Quantum quantities near the Grothendieck bound in a single quantum system

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Abstract. The Grothendieck theorem considers a 'classical' quadratic form $\mathcal{C}$ that uses complex scalars in the unit disc, and the corresponding 'quantum' quadratic form $\mathcal{Q}$ that replaces the scalars with vectors in the unit ball of a Hilbert space. It shows that when $\mathcal{C} \leq 1$ then $\mathcal{Q}$ might take values greater than 1, up to the complex Grothendieck constant k_G. Previous work in a quantum context, used Grothendieck's theorem with multipartite entangled systems, in contrast to the present work which uses it for a single quantum system. The emphasis in the paper is in examples with $\mathcal{Q} \in (1, k_G)$, which is a classically forbidden region in the sense that $\mathcal{C}$ cannot take values in it.

1. Introduction

The Grothendieck inequality [1, 2, 3, 4] 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 leads to the impression that applications in a quantum context should be for multipartite systems described by tensor products of Hilbert spaces. Indeed the Grothendieck theorem has been used with multipartite entangled systems in refs [5, 6, 7, 8, 9, 10, 11, 12] and has been linked to Bell-like inequalities.

All later mathematical work [2, 3, 4] emphasised that the Grothendieck theorem can also be formulated outside the framework of tensor product theory. This motivated the work in ref[13] that uses the Grothendieck bound in a single quantum system. In this paper we present these ideas in a physical way, without the 'destruction' of mathematical proofs.

The Grothendieck theorem considers quadratic forms such that

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

Here θ 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 $H(d)$:

$$\mathcal{Q}(\theta) = \left|\sum_{r,s} \theta_{rs}\lambda_r\mu_s\langle u_r|v_s\rangle\right|; \quad \lambda_r, \mu_r \leq 1. \tag{2}$$

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

$$\mathcal{Q}(\theta) \leq k_G. \tag{3}$$

k_G is the complex Grothendieck constant, for which it is known that $1 < k_G \leq 1.4049$. Its exact value is not known and bounds for its exact value are discussed in [14, 15, 16].

The region $(1, k_G)$ is of special importance because it is classically forbidden in the sense that the classical quantity $\mathcal{C}(\theta)$ cannot take values in it, while the corresponding quantum quantity $\mathcal{Q}(\theta)$ can take values in it. In this paper we are particularly interested in examples where $\mathcal{Q}(\theta) \in (1, k_G)$. These examples are deep into the quantum region, at the 'edge' of quantum mechanics. We note that there is much work in the semiclassical region, between classical and quantum physics. In contrast the present work is in the other end of the spectrum (ultra-quantum region).

We discuss the following:

- In section 2, we express $\mathcal{Q}(\theta)$ as trace of a product of three **arbitrary matrices**, normalised with prefactors. This is more appropriate than Eq.(2) for quantum mechanics. We also show (in section 2.4) that many physically interesting examples give $\mathcal{Q} \leq 1$. In this sense examples where $\mathcal{Q} \in (1, k_G)$ are a new territory of quantum mechanics.
- In section 3, we give some necessary (but not sufficient) conditions for $\mathcal{Q}(\theta) > 1$.
- In section 4, we present families of coherent states that lead to $\mathcal{Q}(\theta) > 1$. These coherent states are unrelated to Heisenberg-Weyl group, SU(2), etc. We discuss the properties of these states that justify the name coherent states, and show that a matrix of their overlaps is a projector, which gives $\mathcal{Q} > 1$.
- In section 5, we present concluding remarks.

2. Grothendieck bound in a single quantum system

2.1. The sets G_d, G'_d of matrices

For any $d \times d$ matrix θ,

$$g(\theta) = \sup\left\{\left|\sum_{r,s=1}^{d} \theta_{rs}a_rb_s\right|; \quad |a_r| \leq 1; \quad |b_s| \leq 1\right\}$$
$$g'(\theta) = \sup\left\{\left|\sum_{r,s=1}^{d} \theta_{rs}a_rb_s\right|; \quad \sum_r |a_r|^2 \leq d; \quad \sum_s |b_s|^2 \leq d\right\} \tag{4}$$

It can be proved that

$$g(\theta) \leq g'(\theta) = d\mathfrak{s}_{\max}, \tag{5}$$

where $\mathfrak{s}_{\max}$ is the largest singular value of θ. For normal matrices $\mathfrak{s}_{\max} = e_{\max}$, where $e_{\max}$ is the largest of the absolute values of the eigenvalues of θ (spectral radius of θ). Therefore for normal matrices

$$g(\theta) \le g'(\theta) = de_{\max}. \tag{6}$$

The following two sets of matrices play an important role in this paper:

- G_d is the set of $d \times d$ complex matrices with

$$\left|\sum_{r,s} \theta_{rs} a_r b_s\right| \le 1; \quad |a_r| \le 1; \quad |b_s| \le 1.$$

By definition, matrices in G_d have $\mathcal{C}(\theta) \le 1$. If θ is an arbitrary matrix, then $\frac{\theta}{g(\theta)} \in G_d$.

