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Bell inequalities and their maximal violation

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Abstract

In this thesis we explore Bell inequalities, a class of inequalities that hold for random variables taking values in $\{1, -1\}$, and the degree to which these can be violated by the results of quantum measurements. We first provide some background knowledge in linear algebra and quantum measurement and prove some preliminary results used in this thesis. The remainder of the thesis can be divided into two parts. In the first part we formally define Bell inequalities and quantify the degree to which they can be violated using the largest violation. Our treatment is based on chapter 5 of [2]. Compared to [2] we provide original proofs of several facts stated without proof in [2] and fill in some details in existing proofs. There are well-known Bell inequalities with a largest violation of $\sqrt{2}$ and theoretical results showing that Bell inequalities with greater largest violation should exist. In the second part of this thesis we address the question of whether we can explicitly find Bell inequalities with a largest violation greater than $\sqrt{2}$. We attempt to find these Bell inequalities by approximating largest violations using optimization algorithms.

Correlation matrices

Central to the topic of Bell inequalities is the concept of correlation matrices. An $N \times N$ matrix $\gamma = (\gamma_{i,j})_{i,j=1}^{N}$ is a correlation matrix if it is of the form $\gamma_{i,j} = \mathbb{E}(P_i Q_j)$. Here $P_1, \dots P_N$ are the measurement results from N measurements on some fixed physical system in some fixed state. Similarly, $Q_1, \dots, Q_N$ are the results from N measurements on a second fixed physical system. Furthermore, $\mathbb{E}$ denotes the expectation. We consider measurements with outcomes in $\{1, -1\}$.

We mainly consider two types of correlation matrices. The first type of correlation matrices, called classical correlation matrices, are those for which the two physical systems and the possible measurements are viewed according to a local hidden variable model. This means that all the measurement outcomes P_i and Q_j can be described as random variables on a single probability space. The second type are the quantum correlation matrices, for which the physical systems and the measurements are described by quantum measurement. We note that we only consider physical systems described by finite dimensional Hilbert spaces, so it would be more accurate to call these correlation matrices quantum correlation matrices of finite dimensional observables. We will refer to these simply as quantum correlation matrices. We write $\mathscr{L}_N$ for the set of classical correlation matrices of size $N \times N$ and $\mathscr{Q}_N$ for the set of quantum correlation matrices (of finite dimensional observables) of size $N \times N$.

We prove that $\mathscr{L}_N$ is a convex set spanned by a finite set of points, or in other words a polytope. The matrices that span $\mathscr{L}_N$ are those with entries of the form $\gamma_{i,j} = t_i s_j$, where $t_i, s_j \in \{1, -1\}$. We have dubbed these matrices deterministic correlation matrices, since these are exactly the matrices obtained when the measurement outcomes P_i and Q_j are deterministic. We also prove

some properties of $\mathscr{Q}_N$, with main results being that $\mathscr{Q}_N$ is convex and that $\mathscr{L}_N \subseteq \mathscr{Q}_N$. Our proof of this last fact is based on a proof provided in [2].

Bell inequalities and largest violation

We define Bell inequalities as follows. Given an $N \times N$ matrix with real entries M and a non-negative constant C, $\left|\sum_{i,j=1}^{N} M_{i,j}\gamma_{i,j}\right| \leq C$ is called a Bell inequality if it holds for all $N \times N$ classical correlation matrices γ. A central question we address is to what degree a Bell inequality can be violated if we instead allow γ to be a quantum correlation matrix. To this end we introduce, given an $N \times N$ matrix M, its classical value

$$\omega(M) = \sup_{\gamma \in \mathscr{L}_N} \left| \sum_{i,j=1}^{N} M_{i,j}\gamma_{i,j} \right|$$

and its quantum value

$$\omega^*(M) = \sup_{\gamma \in \mathscr{Q}_N} \left| \sum_{i,j=1}^{N} M_{i,j}\gamma_{i,j} \right|.$$

Their ratio, the largest violation $LV(M) = \frac{\omega^*(M)}{\omega(M)}$, is our measure for the largest possible violation of a Bell inequality associated with M. Since $\mathscr{L}_N \subseteq \mathscr{Q}_N$, $LV(M) \geq 1$ for any (non-zero) matrix M.

We prove that classical values can be calculated by taking the supremum (or maximum) over all deterministic correlation matrices of appropriate size, rather than all classical correlation matrices. This makes it possible to calculate a classical value by comparing a finite number of values. The calculation of a quantum value is also simplified by using an alternative (but equivalent) definition for quantum correlation matrices. This equivalent definition states that γ is a quantum correlation matrix if and only if its entries have the form $\gamma_{i,j} = \langle x_i, y_j \rangle$ with x_i, y_j unit vectors in some real Hilbert space H. The equivalence of these definitions is known as Tsirelson's theorem which we prove. Our proof is based on a proof in [2] with us filling in some details. We also prove that there are some optional restrictions on the Hilbert space H, which gives additional equivalent definitions. H can be restricted to be finite-dimensional. Instead of an arbitrary real Hilbert space H, $\mathbb{R}^n$ for arbitrary $n \in \mathbb{N}$ gives an equivalent definition. It is also possible to replace H by $\mathbb{R}^{N+1}$.

For the matrix $M_{CHSH} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ we prove that $\omega(M_{CHSH}) = 2$ and $\omega^*(M_{CHSH}) = 2\sqrt{2}$, which implies $LV(M_{CHSH}) = \sqrt{2}$. The associated Bell inequality is known as the CHSH-inequality.

Using the alternative definition from Tsirelson's theorem and the fact that $\omega(M)$ can be calculated by only considering deterministic correlation matrices, it follows from a theorem known as Grothendieck's theorem, that $LV(M)$ is bounded when considering all square matrices with real entries M. The supremum of $LV(M)$ over all these matrices M is known as Grothendieck's constant K_G. No exact value is known for K_G, but 1.67696 and $\frac{\pi}{2\log\left(1+\sqrt{2}\right)} \approx 1.7822139781$ are the current best lower and upper bounds on K_G. We do not prove Grothendieck's theorem or these bounds.

Optimization algorithms

We aim to improve on the CHSH-Inequality, by finding an explicit matrix with largest violation exceeding $\sqrt{2}$. We do this by using optimization algorithms. Given a matrix M we calculate its classical value exactly by comparing $\left|\sum_{i,j=1}^{N} M_{i,j} t_i s_j\right|$ for all different $t_i, s_j \in \{1, -1\}$ (omitting some combinations that always give duplicate results). This process of calculating classical values has a runtime that scales exponentially with the matrix size N, increasing by approximately a factor 4 when N is increased by 1. Quantum values are approximated from below using an optimization algorithm. For fixed dimension n, the vectors x_i, y_j are taken in $\mathbb{R}^n$ and $\sum_{i,j=1}^{N} M_{i,j} \langle x_i, y_j \rangle$ is optimized. For an $N \times N$ matrix M, if we choose $n = N+1$, then $\sup \sum_{i,j=1}^{N} M_{i,j} \langle x_i, y_j \rangle = \omega^*(M)$ with the supremum taken over unit vectors $x_i, y_j \in \mathbb{R}^n$. Therefore, if we choose $n = N + 1$, the optimization algorithm will approximate $\omega^*(N)$. Choosing $n < N + 1$ will improve the runtime of the algorithm, but the result might be approximating a value smaller than $\omega^*(M)$. To ensure that the vectors have unit length, they are expressed using spherical coordinates with radius fixed at 1. The angles are allowed to vary and are used as the variables for the optimization algorithm. For matrices with known quantum values, such as M_{CHSH}, the optimization procedure provides accurate lower bounds (accurate to 11 decimal places for M_{CHSH}). $LV(M)$ is approximated from below by dividing the approximation of $\omega^*(M)$ by the exact value of $\omega(M)$.

For fixed N, (our approximation of) $LV(M)$ is maximized for $N \times N$ matrices M. This is done by using a second layer of optimization, this time using the entries of M as variables. This should provide a lower bound for K_N, which is defined in the same way as K_G only with matrix size fixed at $N \times N$, and for K_G itself. The results of the second layer of optimization depend strongly on the starting values and do not always give an accurate approximation of K_N. Therefore trying several different starting values for the second layer of optimization is advised. The runtime of the algorithm increases drastically in terms of the matrix size N and the vector dimension n. Therefore we were only able to run it for $N \leq 5$ when $n = N + 1$. Choosing smaller n allows to increase N further, up to $N = 10$ when $n = 3$. No matrices with largest violation exceeding $\sqrt{2}$ were found using this procedure.

Further research

We looked at articles [5] and [4] for inspiration, hoping to find explicit matrices with largest violation exceeding $\sqrt{2}$ to use as starting points for further investigation. [5] provides lower bounds for a variation on K_G where the vector dimension n is fixed in the equivalent definition of quantum value from Tsirelson's theorem. The matrices used in proving these lower bounds are difficult to construct explicitly and possibly very large. We have therefore judged them to be unsuitable for finding improvements on them using numerical methods. [4] provides a method of constructing matrices M of which $LV(M)$ can be determined exactly. The smallest matrix provided with largest value exceeding $\sqrt{2}$ is of size 20×20. Since this proves $K_{20} > \sqrt{2}$, the matrix provided in [4] can be used as a starting point to find matrices with even greater largest violation. This can be done by making small adjustments to the matrix provided. 20×20 matrices are too large for our algorithms to calculate classical and quantum values in a reasonable amount of time. If a faster approximation procedure or more powerful hardware is available, we recommend investigating 20×20 matrices to possibly improve on the lower bound for K_{20}.

Contents

1 Introduction

According to the theory of quantum mechanics, the state of a physical system can be described using a wave function. The standard interpretation is that this wave function fully specifies the state of the system. Despite this, the theory tells us that even if the wave function describing the physical state of a system is known, the outcomes of measurements performed on the system will in general be random. In other words, the randomness in the measurement outcomes is not caused by lack of information about the state of the system, but is somehow inherent in nature. This makes quantum mechanics a non-deterministic theory. Many consider the non-deterministic nature of quantum mechanics to be counterintuitive. In addition to this, quantum mechanics has another counterintuitive quality. According to quantum mechanics it is possible to seperate two physical systems over an arbitrary distance and by interacting with the first system, instantly cause changes in the second system. The intuitive belief that it should not be possible to instantaneously cause changes in a physical system from a large distance is known as locality, and this belief is violated by quantum mechanics.

The counterintuitive nature of quantum mechanics has led to skepticism towards the theory and alternative theories have been formulated. Among these are hidden variable models. According to these models, quantum mechanics offers an incomplete description of reality. In other words, the wave function provides some but not all information about the state of a system. There exist certain hidden variables that would provide the missing information. The randomness of measurement outcomes is not inherent in nature, but a consequence of not knowing the hidden variables. When combined with the assumption of locality, these models are known as local hidden variable models and aim to provide an interpretation of quantum mechanics that satisfies the principles of determinism and locality.

Bell has shown that the assumption of a local hidden variable model implies that measurement outcomes must satisfy certain probabilistic inequalities, now known as Bell inequalities. These inequalities are, however, inconsistent with possible measurement outcomes as predicted by quantum mechanics. A well-known example of a Bell inequality is the CHSH-inequality. It states that, given four random variables Q, R, S, T on a single probability space taking values 1 or -1, the following inequality holds:

$$|\mathbb{E}(QS) + \mathbb{E}(RS) + \mathbb{E}(RT) - \mathbb{E}(QT)| \leq 2.$$

Under the assumption of a local hidden variable model, this inequality must hold if Q and R are the outcomes of measurements performed on some physical system and S and T are outcomes of measurements performed on a second physical system (all taking values ± 1). Quantum mechanics predicts that it is theoretically possible to violate the CHSH-inequality in situations where it

should hold according to a local hidden variable model. Experiments have shown that the CHSH-inequality can also be violated in practice. In fact the CHSH-inequality is the Bell inequality usually used in experiments.

Experiments regarding the violation of the CHSH-inequality by quantum measurement generally have the following setup. A source generates pairs of photons in a fixed state. The two photons in such a pair are the physical systems. Each of the photons encounters a polarizer, which allows the photon to enter one of two channels. A detector detects when a photon passes through one of the channels. By assigning the value 1 to one of the channels and -1 to the other, the detection of which channel a photon went through becomes a measurement with outcomes taking values ± 1. By varying the orientation of the polarizers, different measurements can be obtained. Measurements on the first photon using two specific orientations for the first polarizer can be associated with the measurement outcomes Q and R for the first physical system. Similarly, two orientations for the second polarizer can be associated with the measurement outcomes S and T. Under this identification, the CHSH-inequality can be tested experimentally using this setup.

During experiments each expectation on the left-hand side of the CHSH-inequality is approximated by the average of the measurement outcomes and a sufficiently large sample size is needed before drawing conclusions regarding the violation of the CHSH-inequality. Even with a sufficiently large sample size, the approximation of the expectations by measurement averages might not always be considered justified, leading to so-called loopholes that bring the validity of the experiment in question. To give some examples:

- Since not each pair of photons is successfully detected, the question arises if the detected pairs are an adequate sample for approximating the expectations, leading to the detection loophole.
- If the measurements on the two photons are performed too close to each other, the measurement of one photon can influence the outcome of the measurement on the other photon, even with the assumption of locality. This leads to the locality loophole.
- Measurements on subsequent pairs of photons might not be independent, which leads to the memory loophole.

Closing off loopholes such as these presents experimental challenges, which is why many experiments have been performed in an attempt to close off as many loopholes as possible. While the first experiment regarding the CHSH-inequality dates back to a 1982 experiment by Alain Aspect in Orsay [6], the first significant experiments addressing all three of the loopholes we mentioned took place in 2015, including an experiment by Robert Hanson et. al. in Delft [7], which shows that closing these loopholes is no easy task.

Bell inequalities also raise some interesting theoretical questions. Knowing that Bell inequalities can be violated by measurement outcomes in quantum mechanics, the question arises to what degree Bell inequalities can be violated in quantum mechanics. The degree to which a particular Bell inequality can be violated, can be expressed using a quantity known as the largest violation. Generic Bell inequalities are similar in form to the CHSH-inequality and the largest violation is the fraction between the largest value the left-hand side can attain under assumption of quantum mechanics and the largest value it can attain under assumption of a local hidden variable model. For the CHSH-inequality, these values are $2\sqrt{2}$ and 2 respectively, leading to a largest violation of $\sqrt{2}$. Theoretical results show that Bell inequalities with even greater largest violation must exist. In this thesis we address the question of whether we can find explicitly Bell inequalities with a largest violation exceeding $\sqrt{2}$. Such Bell inequalities with a greater largest violation could prove useful experimentally, as they would allow for a greater margin of error. There is, however, a good chance that Bell inequalities with largest violation greater than $\sqrt{2}$ are significantly more complicated and more difficult to build experiments around.

Chapters 2 and 3 of this thesis are meant to provide some background knowledge for the remainder of this thesis, with chapter 2 focusing on linear algebra and chapter 3 on quantum measurement. Chapter 2 also contains the proofs of some preliminary results in linear algebra used in the rest of this thesis. Chapters 2 and 3 can be skipped without loss of continuity and used as reference material when necessary. The remainder of this thesis consists of two parts.

The first part is a theoretical treatment on Bell inequalities based on chapter 5 of [2], but with additional proofs of facts stated in [2] without proof. Chapter 4 introduces and defines Bell inequalities informally and treats the CHSH-inequality as an example of a Bell inequality. In chapters 5 and 6 we introduce and prove properties of classical correlation matrices and quantum correlation matrices, which are needed to formally define Bell inequalities. In chapter 7 we formally define Bell inequalities, define the largest violation of a matrix as a way to quantify the violation of a Bell inequality and show that the matrix associated with the CHSH-inequality has a largest violation of $\sqrt{2}$. In this chapter we also state Grothendieck's theorem, which provides a bound on the largest violation.

In the second part we attempt to find explicit matrices (which represent Bell inequalities), with a largest violation exceeding $\sqrt{2}$. We mainly do this using optimization algorithms, but also look at literature to assist in our search. In chapter 8 we explain our method to approximate the largest violation of a matrix. In chapter 9 we explain our method to maximize the largest violation and discuss our results in trying to find a matrix with largest violation exceeding $\sqrt{2}$. In chapter 10 we discuss two articles we looked into to assist in finding matrices with largest violation exceeding $\sqrt{2}$. In chapter 11 we draw conclusions regarding our research.

2 Linear algebra

This section will first state some of the definitions and theorems (without proof) from linear algebra that are relevant to the contents of this thesis. A more complete treatment of this topic can be found in [1] or most textbooks on linear algebra. In particular we will introduce tensor products. More on tensor products can be found in [1] or [3]. Afterwards we will state and prove a number of more specific theorems from linear algebra that will be used to prove some results in the remainder of this thesis.

Definition 2.1. Inner Product Space. An inner product space is a vector space V over a field F, where F is equal to $\mathbb{R}$ or $\mathbb{C}$ with an operation $\langle \cdot, \cdot \rangle : V \times V \to F$ called the inner product satisfying the following properties for all $x, y, z \in V$ and $a \in F$:

$$\langle x, y \rangle = \langle y, x \rangle^* \tag{1}$$

where a^* denotes the complex conjugate of a. This is called conjugate symmetry. We also have:

$$\langle x, ay \rangle = a \langle x, y \rangle \tag{2}$$

and

$$\langle x, y + z \rangle = \langle x, y \rangle + \langle x, z \rangle . \tag{3}$$

The above two equations express that the inner product is linear in its second argument. Lastly we have:

$$\langle x, x \rangle > 0 \tag{4}$$

where the last equation holds for non-zero $x \in V$ and expresses that the inner product is positive-definite.

Remark. If an operation $\langle \cdot, \cdot \rangle : V \times V \to F$ satisfies all the requirements to be an inner product, except the last requirement is replaced by:

$$\langle x, x \rangle \geq 0 \tag{5}$$

for all $x \in V$ and there exist $0 \neq x \in V$ such that $\langle x, x \rangle = 0$, then this operation is called a degenerate inner product. To stress that $\langle x, x \rangle = 0$ only holds when $x = 0$ for inner products, inner products are sometimes called non-degenerate inner products.

Remark. We note that the (possibly degenerate) inner product as defined above satisfies the following properties for all $x, y, z \in V$ and $a \in F$:

$$\langle ax, y \rangle = a^* \langle x, y \rangle \tag{6}$$

and

$$\langle x+y,z\rangle = \langle x,z\rangle + \langle y,z\rangle\,. \tag{7}$$

This is called conjugate linearity in its first argument. It is also common to define the inner products to be linear in its first argument making it conjugate linear in its second argument. The definition we use, with linearity in the second argument, is standard in the context of quantum mechanics.

Definition 2.2. 2-norm. On an inner product space V the 2-norm is defined as $\|x\|_2 = \sqrt{\langle x,x\rangle}$. This is a norm on V and $d(x,y) = \|x-y\|_2$ defines the associated metric on V.

Remark. Unless otherwise specified, whenever we view an inner product space V as a metric space (such as when discussing convergence) the metric used will be the metric associated with the 2-norm on V.

Theorem 2.1. *Cauchy-Schwarz inequality. Let V be an inner product space over $\mathbb{R}$ or $\mathbb{C}$, then for all $v, w \in V$ the following inequality holds:*

$$|\langle v,w\rangle| \leq \|v\|_2 \|w\|_2. \tag{8}$$

Definition 2.3. Isomorphism. An isomorphism, or unitary map, between inner product space V and W (both over the same field $\mathbb{R}$ or $\mathbb{C}$) is a bijective linear map $F : V \to W$ such that for all scalars $v_1, v_2 \in V$:

$$\langle Fv_1, Fv_2\rangle = \langle v_1, v_2\rangle\,. \tag{9}$$

So F preserves the inner product and as a consequence F also preserves norms:

$$\|Fv\|_2 = \|v\|_2 \tag{10}$$

for all $v \in V$.

Remark. If $F : V \to W$ is an isomorphism, then so is $F^{-1} : W \to V$.

As the following remark and theorem state, finite dimensional inner product spaces can be described using $\mathbb{R}^n$ or $\mathbb{C}^n$.

Remark. Suppose V is an inner product space over F, where F is $\mathbb{R}$ or $\mathbb{C}$, with finite dimension n. Let $B = \{b_1, \ldots, b_n\}$ be a basis of V. Then any vector $v \in V$ can be uniquely written as $v = \sum_{i=1}^n c_i b_i$ with $c_i \in F$. The vector $(c_i)_{i=1}^n \in F^n$ is called the representation of v with respect to the basis B. This representation respects addition and scalar multiplication, so the representation of a sum of vectors v_j is the sum of the representations of those vectors v_j and the representation of a scalar multiple of a vector v is the scalar multiple of the representation of v. If B is an orthonormal basis (so all elements in the basis are orthogonal to each other and have norm equal to 1), then the inner product of two vectors $v, w \in V$ is the same as the inner product of their representations in F^n. An orthonormal basis can always be obtained from a given basis using the Gram-Schmidt process.

Theorem 2.2. *Suppose V, W are inner product spaces over F, where F is $\mathbb{R}$ or $\mathbb{C}$, with finite dimensions n and m respectively. Let $A : V \to W$ be a linear operator. If we fix bases for V and W, then A can be uniquely represented by an $m \times n$ matrix $(a_{i,j})_{(i,j)\in\{1,\ldots,m\}\times\{1,\ldots,n\}}$ with entries in F. Multiplication by this matrix will map the representation of $v \in V$ to the representation of $Av \in W$ using the previously fixed bases.*

Indeed we see that vectors in finite dimensional inner product spaces, the inner products on these spaces and linear operators between these spaces can all be expressed using elements of F^n, the standard inner products on F^n and matrices with entries in F (where F is equal to $\mathbb{R}$ or $\mathbb{C}$).

Definition 2.4. Hilbert space. A Hilbert space is a complete inner product space, so an inner product space where all Cauchy sequences converge.

