculation using the vectors in table I.
- (3) This is seen in the projector in table II below (which is related to $\langle a_i | a_j \rangle$). In each row or in each column of we have one $|\Pi_{ij}| = \frac{3}{9}$, three $|\Pi_{ij}| = \frac{2}{9}$, six $|\Pi_{ij}| = \frac{1}{9}$, and two $|\Pi_{ij}| = 0$. From this follows Eq.(102). \square

An arbitrary state in $H(4)$

$$|f\rangle = \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \end{pmatrix} \quad (103)$$

can be expanded in terms of them as

$$|f\rangle = \sum_{i=0}^{11} f_i |a_i\rangle; \quad f_i = \frac{1}{3} \langle a_i | f \rangle; \quad \langle g | f \rangle = \sum_{i=0}^3 g_i^* f_i = 3 \sum_{i=0}^{11} g_i^* f_i. \quad (104)$$

From this we get 12 relations

$$f_0 = \frac{1}{3\sqrt{3}}(f_0 + f_1 + f_2); \quad f_1 = \frac{1}{3\sqrt{3}}(f_0 + \omega^2 f_1 + \omega f_2); \quad f_2 = \frac{1}{3\sqrt{3}}(f_0 + \omega f_1 + \omega^2 f_2); \quad \text{e.t.c.} \quad (105)$$

and we show that

$$\sum_{i=0}^3 |f_i|^2 = 3 \sum_{i=0}^{11} |f_i|^2. \quad (106)$$

B. The projector Π of overlaps between the coherent states

We introduce the 12×12 projector $\Pi_{ij} = \frac{1}{3} \langle a_i | a_j \rangle$ given in table II (the matrix elements of $9\Pi_{ij}$ are shown). This matrix has the eigenvalues 1 (with multiplicity 4) and 0 (with multiplicity 8).

All columns (and rows) of Π are 12-tuples that span a 4-dimensional space isomorphic to $H(4)$. But we also have the 8-dimensional null space of Π which we denote as $H(8)_{\text{null}}$. The projector $\mathbf{1} - \Pi$ projects into $H(8)_{\text{null}}$. We define the space

$$H(12) = H(4) \oplus H(8)_{\text{null}}. \quad (107)$$

For Π we get $de_{\text{max}} = 12$, and from Eq.(27) it follows that $g(\Pi) \leq 12$.

Lemma VIII.2. *The strict inequality $g(\Pi) < 12$ holds.*

Proof. The proof is similar to the proof of lemma VII.2, and we present briefly the differences. The gist of the proof is that due to the discrete isotropy of the coherent states, the Cauchy-Schwartz inequality cannot become equality in the present context.

We assume that the 12-tuples \mathbf{s}, \mathbf{t} (with $|s_i| \leq 1$ and $|t_i| \leq 1$) give $g(\Pi) = 12$. Then \mathbf{s} and $\mathbf{t}' = \Pi \mathbf{t}$ are proportional to each other, and therefore they both belong in $H(4)$. Since

$$\left| \sum_{i,j} \Pi_{ij} s_i t_j \right| = \left| \sum_{i=0}^{11} s_i t'_i \right| \leq \max \left(\sum_{i=0}^{11} |s_i|^2 \right), \quad (108)$$

it follows that a necessary condition for $g(\Pi) = 12$ is that all $|s_i| = 1$.

Since \mathbf{s} is in $H(4)$, it can be represented with a vector $(\sigma_0, \sigma_1, \sigma_2, \sigma_3)$ (which is not normalised) such that the analogue of Eq.(105) gives 12 inequalities:

$$\begin{aligned} |\sigma_0 + \sigma_1 + \sigma_2| &= 3\sqrt{3}|s_0| = 3\sqrt{3}; & |\sigma_0 + \omega^2\sigma_1 + \omega\sigma_2| &= 3\sqrt{3}|s_1| = 3\sqrt{3} \\ |\sigma_0 + \omega\sigma_1 + \omega^2\sigma_2| &= 3\sqrt{3}|s_2| = 3\sqrt{3}; & \text{e.t.c.} \end{aligned} \quad (109)$$