- G'_d is the set of $d \times d$ complex matrices with

$$\left|\sum_{r,s} \theta_{rs} a_r b_s\right| \le 1; \quad \sum |a_r|^2 \le d; \quad \sum |b_s|^2 \le d.$$

If θ is an arbitrary matrix, then $\frac{\theta}{g'(\theta)} = \frac{\theta}{d\mathfrak{s}_{\max}} \in G'_d$.

Clearly $G'_d \subseteq G_d$. If the strict inequality $g(\theta) < d\mathfrak{s}_{\max}$ holds, then G'_d is a proper subset of G_d. This is needed later.

2.2. *The set $\mathcal{S}_d$ of matrices*

For any $d \times d$ matrix M,

$$\mathcal{N}(M) = \max_i \sqrt{\sum_j |M_{ij}|^2} = \max_i \sqrt{(MM^\dagger)_{ii}} \tag{7}$$

$\mathcal{S}_d$ is the set of matrices M with $\mathcal{N}(M) \le 1$. All unitary matrices belong in $\mathcal{S}_d$.

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

2.3. *$Q(\theta)$ as trace of a product of matrices*

The Grothendieck theorem is equivalent to the following statement[13]. If $\theta \in G_d$ and $V, W \in \mathcal{S}_d$ then

$$\mathcal{Q} = |\mathrm{Tr}(\theta V W^\dagger)| \le k_G. \tag{8}$$

The relationship of this expression to Eq.(2) 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, and W to be a matrix that has the components of $\lambda_r|u_r\rangle$ in the r-row (therefore $W^\dagger$ 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

$$\mathcal{Q} = \left|\mathrm{Tr}\left(\frac{\theta}{g(\theta)} \frac{V}{\mathcal{N}(V)} \frac{W^\dagger}{\mathcal{N}(W^\dagger)}\right)\right| \le k_G. \tag{9}$$

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2.4. Many physical examples give $Q(\theta) \le 1$

Let $|e\rangle, |f\rangle$ be normalised states with components f_r and e_s correspondingly, and U a unitary matrix. We take

$$\theta_{rs} = \frac{f_r e_s}{g(|f\rangle\langle e|)} \in G_d; \quad V = U \in \mathcal{S}_d; \quad W = \mathbf{1}_n \in \mathcal{S}_d. \tag{10}$$

We note that $g(|f\rangle\langle e|) > 1$. Indeed for the matrix $f_r e_s^*$ and for any $|a_r| \le 1$ and $|b_s| \le 1$, we get

$$g(|f\rangle\langle e|)) \ge \left|\sum_{r,s} f_r e_s^* a_r b_s\right|. \tag{11}$$

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

$$g(|f\rangle\langle e|)) \ge \sum_r |f_r| \sum_s |e_s| \ge 1. \tag{12}$$

Therefore

$$\mathcal{Q} = |\mathrm{Tr}(\theta V W^\dagger)| = \frac{|\langle e|U|f\rangle|}{g(|f\rangle\langle e|)} \le 1. \tag{13}$$

Many physically interesting quantities can be written as $\langle e|U|f\rangle$ where U is some unitary operator and they lead to $\mathcal{Q} \le 1$. In this sense physical examples with $\mathcal{Q} > 1$ seem to be rare. In this paper we are interested in examples with $\mathcal{Q} \in (1, k_G)$.

3. Necessary (but not sufficient) condition for $Q(\theta) > 1$

For a normal matrix θ, a necessary (but not sufficient) condition for $Q(\theta) > 1$ is that $\theta \in G_d \setminus G'_d$[13]. We have seen earlier that if the strict inequality $g(\theta) < de_{\max}$ holds (for normal matrices $\mathfrak{s}_{\max} = e_{\max}$), then G'_d is a proper subset of G_d. It follows the following proposition.