Remark. We note that any finite-dimensional inner product space is complete and therefore a Hilbert space.

Definition 2.5. Adjoint. Given an inner product space V with inner product $\langle \cdot, \cdot \rangle$, the adjoint of a linear operator $A : V \to V$ is defined as the unique operator $A^\dagger$ which satisfies $\langle v, Aw \rangle = \langle A^\dagger v, w \rangle$ for all $v, w \in V$.

Remark. The adjoint is conjugate linear in the sense that if V is an inner product space and $A_1, \ldots, A_n$ are operators on V and $a_1, \ldots, a_n$ are scalars, then $(\sum_{i=1}^n a_i A_i)^\dagger = \sum_{i=1}^n a_i^* A_i^\dagger$. We also note that $(A^\dagger)^\dagger = A$ for any operator A. Lastly if A and B are linear operators on a vector space V, then $(AB)^\dagger = B^\dagger A^\dagger$.

Remark. If V is a finite dimensional inner product space over $\mathbb{R}$ or $\mathbb{C}$, a linear operator $A : V \to V$ has a matrix representation with respect to a given basis of V and the matrix representation of $A^\dagger$ is given by the transpose of the complex conjugate of the matrix representation of A.

Definition 2.6. Normal. A linear operator A is called normal if $AA^\dagger = A^\dagger A$.

Definition 2.7. Self-adjoint. A linear operator A is called self-adjoint if $A^\dagger = A$.

Remark. A linear operator A on a finite dimensional inner product space V over $\mathbb{R}$ or $\mathbb{C}$ is self-adjoint if and only if its matrix representation with respect to a given basis of V is Hermitian (equal to the transpose of its complex conjugate).

Definition 2.8. Positive. A linear operator A is called positive if $\langle v, Av \rangle \geq 0$ for all $v \in V$.

Remark. If A is a positive operator and $a \geq 0$ a scalar, then aA is a positive operator.

Definition 2.9. Projector. Let V be a d-dimensional vector space (over $\mathbb{R}$ or $\mathbb{C}$) and $W \subseteq V$ a k-dimensional subspace of V. It is possible to construct an orthonormal basis $B = \{b_1, \ldots, b_d\}$ such that $\{b_1, \ldots, b_k\}$ is a basis for W. The

projector P onto the subspace W is defined by $P\left(\sum_{i=1}^{d} c_i b_i\right) = \sum_{i=1}^{k} c_i b_i$ (with c_i in $\mathbb{R}$ or $\mathbb{C}$ as appropriate). This definition is independent of the chosen basis and P is a linear operator.

Theorem 2.3. *Spectral decomposition. Let V be a finite dimensional vector space and M a normal operator on V. There exists an orthonormal basis for V such that M is diagonal with respect to this basis. This basis consists of eigenvectors of M. Let $\{\lambda_i\}$ be the set of eigenvalues of M, then $M = \sum_i \lambda_i P_i$, where P_i is the projector onto the eigenspace of M associated with the eigenvalue λ_i.*

Definition 2.10. Operator norm. Given a linear operator $A : V \to V$, the norm of A can be defined as:

$$\|A\| = \sup_{v \in V, v \neq 0} \frac{\|Av\|_2}{\|v\|_2} \tag{11}$$

when the supremum in (11) is finite.

Remark. This defines a norm on the space of linear operators $A : V \to V$ for which the supremum in (11) is finite.

Definition 2.11. Trace. The trace of a linear operator $A : V \to V$, where V is a finite dimensional inner product space is defined as follows. A can be represented by a matrix $(a_{i,j})_{i,j=1}^{n}$ with respect to some basis of V and the trace $tr(A)$ of A is defined as the sum of all the elements on the diagonal of that matrix: $tr(A) = \sum_{i=1}^{n} a_{i,i}$.

Remark. This definition turns out to be independent from the chosen basis, so the trace of a linear operator is well-defined. If the chosen basis $\{v_1, \ldots, v_n\}$ of V is orthonormal, then the trace of a linear operator A is given by:

$$tr(A) = \sum_{i=1}^{n} \langle v_i, Av_i \rangle . \tag{12}$$

Remark. The trace is linear, so if V is an inner product space and $A_1, \ldots, A_n$ are operators on V and $a_1, \ldots, a_n$ are scalars, then $tr\left(\sum_{i=1}^{n} a_i A_i\right) = \sum_{i=1}^{n} a_i tr(A_i)$.

Definition 2.12. Direct sum of inner product spaces. If V and W are inner product spaces (over the same field $\mathbb{R}$ or $\mathbb{C}$), then the direct sum $V \oplus W$ of V and W is an inner product space whose elements are the ordered pairs (v, w) with $v \in V$ and $w \in W$. Addition, scalar multiplication and inner product on $V \oplus W$ are defined as:

$$(v_1, w_1) + (v_2, w_2) = (v_1 + v_2, w_1 + w_2), \tag{13}$$

$$a(v, w) = (av, aw) \tag{14}$$

and

$$\langle (v_1, w_1), (v_2, w_2) \rangle = \langle v_1, w_1 \rangle + \langle v_2, w_2 \rangle . \tag{15}$$

It can be verified that this makes $V \oplus W$ into an inner product space with $(0, 0)$ as the zero-element. This definition can be generalized to direct sums of more than two inner product spaces.

Theorem 2.4. *If V and W are inner product spaces (over the same field $\mathbb{R}$ or $\mathbb{C}$) with bases $\{v_i : i \in I\}$ and $\{w_j : j \in J\}$ for V and W respectively, then $\{(v_i, 0) : i \in I\} \cup \{(0, w_j) : j \in J\}$ is a basis for $V \oplus W$. This basis is orthonormal if $\{v_i : i \in I\}$ and $\{w_j : j \in J\}$ are orthonormal.*

Remark. We note that $\mathbb{C}^{n+m}$ can be identified with $\mathbb{C}^n \oplus \mathbb{C}^m$ by identifying $(c_i)_{i=1}^{n+m}$ with $((c_i)_{i=1}^{n}, (c_{i+n})_{i=1}^{m})$.

Definition 2.13. Direct sum of linear operators. If V and W are inner product spaces (over the same field $\mathbb{R}$ or $\mathbb{C}$) and A and B are linear operators on V and W respectively, then the linear operator $A \oplus B$ on $V \oplus W$ is defined as:

$$(A \oplus B)(v, w) = (Av, Bw) \tag{16}$$

and it can be shown that this is indeed a linear operator.

Remark. If V and W are inner product spaces (over the same field $\mathbb{R}$ or $\mathbb{C}$), A and C are linear operators on V and B and D are linear operators on W, then $(A \oplus B)(C \oplus D) = (AC \oplus BD)$.

Definition 2.14. Quotient space. If V is a vector space and $W \subseteq V$ is a subspace of V, then $vRw \iff v - w \in W$ defines an equivalence relation on V. If we write $\overline{v}$ for the equivalence class of v under this equivalence relation, then $V/W = \{\overline{v} : v \in V\}$ is a vector space with $\overline{0}$ as the zero-vector and with addition and scalar multiplication defined as:

$$\overline{v} + \overline{w} = \overline{v + w} \tag{17}$$

and

$$\overline{av} = a\overline{v}. \tag{18}$$

It can be verified that these operations are well-defined and that V/W equipped with these operations is indeed a vector space. V/W is called the quotient vector space of V and W.

Next we will introduce the notion of a tensor product. A tensor product is a way to construct vector spaces using existing vector spaces.

Definition 2.15. Free vector space. Let B be any non-empty set. The free vector space $\mathscr{F}(B)$ of B over a field $\mathbb{R}$ or $\mathbb{C}$ is defined as the vector space with B as its basis. The elements of $\mathscr{F}(B)$ are formal finite sums $\sum_{b \in B} c_b b$ with c_b scalars which are equal to 0 for all but finitely many b. Addition and scalar multiplication are defined component-wise, so $\sum_{b \in B} c_b b + \sum_{b \in B} d_b b = \sum_{b \in B} (c_b + d_b) b$ and $c \sum_{b \in B} c_b b = \sum_{b \in B} c c_b b$.

Remark. We note that the formal sums in the definition of the free vector space are formal in the sense that the summation signs do not indicate the summation of elements of B according to some pre-defined notion of summation in B. The sums serve as a way to suggestively write down the elements of the free vector space. If B is already the underlying set of some vector space, then it should be noted that the free vector space on B does not depend in any way on the vector space structure on B.

Definition 2.16. Tensor product of vector spaces. Given vector spaces V and W (over the same field $\mathbb{R}$ or $\mathbb{C}$), consider the free vector space $\mathscr{F}(V \times W)$ and the linear subspace F of $\mathscr{F}(V \times W)$ spanned by all vectors of the forms $(v, \lambda w) - \lambda(v, w), (\lambda v, w) - \lambda(v, w), (v_1 + v_2, w) - (v_1, w) - (v_2, w), (v, w_1 + w_2) - (v, w_1) - (v, w_2)$ with λ a scalar, $v, v_1, v_2 \in V$ and $w, w_1, w_2 \in W$. We define the tensor product $V \otimes W$ of V and W as the quotient space $V \otimes W = \mathscr{F}(V \times W)/F$. We write $v \otimes w$ for the equivalence class of (v, w) in $V \otimes W$ and call it the tensor product of v and w.

The above definition of the tensor product is rather abstract. One can intuitively think of $V \otimes W$ as the vector space spanned by elements of the form $v \otimes w$ with $v \in V$ and $w \in W$ where the addition and scalar multiplication satisfy the following rules (in addition to the vector space axioms) for all scalars λ, $v, v_1, v_2 \in V$ and $w, w_1, w_2 \in W$:

$$\lambda(v \otimes w) = (\lambda v) \otimes w = v \otimes (\lambda w), \tag{19}$$

$$(v_1 + v_2) \otimes w = (v_1 \otimes w) + (v_2 \otimes w), \tag{20}$$

$$v \otimes (w_1 + w_2) = (v \otimes w_1) + (v \otimes w_2). \tag{21}$$

We note that two elements of $V \otimes W$ are only equal if this follows from the above rules and the vector space axioms. The definition of the tensor product can be extended in case V and W are inner product spaces by defining an inner product on $V \otimes W$.

Definition 2.17. Tensor product of inner product spaces. Given inner product spaces V and W, we define $V \otimes W$ as before making it a vector space. In addition for $v_1, v_2 \in V$ and $w_1, w_2 \in W$ the inner product of $v_1 \otimes w_1$ and $v_2 \otimes w_2$ is defined as:

$$\langle v_1 \otimes w_1, v_2 \otimes w_2 \rangle = \langle v_1, w_1 \rangle \langle v_2, w_2 \rangle . \tag{22}$$

Extending this linearly to $V \otimes W$ defines an inner product (non-degenerate) on $V \otimes W$. This makes $V \otimes W$ into an inner product space.

Just as vector spaces V and W can be used to construct the tensor product $V \otimes W$, linear operators $A : V \to V$ and $B : W \to W$ can be used to construct the tensor product $A \otimes B$ which is a linear operator on $V \otimes W$.

Definition 2.18. Tensor product of operators. Let V, W be vector spaces and A, B linear operators on V and W respectively. The linear operator $A \otimes B$ is defined by letting $(A \otimes B)(v \otimes w) = (Av) \otimes (Bw)$ for all $v \in V$ and $w \in W$ and extending it linearly to $V \otimes W$.

The following theorems state some properties of tensor products that will be relevant to the contents of this thesis.

Theorem 2.5. *Let V, W be vector spaces, A, C linear operators on V and B, D linear operators on W. Then $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$.*

Theorem 2.6. *Let V, W be vector spaces and A, B linear operators on V and W respectively. Then $(A \otimes B)^\dagger = A^\dagger \otimes B^\dagger$.*

Theorem 2.7. *Let V, W be vector spaces and A, B self-adjoint linear operators on V and W respectively. Then $A \otimes B$ is a self-adjoint linear operator on $V \otimes W$.*

Theorem 2.8. *Let V, W be vector spaces and A, B positive linear operators on V and W respectively. Then $A \otimes B$ is a positive linear operator on $V \otimes W$.*

Theorem 2.9. *Let V, W be vector spaces of dimensions n and m respectively and let A, B linear operators on V and W respectively. Let $\{e_i : i \in \{1, \ldots, n\}\}$ and $\{f_j : j \in \{1, \ldots, m\}\}$ be bases for V and W respectively. Let $(a_{i,j})_{i,j=1}^n$ and $(b_{i,j})_{i,j=1}^n$ be the matrix representations of A and B respectively with respect to the given bases. $\{e_i \otimes f_j : (i,j) \in \{1, \ldots, n\} \times \{1, \ldots, m\}\}$ is a basis for $V \otimes W$. If $\{e_i : i \in \{1, \ldots, n\}\}$ and $\{f_j : j \in \{1, \ldots, m\}\}$ are orthonormal bases, then $\{e_i \otimes f_j : (i,j) \in \{1, \ldots, n\} \times \{1, \ldots, m\}\}$ is also an orthonormal basis. $A \otimes B$ will have a matrix representation $(c_{(p,q),(r,s)})_{(p,q),(r,s) \in \{1,\ldots,n\} \times \{1,\ldots,m\}}$ with respect to $\{e_i \otimes f_j : (i,j) \in \{1, \ldots, n\} \times \{1, \ldots, m\}\}$ with:*

$$c_{(p,q),(r,s)} = a_{p,r} b_{q,s}. \tag{23}$$

This representation of $A \otimes B$ is known as the Kronecker product.

We now move on to stating and proving some more specific results.

Theorem 2.10. *Let V be an inner product space over $\mathbb{C}$ and A an operator on V, then there exist self-adjoint operators B and C on V such that $A = B + iC$.*

Proof. Let V be an inner product space over $\mathbb{C}$ and A an operator on V. Let $B = \frac{1}{2}(A + A^\dagger)$ and $C = \frac{1}{2i}(A - A^\dagger)$. Then

$$B + iC = \frac{1}{2}(A + A^\dagger) + \frac{1}{2}(A - A^\dagger) = A. \tag{24}$$

Also

$$B^\dagger = \frac{1}{2}(A^\dagger + (A^\dagger)^\dagger) = \frac{1}{2}(A^\dagger + A) = B \tag{25}$$

and

$$C^\dagger = -\frac{1}{2i}(A^\dagger - (A^\dagger)^\dagger) = -\frac{1}{2i}(A^\dagger - A) = \frac{1}{2i}(A - A^\dagger) = C. \tag{26}$$

So B and C are self-adjoint which completes the proof.

□

Theorem 2.11. *Let V be an inner product space over $\mathbb{C}$ and A a positive operator on V, then A is self-adjoint.*

Proof. Let V be an inner product space over $\mathbb{C}$ and A a positive operator on V. By Theorem 2.10 there exist self-adjoint operators B and C on V such that $A = B + iC$. Let $v \in V$. Since B and C are self-adjoint we have

$$\langle v, Bv\rangle^* = \langle Bv, v\rangle = \left\langle B^\dagger v, v\right\rangle = \langle v, Bv\rangle \tag{27}$$

and

$$\langle v, Cv\rangle^* = \langle Cv, v\rangle = \left\langle C^\dagger v, v\right\rangle = \langle v, Cv\rangle \tag{28}$$

so $\langle v, Bv\rangle$ and $\langle v, Cv\rangle$ are real. Also, since A is positive

$$\langle v, Av\rangle = \langle v, Bv + iCv\rangle = \langle v, Bv\rangle + i\,\langle v, Cv\rangle \tag{29}$$

is positive and therefore real. Since $\langle v, Bv\rangle$ and $\langle v, Cv\rangle$ are real, $\langle v, Av\rangle$ has an imaginary component $\langle v, Cv\rangle$. Since $\langle v, Av\rangle$ is real we must have $\langle v, Cv\rangle = 0$. So $\langle v, Cv\rangle = 0$ for all $v \in V$. This means that

$$\begin{aligned}
&0 = \langle Cv + v, C(Cv + v)\rangle = \langle Cv, C(Cv)\rangle + \langle Cv, Cv\rangle + \langle v, C(Cv)\rangle + \langle v, Cv\rangle = \\
&0 + \langle Cv, Cv\rangle + \langle v, C(Cv)\rangle + 0 = \langle Cv, Cv\rangle + \langle v, C(Cv)\rangle = \\
&\langle Cv, Cv\rangle + \left\langle C^\dagger v, Cv\right\rangle = 2\,\langle Cv, Cv\rangle = 2\|Cv\|_2^2.
\end{aligned} \tag{30}$$

So $\|Cv\|_2 = 0$ and therefore $Cv = 0$. Since this holds for all $v \in V$ we have $C = 0$. But then $A = B$ and B is self-adjoint, so A is self-adjoint. □

Theorem 2.12. *Let V be an inner product space over $\mathbb{C}$ and E a positive operator on V such that $id - E$ is positive. Let $A = id - 2E$, then A is self-adjoint and $\|A\| \leq 1$.*

Proof. Let V be an inner product space over $\mathbb{C}$ and E a positive operator on V such that $id - E$ is positive and let $A = id - 2E$. We note that $E, id - E$ are positive and therefore self-adjoint by Theorem 2.11. The identity is also self-adjoint, so $A^\dagger = id^\dagger - 2E^\dagger = id - 2E = A$ and we see that A is also self-adjoint. We note that $E(id - E) = E - E^2 = (id - E)E$, so E and $id - E$ commute. Let $v \in V$, then

$$
\begin{aligned}
&\|Av\|_2^2 = \langle Av, Av\rangle = \langle (id-2E)v, (id-2E)v\rangle = \langle v-2Ev, v-2Ev\rangle = \\
&\langle v,v\rangle - 2\langle v, Ev\rangle - 2\langle Ev, v\rangle + 4\langle Ev, Ev\rangle = \\
&\langle v,v\rangle - 2\langle v, Ev\rangle - 2\left\langle E^\dagger v, v\right\rangle + 4\langle Ev, Ev\rangle = \\
&\langle v,v\rangle - 2\langle v, Ev\rangle - 2\langle v, Ev\rangle + 4\langle Ev, Ev\rangle = \\
&\langle v,v\rangle - 4\left(\langle v, Ev\rangle - \langle Ev, Ev\rangle\right) = \\
&\langle v,v\rangle - 4\langle v-Ev, Ev\rangle = \langle v,v\rangle - 4\langle (id-E)v, Ev\rangle = \\
&\langle v,v\rangle - 4\left\langle (id-E)^\dagger v, Ev\right\rangle = \langle v,v\rangle - 4\langle v, (id-E)Ev\rangle = \\
&\langle v,v\rangle - 4\langle v, (E+id-E)(id-E)Ev\rangle = \\
&\langle v,v\rangle - 4\langle v, E(id-E)Ev + (id-E)(id-E)Ev\rangle = \\
&\langle v,v\rangle - 4\langle v, E(id-E)Ev + (id-E)E(id-E)v\rangle = \\
&\langle v,v\rangle - 4\left(\langle v, E(id-E)Ev\rangle + \langle v, (id-E)E(id-E)v\rangle\right) = \\
&\langle v,v\rangle - 4\left(\left\langle E^\dagger v, (id-E)Ev\right\rangle + \left\langle (id-E)^\dagger v, E(id-E)v\right\rangle\right) = \\
&\langle v,v\rangle - 4\left(\langle Ev, (id-E)Ev\rangle + \langle (id-E)v, E(id-E)v\rangle\right) \leq \\
&\langle v,v\rangle = \|v\|_2^2
\end{aligned}
\tag{31}
$$

where we used that $\langle Ev, (id-E)Ev\rangle, \langle (id-E)v, E(id-E)v\rangle \geq 0$ because E and $id-E$ are positive. It follows that $\|Av\|_2 \leq \|v\|_2$ and since this holds for all $v \in V$ we have $\|A\| \leq 1$, which completes the proof. □

Theorem 2.13. *Let V be an inner product space over $\mathbb{C}$ and A a self-adjoint operator on V with $\|A\| \leq 1$. Let $E = \frac{1}{2}id - \frac{1}{2}A$, then E and $id-E$ are positive operators.*

Proof. Let V be an inner product space over $\mathbb{C}$ and A a self-adjoint operator on V with $\|A\| \leq 1$ and let $E = \frac{1}{2}id - \frac{1}{2}A$. We note that $id - E = \frac{1}{2}id + \frac{1}{2}A$. Let $v \in V$. Since A is self-adjoint we have

$$
\langle v, Av\rangle^* = \langle Av, v\rangle = \left\langle A^\dagger v, v\right\rangle = \langle v, Av\rangle \tag{32}
$$

so $\langle v, Av\rangle$ is real. Using the fact that $\|A\| \leq 1$ and the Cauchy-Schwarz inequality it follows that:

$$
|\langle v, Av\rangle| \leq \|v\|_2 \|Av\|_2 \leq \|v\|_2 \|A\| \|v\|_2 \leq \|v\|_2^2 = \langle v, v\rangle . \tag{33}
$$

Combining this with the fact that $\langle v, AV\rangle$ is real we find that

$$
-\langle v, v\rangle \leq \langle v, Av\rangle \leq \langle v, v\rangle . \tag{34}
$$

Now it follows that

$$
\begin{aligned}
&\langle v, Ev\rangle = \left\langle v, \left(\frac{1}{2}id - \frac{1}{2}A\right)v\right\rangle = \\
&\frac{1}{2}\langle v, v\rangle - \frac{1}{2}\langle v, Av\rangle \geq \frac{1}{2}\langle v, v\rangle - \frac{1}{2}\langle v, v\rangle = 0
\end{aligned}
\tag{35}
$$

and

$$\begin{aligned}&\langle v, (id - E)v\rangle = \left\langle v, \left(\frac{1}{2}id + \frac{1}{2}A\right) v\right\rangle = \\ &\frac{1}{2}\langle v, v\rangle + \frac{1}{2}\langle v, Av\rangle \geq \frac{1}{2}\langle v, v\rangle - \frac{1}{2}\langle v, v\rangle = 0.\end{aligned} \tag{36}$$