We note that the set of these equations is invariant under permutations of the $(\sigma_0, \sigma_1, \sigma_2, \sigma_3)$. We add the squares all these 12 inequalities. Using the fact that $1 + \omega + \omega^2 = 0$, we find that all terms $\sigma_i\sigma_j^*$ with $i \neq j$, cancel. Therefore we get

$$\sum_{i=0}^3 |\sigma_i|^2 = 36. \quad (110)$$

Due to symmetry, equality in this relation would require that all $|\sigma_i| = 3$. Then from Eqs.(109) we get the 12 equations

$$\begin{aligned} \sigma_0\sigma_1^* + \sigma_1\sigma_2^* + \sigma_2\sigma_0^* + \sigma_0^*\sigma_1 + \sigma_1^*\sigma_2 + \sigma_2^*\sigma_0 &= 0 \\ \sigma_0\sigma_1^*\omega + \sigma_0^*\sigma_1\omega^2 + \sigma_2\sigma_0^*\omega + \sigma_0\sigma_2^*\omega^2 + \sigma_1\sigma_2^*\omega + \sigma_2\sigma_1^*\omega^2 &= 0 \\ \sigma_0\sigma_1^*\omega^2 + \sigma_0^*\sigma_1\omega + \sigma_2\sigma_0^*\omega^2 + \sigma_0\sigma_2^*\omega + \sigma_1^*\sigma_2\omega + \sigma_2^*\sigma_1\omega^2 &= 0; \quad \text{e.t.c.} \end{aligned} \quad (111)$$

We multiply the first three equations by $1, \omega^2, \omega$ correspondingly, and adding them we get:

$$\sigma_0\sigma_1^* + \sigma_1\sigma_2^* + \sigma_2\sigma_0^* = 0. \quad (112)$$

In a similar way we also get

$$\sigma_0\sigma_1^* + \sigma_1\sigma_3^* + \sigma_3\sigma_0^* = 0; \quad \sigma_0\sigma_3^* + \sigma_3\sigma_2^* + \sigma_2\sigma_0^* = 0; \quad \sigma_1\sigma_2^* + \sigma_2\sigma_3^* + \sigma_3\sigma_1^* = 0. \quad (113)$$

We can find solutions for each of these equations. For example if $\sigma_i = 3\exp(i\phi_i)$, Eq.(112) has the solution $\phi_0 - \phi_1 = \frac{2\pi}{3}$ and $\phi_0 = \phi_2$ (and its permutations). But we cannot satisfy simultaneously all these four equations.

We conclude that we cannot have all $|s_i| = 1$ and therefore we cannot have $g(\Pi) = 12$. Throughout the proof we have a symmetry under permutations of the $(\sigma_0, \sigma_1, \sigma_2, \sigma_3)$. This is related to the discrete isotropy of the coherent states. □

C. Example in $H(12)$ that involves the projector Π and takes values in the Grothendieck region $(1, k_G)$

Since $g(\Pi) < 12$, we define

$$\epsilon = \frac{1}{g(\Pi)} - \frac{1}{12} > 0. \quad (114)$$

and then

$$\begin{aligned} \lambda\Pi &\in G_{12} \setminus G'_{12} \quad \text{for } \frac{1}{12} \leq \lambda \leq \frac{1}{12} + \epsilon \\ \lambda\Pi &\in G'_{12} \quad \text{for } \lambda \leq \frac{1}{12}. \end{aligned} \quad (115)$$

We then apply this to a physical example analogous to the one in section VII C (here $\sqrt{3}\Pi \in \mathcal{S}_{12}$) and we show that for $\frac{1}{12} \leq \lambda \leq \frac{1}{12} + \epsilon$ we get \mathcal{Q} within the Grothendieck region $(1, k_G)$.

We do not perform a numerical maximisation in this example (it involves 24 variables).

Remark VIII.3. Both examples in sections 7,8 involve overcomplete sets of states with a resolution of the identity (in Eqs(72), (100)). Overcomplete sets of states with resolution of the identity have been used extensively in the context of coherent states, but we note that here some of these states are orthogonal to each other (there are zeros in the two projectors). These two examples are interesting in their own right, because they might bring a novel aspect in the general area of phase space methods for systems with finite-dimensional Hilbert space.

We also note that the projectors (Eq.(80) and table II) can be linked to reproducing kernels ($\sum \Pi_{ij} f_j = f_i$). The reproducing kernel formalism has been used extensively in maximisation problems (e.g., in the context of Machine Learning and Artificial Intelligence[26–28]), and this might provide a deeper understanding of why these two examples lead to values within the Grothendieck region, which is on the edge of the Hilbert space formalism and consequently of the Quantum formalism.