Proposition 3.1. *For a normal matrix θ, a necessary (but not sufficient) condition for $Q(\theta) > 1$ is that the strict inequality $g(\theta) < de_{\max}$ holds. In this case*

$$\lambda \le \frac{1}{de_{\max}} \;\Rightarrow\; \lambda\theta \in G'_d \Rightarrow Q(\lambda\theta) < 1. \tag{14}$$

Also

$$\frac{1}{de_{\max}} < \lambda \le \frac{1}{g(\theta)} \Rightarrow \lambda\theta \in G_d \setminus G'_d \Rightarrow \text{may be } Q(\lambda\theta) > 1. \tag{15}$$

4. Family of coherent states in $H(3)$ with $\mathcal{Q} \ge 1$

In $H(3)$ we consider the 6 states

$$|a_z(0)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\z\\0\end{pmatrix}; \; |a_z(1)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}z\\0\\1\end{pmatrix}; \; |a_z(2)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\z\end{pmatrix}$$
$$|a_z(3)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-z\\0\end{pmatrix}; \; |a_z(4)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}-z\\0\\1\end{pmatrix}; \; |a_z(5)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-z\end{pmatrix} \tag{16}$$

z is constant with $|z| = 1$. They are coherent states in the sense that they have the following properties:

- **resolution of the identity:** It is easily seen that

$$\frac{1}{2}\sum_{r=0}^{5}|a_z(r)\rangle\langle a_z(r)| = \mathbf{1}. \tag{17}$$

- **The set of coherent states is invariant under transformations in the group $\mathcal{G}_3$:** Let X be the 'upwards displacement' matrix:

$$X = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}; \quad X^3 = \mathbf{1}. \tag{18}$$

$\mathcal{G}_3$ is the cyclic group $\{\mathbf{1}, X, X^2\}$ with the operation of matrix multiplication (it is isomorphic to $\mathbb{Z}_3$).
Action of $\mathcal{G}_3$ on the set of coherent states leaves it invariant. But we note that action of $\mathcal{G}_3$ on the set of coherent states is not transitive. It leads to two orbits as follows:

$$\begin{aligned} &|a_z(0)\rangle \xrightarrow{X} |a_z(1)\rangle \xrightarrow{X} |a_z(2)\rangle \xrightarrow{X} |a_z(0)\rangle; \\ &|a_z(3)\rangle \xrightarrow{X} |a_z(4)\rangle \xrightarrow{X} |a_z(5)\rangle \xrightarrow{X} |a_z(3)\rangle. \end{aligned} \tag{19}$$

- **discrete isotropy:** The set of 6 probabilities

$$A_r = \{|\langle a_z(r)|a_z(s)\rangle|^2 \mid s = 0, ...5\}, \tag{20}$$

is the same for all r. The following sum does not depend on r:

$$S(\nu) = \sum_{s=0}^{5}|\langle a_z(r)|a_z(s)\rangle|^\nu = 1 + \frac{1}{2^{\nu-2}}; \quad \nu = 1, 2, ... \tag{21}$$

- **Bargmann 6-tuple representation of states in $H(3)$:** We can define an analogue of the Bargmann representation in the present context. Of course here there is no analyticity. Let $|f\rangle$ be an arbitrary state in $H(3)$:

$$|f\rangle = \begin{pmatrix} f_0 \\ f_1 \\ f_2 \end{pmatrix}; \quad \sum_{i=0}^{2}|f_i|^2 = 1 \tag{22}$$

Using the resolution of the identity, we can write it as

$$|f\rangle = \sqrt{\frac{1}{2}}\sum_{r=0}^{5}\widetilde{f}_r|a_z(r)\rangle; \quad \widetilde{f}_r = \sqrt{\frac{1}{2}}\langle a_z(r)|f\rangle; \quad \sum_{r=0}^{5}|\widetilde{f}_r|^2 = 1. \tag{23}$$

Here we represent vectors in $H(3)$ with the 6 components $\widetilde{f}_r$. There is merit in having this redundancy in noisy situations. Adding noise to $\widetilde{f}_r$, will lead to a state $|f'\rangle$ which is closer to $|f\rangle$, than if we do the same process with an orthonormal basis.

- **The 6×6 projector of overlaps of coherent states:** We consider the following matrix of overlaps of coherent states:

$$\Pi_{rs} = \frac{1}{2}\langle a_r|a_s\rangle = \frac{1}{4}\begin{pmatrix} 2 & z & z^* & 0 & -z & z^* \\ z^* & 2 & z & z^* & 0 & -z \\ z & z^* & 2 & -z & z^* & 0 \\ 0 & z & -z^* & 2 & -z & -z^* \\ -z^* & 0 & z & -z^* & 2 & -z \\ z & -z^* & 0 & -z & -z^* & 2 \end{pmatrix} \tag{24}$$

Using the resolution of the identity we easily see that it is a projector. Its eigenvalues are 1 (with multiplicity 3) and 0 (with multiplicity 3). Π acts on vectors in $H(6)$ which can be written as

$$H(6) = H(3) \oplus H(3)_{\text{null}}. \tag{25}$$

Here $H(3)_{\text{null}}$ is the null space of Π. A vector in $H(6)$, can be written as $\widetilde{f}_r + \widetilde{\phi}_r$, where

$$\sum_{r=0}^{5} \Pi_{sr}\widetilde{f}_r = \widetilde{f}_s; \quad \widetilde{f}_r \in H(3)$$
$$\sum_{r=0}^{5} \Pi_{sr}\widetilde{\phi}_r = 0; \quad \widetilde{\phi}_r \in H(3)_{\text{null}}.$$

The first of these relations is the reproducing kernel relation in the present context.