This holds for all $v \in V$, so E and $id - E$ are positive operators which completes the proof. □

Theorem 2.14. *Let V, W be finite dimensional inner product spaces. Let $A : V \to V$ and $B : W \to W$ be normal operators of finite norm. Then $\|A \otimes B\| = \|A\|\|B\|$.*

Proof. Let V, W be finite dimensional inner product spaces. Let $A : V \to V$ and $B : W \to W$ be normal operators of finite norm. Let n and m be the dimensions of V and W respectively. Since A is normal, there exists an orthonormal basis $\{v_1, \ldots, v_n\}$ of V such that v_i is an eigenvector of A with eigenvalue a_i. Similarly, because B is normal, there exists an orthonormal basis $\{w_1, \ldots, w_m\}$ of W such that w_j is an eigenvector of B with eigenvalue b_j. We note that for all $i \in \{1, \ldots, n\}$ and $j \in \{1, \ldots, m\}$:

$$|a_i| = \frac{|a_i|\|v_i\|_2}{\|v_i\|_2} = \frac{\|a_i v_i\|_2}{\|v_i\|_2} = \frac{\|Av_i\|_2}{\|v_i\|_2} \leq \|A\| \tag{37}$$

and

$$|b_j| = \frac{|b_j|\|w_j\|_2}{\|w_j\|_2} = \frac{\|b_j w_j\|_2}{\|w_j\|_2} = \frac{\|Bw_j\|_2}{\|w_j\|_2} \leq \|B\|. \tag{38}$$

Now $\{v_i \otimes w_j : i \in \{1, \ldots, n\}, j \in \{1, \ldots, m\}\}$ is a basis for $V \otimes W$, so an arbitrary element of $V \otimes W$ can be written as $\sum_{i=1}^{n}\sum_{j=1}^{m} c_{i,j}(v_i \otimes w_j)$ for unique scalars $c_{i,j}$. Now we have for any choice of scalars $c_{i,j}$:

$$\left\|(A\otimes B)\sum_{i=1}^{n}\sum_{j=1}^{m}c_{i,j}(v_i\otimes w_j)\right\|_2=\left\|\sum_{i=1}^{n}\sum_{j=1}^{m}c_{i,j}(Av_i\otimes Bw_j)\right\|_2=$$

$$\left\|\sum_{i=1}^{n}\sum_{j=1}^{m}c_{i,j}(a_iv_i\otimes b_jw_j)\right\|_2=\left\|\sum_{i=1}^{n}\sum_{j=1}^{m}c_{i,j}a_ib_j(v_i\otimes w_j)\right\|_2=$$

$$\sqrt{\left\langle\sum_{i=1}^{n}\sum_{j=1}^{m}c_{i,j}a_ib_j(v_i\otimes w_j),\sum_{k=1}^{n}\sum_{l=1}^{m}c_{k,l}a_kb_l(v_k\otimes w_l)\right\rangle}=$$

$$\sqrt{\sum_{i=1}^{n}\sum_{j=1}^{m}\sum_{k=1}^{n}\sum_{l=1}^{m}c_{i,j}^*a_i^*b_j^*c_{k,l}a_kb_l\left\langle v_i,v_k\right\rangle\left\langle w_j,w_l\right\rangle}=$$

$$\sqrt{\sum_{i=1}^{n}\sum_{j=1}^{m}|c_{i,j}|^2|a_i|^2|b_j|^2}\leq\sqrt{\sum_{i=1}^{n}\sum_{j=1}^{m}|c_{i,j}|^2\|A\|^2\|B\|^2}= \tag{39}$$

$$\|A\|\|B\|\sqrt{\sum_{i=1}^{n}\sum_{j=1}^{m}|c_{i,j}|^2}=$$

$$\|A\|\|B\|\sqrt{\sum_{i=1}^{n}\sum_{j=1}^{m}\sum_{k=1}^{n}\sum_{l=1}^{m}\langle c_{i,j}(v_i\otimes w_j),c_{k,l}(v_k\otimes w_l)\rangle}=$$

$$\|A\|\|B\|\sqrt{\left\langle\sum_{i=1}^{n}\sum_{j=1}^{m}c_{i,j}(v_i\otimes w_j),\sum_{k=1}^{n}\sum_{l=1}^{m}c_{k,l}(v_k\otimes w_l)\right\rangle}=$$

$$\|A\|\|B\|\left\|\sum_{i=1}^{n}\sum_{j=1}^{m}c_{i,j}(v_i\otimes w_j)\right\|_2.$$

This means that $\|A\otimes B\|\leq\|A\|\|B\|$. In case $\|A\|=0$ or $\|B\|=0$ it follows that $0\leq\|A\otimes B\|\leq\|A\|\|B\|=0$, so $\|A\otimes B\|=0=\|A\|\|B\|$. Suppose instead that $\|A\|,\|B\|>0$ and let $\epsilon>0$. Let $\delta=\min\left\{\frac{\epsilon}{\|A\|+\|B\|+1},\|A\|,\|B\|\right\}>0$. Let $v\in V$ and $w\in W$ be such that $\frac{\|Av\|_2}{\|v\|_2}>\|A\|-\delta$ and $\frac{\|Bw\|_2}{\|w\|_2}>\|B\|-\delta$. We then have:

$$\|A \otimes B\| \geq \frac{\|(A \otimes B)(v \otimes w)\|_2}{\|v \otimes w\|_2} = \frac{\|Av \otimes Bw)\|_2}{\|v \otimes w\|_2} = \frac{\sqrt{\langle Av \otimes Bw, Av \otimes Bw\rangle}}{\sqrt{\langle v \otimes w, v \otimes w\rangle}} =$$
$$\frac{\sqrt{\langle Av, Av\rangle}\sqrt{\langle Bw, Bw\rangle}}{\sqrt{\langle v, v\rangle}\sqrt{\langle w, w\rangle}} = \frac{\|Av\|_2}{\|v\|_2}\frac{\|Bw\|_2}{\|w\|_2} > (\|A\| - \delta)(\|B\| - \delta) =$$
$$\|A\|\|B\| - \delta(\|A\| + \|B\|) + \delta^2 > \|A\|\|B\| - \delta(\|A\| + \|B\|) \geq$$
$$\|A\|\|B\| - \frac{\epsilon}{\|A\| + \|B\| + 1}(\|A\| + \|B\|) > \|A\|\|B\| - \epsilon. \tag{40}$$

This holds for all $\epsilon > 0$ so $\|A \otimes B\| \geq \|A\|\|B\|$, so we see that $\|A \otimes B\| = \|A\|\|B\|$. □

Theorem 2.15. *Let V be an inner product space of finite dimension n and $A : V \to V$ a linear operator. Let $(a_{i,j})_{i,j=1}^n$ be the matrix representation of A with respect to an orthonormal basis $\{v_1, \ldots, v_n\}$ of V. Then $|a_{i,j}| \leq \|A\|$ for all $i, j \in \{1, \ldots, n\}$.*

Proof. Let V be an inner product space of finite dimension n. Let $A : V \to V$ be a linear operator of finite norm $\|A\|$. Let $(a_{i,j})_{i,j=1}^n$ be the matrix representation of A with respect to an orthonormal basis $\{v_1, \ldots, v_n\}$ of V. We note that the basis vectors v_i have representations $(\delta_{i,j})_{j=1}^n$ with respect to the given basis. Now we have for all $i, j \in \{1, \ldots, n\}$, using the Cauchy-Schwarz inequality:

$$|a_{i,j}| = \left|\sum_{k=1}^n \delta_{i,k} a_{k,j}\right| = |\langle (\delta_{i,k})_{k=1}^n, (a_{k,j})_{k=1}^n\rangle| =$$
$$\left|\left\langle (\delta_{i,k})_{k=1}^n, \left(\sum_{l=1}^n \delta_{j,l} a_{k,l}\right)_{k=1}^n \right\rangle\right| = \left|\left\langle (\delta_{i,k})_{k=1}^n, (a_{k,l})_{k,l=1}^n (\delta_{j,l})_{l=1}^n \right\rangle\right| = \tag{41}$$
$$|\langle v_i, Av_j\rangle| \leq \|v_i\|_2 \|Av_j\|_2 \leq \|v_i\|_2 \|A\| \|v_j\|_2 = \|A\|$$

which completes the proof. □

Theorem 2.16. *Let V be an inner product space of finite dimension n. Let $A : V \to V$ be a positive linear operator. Let $(a_{i,j})_{i,j=1}^n$ be the matrix representation of A with respect to an orthonormal basis $\{v_1, \ldots, v_n\}$ of V. Then $a_{i,i} \geq 0$ for all $i \in \{1, \ldots, n\}$.*

Proof. Let V be an inner product space of finite dimension n. Let $A : V \to V$ be a positive linear operator. Let $(a_{i,j})_{i,j=1}^n$ be the matrix representation of A with respect to an orthonormal basis $\{v_1, \ldots, v_n\}$ of V. We note that the basis vectors v_i have representations $(\delta_{i,j})_{j=1}^n$ with respect to the given basis. Now we have for all $i \in \{1, \ldots, n\}$:

$$a_{i,i} = \sum_{k=1}^{n} \delta_{i,k} a_{k,i} = \langle (\delta_{i,k})_{k=1}^{n}, (a_{k,i})_{k=1}^{n} \rangle = \\ \left\langle (\delta_{i,k})_{k=1}^{n}, \left(\sum_{l=1}^{n} \delta_{i,l} a_{k,l} \right)_{k=1}^{n} \right\rangle = \left\langle (\delta_{i,k})_{k=1}^{n}, (a_{k,l})_{k,l=1}^{n} (\delta_{i,l})_{l=1}^{n} \right\rangle = \\ \langle v_i, A v_i \rangle \geq 0 \tag{42}$$

which completes the proof. □

Theorem 2.17. *Let V be an inner product space of finite dimension n. Let $A, B : V \to V$ be self-adjoint operators, then $tr(AB) \in \mathbb{R}$. If furthermore B is positive, then $|tr(AB)| \leq \|A\| tr(B)$.*

Proof. Let V be an inner product space of finite dimension n. Let $A, B : V \to V$ be self-adjoint operators. Since A is normal, there exists an orthonormal basis $\{v_1, \ldots, v_n\}$ of V such that A is diagonal with respect to this basis. Let $(a_{i,j})_{i,j=1}^{n}$ and $(b_{i,j})_{i,j=1}^{n}$ be the matrix representations of A and B respectively with respect to the given basis. A is diagonal with respect to this basis, so $a_{i,j} = 0$ if $i \neq j$. A and B are self-adjoint, so $a_{i,i}^{*} = a_{i,i}$ and $b_{i,i}^{*} = b_{i,i}$ for all $i \in \{1, \ldots, n\}$ so the $a_{i,i}$ and $b_{i,i}$ are real. This means that

$$tr(AB) = tr((a_{i,k})_{i,k=1}^{n} (b_{k,j})_{k,j=1}^{n}) = tr\left(\left(\sum_{k=1}^{n} a_{i,k} b_{k,j} \right)_{i,j=1}^{n} \right) = \\ tr\left((a_{i,i} b_{i,j})_{i,j=1}^{n} \right) = \sum_{i=1}^{n} a_{i,i} b_{i,i} \in \mathbb{R} \tag{43}$$

because all the $a_{i,i}$ and $b_{i,i}$ are real. Now suppose that B is positive. Then $|a_{i,i}| \leq \|A\|$ and $b_{i,i} \geq 0$ for all $i \in \{1, \ldots, n\}$ by Theorems 2.15 and 2.16 respectively. It follows that

$$|tr(AB)| = \left| \sum_{i=1}^{n} a_{i,i} b_{i,i} \right| \leq \sum_{i=1}^{n} |a_{i,i}||b_{i,i}| = \sum_{i=1}^{n} |a_{i,i}| b_{i,i} \leq \sum_{i=1}^{n} \|A\| b_{i,i} = \\ \|A\| \sum_{i=1}^{n} b_{i,i} = \|A\| tr(B) \tag{44}$$

which completes the proof. □

Theorem 2.18. *If $F : V \to W$ is an isomorphism and A is a linear operator on V, then*

$$(F A F^{-1})^{\dagger} = F A^{\dagger} F^{-1}. \tag{45}$$

Proof. Let $F : V \to W$ an isomorphism and A a linear operator on V. Then for all $v, w \in W$ we have:

$$\left\langle FA^\dagger F^{-1}v, w\right\rangle = \left\langle A^\dagger F^{-1}v, F^{-1}w\right\rangle = \left\langle F^{-1}v, AF^{-1}w\right\rangle = \left\langle v, FAF^{-1}w\right\rangle \quad (46)$$

so $(FAF^{-1})^\dagger = FA^\dagger F^{-1}$. □

Corollary 2.18.1. *If $F : V \to W$ is an isomorphism and A is a self-adjoint operator on V, then FAF^{-1} is self-adjoint.*

Proof. Let $F : V \to W$ an isomorphism and A a self-adjoint operator on V, then $(FAF^{-1})^\dagger = FA^\dagger F^{-1} = FAF^{-1}$, so FAF^{-1} is self-adjoint. □

Theorem 2.19. *If $F : V \to W$ is an isomorphism and A is a linear operator on V with finite norm $\|A\|$, then $\left\|FAF^{-1}\right\| = \|A\|$.*

Proof. Let $F : V \to W$ an isomorphism and A a linear operator on V with finite norm $\|A\|$. For all $w \in W$ we have:

$$\left\|FAF^{-1}w\right\|_2 = \left\|AF^{-1}w\right\|_2 \leq \|A\|\left\|F^{-1}w\right\|_2 = \|A\|\|w\|_2, \quad (47)$$

so FAF^{-1} has a finite norm $\left\|FAF^{-1}\right\| \leq \|A\|$. Also, for all $v \in V$ we have:

$$\|Av\|_2 = \left\|AF^{-1}Fv\right\|_2 = \left\|FAF^{-1}Fv\right\|_2 \leq \left\|FAF^{-1}\right\|\|Fv\|_2 = \left\|FAF^{-1}\right\|\|v\|_2, \quad (48)$$

so $\|A\| \leq \left\|FAF^{-1}\right\|$ and we conclude that $\left\|FAF^{-1}\right\| = \|A\|$. □

Theorem 2.20. *If $F : V \to W$ is an isomorphism and A is a positive operator on V, then FAF^{-1} is a positive operator.*

Proof. Let $F : V \to W$ an isomorphism and A a positive operator on V. For all $w \in W$ we have:

$$\left\langle w, FAF^{-1}w\right\rangle = \left\langle F^{-1}w, AF^{-1}w\right\rangle \geq 0 \quad (49)$$

because A is positive, so FAF^{-1} is also positive. □

Theorem 2.21. *If $F : V \to W$ is an isomorphism and $\{v_i : i \in I\}$ is a basis for V, then $\{Fv_i : i \in I\}$ is a basis for W. In addition if $\{v_i : i \in I\}$ is orthonormal, then so is $\{Fv_i : i \in I\}$.*

Proof. Let $F : V \to W$ an isomorphism and $\{v_i : i \in I\}$ a basis for V, then $\{v_i : i \in I\}$ spans V and is linearly independent. Let $w \in W$, then $w = FF^{-1}w$. $F^{-1}w \in V$ so there exist scalars a_i, all but finitely many equal to 0, such that $F^{-1}w = \sum_{i\in I} a_i v_i$. But then:

$$w = FF^{-1}w = F\sum_{i\in I} a_i v_i = \sum_{i\in I} a_i Fv_i, \quad (50)$$

so $\{Fv_i : i \in I\}$ spans W. Also if a_i are scalars, all but finitely many equal to 0, such that $\sum_{i\in I} a_i F v_i = 0$, then:

$$0 = F^{-1}0 = F^{-1}\sum_{i\in I} a_i F v_i = \sum_{i\in I} a_i F^{-1} F v_i = \sum_{i\in I} a_i v_i. \tag{51}$$

Now the linear independence of $\{v_i : i \in I\}$ implies that $a_i = 0$ for all i. This means that $\{Fv_i : i \in I\}$ is linearly independent, so $\{Fv_i : i \in I\}$ is a basis for W. Suppose in addition that $\{v_i : i \in I\}$ is orthonormal, so $\langle v_i, v_j\rangle = \delta_{i,j}$. Then we have:

$$\langle Fv_i, Fv_j\rangle = \langle v_i, v_j\rangle = \delta_{i,j}, \tag{52}$$

so $\{Fv_i : i \in I\}$ is orthonormal which completes the proof. □

Theorem 2.22. *If $F : V \to W$ is an isomorphism, V has a finite dimension n and A is a linear operator on V, then $tr(FAF^{-1}) = tr(A)$.*

Proof. Let $F : V \to W$ an isomorphism with V of finite dimension n and A a linear operator on V. Let $\{v_1, \ldots, v_n\}$ be an orthonormal basis for V. Then by Theorem 2.21 $\{Fv_1, \ldots, Fv_n\}$ is an orthonormal basis for W and therefore:

$$tr(FAF^{-1}) = \sum_{i=1}^{n} \left\langle Fv_i, FAF^{-1}Fv_i\right\rangle = \sum_{i=1}^{n} \langle Fv_i, FAv_i\rangle = \sum_{i=1}^{n} \langle v_i, Av_i\rangle = tr(A) \tag{53}$$

which completes the proof. □

Theorem 2.23. *Let V and W be inner product spaces (over the same field $\mathbb{R}$ or $\mathbb{C}$) with orthonormal bases $\{v_i : i \in I\}$ and $\{w_i : i \in I\}$. Let $F : V \to W$ be defined as:*

$$F\left(\sum_{i\in I} a_i v_i\right) = \sum_{i\in I} a_i w_i, \tag{54}$$

then F is an isomorphism.

Proof. Let V, W, $\{v_i : i \in I\}$, $\{w_i : i \in I\}$ and F as defined in the theorem. We can define $G : W \to V$ as:

$$G\left(\sum_{i\in I} a_i w_i\right) = \sum_{i\in I} a_i v_i. \tag{55}$$

Now

$$(F \circ G)\left(\sum_{i\in I} a_i w_i\right) = F\left(\sum_{i\in I} a_i v_i\right) = \sum_{i\in I} a_i w_i \tag{56}$$

and

$$(G \circ F)\left(\sum_{i\in I} a_i v_i\right) = G\left(\sum_{i\in I} a_i w_i\right) = \sum_{i\in I} a_i v_i, \tag{57}$$

so $G = F^{-1}$, the two-sided inverse of F and F is therefore bijective. F is also a linear map preserving inner products, since for all scalars a, a_i, b_i for $i \in I$ we have:

$$\begin{aligned} &F\left(\sum_{i\in I} a_i v_i + \sum_{i\in I} b_i v_i\right) = F\left(\sum_{i\in I}(a_i + b_i)v_i\right) = \sum_{i\in I}(a_i + b_i)w_i = \\ &\sum_{i\in I} a_i w_i + \sum_{i\in I} w_i v_i = F\left(\sum_{i\in I} a_i v_i\right) + F\left(\sum_{i\in I} b_i v_i\right), \end{aligned} \tag{58}$$

$$F\left(a\sum_{i\in I} a_i v_i\right) = F\left(\sum_{i\in I}(aa_i)v_i\right) = \sum_{i\in I}(aa_i)w_i = a\sum_{i\in I} a_i w_i = aF\left(\sum_{i\in I} a_i v_i\right) \tag{59}$$

and

$$\begin{aligned} &\left\langle F\left(\sum_{i\in I} a_i v_i\right), F\left(\sum_{j\in I} b_j v_j\right)\right\rangle = \left\langle \sum_{i\in I} a_i w_i, \sum_{j\in I} b_j w_j \right\rangle = \\ &\sum_{i\in I}\sum_{j\in I} a_i^* b_j \left\langle w_i, w_j\right\rangle = \sum_{i\in I}\sum_{j\in I} a_i^* b_j \delta_{i,j} = \sum_{i\in I}\sum_{j\in I} a_i^* b_j \left\langle v_i, v_j\right\rangle = \\ &\left\langle \sum_{i\in I} a_i v_i, \sum_{j\in I} b_j v_j \right\rangle. \end{aligned} \tag{60}$$

So F is an isomorphism, which completes the proof. □

Theorem 2.24. *If V and W are inner product spaces (over the same field $\mathbb{R}$ or $\mathbb{C}$) and A and B are linear operators on V and W respectively, then $(A \oplus B)^\dagger = A^\dagger \oplus B^\dagger$.*

Proof. Let V and W inner product spaces (over the same field $\mathbb{R}$ or $\mathbb{C}$) and A and B linear operators on V and W respectively. For all $(v, w) \in V \oplus W$ we have:

$$\begin{aligned} &\left\langle (A^\dagger \oplus B^\dagger)(v,w), (v,w)\right\rangle = \left\langle (A^\dagger v, B^\dagger w), (v,w)\right\rangle = \left\langle A^\dagger v, v\right\rangle + \left\langle B^\dagger w, w\right\rangle = \\ &\langle v, Av\rangle + \langle w, Bw\rangle = \langle (v,w), (Av, Bw)\rangle = \langle (v,w), (A\oplus B)(v,w)\rangle, \end{aligned} \tag{61}$$

so $(A \oplus B)^\dagger = A^\dagger \oplus B^\dagger$. □

Corollary 2.24.1. *If V and W are inner product spaces (over the same field $\mathbb{R}$ or $\mathbb{C}$) and A and B are self-adjoint operators on V and W respectively, then $A \oplus B$ is self-adjoint.*

Proof. Let V and W inner product spaces (over the same field $\mathbb{R}$ or $\mathbb{C}$) and A and B self-adjoint operators on V and W respectively. Now by Theorem 2.24 $(A \oplus B)^\dagger = A^\dagger \oplus B^\dagger = A \oplus B$, so $A \oplus B$ is self-adjoint. □