IX. DISCUSSION

We have used the Grothendieck theorem in the context of a single quantum system, in contrast to previous work that used it in the context of multipartite entangled systems. In this paper:

- We have reformulated the Grothendieck theorem in terms of products of normalised matrices so that it can be used with measurable quantum mechanical quantities. The normalisation factors and their properties have been discussed in sections 3,4.
- We are particularly interested in the Grothendieck region $(1, k_G)$, which is a kind of ‘quantum ceiling’. We have shown that there are large families of examples with \mathcal{Q} that cannot take values in the Grothendieck region $(1, k_G)$. We also gave necessary (but not sufficient) conditions for \mathcal{Q} taking values in the Grothendieck region (corollary V.2 and proposition VI.1). In Mathematics sometimes the interesting features are found in rare examples on the ‘edge’ (which here is the Grothendieck bound k_G). Section 6 indicates that examples with $\mathcal{Q} \in (1, k_G)$ might be rare. Further work with random sampling of matrices, can quantify how rare are the examples with $\mathcal{Q} \in (1, k_G)$.
- A physical example in the Hilbert space $H(6)$, that leads to $\mathcal{Q} = \frac{6}{5}$ has been discussed in section 7. We presented both an analytical method which shows that \mathcal{Q} enters the Grothendieck region $(1, k_G)$, and a numerical method that gives the maximum value $\mathcal{Q} = \frac{6}{5}$. A similar example in the Hilbert space $H(12)$ has been discussed in section 8 (the analytical approach only).

These two examples use $d(d-1)$ novel generalised coherent states in $H(d)$, which resolve the identity and have a discrete isotropy (with $d = 3, 4$). Their overlaps define a $(d^2 - d) \times (d^2 - d)$ projector. We considered its null space $H(d^2 - 2d)_{\text{null}}$ and the space $H(d^2 - d) = H(d) \oplus H(d^2 - 2d)_{\text{null}}$. We then proved that for $d = 3, 4$ we get the strict inequality $g(\Pi) < d^2 - d$ and this led to values in the Grothendieck region. These examples might be generalised into $d \geq 5$.

More work is needed on examples that take values very close to $k(d) \leq k_G \leq 1.4049$. The present work indicates that they might be related to generalised coherent states with discrete isotropy as symmetry. Helpful in this direction is the link between coherent states with the reproducing formalism and in turn with maximisation problems. Such examples illuminate a new territory at the edge of quantum mechanics. Another related problem is to find better estimates of $k(d)$ and for k_G and improve the results in [11–13].

The work explores the Grothendieck theorem in the context of a single quantum system, with emphasis on the Grothendieck region $(1, k_G)$ which is on the edge of the Hilbert space formalism and the quantum formalism.

TABLE I: 12 vectors $|a_i\rangle$ in $H(4)$. The components of $\sqrt{3}|a_i\rangle$ are shown. Here $\omega = \exp(i\frac{2\pi}{3})$.

$\sqrt{3} a_0\rangle$	$\sqrt{3} a_1\rangle$	$\sqrt{3} a_2\rangle$	$\sqrt{3} a_3\rangle$	$\sqrt{3} a_4\rangle$	$\sqrt{3} a_5\rangle$	$\sqrt{3} a_6\rangle$	$\sqrt{3} a_7\rangle$	$\sqrt{3} a_8\rangle$	$\sqrt{3} a_9\rangle$	$\sqrt{3} a_{10}\rangle$	$\sqrt{3} a_{11}\rangle$
1	1	1	0	0	0	1	ω^2	ω	1	ω	ω^2
1	ω	ω^2	1	1	1	0	0	0	1	ω^2	ω
1	ω^2	ω	1	ω	ω^2	1	1	1	0	0	0
0	0	0	1	ω^2	ω	1	ω	ω^2	1	1	1

TABLE II: The projector $\Pi_{ij} = \frac{1}{3}\langle a_i|a_j\rangle$ where $|a_i\rangle$ are the vectors in table I. The matrix elements of $9\Pi_{ij}$ are shown. Here $\omega = \exp(i\frac{2\pi}{3})$.