For $\theta = \Pi$ the relation $g(\theta) \le de_{\max}$ gives $g(\Pi) \le 6$. It can be proved analytically[13] that for $z \ne \pm i$ we get the strict inequality $g(\Pi) < 6$. According to Eq.(15) in this case we might get $\mathcal{Q} > 1$.

Indeed we use Eq.(13) with the matrices

$$\theta = \lambda\Pi; \quad V = W = \sqrt{2}\Pi \in \mathcal{S}_6 \tag{26}$$

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

$$\epsilon = \frac{1}{g(\Pi)} - \frac{1}{6} > 0. \tag{27}$$

Therefore Eqs(14), (15) give

$$\begin{aligned} &\lambda \le \frac{1}{6} \to \lambda\Pi \in G_6' \to \mathcal{Q} = |\mathrm{Tr}(\theta V W^\dagger)| = 2\lambda\mathrm{Tr}(\Pi) = 6\lambda \le 1 \\ &\frac{1}{6} < \lambda \le \frac{1}{6} + \epsilon \to \lambda\Pi \in G_6 \setminus G_6' \to \mathcal{Q} = |\mathrm{Tr}(\theta V W^\dagger)| = 2\lambda\mathrm{Tr}(\Pi) = 6\lambda > 1 \end{aligned} \tag{28}$$

It is seen that for $\lambda \le \frac{1}{6}$ (in which case $\theta = \lambda\Pi \in G_6'$) we get $\mathcal{Q} \in (0, 1)$, and for $\frac{1}{6} \le \lambda \le \frac{1}{6} + \epsilon$ (in which case $\theta = \lambda\Pi \in G_6 \setminus G_6'$) we get $\mathcal{Q} \in (1, 1 + 6\epsilon)$.

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5. 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 expressed $\mathcal{Q}(\theta)$ as trace of products of **arbitrary matrices** normalised with prefactor. This is more appropriate than Eq.(2) for quantum mechanics.
- We gave some necessary (but not sufficient) conditions for $\mathcal{Q}(\theta) > 1$.
- We presented a family coherent states. The overlap of these coherent states is a projector with $\mathcal{Q}(\Pi) > 1$.

The presentation emphasised the physical aspects, and the mathematical proof of many of the statements is given in [13]. The work explores the Grothendieck theorem in the context of a single quantum system. The emphasis is on examples with $\mathcal{Q} \in (1, k_G)$ which is on the edge of the Hilbert space formalism and the quantum formalism.

6. References

[1] Grothendieck A. (1953) Bol. Soc. Mat. Sao Paolo **8** 1
[2] Lindenstrauss J. and Pelczynski A (1968) Studia Mathematica **29** 275
[3] Diestel J., Fourie J.and Swart J. (2008) The metric theory of tensor products: Grothendieck's resume revisited (Rhode Island: AMS)
[4] Pisier G (2012) Bull. Amer. Math. Soc. **49** 237
[5] Tsirelson B.S. (1980) Lett. Math. Phys. **4** 93
[6] Tsirelson B.S. (1987) J. Sov. Math. **36** 557
[7] Acin A., Gisin N. and Toner B. (2006), Phys. Rev. A **73** 062105
[8] Heydari H. (2006) J. Phys. A **39** 11869
[9] Pitowski I. (2008) J. Math. Phys. **49** 012101
[10] Briet J., Buhrman H.and Toner B. (2011) Commun. Math. Phys. **205** 827
[11] Hua B., Li M., Zhang T., Zhou C., Li-Jost X and Fei S.M. (2015) J. Phys. A **48**, 065302
[12] Hirsch F., Quintino M.T., Vertesi T., Navascues M. and Brunner N. (2017), Quantum **1** 3
[13] Vourdas A. (2022) J. Phys. A **55** 435206 (and corrigendum Vourdas A. (2023) J. Phys. A **56** 169501)
[14] Fishburn P.C. and Reeds J.A. (1994) SIAM J. Discr. Math. **7** 48
[15] Krivine J.L. (1977) C.R. Acad. Sci. Paris A **284** 445
[16] Haagerup U. (1987) Isr. J. Math. **60** 199