Theorem 2.25. *If V and W are inner product spaces (over the same field $\mathbb{R}$ or $\mathbb{C}$) and A and B are linear operators on V and W respectively with finite norms, then:*

$$\|A \oplus B\| = \max\{\|A\|, \|B\|\}. \tag{62}$$

Proof. Let V and W inner product spaces (over the same field $\mathbb{R}$ or $\mathbb{C}$) and A and B linear operators on V and W respectively with finite norms. For all $(v, w) \in V \oplus W$ we have:

$$\begin{aligned}
&\|(A \oplus B)(v, w)\|_2 = \|(Av, Bw)\|_2 = \sqrt{\langle (Av, Bw), (Av, Bw)\rangle} = \\
&\sqrt{\langle Av, Av\rangle + \langle Bw, Bw\rangle} = \sqrt{\|Av\|_2^2 + \|Bw\|_2^2} \leq \\
&\sqrt{\|A\|^2\|v\|_2^2 + \|B\|^2\|w\|_2^2} \leq \sqrt{(\max\{\|A\|, \|B\|\})^2(\|v\|_2^2 + \|w\|_2^2)} = \\
&\max\{\|A\|, \|B\|\}\sqrt{\|v\|_2^2 + \|w\|_2^2} = \max\{\|A\|, \|B\|\}\sqrt{\langle v, v\rangle + \langle w, w\rangle} = \\
&\max\{\|A\|, \|B\|\}\sqrt{\langle (v, w), (v, w)\rangle} = \max\{\|A\|, \|B\|\}\|(v, w)\|_2,
\end{aligned} \tag{63}$$

so we see that $A \oplus B$ has a finite norm $\|A \oplus B\| \leq \max\{\|A\|, \|B\|\}$. Now for all $v \in V$ we have:

$$\begin{aligned}
&\|Av\|_2 = \sqrt{\langle Av, Av\rangle} = \sqrt{\langle Av, Av\rangle + \langle B0, B0\rangle} = \sqrt{\langle (Av, B0), (Av, B0)\rangle} = \\
&\|(Av, B0)\|_2 = \|(A \oplus B)(v, 0)\|_2 \leq \|A \oplus B\|\|(v, 0)\|_2 = \\
&\|A \oplus B\|\sqrt{\langle (v, 0), (v, 0)\rangle} = \|A \oplus B\|\sqrt{\langle v, v\rangle + \langle 0, 0\rangle} = \|A \oplus B\|\sqrt{\langle v, v\rangle} = \\
&\|A \oplus B\|\|v\|_2,
\end{aligned} \tag{64}$$

so $\|A\| \leq \|A \oplus B\|$. Similarly for all $w \in W$ we have:

$$\begin{aligned}
&\|Bw\|_2 = \sqrt{\langle Bw, Bw\rangle} = \sqrt{\langle A0, A0\rangle + \langle Bw, Bw\rangle} = \sqrt{\langle (A0, Bw), (A0, Bw)\rangle} = \\
&\|(A0, Bw)\|_2 = \|(A \oplus B)(0, w)\|_2 \leq \|A \oplus B\|\|(0, w)\|_2 = \\
&\|A \oplus B\|\sqrt{\langle (0, w), (0, w)\rangle} = \|A \oplus B\|\sqrt{\langle 0, 0\rangle + \langle w, w\rangle} = \|A \oplus B\|\sqrt{\langle w, w\rangle} = \\
&\|A \oplus B\|\|w\|_2,
\end{aligned} \tag{65}$$

so $\|B\| \leq \|A \oplus B\|$. Combining these last two results we find that $\max\{\|A\|, \|B\|\} \leq \|A \oplus B\|$, so we conclude that $\|A \oplus B\| = \max\{\|A\|, \|B\|\}$. □

Theorem 2.26. *If V and W are inner product spaces (over the same field $\mathbb{R}$ or $\mathbb{C}$) and A and B are positive operators on V and W respectively, then $A \oplus B$ is positive.*

Proof. Let V and W inner product spaces (over the same field $\mathbb{R}$ or $\mathbb{C}$) and A and B positive operators on V and W respectively. Then for all $(v, w) \in V \oplus W$ we have:

$$\langle (v,w), (A \oplus B)(v,w) \rangle = \langle (v,w), (Av, Bw) \rangle = \langle v, Av \rangle + \langle w, Bw \rangle \geq 0 + 0 = 0, \tag{66}$$

where we used the positivity of A and B, so we conclude that $A \oplus B$ is positive. □

Theorem 2.27. *If V and W are inner product spaces (over the same field $\mathbb{R}$ or $\mathbb{C}$) of finite dimensions n and m respectively and A and B are positive operators on V and W respectively, then:*

$$tr(A \oplus B) = tr(A) + tr(B). \tag{67}$$

Proof. Let V and W inner product spaces (over the same field $\mathbb{R}$ or $\mathbb{C}$) of finite dimensions n and m respectively and A and B positive operators on V and W respectively. Let $\{v_1, \ldots, v_n\}$ and $\{w_1, \ldots, w_m\}$ be orthonormal bases of V and W respectively. Then $\{(v_1, 0), \ldots, (v_n, 0)\} \cup \{(0, w_1), \ldots, (0, w_m)\}$ is an orthonormal basis for $V \oplus W$. Therefore we can used these orthonormal bases to calculate traces:

$$\begin{aligned}
&tr(A \oplus B) = \sum_{i=1}^{n} \langle (v_i, 0), (A \oplus B)(v_i, 0) \rangle + \sum_{j=1}^{m} \langle (0, w_j), (A \oplus B)(0, w_j) \rangle = \\
&\sum_{i=1}^{n} \langle (v_i, 0), (Av_i, 0) \rangle + \sum_{j=1}^{m} \langle (0, w_j), (0, Bw_j) \rangle = \\
&\sum_{i=1}^{n} (\langle v_i, Av_i \rangle + \langle 0, 0 \rangle) + \sum_{j=1}^{m} (\langle 0, 0 \rangle + \langle w_j, Bw_j \rangle) = \\
&\sum_{i=1}^{n} \langle v_i, Av_i \rangle + \sum_{j=1}^{m} \langle w_j, Bw_j \rangle = tr(A) + tr(B)
\end{aligned} \tag{68}$$

which completes the proof. □

Theorem 2.28. *Let V be a finite dimensional inner product space and A a normal operator on V, then $\left\|A^2\right\| = \|A\|^2$.*

Proof. Let V be a finite dimensional inner product space and A a normal operator on V. Let $v \in V$, then:

$$\left\|A^2 v\right\|_2 = \|A(Av)\|_2 \leq \|A\|\|Av\|_2 \leq \|A\|^2 \|v\|_2. \tag{69}$$

Since this holds for all $v \in V$ we have $\left\|A^2\right\| \leq \|A\|^2$. A is normal, so there exists an orthonormal basis $\{v_1, \ldots, v_n\}$ for V such that each v_i is an eigenvector of A with eigenvalue a_i. Let $m \in \{1, \ldots, n\}$ be such that $|a_m| \geq |a_i|$ for all $i \in \{1, \ldots, n\}$. For any $v = \sum_{i=1}^n c_i v_i \in V$ we have:

$$\begin{aligned}
&\|Av\|_2 = \left\|A\sum_{i=1}^n c_i v_i\right\|_2 = \left\|\sum_{i=1}^n c_i A v_i\right\|_2 = \left\|\sum_{i=1}^n c_i a_i v_i\right\|_2 = \\
&\sqrt{\left\langle \sum_{i=1}^n c_i a_i v_i, \sum_{j=1}^n c_j a_j v_j \right\rangle} = \sqrt{\sum_{i=1}^n \sum_{j=1}^n c_i^* c_j a_i^* a_j \left\langle v_i, v_j \right\rangle} = \\
&\sqrt{\sum_{i=1}^n \sum_{j=1}^n c_i^* c_j a_i^* a_j \delta_{i,j}} = \sqrt{\sum_{i=1}^n |c_i|^2 |a_i|^2} \leq \sqrt{\sum_{i=1}^n |c_i|^2 |a_m|^2} = \\
&\sqrt{|a_m|^2 \sum_{i=1}^n |c_i|^2} = |a_m| \sqrt{\sum_{i=1}^n \sum_{j=1}^n c_i^* c_j \delta_{i,j}} = |a_m| \sqrt{\sum_{i=1}^n \sum_{j=1}^n c_i^* c_j \left\langle v_i, v_j \right\rangle} = \\
&|a_m| \sqrt{\left\langle \sum_{i=1}^n c_i v_i, \sum_{j=1}^n c_j v_j \right\rangle} = |a_m| \sqrt{\langle v, v \rangle} = |a_m| \|v\|_2.
\end{aligned} \tag{70}$$

So we see that $\|A\| \leq |a_m|$. We also have:

$$\|Av_m\|_2 = \|a_m v_m\|_2 = |a_m| \|v_m\|_2 \tag{71}$$

so in fact $\|A\| = |a_m|$. Therefore we have:

$$\left\|A^2 v_m\right\|_2 = \|a_m A v_m\|_2 = \left\|a_m^2 v_m\right\|_2 = |a_m|^2 \|v_m\|_2. \tag{72}$$

So we see that $\left\|A^2\right\| \geq |a_m|^2 = \|A\|^2$. We conclude that $\left\|A^2\right\| = \|A\|^2$. □

Theorem 2.29. *Let V be a finite dimensional vector space and A and B linear operators on V, then $tr(AB) = tr(BA)$.*

Proof. Let V be a finite dimensional vector space and A and B linear operators on V. Let $(a_{i,j})_{i,j=1}^n$ and $(b_{i,j})_{i,j=1}^n$ be the matrix representations of A and B with respect to some fixed basis of V. We have:

$$tr(AB) = tr((a_{i,j})_{i,j=1}^{n}(b_{j,k})_{j,k=1}^{n}) = tr\left(\left(\sum_{j=1}^{n} a_{i,j}b_{j,k}\right)_{i,k=1}^{n}\right) =$$
$$\sum_{i=1}^{n}\sum_{j=1}^{n} a_{i,j}b_{j,i} = \sum_{j=1}^{n}\sum_{i=1}^{n} b_{j,i}a_{i,j} = \sum_{i=1}^{n}\sum_{j=1}^{n} b_{i,j}a_{j,i} = \tag{73}$$
$$tr\left(\left(\sum_{j=1}^{n} b_{i,j}a_{j,k}\right)_{i,k=1}^{n}\right) = tr((b_{i,j})_{i,j=1}^{n}(a_{j,k})_{j,k=1}^{n})) = tr(BA).$$

□

Theorem 2.30. *Let V be a finite dimensional vector space and A a linear operator on V, then $tr(A^\dagger) = tr(A)^*$.*

Proof. Let V be a finite dimensional vector space and A a linear operator on V. By Theorem 2.10 there exist self-adjoint operators B and C such that $A = B + iC$. Matrix representations of B and C (with respect to any basis) are hermitian and therefore have real entries on the diagonal. It follows that their trace is real. Using the linearity of the trace and the conjugate linearity of the adjoint it follows that:

$$\begin{aligned} &tr(A^\dagger) = tr((B + iC)^\dagger) = tr(B^\dagger - iC^\dagger) = tr(B - iC) = \\ &tr(B) - itr(C) = (tr(B) + itr(C))^* = tr(A)^* \end{aligned} \tag{74}$$

□

which completes the proof.

Theorem 2.31. *Let V be a finite dimensional vector space and A, B and C self-adjoint operators on V, then $tr(BAC) = (tr(ABC))^*$.*

Proof. Let V be a finite dimensional vector space and A, B and C self-adjoint operators on V. Using Theorems 2.29 and 2.30 it follows that:

$$(tr(ABC))^* = tr((ABC)^\dagger) = tr(C^\dagger B^\dagger A^\dagger) = tr(CBA) = tr(BAC) \tag{75}$$

which completes the proof. □

Theorem 2.32. *Let V be a finite dimensional vector space, A a self-adjoint operator on V and B a positive operator on V, then $tr(A^2B) \geq 0$.*

Proof. Let V be a finite dimensional vector space, A a self-adjoint operator on V and B a positive operator on V. B is positive and therefore normal so there exists an orthonormal basis of V such that B is diagonal with respect to

this basis. Let $(a_{i,j})_{i,j=1}^n$ and $(b_{i,j})_{i,j=1}^n$ be the matrix representations of A and B with respect to this basis. A is self-adjoint so its matrix representation is Hermitian, which means that $a_{i,j} = a_{j,i}^*$ for all $i, j \in \{1, \ldots, n\}$. The matrix representation of B is diagonal so $b_{i,j} = 0$ for $i \neq j$. Also, since B is positive, by Theorem 2.16 we have $b_{i,i} \geq 0$ for all $i \in \{1, \ldots, n\}$. From this it follows that:

$$\begin{aligned}
&tr(A^2B) = tr\left((a_{i,j})_{i,j=1}^n (a_{j,k})_{j,k=1}^n (b_{k,l})_{k,l=1}^n\right) = \\
&tr\left(\left(\sum_{j=1}^n a_{i,j}a_{j,k}\right)_{i,k=1}^n (b_{k,l})_{k,l=1}^n\right) = tr\left(\left(\sum_{j=1}^n \sum_{k=1}^n a_{i,j}a_{j,k}b_{k,l}\right)_{i,l=1}^n\right) = \\
&\sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n a_{i,j}a_{j,k}b_{k,i} = \sum_{i=1}^n \sum_{j=1}^n a_{i,j}a_{j,i}b_{i,i} = \sum_{i=1}^n \sum_{j=1}^n a_{i,j}a_{i,j}^* b_{i,i} = \\
&\sum_{i=1}^n \sum_{j=1}^n |a_{i,j}|^2 b_{i,i} \geq 0
\end{aligned} \tag{76}$$

since $|a_{i,j}|^2 \geq 0$ and $b_{i,i} \geq 0$. □

Theorem 2.33. *Let V be a vector space over a field F, where F is equal to $\mathbb{R}$ or $\mathbb{C}$, and let $\langle \cdot, \cdot \rangle : V \times V \to F$ be a (possibly degenerate) inner product. Then for all $v \in V$ such that $\langle v, v \rangle = 0$ we have that $\langle v, w \rangle = 0$ for all $w \in V$.*

Remark. We note that this result follows from the Cauchy-Schwarz inequality which holds for both degenerate and non-degenerate inner products. The proof below essentially shows that the Cauchy-Schwarz inequality holds in case one or both vectors have an inner product with themselves equal to 0.

Proof. Let V be a vector space over a field F, where F is equal to $\mathbb{R}$ or $\mathbb{C}$, and let $\langle \cdot, \cdot \rangle : V \times V \to F$ be a (possibly degenerate) inner product. Suppose first that $\langle v, v \rangle = 0$ for all $v \in V$. Let $v, w \in V$, then we have:

$$\begin{aligned}
&0 = \langle v + w, v + w \rangle = \langle v, v \rangle + \langle v, w \rangle + \langle w, v \rangle + \langle w, w \rangle = \langle v, w \rangle + \langle v, w \rangle^* = \\
&2\mathrm{Re}(\langle v, w \rangle).
\end{aligned} \tag{77}$$

If $F = \mathbb{R}$, then $\langle v, w \rangle \in \mathbb{R}$ and we conclude that $\langle v, w \rangle = 0$. If $F = \mathbb{C}$ we note that $iw \in V$, so we also have:

$$0 = \langle v + iw, v + iw \rangle = 2\mathrm{Re}(\langle v, iw \rangle) = 2\mathrm{Re}(i \langle v, w \rangle) = -2\mathrm{Im}(\langle v, w \rangle). \tag{78}$$

Again we can conclude that $\langle v, w \rangle = 0$. So the theorem holds in case $\langle v, v \rangle = 0$ for all $v \in V$. Suppose instead that this is not the case, so there exist $u \in V$

with $\langle u, u\rangle > 0$. Suppose $v, w \in V$ such that $\langle v, v\rangle = 0$ and $\langle w, w\rangle > 0$. We note that we can write:

$$v = \frac{\langle w, v\rangle}{\langle w, w\rangle} w + v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w. \tag{79}$$

We have:

$$\left\langle \frac{\langle w, v\rangle}{\langle w, w\rangle} w, w \right\rangle = \left(\frac{\langle w, v\rangle}{\langle w, w\rangle} \right)^* \langle w, w\rangle = \frac{\langle w, v\rangle^*}{\langle w, w\rangle} \langle w, w\rangle = \frac{\langle v, w\rangle}{\langle w, w\rangle} \langle w, w\rangle = \langle v, w\rangle \tag{80}$$

and therefore:

$$\left\langle v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w, w \right\rangle = \langle v, w\rangle - \left\langle \frac{\langle w, v\rangle}{\langle w, w\rangle} w, w \right\rangle = \langle v, w\rangle - \langle v, w\rangle = 0. \tag{81}$$

From this it follows that:

$$\begin{aligned}
&0 = \langle v, v\rangle = \left\langle \frac{\langle w, v\rangle}{\langle w, w\rangle} w + v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w, \frac{\langle w, v\rangle}{\langle w, w\rangle} w + v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w \right\rangle = \\
&\left\langle \frac{\langle w, v\rangle}{\langle w, w\rangle} w, \frac{\langle w, v\rangle}{\langle w, w\rangle} w \right\rangle + \left\langle \frac{\langle w, v\rangle}{\langle w, w\rangle} w, v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w \right\rangle + \\
&\left\langle v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w, \frac{\langle w, v\rangle}{\langle w, w\rangle} w \right\rangle + \left\langle v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w, v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w \right\rangle = \\
&\left(\frac{\langle w, v\rangle}{\langle w, w\rangle} \right)^* \frac{\langle w, v\rangle}{\langle w, w\rangle} \langle w, w\rangle + \left(\frac{\langle w, v\rangle}{\langle w, w\rangle} \right)^* \left\langle w, v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w \right\rangle + \\
&\frac{\langle w, v\rangle}{\langle w, w\rangle} \left\langle v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w, w \right\rangle + \left\langle v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w, v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w \right\rangle = \\
&\frac{|\langle v, w\rangle|^2}{\langle w, w\rangle^2} \langle w, w\rangle + \frac{\langle v, w\rangle}{\langle w, w\rangle} \left\langle v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w, w \right\rangle^* + \\
&\frac{\langle w, v\rangle}{\langle w, w\rangle} \left\langle v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w, w \right\rangle + \left\langle v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w, v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w \right\rangle = \\
&\frac{|\langle v, w\rangle|^2}{\langle w, w\rangle} + \left\langle v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w, v - \frac{\langle w, v\rangle}{\langle w, w\rangle} w \right\rangle \geq \frac{|\langle v, w\rangle|^2}{\langle w, w\rangle}.
\end{aligned} \tag{82}$$

Since $\langle w, w\rangle > 0$ it follows that $|\langle v, w\rangle|^2 \leq 0$ and therefore $\langle v, w\rangle = 0$. So if $\langle v, v\rangle = 0$ and $\langle w, w\rangle > 0$ then $\langle v, w\rangle = 0$. Now suppose $v, w \in V$ with $\langle v, v\rangle = \langle w, w\rangle = 0$. We assumed that there exists a $u \in V$ with $\langle u, u\rangle > 0$. Since $\langle w, w\rangle = 0$ it follows that:

$$\begin{aligned}
&\langle w + u, w + u\rangle = \langle w, w\rangle + \langle w, u\rangle + \langle u, w\rangle + \langle u, u\rangle = \\
&\langle w, w\rangle + \langle w, u\rangle + \langle w, u\rangle^* + \langle u, u\rangle = 0 + 0 + 0 + \langle u, u\rangle = \langle u, u\rangle > 0.
\end{aligned} \tag{83}$$

Since $\langle v, v\rangle = 0$ and $\langle u, u\rangle = \langle w + u, w + u\rangle > 0$ it follows that:

$$\langle v, w\rangle = \langle v, w + u - u\rangle = \langle v, w + u\rangle - \langle v, u\rangle = 0 - 0 = 0. \tag{84}$$

So we see that $\langle v, w\rangle = 0$ also when $\langle w, w\rangle = 0$. We conclude that $\langle v, w\rangle = 0$ for all $v, w \in V$ with $\langle v, v\rangle = 0$. □

Theorem 2.34. *Let V be a vector space over a field F, where F is equal to $\mathbb{R}$ or $\mathbb{C}$, and let $\langle \cdot, \cdot\rangle : V \times V \to F$ be a (possibly degenerate) inner product. Let $G = \{v \in V : \langle v, v\rangle = 0\}$. Then G is a subspace of V and $\langle \cdot, \cdot\rangle : V/G \times V/G \to F$ defined as $\langle \overline{v}, \overline{w}\rangle = \langle v, w\rangle$ is a non-degenerate inner product on the quotient vector space V/G.*