3	0	0	2	$-\omega^2$	$-\omega$	2	$-\omega$	$-\omega^2$	2	-1	-1
0	3	0	-1	$2\omega^2$	$-\omega$	$-\omega^2$	-1	2ω	$-\omega$	2ω	$-\omega$
0	0	3	-1	$-\omega^2$	2ω	$-\omega$	$2\omega^2$	-1	$-\omega^2$	$-\omega^2$	$2\omega^2$
2	-1	-1	3	0	0	2	$-\omega^2$	$-\omega$	2	$-\omega$	$-\omega^2$
$-\omega$	2ω	$-\omega$	0	3	0	-1	$2\omega^2$	$-\omega$	$-\omega^2$	-1	2ω
$-\omega^2$	$-\omega^2$	$2\omega^2$	0	0	3	-1	$-\omega^2$	2ω	$-\omega$	$2\omega^2$	-1
2	$-\omega$	$-\omega^2$	2	-1	-1	3	0	0	2	$-\omega^2$	$-\omega$
$-\omega^2$	-1	2ω	$-\omega$	2ω	$-\omega$	0	3	0	-1	$2\omega^2$	$-\omega$
$-\omega$	$2\omega^2$	-1	$-\omega^2$	$-\omega^2$	$2\omega^2$	0	0	3	-1	$-\omega^2$	2ω
2	$-\omega^2$	$-\omega$	2	$-\omega$	$-\omega^2$	2	-1	-1	3	0	0
-1	$2\omega^2$	$-\omega$	$-\omega^2$	-1	2ω	$-\omega$	2ω	$-\omega$	0	3	0
-1	$-\omega^2$	2ω	$-\omega$	$2\omega^2$	-1	$-\omega^2$	$-\omega^2$	$2\omega^2$	0	0	3

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- [1] E. H. Lieb Commun. Math. Phys. 31, 327 (1973)
[2] K. Ball, E. Carlen, E. Lieb, Invent. Math. 115, 463 (1994)
[3] E. Carlen, Contemp. Math. 529, 73 (2009)
[4] J.S. Bell, Physics 1, 195 (1964)
[5] J.F. Clauser, M.A. Horne, A. Shimony, R.A. Holt, Phys. Rev. Lett., 23, 880 (1969)
[6] A. Vourdas, J. Phys. A52, 085301 (2019)
[7] A. Grothendieck, Bol. Soc. Mat. Sao Paulo 8, 1 (1953)
[8] J. Lindenstrauss, A. Pelczynski, Studia Mathematica 29, 275 (1968)
[9] J. Diestel, J. Fourie, J. Swart, 'The metric theory of tensor products: Grothendieck's resume revisited' (AMS, Rhode Island, 2008)

- [10] G. Pisier, *Bull. Amer. Math. Soc.* 49, 237 (2012)
- [11] P.C. Fishburn, J.A. Reeds, *SIAM J. Discr. Math.* 7,48 (1994)
- [12] J.L. Krivine, *C.R. Acad. Sci. Paris A284*, 445 (1977)
- [13] U. Haagerup, *Isr. J. Math.* 60, 199 (1987)
- [14] N. Alon, K. Makarychev, Y. Makarychev, A. Naor, *Invent. Math.* 163, 499 (2006)
- [15] B.S. Tsirelson, *Lett. Math. Phys.* 4, 93 (1980)
- [16] B.S. Tsirelson, *J. Sov. Math.* 36, 557 (1987)
- [17] A. Acin, N. Gisin, B. Toner, *Phys. Rev. A*73, 062105 (2006)
- [18] H. Heydari, *J. Phys.* A39, 11869 (2006)
- [19] I. Pitowski, *J. Math. Phys.* 49, 012101 (2008)
- [20] J. Briet, H. Buhrman, B. Toner, *Commun. Math. Phys.* 205, 827 (2011)
- [21] B. Hua, M. Li, T. Zhang, C. Zhou, X. Li-Jost, S.M. Fei, *J. Phys.* A48 065302 (2015)
- [22] F. Hirsch, M.T. Quintino, T. Vertesi, M. Navascues, N. Brunner, *Quantum* 1,3 (2017)
- [23] B.E. Sagan, 'the symmetric group' (Springer, Berlin, 2001)
- [24] A. Vourdas, *Rep. Prog. Phys.* 67, 267 (2004)
- [25] A. Vourdas, 'Finite and profinite quantum systems' (Springer, Berlin, 2017)
- [26] F. Cucker, S. Smale, *Bull. Amer. Math. Soc.* 39, 1 (2002)
- [27] H. Zhang, Y. Xu, J. Zhang, *J. Machine Learning Res.* 10, 2741 (2009)
- [28] A. Berlinet, C. Thomas-Agnan 'Reproducing Kernel Hilbert Spaces in Probability and Statistics' (Springer Science and Business Media, New York, 2004)