Proof. Let V be a vector space over a field F, where F is equal to $\mathbb{R}$ or $\mathbb{C}$, and let $\langle \cdot, \cdot\rangle : V \times V \to F$ be a (possibly degenerate) inner product. Let $G = \{v \in V : \langle v, v\rangle = 0\}$. We note that by Theorem 2.33 $\langle v, w\rangle = \langle w, v\rangle^* = 0$ whenever $\langle v, v\rangle = 0$ or $\langle w, w\rangle = 0$. If $v \in G$ and $a \in F$ then:

$$\langle av, av\rangle = |a|^2 \langle v, v\rangle = 0 \tag{85}$$

so $av \in G$. If $v, w \in G$, then:

$$\langle v + w, v + w\rangle = \langle v, v\rangle + \langle v, w\rangle + \langle w, v\rangle + \langle w, w\rangle = 0 + 0 + 0 + 0 = 0 \tag{86}$$

so $v + w \in G$. We see that G is indeed a subspace of V. On the quotient vector space V/G we define the operation $\langle \cdot, \cdot\rangle : V/G \times V/G \to F$ by letting:

$$\langle \overline{v}, \overline{w}\rangle = \langle v, w\rangle . \tag{87}$$

We will verify that this operation is well-defined and that it is a non-degenerate inner product on V/G. To show that the operation is well-defined we need to show that it does not depend on the choice of representative of the equivalence classes. So we need to show that if $\overline{v_1} = \overline{v_2}$ and $\overline{w_1} = \overline{w_2}$, then $\langle v_1, w_1\rangle = \langle v_2, w_2\rangle$. So suppose $\overline{v_1} = \overline{v_2}$ and $\overline{w_1} = \overline{w_2}$, then $v_1 - v_2, w_1 - w_2 \in G$ and therefore $\langle v_1 - v_2, v_1 - v_2\rangle = \langle w_1 - w_2, w_1 - w_2\rangle = 0$. Using Theorem 2.33 it follows that:

$$\begin{aligned} &\langle v_1, w_1\rangle = \langle v_1 - v_2 + v_2, w_1 - w_2 + w_2\rangle = \\ &\langle v_1 - v_2, w_1 - w_2\rangle + \langle v_1 - v_2, w_2\rangle + \langle v_2, w_1 - w_2\rangle + \langle v_2, w_2\rangle = \\ &0 + 0 + 0 + \langle v_2, w_2\rangle = \langle v_2, w_2\rangle . \end{aligned} \tag{88}$$

So we see that the operation is well-defined. Let $\overline{v}, \overline{w} \in V/G$, then we have:

$$\langle \overline{v}, \overline{w}\rangle = \langle v, w\rangle = \langle w, v\rangle^* = \langle \overline{w}, \overline{v}\rangle^* . \tag{89}$$

Also for all $\overline{v}, \overline{w}, \overline{u} \in V/G$ and $a \in F$:

$$\langle \overline{v}, a\overline{w} \rangle = \langle \overline{v}, \overline{aw} \rangle = \langle v, aw \rangle = a \langle v, w \rangle = a \langle \overline{v}, \overline{w} \rangle \tag{90}$$

and

$$\begin{aligned} &\langle \overline{v}, \overline{w} + \overline{u} \rangle = \langle \overline{v}, \overline{w+u} \rangle = \langle v, w+u \rangle = \langle v, w \rangle + \langle v, u \rangle = \\ &\langle \overline{v}, \overline{w} \rangle + \langle \overline{v}, \overline{u} \rangle . \end{aligned} \tag{91}$$

Let $\overline{v} \in V/G$, then:

$$\langle \overline{v}, \overline{v} \rangle = \langle v, v \rangle \geq 0. \tag{92}$$

We can now conclude that the operation we defined on V/G is a (possibly degenerate) inner product. To show that it is a non-degenerate inner product, we need to show that $\langle \overline{v}, \overline{v} \rangle = 0$ only if $\overline{v} = \overline{0}$. Suppose $\langle \overline{v}, \overline{v} \rangle = 0$, then:

$$\langle v, v \rangle = \langle \overline{v}, \overline{v} \rangle = 0 \tag{93}$$

so $v - 0 = v \in G$ and therefore $\overline{v} = \overline{0}$. We conclude that the operation we defined on V/G is a non-degenerate inner product, so V/G is an inner product space. This completes the proof. □

3 Formalism of quantum mechanics

Similarly to the previous section, this section will state the quantum mechanical formalism relevant to the contents of this thesis. A more complete treatment can again be found in [1], on which this section is based.

The formalism of quantum mechanics states that an isolated physical system can be described using a Hilbert space V over $\mathbb{C}$. At any point in time the state of the system can be fully described by some vector in V [1].

A measurement performed on the system is described by a collection $\{M_m\}$. The M_m are linear operators on V known as measurement operators and the indices m refer to the possible measurement outcomes. If $v \in V$ is the state of the system before the measurement is performed, then the probability of obtaining outcome m upon measuring is given by

$$p(m) = \left\langle v, M_m^\dagger M_m v \right\rangle \tag{94}$$

and if m is the obtained outcome of the measurement, then the state of the system after the measurement is given by

$$\frac{M_m v}{\sqrt{\left\langle v, M_m^\dagger M_m v \right\rangle}}. \tag{95}$$

The measurement operators have to satisfy the completeness equation

$$\sum_m M_m^\dagger M_m = id \tag{96}$$

to ensure that the probabilities of the different measurement outcomes sum to 1 [1].

An important subclass of quantum measurements consists of projective measurements. In the case of projective measurements, the measurement operators must have two additional properties. Each M_m must be self-adjoint and $M_m M_{m'} = \delta_{m,m'} M_m$. Projective measurements can be described by an observable M, which is a self-adjoint operator. The fact that M is self-adjoint implies that M is normal, so it has a spectral decomposition $M = \sum_m m P_m$, where P_m is the projector on the eigenspace of M associated with the eigenvalue m. When measuring a state v, the possible outcomes are given by the eigenvalues m. Outcome m is measured with probability

$$p(m) = \langle v, P_m v \rangle \tag{97}$$

and the post-measurement state after measuring outcome m is given by

$$\frac{P_m v}{\langle v, P_m v \rangle}. \tag{98}$$

Projective measurements have the nice property that the expectation value of the measurement outcome has a simple expression:

$$\mathbb{E}(M) = \langle v, Mv \rangle . \tag{99}$$

We note that in the description of quantum measurement, the measurement operators M_m themselves are needed only to describe the post-measurement state. The probabilities of the measurement outcomes and the completeness equation can be formulated in terms of the operators $E_m = M_m^\dagger M_m$. The operators $E_m = M_m^\dagger M_m$ are positive and satisfy $\sum_m E_m = id$. Conversely, if $\{E_m\}$ is a collection of positive operators satisfying $\sum_m E_m = id$, it can be shown that there exists a family M_m of measurement operators such that $E_m = M_m^\dagger M_m$.

Definition 3.1. POVM. A collection $\{E_m\}$ of positive operators satisfying $\sum_m E_m = id$ is called a POVM.

POVM's play a central role in the POVM formalism, which states that a measurement performed on an isolated physical system is described by a POVM $\{E_m\}$ and the probability of obtaining outcome m upon measuring the system in state v is given by

$$p(m) = \langle v, E_m v \rangle . \tag{100}$$

The fact that any set of measurement operators has an associated POVM and vice versa shows that the POVM formalism is a special case of the general measurement formalism, giving the measurement probabilities but not the post-measurement states of the system. The POVM formalism is useful when the post-measurement states are not relevant [1].

There exists an alternative method to describe the state of a physical system. Instead of representing the state of a system using a vector $v \in V$, the state is represented using a density operator $\rho : V \to V$.

Definition 3.2. Density operator. A linear operator $\rho : V \to V$ with V a finite dimensional Hilbert space, is called a density operator when ρ is positive and $tr(\rho) = 1$.

This density operator formalism can be used to describe any state of the system which can also be described be a vector $v \in V$. Such a state is known as a pure state. If the state of a system is described using the vector v, then in the density operator formalism this state is described by the density operator ρ_v defined as:

$$\rho_v(w) = \langle v, w \rangle \, v. \tag{101}$$

The density operator formalism can, however, also be used to describe a mixed state. A mixed state is a state that is not fully known. For example if you have a collection of systems, half of which is prepared in state a and the rest in state b, then an arbitrary system from this collection can be described by a mixed

state that is equal to state a or b each with probability $\frac{1}{2}$. Such a state can be described using a density operator, which is one of the main selling points of the density operator formalism. Measurements in the density operator formalism are described by a collection of measurement operators $\{M_m\}$ subject to the same conditions. In this case the probabilities are given by

$$p(m) = tr(M_m^\dagger M_m \rho) \tag{102}$$

and the post-measurement state by

$$\frac{M_m \rho M_m^\dagger}{tr(M_m^\dagger M_m \rho)}. \tag{103}$$

The POVM formalism can also be applied in the context of the density operator formalism. In this case measurements are described by a POVM $\{E_m\}$ and the measurement probabilities are given by [1]

$$p(m) = tr(E_m \rho). \tag{104}$$

So far all the formalism we introduced was used to describe states of a single system and measurements on those states. The last bit of formalism we will discuss deals with the description of multiple systems. If V and W are Hilbert spaces used to describe two physical systems, then the tensor product $V \otimes W$ can be used to describe the composite system consisting of these two systems. If the first system is in the state $v \in V$ and the second system in the state $w \in W$, then the composite system is in the state $v \otimes w$. Linear combinations of such states are also possible and not every state of the composite system is the tensor product of two states of the individual systems. A state that cannot be written as the tensor product of two states of the individual systems is known as an entangled state. A composite system can also be described using the density operator formalism, in which if the first system is in the state $\rho : V \to V$ and the second system in the state $\sigma : W \to W$, then the composite system is in the state $\rho \otimes \sigma$. If $\{M_m\}$ is a collection of measurement operators on V and $\{N_n\}$ a collection of measurement operators on W, then $\{M_m \otimes N_n\}$ is a collection of measurement operators on $V \otimes W$. This collection of measurement operators describes a measurement on a state of the composite system where the measurements described by $\{M_m\}$ and $\{N_n\}$ are carried out simultaneously on the individual systems. This simultaneous combination of measurements also occurs in the context of either projective measurements or POVM's. Observables M on V and N on W give rise to an observable $M \otimes N$ on $V \otimes W$ and POVM's $\{E_m\}$ on V and $\{F_n\}$ on W give rise to a POVM $\{E_m \otimes F_n\}$ on $V \otimes W$.

Lastly in this section we introduce the Pauli-matrices, which are (matrix representations of) self-adjoint operators on $\mathbb{C}^2$. The three Pauli-matrices are given by:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{105}$$

$$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{106}$$

and

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{107}$$

Since these operators are self-adjoint, they can be used to represent observables in the context of projective measurements. The Pauli-matrices will be used on multiple occasions throughout the remainder of this thesis. By multiplying the Pauli-matrices it can be verified that they satisfy the following properties:

$$X^2 = Y^2 = Z^2 = id, \tag{108}$$

$$XY = -YX = iZ, \tag{109}$$

$$YZ = -ZY = iX \tag{110}$$

and

$$ZX = -XZ = iY. \tag{111}$$

We note in particular that if A and B are two different Pauli-matrices, that $AB = -BA$.

4 Bell inequalities

Bell inequalities are, roughly speaking, inequalities that hold in classical probability but are violated in quantum probability. To explain how this can happen, suppose we have some physical system and a number of different measurements that can be performed on the system. According to the standard formalism of quantum mechanics, the system can be associated with a complex Hilbert space V and the state of the system is fully described by a vector in V. Even if this state vector is known, the outcomes of the measurements that can be performed on the system are, in general, random. So according to the standard formalism of quantum mechanics, there is an inherent randomness in nature. Alternatively, there exist hidden variable models. According to those models the state vector does not fully specify the state of a system. Instead there exist certain hidden variables, which determine the outcomes of the possible measurements on the system. This would make the outcomes of the measurements deterministic in case the hidden variables are known. These hidden variables are, however, in general not known. All that is known is the state vector and this incomplete knowledge is responsible for the randomness in quantum mechanics. Under the assumption of such a hidden variable model, there should be a probability space associated with a given state vector and the outcomes of the possible measurements on this state are described by random variables on the underlying probability space. This means these measurement outcomes should satisfy inequalities that hold in general for random variables on some probability space. For some states the probabilities of the measurement outcomes as predicted by the formalism of quantum measurement happen to violate an inequality in classical probability that should be applicable under the assumption of a hidden variable model. Inequalities in classical probability that can be violated by the outcomes of quantum measurements even though these inequalities should be applicable under the assumption of a hidden variable model are known as Bell inequalities. The fact that these Bell inequalities can be violated indicates that hidden variable models are not compatible with the formalism of quantum measurement. In order to make the concept of a Bell inequality more tangible, we will provide an example. First we will derive the inequality in classical probability known as the CHSH-inequality and afterwards we show the quantum mechanical context in which it should apply assuming a hidden variable model, but is violated according to quantum measurement formalism. This treatment of the CHSH-inequality is based on chapter 5 of [2].

Theorem 4.1. *Let $(\Omega, \mathscr{A}, \mathbb{P})$ be a probability space and $Q, R, S, T : \Omega \to \{1, -1\}$ random variables, then the following inequality holds:*

$$|\mathbb{E}(QS) + \mathbb{E}(RS) + \mathbb{E}(RT) - \mathbb{E}(QT)| \leq 2. \tag{112}$$

Proof. Let $(\Omega, \mathscr{A}, \mathbb{P})$ be a probability space and $Q, R, S, T : \Omega \to \{1, -1\}$ random variables. Now, for all $q, r, s, t \in \{1, -1\}$ we have

$$qs + rs + rt - qt = (q + r)s + (r - q)t. \tag{113}$$

Now if $q = r$, then $r - q = 0$ and $q + r \in \{2, -2\}$ and since $s \in \{1, -1\}$ we have $qs + rs + rt - qt \in \{2, -2\}$ in this case. If $q \neq r$, then $q = -r$ and we have $q + r = 0$ and $r - q \in \{2, -2\}$. Since $t \in \{1, -1\}$ we again have $qs + rs + rt - qt \in \{2, -2\}$, so $qs + rs + rt - qt \in \{2, -2\}$ holds for all $q, r, s, t \in \{1, -1\}$. For $(q, r, s, t) \in \{1, -1\}^4$ we define:

$$\Omega_{q,r,s,t} = \{\omega \in \Omega : Q(\omega) = q, R(\omega) = r, S(\omega) = s, T(\omega) = t\}. \tag{114}$$

This defines a collection of disjoint measurable subsets of Ω. The sets are measurable as they are finite intersections of the inverse images under random variables of $\{1\}$ or $\{-1\}$. These sets cover all different combinations of possible values of the four random variables, so we have the disjoint union:

$$\Omega = \cup_{(q,r,s,t)\in\{1,-1\}^4}\Omega_{q,r,s,t}. \tag{115}$$

Using this it follows that:

$$\begin{aligned}
&|\mathbb{E}(QS) + \mathbb{E}(RS) + \mathbb{E}(RT) - \mathbb{E}(QT)| = |\mathbb{E}(QS + RS + RT - QT)| = \\
&\left|\int_\Omega Q(\omega)S(\omega) + R(\omega)S(\omega) + R(\omega)T(\omega) - Q(\omega)T(\omega)d\mathbb{P}(\omega)\right| = \\
&\left|\sum_{(q,r,s,t)\in\{1,-1\}^4}\int_{\Omega_{q,r,s,t}} Q(\omega)S(\omega) + R(\omega)S(\omega) + R(\omega)T(\omega) - Q(\omega)T(\omega)d\mathbb{P}(\omega)\right| = \\
&\left|\sum_{(q,r,s,t)\in\{1,-1\}^4}\int_{\Omega_{q,r,s,t}} qs + rs + rt - qtd\mathbb{P}(\omega)\right| = \\
&\left|\sum_{(q,r,s,t)\in\{1,-1\}^4}(qs + rs + rt - qt)\mathbb{P}(\Omega_{q,r,s,t})\right| \leq \\
&\sum_{(q,r,s,t)\in\{1,-1\}^4}|qs + rs + rt - qt|\mathbb{P}(\Omega_{q,r,s,t}) = \\
&2\sum_{(q,r,s,t)\in\{1,-1\}^4}\mathbb{P}(\Omega_{q,r,s,t}) = 2\mathbb{P}(\Omega) = 2,
\end{aligned} \tag{116}$$

which completes the proof. □

If we have a quantum mechanical system and four measurements we can perform on said system each with possible outcomes 1 or -1, then according to a hidden variable model the outcomes of these measurements can be described by random variables Q, R, S, T on some probability space and the CHSH-inequality must hold for these random variables. In order to violate the CHSH-inequality we consider a physical system described by the Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^2$ and the state $\psi = \frac{1}{\sqrt{2}}(e_1 \otimes e_2 - e_2 \otimes e_1)$ with $e_i = (\delta_{i,j})_{j=1}^2$. The measurements we consider will be projective measurements. Using the Pauli-matrices we define

the following self-adjoint operators on $\mathbb{C}^2 \otimes \mathbb{C}^2$: $Q = Z \otimes id$, $R = X \otimes id$, $S = id \otimes \frac{-Z-X}{\sqrt{2}}$ and $T = id \otimes \frac{Z-X}{\sqrt{2}}$. These operators define observables which can be measured. Products of these operators are also self-adjoint and represent observables as well. We note that $Xe_1 = e_2$, $Xe_2 = e_1$, $Ze_1 = e_1$ and $Ze_2 = -e_2$. This can be used to calculate the expectation values of the observables QS, RS, RT, QT when measuring these on the state ψ defined earlier. We note that $\langle e_i \otimes e_j, e_k \otimes e_l \rangle = \langle e_i, e_k \rangle \langle e_j, e_l \rangle = \delta_{i,k}\delta_{j,l}$. We have:

$$
\begin{aligned}
&\mathbb{E}(QS) = \langle \psi, QS\psi \rangle = \left\langle \psi, (Z \otimes id) \left(id \otimes \frac{-Z-X}{\sqrt{2}} \right) \psi \right\rangle = \\
&\left\langle \frac{1}{\sqrt{2}}(e_1 \otimes e_2 - e_2 \otimes e_1), \left(Z \otimes \frac{-Z-X}{\sqrt{2}} \right) \frac{1}{\sqrt{2}}(e_1 \otimes e_2 - e_2 \otimes e_1) \right\rangle = \\
&\frac{1}{2} \left\langle e_1 \otimes e_2 - e_2 \otimes e_1, Ze_1 \otimes \frac{-Z-X}{\sqrt{2}} e_2 - \left(Ze_2 \otimes \frac{-Z-X}{\sqrt{2}} e_1 \right) \right\rangle = \\
&\frac{1}{2} \left\langle e_1 \otimes e_2 - e_2 \otimes e_1, e_1 \otimes \frac{1}{\sqrt{2}}(e_2 - e_1) - \left(-e_2 \otimes \frac{1}{\sqrt{2}}(-e_1 - e_2) \right) \right\rangle = \\
&\frac{1}{2} \left\langle e_1 \otimes e_2 - e_2 \otimes e_1, \frac{1}{\sqrt{2}}(e_1 \otimes e_2 - e_1 \otimes e_1 - e_2 \otimes e_1 - e_2 \otimes e_2) \right\rangle = \\
&\frac{1}{2\sqrt{2}} \langle e_1 \otimes e_2 - e_2 \otimes e_1, e_1 \otimes e_2 - e_1 \otimes e_1 - e_2 \otimes e_1 - e_2 \otimes e_2 \rangle = \\
&\frac{1}{2\sqrt{2}}(1+1) = \frac{1}{\sqrt{2}},
\end{aligned}
\tag{117}
$$

$$
\begin{aligned}
&\mathbb{E}(RS) = \langle \psi, RS\psi \rangle = \left\langle \psi, (X \otimes id) \left(id \otimes \frac{-Z-X}{\sqrt{2}} \right) \psi \right\rangle = \\
&\left\langle \frac{1}{\sqrt{2}}(e_1 \otimes e_2 - e_2 \otimes e_1), \left(X \otimes \frac{-Z-X}{\sqrt{2}} \right) \frac{1}{\sqrt{2}}(e_1 \otimes e_2 - e_2 \otimes e_1) \right\rangle = \\
&\frac{1}{2} \left\langle e_1 \otimes e_2 - e_2 \otimes e_1, Xe_1 \otimes \frac{-Z-X}{\sqrt{2}} e_2 - \left(Xe_2 \otimes \frac{-Z-X}{\sqrt{2}} e_1 \right) \right\rangle = \\
&\frac{1}{2} \left\langle e_1 \otimes e_2 - e_2 \otimes e_1, e_2 \otimes \frac{1}{\sqrt{2}}(e_2 - e_1) - \left(e_1 \otimes \frac{1}{\sqrt{2}}(-e_1 - e_2) \right) \right\rangle = \\
&\frac{1}{2} \left\langle e_1 \otimes e_2 - e_2 \otimes e_1, \frac{1}{\sqrt{2}}(e_2 \otimes e_2 - e_2 \otimes e_1 + e_1 \otimes e_1 + e_1 \otimes e_2) \right\rangle = \\
&\frac{1}{2\sqrt{2}} \langle e_1 \otimes e_2 - e_2 \otimes e_1, e_2 \otimes e_2 - e_2 \otimes e_1 + e_1 \otimes e_1 + e_1 \otimes e_2 \rangle = \\
&\frac{1}{2\sqrt{2}}(1+1) = \frac{1}{\sqrt{2}},
\end{aligned}
\tag{118}
$$

$$\mathbb{E}(RT) = \langle \psi, RT\psi \rangle = \left\langle \psi, (X \otimes id)\left(id \otimes \frac{Z-X}{\sqrt{2}}\right)\psi \right\rangle =$$
$$\left\langle \frac{1}{\sqrt{2}}(e_1 \otimes e_2 - e_2 \otimes e_1), \left(X \otimes \frac{Z-X}{\sqrt{2}}\right)\frac{1}{\sqrt{2}}(e_1 \otimes e_2 - e_2 \otimes e_1) \right\rangle =$$
$$\frac{1}{2}\left\langle e_1 \otimes e_2 - e_2 \otimes e_1, Xe_1 \otimes \frac{Z-X}{\sqrt{2}}e_2 - \left(Xe_2 \otimes \frac{Z-X}{\sqrt{2}}e_1\right) \right\rangle =$$
$$\frac{1}{2}\left\langle e_1 \otimes e_2 - e_2 \otimes e_1, e_2 \otimes \frac{1}{\sqrt{2}}(-e_2 - e_1) - \left(e_1 \otimes \frac{1}{\sqrt{2}}(e_1 - e_2)\right) \right\rangle = \quad (119)$$
$$\frac{1}{2}\left\langle e_1 \otimes e_2 - e_2 \otimes e_1, \frac{1}{\sqrt{2}}(-e_2 \otimes e_2 - e_2 \otimes e_1 - e_1 \otimes e_1 + e_1 \otimes e_2) \right\rangle =$$
$$\frac{1}{2\sqrt{2}}\langle e_1 \otimes e_2 - e_2 \otimes e_1, -e_2 \otimes e_2 - e_2 \otimes e_1 - e_1 \otimes e_1 + e_1 \otimes e_2 \rangle =$$
$$\frac{1}{2\sqrt{2}}(1+1) = \frac{1}{\sqrt{2}}$$

and

$$\mathbb{E}(QT) = \langle \psi, QT\psi \rangle = \left\langle \psi, (Z \otimes id)\left(id \otimes \frac{Z-X}{\sqrt{2}}\right)\psi \right\rangle =$$
$$\left\langle \frac{1}{\sqrt{2}}(e_1 \otimes e_2 - e_2 \otimes e_1), \left(Z \otimes \frac{Z-X}{\sqrt{2}}\right)\frac{1}{\sqrt{2}}(e_1 \otimes e_2 - e_2 \otimes e_1) \right\rangle =$$
$$\frac{1}{2}\left\langle e_1 \otimes e_2 - e_2 \otimes e_1, Ze_1 \otimes \frac{Z-X}{\sqrt{2}}e_2 - \left(Ze_2 \otimes \frac{Z-X}{\sqrt{2}}e_1\right) \right\rangle =$$
$$\frac{1}{2}\left\langle e_1 \otimes e_2 - e_2 \otimes e_1, e_1 \otimes \frac{1}{\sqrt{2}}(-e_2 - e_1) - \left(-e_2 \otimes \frac{1}{\sqrt{2}}(e_1 - e_2)\right) \right\rangle = \quad (120)$$
$$\frac{1}{2}\left\langle e_1 \otimes e_2 - e_2 \otimes e_1, \frac{1}{\sqrt{2}}(-e_1 \otimes e_2 - e_1 \otimes e_1 + e_2 \otimes e_1 - e_2 \otimes e_2) \right\rangle =$$
$$\frac{1}{2\sqrt{2}}\langle e_1 \otimes e_2 - e_2 \otimes e_1, -e_1 \otimes e_2 - e_1 \otimes e_1 + e_2 \otimes e_1 - e_2 \otimes e_2 \rangle =$$
$$\frac{1}{2\sqrt{2}}(-1-1) = -\frac{1}{\sqrt{2}}.$$

Now we see that for this choice of measurements and the state ψ we have:

$$|\mathbb{E}(QS) + \mathbb{E}(RS) + \mathbb{E}(RT) - \mathbb{E}(QT)| = \left|\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}}\right| = 2\sqrt{2} > 2 \quad (121)$$

which violates the CHSH-inequality. So the CHSH-inequality is indeed a Bell inequality as it holds in classical probability but fails in the context of quantum measurement even though it should be applicable according to a hidden variable model. Bell inequalities by their very nature can be violated in the context of quantum measurement and we might ask to what extent a Bell inequality can be violated. In order to properly address this question we will spend the next few chapters, which are also based on chapter 5 of [2], giving a more precise mathematical definition of Bell inequalities. In some sense we will be generalizing the

CHSH-inequality by starting from a similar quantum mechanical context. The CHSH-inequality will be a specific instance of the more general Bell inequalities we will consider.

5 Classical correlation matrix

The quantum mechanical setting we will consider is as follows. We consider a composite physical system consisting of two systems. This system will be in some state. For some $N \in \mathbb{N}$ we have N measurements $P_1, \ldots, P_N$ we can perform on the first of these systems and N measurements $Q_1, \ldots, Q_N$ we can perform on the second system. All of these measurements will have possible outcomes in $\{1, -1\}$. We will eventually look at inequalities involving terms of the form $\mathbb{E}(P_i Q_j)$ similar to the CHSH-inequality. We will consider terms of the form $\mathbb{E}(P_i Q_j)$ both from the perspective of a hidden variable model and from the perspective of quantum measurement.

We will first look at this scenario from the perspective of a hidden variable model. According to such a model there is a probability space $(\Omega, \mathscr{A}, \mathbb{P})$ such that the measurement outcomes $P_1, \ldots, P_N$ and $Q_1, \ldots, Q_N$ are random variables on $(\Omega, \mathscr{A}, \mathbb{P})$. In this section we will define classical correlation matrices as a convenient way to view the terms $\mathbb{E}(P_i Q_j)$ from a hidden variable perspective as a single object. We will also derive some properties of the set of classical correlation matrices, appearing as remarks in chapter 5 of [2], which will be useful when exploring to what degree Bell inequalities can be violated by quantum mechanics. We have the following definition which can also be found in chapter 5 of [2].

Definition 5.1. Classical correlation matrix. The set $\mathscr{L}_N$ is defined, for $N \in \mathbb{N}$, as the set of $N \times N$ matrices $\gamma = (\gamma_{i,j})_{i,j=1}^N$ whose elements have the following form:

$$\gamma_{i,j} = \mathbb{E}(A_i B_j) = \int_\Omega A_i(\omega) B_j(\omega) d\mathbb{P}(\omega) \tag{122}$$

where $(\Omega, \mathscr{A}, \mathbb{P})$ is a probability space and A_i, B_j for $i, j \in \{1, \ldots, N\}$ are random variables on Ω taking values in $\{1, -1\}$. The matrices $\gamma \in \mathscr{L}_N$ are called classical correlation matrices.

An important subset of $\mathscr{L}_N$ consists of the correlation matrices obtained from probability spaces where each of the random variables A_i and B_j is deterministic. In other words there exist constants $a_i, b_j \in \{1, -1\}$ for each $i, j \in \{1, \ldots, N\}$ such that $A_i(\omega) = a_i$ and $B_j(\omega) = b_j$ for all $\omega \in \Omega$. In this case the elements of the correlation matrix take the form:

$$\gamma_{i,j} = \mathbb{E}(A_i B_j) = \int_\Omega A_i(\omega) B_j(\omega) d\mathbb{P}(\omega) = \int_\Omega a_i b_j d\mathbb{P}(\omega) = a_i b_j \mathbb{P}(\Omega) = a_i b_j. \tag{123}$$

So in the special case of deterministic random variables the correlation matrices have the form $\gamma = (\gamma_{i,j})_{i,j=1}^N = (t_i s_j)_{i,j=1}^N$ with $t_i, s_j \in \{1, -1\}$ (and conversely every correlation matrix of this form can be obtained from a probability space with deterministic random variables taking values in $\{1, -1\}$ by choosing the

values $a_i = t_i$ and $b_j = s_j$ for the constants). We will from now on refer to the matrices $\gamma = (\gamma_{i,j})_{i,j=1}^N = (t_i s_j)_{i,j=1}^N$ with $t_i, s_j \in \{1, -1\}$ as deterministic correlation matrices, so we have the following definition:

Definition 5.2. Deterministic correlation matrix. An $N \times N$ deterministic correlation matrix is an $N \times N$ matrix $\gamma = (\gamma_{i,j})_{i,j=1}^N = (t_i s_j)_{i,j=1}^N$ with $t_i, s_j \in \{1, -1\}$

We note that for any fixed N, the number of deterministic correlation matrices is finite. In fact since there are 2 possible values for each t_i and s_j, there are no more than 2^{2N} different deterministic correlation matrices. The exact number is actually 2^{2N-1} which we will prove.

Theorem 5.1. *There exist 2^{2N-1} deterministic correlation matrices of size $N \times N$.*

Proof. Suppose we fix $s_1 = 1$. In this case the first column of the correlation matrix is given by $(t_i)_{i=1}^N$ and each different choice of $t_i \in \{1, -1\}$ results in a different first column. Now the j-th column (for $j \in \{2, \ldots, N\}$) is given by $(t_i s_j)_{i=1}^N = s_j (t_i)_{i=1}^N$, so the j-th column is either equal to the first column (if $s_j = 1$) or equal to its opposite (if $s_j = -1$). We now consider two deterministic correlation matrices $(t_i s_j)_{i,j=1}^N$ and $(t'_i s'_j)_{i,j=1}^N$ with $s_1 = s'_1 = 1$ but such that $t_i \neq t'_i$ for some $i \in \{1, \ldots, N\}$ or $s_j \neq s'_j$ for some $j \in \{2, \ldots, N\}$. These matrices will be different. This is because if $t_i \neq t'_i$ for some $i \in \{1, \ldots, N\}$ then the first columns of the matrices will be different. On the other hand, if $t_i = t'_i$ for all $i \in \{1, \ldots, N\}$, then the first columns of the matrices will be identical, but $s_j \neq s'_j$ for some $j \in \{2, \ldots, N\}$ and the j-th columns of the matrices will be each others' opposites and therefore different. This argument shows that once $s_1 = 1$ is fixed, each different choice of the other t_i and s_j will correspond to a different deterministic correlation matrix. There are 2^{2N-1} different ways of choosing the remaining t_i and s_j and therefore at least 2^{2N-1} different deterministic correlation matrices. To show that there aren't any more deterministic correlation matrices, we consider a deterministic correlation matrix $(t_i s_j)_{i,j=1}^N$ where $s_1 = -1$. We note that changing each t_i to $-t_i$ and each s_j to $-s_j$ will not change the overall matrix. So this matrix is also of the form $(t'_i s'_j)_{i,j=1}^N$ where $s'_1 = 1$ and therefore among the 2^{2N-1} matrices we already counted. So allowing $s_1 = -1$ does not give any new matrices, so we conclude that there are 2^{2N-1} deterministic correlation matrices of size $N \times N$.

□

Definition 5.3. Convex combination. Given a finite number of points x_i for $i \in \{1, \ldots, n\}$ in a vector space V over $\mathbb{R}$ or $\mathbb{C}$, a convex combination of these points is any point of the form

$$x = \sum_{i=1}^n a_i x_i \tag{124}$$

with $a_i \geq 0$ and $\sum_{i=1}^n a_i = 1$.

Remark. The requirement that all the x_i should be distinct can be added to the above definition to make sure each point can only appear once in the convex combination. This would ensure that the definition does not depend on the representation of the set $\{x_i : i \in \{1, \ldots, n\}\}$. However, a convex combination where not all points x_i are distinct is also a convex combination using only distinct points, which can be shown by grouping together all terms using the same point. The corresponding coefficients will be added together resulting in new coefficients which are still non-negative and sum to 1. This argument shows that we can safely use the definition of a convex combination without having to worry whether all the x_i are distinct. This is useful because in our situation each deterministic correlation matrix has two different representations.

The importance of the deterministic correlation matrices lies in the following theorem:

Theorem 5.2. *$\mathscr{L}_N$ is equal to the set of convex combinations of the $N \times N$ deterministic correlation matrices.*

This means that $\mathscr{L}_N$ is fully determined by the deterministic correlation matrices which are finite in number and can be explicitly calculated. This characterization can in some ways be easier to work with than the original definition.

Proof. We will first show that $\mathscr{L}_N$ is a subset of the set of convex combinations of $N \times N$ deterministic correlation matrices. We consider a classical correlation matrix $\gamma = (\gamma_{i,j})_{i,j=1}^N \in \mathscr{L}_N$ along with the probability space $(\Omega, \mathscr{A}, \mathbb{P})$ and random variables A_i, B_j such that the elements of γ are given by (122). For $(t_1, \ldots, t_N, s_1, \ldots, s_N) \in \{1, -1\}^{2N}$ we define:

$$\begin{aligned} &\Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N} = (\cap_{i=1}^N A_i^{-1}[\{t_i\}]) \cap (\cap_{j=1}^N B_j^{-1}[\{s_j\}]) = \\ &\{\omega \in \Omega : (\forall i, j \in \{1, \ldots, N\})(A_i(\omega) = t_i, B_j(\omega) = s_j)\}. \end{aligned} \tag{125}$$

We note that the $\Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}$ are distinct and disjoint subsets of Ω, since if $(t_1, \ldots, t_N, s_1, \ldots, s_N) \neq (t'_1, \ldots, t'_N, s'_1, \ldots, s'_N)$, then $t_i \neq t'_i$ for some i or $s_j \neq s'_j$ for some j. Now if $\omega \in \Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N} \cap \Omega_{t'_1,\ldots,t'_N,s'_1,\ldots,s'_N}$, then $A_i(\omega) = t_i = t'_i$ for all i and $B_j(\omega) = s_j = s'_j$ for all j which would lead to a contradiction, so no such ω exists and $\Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N} \cap \Omega_{t'_1,\ldots,t'_N,s'_1,\ldots,s'_N} = \emptyset$. Also, if $\omega \in \Omega$, then $(A_1(\omega), \ldots, A_N(\omega), B_1(\omega), \ldots, B_N(\omega)) = (t_1, \ldots, t_N, s_1, \ldots, s_N)$ for some $(t_1, \ldots, t_N, s_1, \ldots, s_N) \in \{1, -1\}^{2N}$ and therefore $\omega \in \Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}$. Each $\Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}$ is also measurable, because it is a finite intersection of inverse images under random variables of $\{1\}$ or $\{-1\}$. Combining these results we find that we have the following disjoint union of measurable sets:

$$\Omega = \cup_{(t_1,\ldots,t_N,s_1,\ldots,s_N) \in \{1,-1\}^{2N}} \Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}. \tag{126}$$

Using this, along with the fact that on each $\Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}$ the random variables are constant (A_i takes value t_i and B_j takes value s_j), we find that

$$\gamma = (\gamma_{i,j})_{i,j=1}^{N} = \left(\int_{\Omega} A_i(\omega) B_j(\omega) d\mathbb{P}(\omega) \right)_{i,j=1}^{N} =$$
$$\left(\int_{\cup_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} \Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}} A_i(\omega) B_j(\omega) d\mathbb{P}(\omega) \right)_{i,j=1}^{N} =$$
$$\left(\sum_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} \int_{\Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}} A_i(\omega) B_j(\omega) d\mathbb{P}(\omega) \right)_{i,j=1}^{N} =$$
$$\left(\sum_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} \int_{\Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}} t_i s_j d\mathbb{P}(\omega) \right)_{i,j=1}^{N} =$$
$$\left(\sum_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} \mathbb{P}(\Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}) t_i s_j \right)_{i,j=1}^{N} =$$
$$\sum_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} \mathbb{P}(\Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}) \, (t_i s_j)_{i,j=1}^{N} \tag{127}$$

which is a convex combination of the deterministic correlation matrices because $\mathbb{P}(\Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}) \geq 0$ for each $(t_1,\ldots,t_N,s_1,\ldots,s_N) \in \{1,-1\}^{2N}$ and

$$\sum_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} \mathbb{P}(\Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}) =$$
$$\mathbb{P}(\cup_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} \Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}) = \mathbb{P}(\Omega) = 1. \tag{128}$$

So we see that $\mathscr{L}_N$ is indeed a subset of the set of convex combinations of $N \times N$ deterministic correlation matrices. We will now show that the set of convex combinations of $N \times N$ deterministic correlation matrices is also a subset of $\mathscr{L}_N$ from which we will be able to conclude that these two sets are the same. We consider an arbitrary convex combination of the deterministic correlation matrices:

$$\gamma = \sum_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} a_{(t_1,\ldots,t_N,s_1,\ldots,s_N)} \, (t_i s_j)_{i,j=1}^{N} \tag{129}$$

with each $a_{(t_1,\ldots,t_N,s_1,\ldots,s_N)} \geq 0$ and $\sum_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} a_{(t_1,\ldots,t_N,s_1,\ldots,s_N)} = 1$ and we will show that γ is a classical correlation matrix. To this end we consider the probability space $(\Omega, \mathscr{A}, \mathbb{P})$, where $\Omega = (0,1]$, $\mathscr{A}$ is the Borel σ-algebra on $(0,1]$ and $\mathbb{P} = \lambda$, the Lebesgue measure (restricted to $(0,1]$). The Lebesgue measure is a measure and since $\lambda((0,1]) = 1 - 0 = 1$ it is also a probability measure. Since $\left|\{1,-1\}^{2N}\right| = 2^{2N}$, there exists a bijection $f : \{1,\ldots,2^{2N}\} \to \{1,-1\}^{2N}$. For $k \in \{1,\ldots,2^{2N}\}$ we define the following sets:

$$\Omega_{f(k)} = \left(\sum_{l=1}^{k-1} a_{f(l)}, \sum_{l=1}^{k} a_{f(l)} \right] \tag{130}$$

where we use the convention that $(a, b] = \emptyset$ if $b \leq a$. Since each $a_{f(l)} \geq 0$ and $\sum_{l=1}^{2^{2N}} a_{f(a)} = \sum_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} a_{(t_1,\ldots,t_N,s_1,\ldots,s_N)} = 1$ it follows that the $\Omega_{f(k)}$ are disjoint subsets of Ω and $\Omega = (0, 1] = \cup_{l=1}^{2^{2N}} \Omega_{f(k)}$ is a disjoint union. We also note that each $\Omega_{f(k)}$, being a half-open interval (or empty) is Lebesgue-measurable. Moreover we have $\mathbb{P}(\Omega_{f(k)}) = \lambda\left(\left(\sum_{l=1}^{k-1} a_{f(l)}, \sum_{l=1}^{k} a_{f(l)}\right]\right) = a_{f(k)}$ So far we have constructed a probability space $(\Omega, \mathscr{A}, \mathbb{P})$ with subsets $\Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}$ such that $\Omega = \cup_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} \Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}$ is a disjoint union and $\mathbb{P}(\Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}) = a_{(t_1,\ldots,t_N,s_1,\ldots,s_N)}$. We can now define random variables A_i and B_j for $i, j \in \{1, \ldots, N\}$ as follows. For $\omega \in \Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}$ we define $A_i(\omega) = t_i$ and $B_j(\omega) = s_j$. Since the sets $\Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}$ are disjoint and their union is Ω, the functions A_i and B_j are well-defined on Ω. Moreover, since A_i and B_j are constant on each $\Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}$ (which are measurable sets), A_i and B_j are measurable functions and therefore random variables. Since $t_i, s_j \in \{1, -1\}$, A_i and B_j takes values in $\{1, -1\}$. We have constructed a probability space with random variables meeting all the requirements in the definition of $\mathscr{L}_N$, so the matrix with elements $\int_\Omega A_i(\omega)B_j(\omega)d\mathbb{P}(\omega)$ is a classical correlation matrix. We will now show that γ is this matrix. We note that the sets $\Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}$ agree with the definition given in (125). Now it follows from (127) that

$$\begin{aligned}\left(\int_\Omega A_i(\omega)B_j(\omega)d\mathbb{P}(\omega)\right)_{i,j=1}^{N} = \\ \sum_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} \mathbb{P}(\Omega_{t_1,\ldots,t_N,s_1,\ldots,s_N}) \, (t_i s_j)_{i,j=1}^{N} = \\ \sum_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} a_{(t_1,\ldots,t_N,s_1,\ldots,s_N)} \, (t_i s_j)_{i,j=1}^{N} = \gamma.\end{aligned} \tag{131}$$

So γ is a classical correlation matrix. This completes the proof that $\mathscr{L}_N$ is the set of all convex combinations of $N \times N$ deterministic correlation matrices. □

Definition 5.4. Convex set. A convex set C is a subset of some vector space V over $\mathbb{R}$ or $\mathbb{C}$ such that for all $x, y \in C$ and $t \in [0, 1]$ we have $(1-t)x+ty \in C$.

Theorem 5.3. *If V is a vector space over $\mathbb{R}$ or $\mathbb{C}$ and C is the set of all convex combinations of the points in $\{c_1, \ldots, c_n\} \subseteq V$, then C is a convex set.*

Proof. Suppose C is the set of all convex combinations of the points in $\{c_1, \ldots, c_n\} \subseteq V$. Let $x, y \in C$ and $t \in [0, 1]$. Then $x = \sum_{i=1}^{n} a_i c_i$ and $y = \sum_{i=1}^{n} b_i c_i$ for some $a_i, b_i \geq 0$ with $\sum_{i=1}^{n} a_i = \sum_{i=1}^{n} b_i = 1$. Now we have:

$$(1-t)x + ty = (1-t)\sum_{i=1}^{n} a_i c_i + t\sum_{i=1}^{n} b_i c_i = \sum_{i=1}^{n}(1-t)a_i c_i + \sum_{i=1}^{n} t b_i c_i = \sum_{i=1}^{n}((1-t)a_i + tb_i)c_i \tag{132}$$

where $(1-t), t, a_i, b_i \geq 0$, so $(1-t)a_i + tb_i \geq 0$ and

$$\sum_{i=1}^{n}((1-t)a_i + tb_i) = (1-t)\sum_{i=1}^{n} a_i + t\sum_{i=1}^{n} b_i = (1-t) + t = 1. \tag{133}$$

So $(1-t)x + ty$ is a convex combination of the points in $\{c_1, \ldots, c_n\}$ and we see that $(1-t)x + ty \in C$. We conclude that C is a convex set. □

Theorems 5.2 and 5.3 together imply the following corollary:

Corollary 5.3.1. *$\mathscr{L}_N$ is a convex set.*

6 Quantum correlation matrix

We will now take another look at the terms of the form $\mathbb{E}(P_iQ_j)$ but from the point of view of quantum measurement. As before we still consider some state of a system composed of two systems with $P_1, \ldots, P_N$ measurements on the first system and $Q_1, \ldots, Q_N$ measurements on the second system, all having possible outcomes in $\{1, -1\}$. Similarly to the previous chapter, we want to define quantum correlation matrices as matrices with elements of the form $\mathbb{E}(P_iQ_j)$, but now from the point of view of quantum measurement. Just as in the case of the classical correlation matrices we will first translate this to a more explicit definition. Back when we violated the CHSH-inequality we only considered one specific state of a specific system and a specific set of measurements. This was sufficient, since we only wanted to show that the CHSH-inequality can be violated. Now we want to address the question to what degree a Bell inequality can be violated, so we must clearly define which systems, states and measurements we allow.

As stated before we consider a composition of two systems. Each of those two systems can in general be described by some complex Hilbert space. We will restrict ourselves to the case where both systems can be described by the finite-dimensional complex Hilbert space $\mathbb{C}^n$. Here $n \in \mathbb{N}$ is arbitrary and can vary but is always equal for both systems. The composite systems are then described by $\mathbb{C}^n \otimes \mathbb{C}^n$ for some $n \in \mathbb{N}$. We will consider states of these composite systems described by density operators $\rho : \mathbb{C}^n \otimes \mathbb{C}^n \to \mathbb{C}^n \otimes \mathbb{C}^n$. So we will be using the density operator formalism and will allow mixed states. As stated before we will consider measurements $P_1, \ldots, P_N$ on the first system and $Q_1, \ldots, Q_N$ on the second system with outcomes in $\{1, -1\}$ for some $N \in \mathbb{N}$ which will determine the size of the quantum correlation matrices. Aside from the outcomes being in $\{1, -1\}$ we will consider general measurements and since we are not interested in the post-measurement state of the system we will use the POVM formalism. Since each measurement has two outcomes, each POVM will have two elements which sum to the identity. The POVM for P_i will be $\{E_i, id - E_i\}$ with E_i associated to 1 and $id - E_i$ associated to -1. Similarly the POVM for Q_j will be $\{F_j, id - F_j\}$ with F_j associated to 1 and $id - F_j$ associated to -1. We note that, as part of POVM's, $E_i, id - E_i, F_j, id - F_j$ will all be positive operators on $\mathbb{C}^n$. Now that we have specified which systems, states and measurements we allow, we can derive a more explicit expression for $\mathbb{E}(P_iQ_j)$. This derivation is based on a similar derivation in chapter 5 of [2].

The combined measurement of P_i and Q_j is described by the POVM $\{E_i \otimes F_j, E_i \otimes (id - F_j), (id - E_i) \otimes F_j, (id - E_i) \otimes (id - F_j)\}$, where the positive operators are associated to outcomes $(1, 1), (1, -1), (-1, 1), (-1, -1)$ respectively. From this it follows that

$$\begin{aligned}
&\mathbb{E}(P_iQ_j) = (1\cdot 1)p(P_i=1,Q_j=1) + (1\cdot -1)p(P_i=1,Q_j=-1) + \\
&(-1\cdot 1)p(P_i=-1,Q_j=1) + (-1\cdot -1)p(P_i=-1,Q_j=-1) = \\
&p(P_i=1,Q_j=1) - p(P_i=1,Q_j=-1) - \\
&p(P_i=-1,Q_j=1) + p(P_i=-1,Q_j=-1) = \\
&tr((E_i\otimes F_j)\rho) - tr((E_i\otimes(id-F_j))\rho) - \\
&tr(((id-E_i)\otimes F_j)\rho) + tr(((id-E_i)\otimes(id-F_j))\rho) = \\
&tr((E_i\otimes F_j - E_i\otimes(id-F_j) - (id-E_i)\otimes F_j + (id-E_i)\otimes(id-F_j))\rho) = \\
&tr((E_i\otimes F_j - E_i\otimes id + E_i\otimes F_j - id\otimes F_j + E_i\otimes F_j + \\
&id\otimes id - id\otimes F_j - E_i\otimes id + E_i\otimes F_j)\rho) = \\
&tr((id\otimes id - 2(id\otimes F_j) - 2(E_i\otimes id) + 4(E_i\otimes F_j))\rho) = \\
&tr(((id-2E_i)\otimes(id-2F_j)\rho).
\end{aligned} \tag{134}$$

So the elements of the quantum correlation matrices will be of the form $tr(((id-2E_i)\otimes(id-2F_j))\rho)$ with E_i, F_j positive operators on $\mathbb{C}^n$ for some $n\in\mathbb{N}$ such that $id-E_i, id-F_j$ are also positive and ρ a density operator on $\mathbb{C}^n\otimes\mathbb{C}^n$. Theorems 2.12 and 2.13 now tell us that elements of the form $tr(((id-2E_i)\otimes(id-2F_j))\rho)$, with E_i, F_j positive operators on $\mathbb{C}^n$ for some $n\in\mathbb{N}$ such that $id-E_i, id-F_j$ are also positive and ρ a density operator on $\mathbb{C}^n\otimes\mathbb{C}^n$, are exactly the same as the elements of the form $tr(A_i\otimes B_j\rho)$ with A_i, B_j self-adjoint operators on $\mathbb{C}^n$ for some $n\in\mathbb{N}$ with $\|A_i\|, \|B_j\|\leq 1$ and ρ a density operator on $\mathbb{C}^n\otimes\mathbb{C}^n$. We now use this simplified expression to define the quantum correlation matrices, as in chapter 5 of [2], and we will spend the remainder of this chapter stating and proving some properties of the set of quantum correlation matrices. Most of these properties are also stated in chapter 5 of [2] but often without proof.

Definition 6.1. Quantum correlation matrix. The set $\mathscr{Q}_N$ of quantum correlation matrices is defined, for $N\in\mathbb{N}$, as the set of $N\times N$ matrices $\gamma=(\gamma_{i,j})_{i,j=1}^N$ whose elements have the following form:

$$\gamma_{i,j} = tr(A_i\otimes B_j\rho) \tag{135}$$

where A_i, B_j for $i,j\in\{1,\dots,N\}$ are self-adjoint operators acting on a Hilbert space $\mathbb{C}^n$ for some $n\in\mathbb{N}$ with $\max\{\|A_1\|,\dots,\|A_N\|,\|B_1\|,\dots,\|B_N\|\}\leq 1$ and ρ a density operator acting on $\mathbb{C}^n\otimes\mathbb{C}^n$.

The following theorem states that the elements of a quantum correlation matrix are real numbers between -1 and 1. This is not surprising since the elements of the quantum correlation matrices are constructed to be of the form $\mathbb{E}(P_iQ_j)$, where P_i and Q_j are measurements with outcomes in $\{1,-1\}$.

Theorem 6.1. *Let $(\gamma_{i,j})_{i,j=1}^N\in\mathscr{Q}_N$, then for all $i,j\in\{1,\dots,N\}$, $\gamma_{i,j}$ is real and $|\gamma_{i,j}\leq 1|$.*

Proof. Let $(\gamma_{i,j})_{i,j=1}^N \in \mathscr{Q}_N$. There exists an $n \in \mathbb{N}$, self-adjoint operators $A_1, \ldots, A_N, B_1, \ldots, B_N : \mathbb{C}^n \to \mathbb{C}^n$ with $\|A_i\|, \|B_j\| \leq 1$ for all $i, j \in \{1, \ldots, N\}$ and a density operator $\rho : \mathbb{C}^n \otimes \mathbb{C}^n \to \mathbb{C}^n \otimes \mathbb{C}^n$ such that $\gamma_{i,j} = tr(A_i \otimes B_j \rho)$. ρ is positive and $tr(\rho) = 1$. Let $i, j \in \{1, \ldots, N\}$, then by Theorem 2.14

$$\|A_i \otimes B_j\| = \|A_i\|\|B_j\| \leq 1 \cdot 1 = 1 \tag{136}$$

and $A_i \otimes B_j$ is self-adjoint. Now by Theorem 2.17 $\gamma_{i,j} = tr(A_i \otimes B_j \rho)$ is real and

$$|\gamma_{i,j}| = |tr(A_i \otimes B_j \rho)| \leq \|A_i \otimes B_j\| tr(\rho) \leq tr(\rho) = 1 \tag{137}$$

which completes the proof. □

The following theorem tells us that the classical correlation matrices form a subset of the quantum correlation matrices. This result is also stated and proved in chapter 5 of [2]. The proof we give is similar but fills in the details omitted from the original proof.

Theorem 6.2. $\mathscr{L}_N \subseteq \mathscr{Q}_N$

Before proving this theorem we would like to make the following remark

Remark. For $n \in \mathbb{N}$, $\mathbb{C}^n$ has a standard orthonormal basis $\{e_k = (\delta_{k,l})_{l=1}^n : k \in \{1, \ldots, n\}\}$. Therefore by Theorem 2.9 $\{e_k \otimes e_l : k, l \in \{1, \ldots, n\}\}$ is an orthonormal basis for $\mathbb{C}^n \otimes \mathbb{C}^n$ which we will refer to as the standard basis for $\mathbb{C}^n \otimes \mathbb{C}^n$. If $A, B : \mathbb{C}^n \to \mathbb{C}^n$ are linear operators with matrix representations $(a_{k,l})_{k,l=1}^n, (b_{k,l})_{k,l=1}^n$ with respect to the standard basis, then $A \otimes B : \mathbb{C}^n \otimes \mathbb{C}^n \to \mathbb{C}^n \otimes \mathbb{C}^n$ will have a matrix representation $(c_{(p,q),(r,s)})_{(p,q),(r,s) \in \{1,\ldots,n\}^2}$ with respect to the standard basis of $\mathbb{C}^n \otimes \mathbb{C}^n$ with:

$$c_{(p,q),(r,s)} = a_{p,r} b_{q,s}. \tag{138}$$

Because the standard basis of $\mathbb{C}^n \otimes \mathbb{C}^n$ is orthonormal, any inner products between vectors in $\mathbb{C}^n \otimes \mathbb{C}^n$ are equal to the inner products of their representations with respect to the standard basis.

Proof. Let $\gamma = (\gamma_{i,j})_{i,j=1}^N \in \mathscr{L}_N$. Since $\mathscr{L}_N$ consists of all convex combinations of the deterministic correlation matrices, γ is as in (129) with non-negative coefficients that sum to 1. Let $f : \{1, \ldots, 2^{2N}\} \to \{1, -1\}^{2N}$ be a bijection, then we can write

$$\gamma = \sum_{k=1}^{2^{2N}} a_{f(k)} (t_i(k) s_j(k))_{i,j=1}^N \tag{139}$$

with $t_i(k), s_j(k) \in \{1, -1\}$ such that $f(k) = (t_1(k), \ldots, t_N(k), s_1(k), \ldots, s_N(k))$. We now define the operators A_i and B_j for $i, j \in \{1, \ldots, N\}$ on $\mathbb{C}^{2^{2N}}$ using matrix representations $(\delta_{k,l} t_i(k))_{k,l=1}^{2^{2N}}$ and $(\delta_{k,l} s_j(k))_{k,l=1}^{2^{2N}}$ with respect to the standard basis. We note that these are diagonal matrices with real elements

(1 or -1) on the diagonal. This means the matrices are Hermitian and the corresponding operators are self-adjoint. Now for any vector $(c_l)_{l=1}^{2^{2N}} \in \mathbb{C}^{2^{2N}}$ we have:

$$\left\|(\delta_{k,l}t_i(k))_{k,l=1}^{2^{2N}}(c_l)_{l=1}^{2^{2N}}\right\|_2 = \left\|\left(\sum_{l=1}^{2^{2N}}\delta_{k,l}t_i(k)c_l\right)_{k=1}^{2^{2N}}\right\|_2 = \left\|(t_i(k)c_k)_{k=1}^{2^{2N}}\right\|_2 =$$
$$\sqrt{\sum_{k=1}^{2^{2N}}|t_i(k)c_k|^2} = \sqrt{\sum_{k=1}^{2^{2N}}|t_i(k)|^2|c_k|^2} = \sqrt{\sum_{k=1}^{2^{2N}}|c_k|^2} = \left\|(c_l)_{l=1}^{2^{2N}}\right\|_2 \tag{140}$$

and

$$\left\|(\delta_{k,l}s_j(k))_{k,l=1}^{2^{2N}}(c_l)_{l=1}^{2^{2N}}\right\|_2 = \left\|\left(\sum_{l=1}^{2^{2N}}\delta_{k,l}s_j(k)c_l\right)_{k=1}^{2^{2N}}\right\|_2 = \left\|(s_j(k)c_k)_{k=1}^{2^{2N}}\right\|_2 =$$
$$\sqrt{\sum_{k=1}^{2^{2N}}|s_j(k)c_k|^2} = \sqrt{\sum_{k=1}^{2^{2N}}|s_j(k)|^2|c_k|^2} = \sqrt{\sum_{k=1}^{2^{2N}}|c_k|^2} = \left\|(c_l)_{l=1}^{2^{2N}}\right\|_2. \tag{141}$$

So it follows that $\|A_i\| = \|B_j\| = 1$ for all $i,j \in \{1,\ldots,N\}$ and therefore $\max\{\|A_1\|,\ldots,\|A_N\|,\|B_1\|,\ldots,\|B_N\|\} = 1$. We see that the operators satisfy all requirements in the definition of the quantum correlation matrices.
With respect to the standard basis $A_i \otimes B_j$ has a matrix representation $\left(d^{(i,j)}_{(m,n),(q,r)}\right)_{(m,n),(q,r)\in\{1,\ldots,2^{2N}\}^2}$ with:

$$d^{(i,j)}_{(m,n),(q,r)} = (A_i)_{m,q}(B_j)_{n,r} = \delta_{m,q}t_i(m)\delta_{n,r}s_j(n). \tag{142}$$

We now define the operator $\rho : \mathbb{C}^{2^{2N}} \otimes \mathbb{C}^{2^{2N}} \to \mathbb{C}^{2^{2N}} \otimes \mathbb{C}^{2^{2N}}$ using a matrix representation $\left(\rho_{(m,n),(q,r)}\right)_{(m,n),(q,r)\in\{1,\ldots,2^{2N}\}^2}$ with respect to the standard basis with:

$$\rho_{(m,n),(q,r)} = \delta_{m,n}\delta_{q,r}\delta_{m,q}a_{f(m)}. \tag{143}$$

Let $c \in \mathbb{C}^{2^{2N}} \otimes \mathbb{C}^{2^{2N}}$ and $(c_{(q,r)})_{(q,r)\in\{1,\ldots,2^{2N}\}^2}$ its representation in the standard basis. We see that:

$$
\begin{aligned}
&\langle c, \rho c\rangle = \\
&\left\langle \left(c_{(m,n)}\right)_{(m,n)\in\{1,\ldots,2^{2N}\}^2}, \left(\rho_{(m,n),(q,r)}\right)_{(m,n),(q,r)\in\{1,\ldots,2^{2N}\}^2} \left(c_{(q,r)}\right)_{(q,r)\in\{1,\ldots,2^{2N}\}^2} \right\rangle = \\
&\left\langle \left(c_{(m,n)}\right)_{(m,n)\in\{1,\ldots,2^{2N}\}^2}, \left(\sum_{q=1}^{2^{2N}} \sum_{r=1}^{2^{2N}} \rho_{(m,n),(q,r)} c_{(q,r)} \right)_{(m,n)\in\{1,\ldots,2^{2N}\}^2} \right\rangle = \\
&\sum_{m=1}^{2^{2N}} \sum_{n=1}^{2^{2N}} c^*_{(m,n)} \sum_{q=1}^{2^{2N}} \sum_{r=1}^{2^{2N}} \rho_{(m,n),(q,r)} c_{(q,r)} = \sum_{m=1}^{2^{2N}} \sum_{n=1}^{2^{2N}} \sum_{q=1}^{2^{2N}} \sum_{r=1}^{2^{2N}} \rho_{(m,n),(q,r)} c^*_{(m,n)} c_{(q,r)} = \\
&\sum_{m=1}^{2^{2N}} \sum_{n=1}^{2^{2N}} \sum_{q=1}^{2^{2N}} \sum_{r=1}^{2^{2N}} \delta_{m,n}\delta_{q,r}\delta_{m,q} a_{f(m)} c^*_{(m,n)} c_{(q,r)} = \\
&\sum_{m=1}^{2^{2N}} \sum_{n=1}^{2^{2N}} \sum_{q=1}^{2^{2N}} \delta_{m,n}\delta_{m,q} a_{f(m)} c^*_{(m,n)} c_{(q,q)} = \sum_{m=1}^{2^{2N}} \sum_{n=1}^{2^{2N}} \delta_{m,n} a_{f(m)} c^*_{(m,n)} c_{(m,m)} = \\
&\sum_{m=1}^{2^{2N}} a_{f(m)} c^*_{(m,m)} c_{(m,m)} = \sum_{m=1}^{2^{2N}} a_{f(m)} \left|c_{(m,m)}\right|^2 \geq 0
\end{aligned}
\tag{144}
$$

because $\left|c_{(m,m)}\right|^2 \geq 0$ and $a_{f(m)} \geq 0$ for all $m \in \{1, \ldots, 2^{2N}\}$. This shows that ρ is a positive operator. We also have:

$$
\begin{aligned}
&tr(\rho) = tr((\rho_{(m,n),(q,r)})_{(m,n),(q,r)\in\{1,\ldots,2^{2N}\}^2}) = \sum_{m=1}^{2^{2N}} \sum_{n=1}^{2^{2N}} \rho_{(m,n),(m,n)} = \\
&\sum_{m=1}^{2^{2N}} \sum_{n=1}^{2^{2N}} \delta_{m,n}\delta_{m,n}\delta_{m,m} a_{f(m)} = \sum_{m=1}^{2^{2N}} \sum_{n=1}^{2^{2N}} \delta_{m,n} a_{f(m)} = \sum_{m=1}^{2^{2N}} a_{f(m)} = 1.
\end{aligned}
\tag{145}
$$

So ρ satisfies all requirements in the definition of the quantum correlation matrices. This means the matrix $(tr(A_i \otimes B_j \rho))_{i,j=1}^N$ is a quantum correlation matrix. Now

$$
\begin{aligned}
&tr(A_i \otimes B_j \rho) = \\
&tr\left(\left(d^{(i,j)}_{(m,n),(p,s)}\right)_{(m,n),(p,s)\in\{1,\ldots,2^{2N}\}^2} \left(\rho_{(p,s),(q,r)}\right)_{(p,s),(q,r)\in\{1,\ldots,2^{2N}\}^2}\right) = \\
&tr\left(\left(\sum_{p=1}^{2^{2N}}\sum_{s=1}^{2^{2N}} d^{(i,j)}_{(m,n),(p,s)}\rho_{(p,s),(q,r)}\right)_{(m,n),(q,r)\in\{1,\ldots,2^{2N}\}^2}\right) = \\
&\sum_{m=1}^{2^{2N}}\sum_{n=1}^{2^{2N}}\sum_{p=1}^{2^{2N}}\sum_{s=1}^{2^{2N}} d^{(i,j)}_{(m,n),(p,s)}\rho_{(p,s),(m,n)} = \\
&\sum_{m=1}^{2^{2N}}\sum_{n=1}^{2^{2N}}\sum_{p=1}^{2^{2N}}\sum_{s=1}^{2^{2N}} \delta_{m,p}t_i(m)\delta_{n,s}s_j(n)\delta_{p,s}\delta_{m,n}\delta_{p,m}a_{f(p)} = \\
&\sum_{m=1}^{2^{2N}}\sum_{n=1}^{2^{2N}}\sum_{p=1}^{2^{2N}}\sum_{s=1}^{2^{2N}} \delta_{m,p}\delta_{n,s}\delta_{p,s}\delta_{m,n}a_{f(p)}t_i(m)s_j(n) = \\
&\sum_{m=1}^{2^{2N}}\sum_{n=1}^{2^{2N}}\sum_{p=1}^{2^{2N}} \delta_{m,p}\delta_{p,n}\delta_{m,n}a_{f(p)}t_i(m)s_j(n) = \\
&\sum_{m=1}^{2^{2N}}\sum_{n=1}^{2^{2N}} \delta_{m,n}a_{f(m)}t_i(m)s_j(n) = \sum_{m=1}^{2^{2N}} a_{f(m)}t_i(m)s_j(m) = \gamma_{i,j}.
\end{aligned}
\tag{146}
$$

So this quantum correlation matrix is actually equal to γ, so $\gamma \in \mathscr{Q}_N$. This proves that $\mathscr{L}_N \subseteq \mathscr{Q}_N$. □

As the following theorem states, classical correlation matrices and quantum correlation matrices are the same in case $N = 1$.

Theorem 6.3. $\mathscr{L}_1 = \mathscr{Q}_1$

Proof. $\mathscr{L}_1 \subseteq \mathscr{Q}_1$ is a special case of the previous theorem. Let $\gamma = (\gamma_{1,1}) \in \mathscr{Q}_1$. As we have seen before, $\gamma_{1,1} \in [-1, 1]$. Now

$$
\gamma_{1,1} = \frac{1}{2}(1 + \gamma_{1,1}) \cdot 1 + \frac{1}{2}(1 - \gamma_{1,1}) \cdot -1 \tag{147}
$$

where $\frac{1}{2}(1 \pm \gamma_{1,1}) \geq 0$ and $\frac{1}{2}(1 + \gamma_{1,1}) + \frac{1}{2}(1 - \gamma_{1,1}) = 1$. So γ is a convex combination of the deterministic correlation matrices (1) and (-1) and therefore $\gamma \in \mathscr{L}_1$. So $\mathscr{Q}_1 \subseteq \mathscr{L}_1$ and we conclude that $\mathscr{L}_1 = \mathscr{Q}_1$. □

Our next theorem tells us that the set of quantum correlation matrices is convex, just like the set of classical correlation matrices. This result is stated but not proved in chapter 5 of [2].

Theorem 6.4. *$\mathscr{Q}_N$ is a convex set.*

Proof. Let $\gamma = (\gamma_{i,j})_{i,j=1}^N, \beta = (\beta_{i,j})_{i,j=1}^N) \in \mathscr{Q}_N$ and $t \in [0,1]$. This means there exist natural numbers n, m; self-adjoint operators A_i, B_j for $i, j \in \{1, \ldots, N\}$ acting on $\mathbb{C}^n$ with $\max\{\|A_1\|, \ldots, \|A_N\|, \|B_1\|, \ldots, \|B_N\|\} \leq 1$; a density operator ρ acting on $\mathbb{C}^n \otimes \mathbb{C}^n$; self-adjoint operators C_i, D_j for $i, j \in \{1, \ldots, N\}$ acting on $\mathbb{C}^m$ with $\max\{\|C_1\|, \ldots, \|C_N\|, \|D_1\|, \ldots, \|D_N\|\} \leq 1$; and a density operator σ acting on $\mathbb{C}^m \otimes \mathbb{C}^m$ such that $\gamma_{i,j} = tr(A_i \otimes B_j \rho)$ and $\beta_{i,j} = tr(C_i \otimes D_j \sigma)$. In order to prove the convexity of $\mathscr{Q}_N$ we need to show that $(1-t)\gamma + t\beta \in \mathscr{Q}_N$. To do this we will define self-adjoint operators E_i, F_j for $i, j \in \{1, \ldots, N\}$ on $\mathbb{C}^{n+m}$ with $\|E_i\|, \|F_j\| \leq 1$ and a density operator τ on $\mathbb{C}^{n+m} \otimes \mathbb{C}^{n+m}$ such that $tr(E_i \otimes F_j \tau) = (1-t)\gamma_{i,j} + t\beta_{i,j}$ which will prove that $(1-t)\gamma + t\beta \in \mathscr{Q}_N$. Using the identification $\mathbb{C}^{n+m} = \mathbb{C}^n \oplus \mathbb{C}^m$ we define the linear operators:

$$E_i = A_i \oplus C_i \tag{148}$$

and

$$F_j = B_j \oplus D_j. \tag{149}$$

A_i, B_j, C_i, D_j are all self-adjoint so E_i and F_j are self-adjoint by Corollary 2.24.1. We also have by Theorem 2.25 that

$$\|E_i\| = \max\{\|A_i\|, \|C_i\|\} \leq 1 \tag{150}$$

and

$$\|F_j\| = \max\{\|B_j\|, \|D_j\|\} \leq 1. \tag{151}$$

This shows that the linear operators E_i and F_j meet all requirements in the definition of $\mathscr{Q}_N$. In order to define τ we will need an isomorphism $G : (\mathbb{C}^n \oplus \mathbb{C}^m) \otimes (\mathbb{C}^n \oplus \mathbb{C}^m) \to (\mathbb{C}^n \otimes \mathbb{C}^n) \oplus (\mathbb{C}^n \otimes \mathbb{C}^m) \oplus (\mathbb{C}^m \otimes \mathbb{C}^n) \oplus (\mathbb{C}^m \otimes \mathbb{C}^m)$. In order to define G we will use orthonormal bases of the two spaces. We will write e_k^n and e_k^m for the elements of the standard bases of $\mathbb{C}^n$ and $\mathbb{C}^m$ respectively. These bases are orthonormal. Now $\{(e_k^n, 0) : k \in \{1, \ldots, n\}\} \cup \{(0, e_k^m) : k \in \{1, \ldots, m\}$ is an orthonormal basis for $\mathbb{C}^n \oplus \mathbb{C}^m$ and it follows that $\{(e_k^n, 0) \otimes (e_l^n, 0) : k, l \in \{1, \ldots, n\}\} \cup \{(e_k^n, 0) \otimes (0, e_l^m) : k \in \{1, \ldots, n\}, l \in \{1, \ldots, m\}\} \cup \{(0, e_k^m) \otimes (e_l^n, 0) : k \in \{1, \ldots, m\}, l \in \{1, \ldots, n\}\} \cup \{0, (e_k^n) \otimes (0, e_l^n) : k, l \in \{1, \ldots, m\}\}$ is an orthonormal basis for $(\mathbb{C}^n \oplus \mathbb{C}^m) \otimes (\mathbb{C}^n \oplus \mathbb{C}^m)$. We also have the orthonormal bases $\{e_k^n \otimes e_l^n : k, l \in \{1, \ldots, n\}\}$, $\{e_k^n \otimes e_l^m : k \in \{1, \ldots, n\}, l \in \{1, \ldots, m\}\}$, $\{e_k^m \otimes e_l^n : k \in \{1, \ldots, m\}, l \in \{1, \ldots, n\}\}$ and $\{e_k^m \otimes e_l^m : k, l \in \{1, \ldots, m\}\}$ for $\mathbb{C}^n \otimes \mathbb{C}^n$, $\mathbb{C}^n \otimes \mathbb{C}^m$, $\mathbb{C}^m \otimes \mathbb{C}^n$ and $\mathbb{C}^m \otimes \mathbb{C}^m$ respectively. This gives us the orthonormal basis $\{(e_k^n \otimes e_l^n, 0, 0, 0) : k, l \in \{1, \ldots, n\}\} \cup \{(0, e_k^n \otimes e_l^m, 0, 0) : k \in \{1, \ldots, n\}, l \in \{1, \ldots, m\}\} \cup \{(0, 0, e_k^m \otimes e_l^n, 0) : k \in \{1, \ldots, m\}, l \in \{1, \ldots, n\}\} \cup \{(0, 0, 0, e_k^m \otimes e_l^m) : k, l \in \{1, \ldots, m\}\}$ for $(\mathbb{C}^n \otimes \mathbb{C}^n) \oplus (\mathbb{C}^n \otimes \mathbb{C}^m) \oplus (\mathbb{C}^m \otimes \mathbb{C}^n) \oplus (\mathbb{C}^m \otimes \mathbb{C}^m)$. Using these bases we define G as:

$$
\begin{aligned}
&G(\sum_{k=1}^{n}\sum_{l=1}^{n} a_{k,l}(e_k^n,0)\otimes(e_l^n,0)+\sum_{k=1}^{n}\sum_{l=1}^{m} b_{k,l}(e_k^n,0)\otimes(0,e_l^m)+\\
&\sum_{k=1}^{m}\sum_{l=1}^{n} c_{k,l}(0,e_k^m)\otimes(e_l^n,0)+\sum_{k=1}^{m}\sum_{l=1}^{m} d_{k,l}(0,e_k^m)\otimes(0,e_l^m))=\\
&\sum_{k=1}^{n}\sum_{l=1}^{n} a_{k,l}(e_k^n\otimes e_l^n,0,0,0)+\sum_{k=1}^{n}\sum_{l=1}^{m} b_{k,l}(0,e_k^n\otimes e_l^m,0,0)+\\
&\sum_{k=1}^{m}\sum_{l=1}^{n} c_{k,l}(0,0,e_k^m\otimes e_l^n,0)+\sum_{k=1}^{m}\sum_{l=1}^{m} d_{k,l}(0,0,0,e_k^m\otimes e_l^m)
\end{aligned}
\tag{152}
$$

for any choice of $a_{k,l}, b_{k,l}, c_{k,l}, d_{k,l} \in \mathbb{C}$ and Theorem 2.23 ensures that G is an isomorphism. This definition of G is not the most practical to work with, so we will first show that for all $v, w \in \mathbb{C}^n$ and $x, y \in \mathbb{C}^m$ we have

$$G((v,x)\otimes(w,y)) = (v\otimes w, v\otimes y, x\otimes w, x\otimes y). \tag{153}$$

To show this we express v, w, x, y as linear combinations of basis vectors:

$$v = \sum_{k=1}^{n} a_k e_k^n, \tag{154}$$

$$w = \sum_{k=1}^{n} b_k e_k^n, \tag{155}$$

$$x = \sum_{k=1}^{m} c_k e_k^m \tag{156}$$

and

$$y = \sum_{k=1}^{m} d_k e_k^m. \tag{157}$$

Using the definition of G we find that:

$$
\begin{aligned}
&G((v,x)\otimes(w,y)) = \\
&G((v,0)\otimes(w,0)+(v,0)\otimes(0,y)+(0,x)\otimes(w,0)+(0,x)\otimes(0,y)) = \\
&G((\sum_{k=1}^{n} a_k e_k^n,0)\otimes(\sum_{l=1}^{n} b_l e_l^n,0)+(\sum_{k=1}^{n} a_k e_k^n,0)\otimes(0,\sum_{l=1}^{m} d_l e_l^m)+ \\
&(0,\sum_{k=1}^{m} c_k e_k^m)\otimes(\sum_{l=1}^{n} b_l e_l^n,0)+(0,\sum_{k=1}^{m} c_k e_k^m)\otimes(0,\sum_{l=1}^{m} d_l e_l^m)) = \\
&G(\sum_{k=1}^{n}\sum_{l=1}^{n} a_k b_l (e_k^n,0)\otimes(e_l^n,0)+\sum_{k=1}^{n}\sum_{l=1}^{m} a_k d_l (e_k^n,0)\otimes(0,e_l^m)+ \\
&\sum_{k=1}^{m}\sum_{l=1}^{n} c_k b_l (0,e_k^m)\otimes(e_l^n,0)+\sum_{k=1}^{m}\sum_{l=1}^{m} c_k d_l (0,e_k^m)\otimes(0,e_l^m)) = \\
&\sum_{k=1}^{n}\sum_{l=1}^{n} a_k b_l (e_k^n\otimes e_l^n,0,0,0)+\sum_{k=1}^{n}\sum_{l=1}^{m} a_k d_l (0,e_k^n\otimes e_l^m,0,0)+ \\
&\sum_{k=1}^{m}\sum_{l=1}^{n} c_k b_l (0,0,e_k^m\otimes e_l^n,0)+\sum_{k=1}^{m}\sum_{l=1}^{m} c_k d_l (0,0,0,e_k^m\otimes e_l^m) = \\
&(\sum_{k=1}^{n} a_k e_k^n\otimes\sum_{l=1}^{n} b_l e_l^n,0,0,0)+(0,\sum_{k=1}^{n} a_k e_k^n\otimes\sum_{l=1}^{m} d_l e_l^m,0,0)+ \\
&(0,0,\sum_{k=1}^{m} c_k e_k^m\otimes\sum_{l=1}^{n} b_l e_l^n,0)+(0,0,0,\sum_{k=1}^{m} c_k e_k^m\otimes\sum_{l=1}^{m} d_l e_l^m) = \\
&(v\otimes w,0,0,0)+(0,v\otimes y,0,0)+(0,0,x\otimes w,0)+(0,0,0,x\otimes y) = \\
&(v\otimes w, v\otimes y, x\otimes w, x\otimes y)
\end{aligned}
\tag{158}
$$

which is what we wanted to show. Next we will show that $G(E_i\otimes F_j)G^{-1} = (A_i\otimes B_j)\oplus(A_i\otimes D_j)\oplus(C_i\otimes B_j)\oplus(C_i\otimes D_j)$. For any choice of $a_{k,l}, b_{k,l}, c_{k,l}, d_{k,l}\in\mathbb{C}$ we have:

$$
\begin{aligned}
&G(E_i\otimes F_j)G^{-1}(\sum_{k=1}^{n}\sum_{l=1}^{n} a_{k,l}(e_k^n\otimes e_l^n,0,0,0)+\sum_{k=1}^{n}\sum_{l=1}^{m} b_{k,l}(0,e_k^n\otimes e_l^m,0,0)+ \\
&\sum_{k=1}^{m}\sum_{l=1}^{n} c_{k,l}(0,0,e_k^m\otimes e_l^n,0)+\sum_{k=1}^{m}\sum_{l=1}^{m} d_{k,l}(0,0,0,e_k^m\otimes e_l^m)) = \\
&G(E_i\otimes F_j)(\sum_{k=1}^{n}\sum_{l=1}^{n} a_{k,l}(e_k^n,0)\otimes(e_l^n,0)+\sum_{k=1}^{n}\sum_{l=1}^{m} b_{k,l}(e_k^n,0)\otimes(0,e_l^m)+ \\
&\sum_{k=1}^{m}\sum_{l=1}^{n} c_{k,l}(0,e_k^m)\otimes(e_l^n,0)+\sum_{k=1}^{m}\sum_{l=1}^{m} d_{k,l}(0,e_k^m)\otimes(0,e_l^m)) =
\end{aligned}
$$

$$G(\sum_{k=1}^{n}\sum_{l=1}^{n} a_{k,l}E_i(e_k^n,0)\otimes F_j(e_l^n,0)+\sum_{k=1}^{n}\sum_{l=1}^{m} b_{k,l}E_i(e_k^n,0)\otimes F_j(0,e_l^m)+$$
$$\sum_{k=1}^{m}\sum_{l=1}^{n} c_{k,l}E_i(0,e_k^m)\otimes F_j(e_l^n,0)+\sum_{k=1}^{m}\sum_{l=1}^{m} d_{k,l}E_i(0,e_k^m)\otimes F_j(0,e_l^m))=$$
$$G(\sum_{k=1}^{n}\sum_{l=1}^{n} a_{k,l}(A_ie_k^n,0)\otimes (B_je_l^n,0)+\sum_{k=1}^{n}\sum_{l=1}^{m} b_{k,l}(A_ie_k^n,0)\otimes (0,D_je_l^m)+$$
$$\sum_{k=1}^{m}\sum_{l=1}^{n} c_{k,l}(0,C_ie_k^m)\otimes (B_je_l^n,0)+\sum_{k=1}^{m}\sum_{l=1}^{m} d_{k,l}(0,C_ie_k^m)\otimes (0,D_je_l^m))=$$
$$\sum_{k=1}^{n}\sum_{l=1}^{n} a_{k,l}G((A_ie_k^n,0)\otimes (B_je_l^n,0))+\sum_{k=1}^{n}\sum_{l=1}^{m} b_{k,l}G((A_ie_k^n,0)\otimes (0,D_je_l^m))+$$
$$\sum_{k=1}^{m}\sum_{l=1}^{n} c_{k,l}G((0,C_ie_k^m)\otimes (B_je_l^n,0))+\sum_{k=1}^{m}\sum_{l=1}^{m} d_{k,l}G((0,C_ie_k^m)\otimes (0,D_je_l^m))=$$
$$\sum_{k=1}^{n}\sum_{l=1}^{n} a_{k,l}(A_ie_k^n\otimes B_je_l^n,0,0,0)+\sum_{k=1}^{n}\sum_{l=1}^{m} b_{k,l}(0,A_ie_k^n\otimes D_je_l^m,0,0)+$$
$$\sum_{k=1}^{m}\sum_{l=1}^{n} c_{k,l}(0,0,C_ie_k^m\otimes B_je_l^n,0)+\sum_{k=1}^{m}\sum_{l=1}^{m} d_{k,l}(0,0,0,C_ie_k^m\otimes D_je_l^m)=$$
$$((A_i\otimes B_j)\sum_{k=1}^{n}\sum_{l=1}^{n} a_{k,l}e_k^n\otimes e_l^n,0,0,0)+(0,(A_i\otimes D_j)\sum_{k=1}^{n}\sum_{l=1}^{m} b_{k,l}e_k^n\otimes e_l^m,0,0)+$$
$$(0,0,(C_i\otimes B_j)\sum_{k=1}^{m}\sum_{l=1}^{n} c_{k,l}e_k^m\otimes e_l^n,0)+(0,0,0,(C_i\otimes D_j)\sum_{k=1}^{m}\sum_{l=1}^{m} d_{k,l}e_k^m\otimes e_l^m)=$$
$$((A_i\otimes B_j)\sum_{k=1}^{n}\sum_{l=1}^{n} a_{k,l}e_k^n\otimes e_l^n,(A_i\otimes D_j)\sum_{k=1}^{n}\sum_{l=1}^{m} b_{k,l}e_k^n\otimes e_l^m,$$
$$(C_i\otimes B_j)\sum_{k=1}^{m}\sum_{l=1}^{n} c_{k,l}e_k^m\otimes e_l^n,(C_i\otimes D_j)\sum_{k=1}^{m}\sum_{l=1}^{m} d_{k,l}e_k^m\otimes e_l^m)=$$
$$((A_i\otimes B_j)\oplus(A_i\otimes D_j)\oplus(C_i\otimes B_j)\oplus(C_i\otimes D_j))(\sum_{k=1}^{n}\sum_{l=1}^{n} a_{k,l}(e_k^n\otimes e_l^n,0,0,0)+$$
$$\sum_{k=1}^{n}\sum_{l=1}^{m} b_{k,l}(0,e_k^n\otimes e_l^m,0,0)+\sum_{k=1}^{m}\sum_{l=1}^{n} c_{k,l}(0,0,e_k^m\otimes e_l^n,0)+$$
$$\sum_{k=1}^{m}\sum_{l=1}^{m} d_{k,l}(0,0,0,e_k^m\otimes e_l^m)) \tag{159}$$

which gives us the desired result. We now consider the linear operator $(1-$

$t)\rho \oplus 0 \oplus 0 \oplus t\sigma$ on $(\mathbb{C}^n \otimes \mathbb{C}^n) \oplus (\mathbb{C}^n \otimes \mathbb{C}^m) \oplus (\mathbb{C}^m \otimes \mathbb{C}^n) \oplus (\mathbb{C}^m \otimes \mathbb{C}^m)$ with 0 being the zero-operator which sends every element to 0. ρ and σ are positive and $(1-t), t \geq 0$ so $(1-t)\rho$ and $t\sigma$ are positive. Since 0 is also positive, it follows from Theorem 2.26 that $(1-t)\rho \oplus 0 \oplus 0 \oplus t\sigma$ is a positive operator. By Theorem 2.27 we also have:

$$\begin{aligned} &tr((1-t)\rho \oplus 0 \oplus 0 \oplus t\sigma) = tr((1-t)\rho) + tr(0) + tr(0) + tr(t\sigma) = \\ &(1-t)tr(\rho) + 0 + 0 + ttr(\sigma) = (1-t) + t = 1. \end{aligned} \tag{160}$$

□

We define the linear operator $\tau = G^{-1}((1-t)\rho \oplus 0 \oplus 0 \oplus t\sigma)G$ on $(\mathbb{C}^n \oplus \mathbb{C}^m) \otimes (\mathbb{C}^n \oplus \mathbb{C}^m)$ and note that because G is an isomorphism and $(1-t)\rho \oplus 0 \oplus 0 \oplus t\sigma$ is a positive operator with trace equal to 1, that τ is also positive and $tr(\tau) = 1$ by Theorems 2.20 and 2.22, so τ is a density operator. Now, using the fact that G is an isomorphism we have by Theorems 2.22 and 2.27:

$$\begin{aligned} &tr((E_i \otimes F_j)\tau) = tr(G(E_i \otimes F_j)\tau G^{-1}) = \\ &tr(G(E_i \otimes F_j)G^{-1}((1-t)\rho \oplus 0 \oplus 0 \oplus t\sigma)GG^{-1}) = \\ &tr((A_i \otimes B_j) \oplus (A_i \otimes D_j) \oplus (C_i \otimes B_j) \oplus (C_i \otimes D_j)((1-t)\rho \oplus 0 \oplus 0 \oplus t\sigma)) = \\ &tr((1-t)(A_i \otimes B_j)\rho \oplus 0 \oplus 0 \oplus t(C_i \otimes D_j)\sigma) = \\ &tr((1-t)(A_i \otimes B_j)\rho) + tr(0) + tr(0) + tr(t(C_i \otimes D_j)\sigma) = \\ &(1-t)tr((A_i \otimes B_j)\rho) + 0 + 0 + ttr((C_i \otimes D_j)\sigma) = (1-t)\gamma_{i,j} + t\beta_{i,j} \end{aligned} \tag{161}$$

which completes the proof. We also give a second proof that does not rely on isomorphisms or direct sums and instead relies on the Kronecker product to represent all operators using matrices.

Proof. Let $\gamma = (\gamma_{i,j})_{i,j=1}^N, \beta = (\beta_{i,j})_{i,j=1}^N \in \mathscr{Q}_N$ and $t \in [0,1]$. This means there exist natural numbers n, m; self-adjoint operators A_i, B_j for $i, j \in \{1, \ldots, N\}$ acting on $\mathbb{C}^n$ with $\max\{\|A_1\|, \ldots, \|A_N\|, \|B_1\|, \ldots, \|B_N\|\} \leq 1$; a density operator ρ acting on $\mathbb{C}^n \otimes \mathbb{C}^n$; self-adjoint operators C_i, D_j for $i, j \in \{1, \ldots, N\}$ acting on $\mathbb{C}^m$ with $\max\{\|C_1\|, \ldots, \|C_N\|, \|D_1\|, \ldots, \|D_N\|\} \leq 1$; and a density operator σ acting on $\mathbb{C}^m \otimes \mathbb{C}^m$ such that $\gamma_{i,j} = tr(A_i \otimes B_j \rho)$ and $\beta_{i,j} = tr(C_i \otimes D_j \sigma)$. Let $(a_{k,l}^{(i)})_{k,l=1}^n, (b_{k,l}^{(j)})_{k,l=1}^n$, $(\rho_{(p,q),(r,s)})_{(p,q),(r,s)\in\{1,\ldots,n\}^2}$, $(c_{k,l}^{(i)})_{k,l=1}^m$, $(d_{k,l}^{(j)})_{k,l=1}^m$, $(\sigma_{(p,q),(r,s)})_{(p,q),(r,s)\in\{1,\ldots,m\}^2}$ be the matrix representations of $A_i, B_j, \rho, C_i, B_j, \sigma$ respectively with respect to the appropriate standard bases. Let $(x_{(p,q),(r,s)}^{(i,j)})_{(p,q),(r,s)\in\{1,\ldots,n\}^2}$, $(y_{(p,q),(r,s)}^{(i,j)})_{(p,q),(r,s)\in\{1,\ldots,m\}^2}$ be the matrix representations of $A_i \otimes B_j$ and $C_i \otimes D_j$ respectively with respect to the appropriate standard bases. Then we have by Theorem 2.9:

$$x_{(p,q),(r,s)}^{(i,j)} = a_{p,r}^{(i)} b_{q,s}^{(j)}. \tag{162}$$

and:

$$y^{(i,j)}_{(p,q),(r,s)} = c^{(i)}_{p,r} d^{(j)}_{q,s}. \tag{163}$$

From this it follows that

$$\begin{aligned}
&\gamma_{i,j} = tr(A_i \otimes B_j \rho) = \\
&tr\left((x^{(i,j)}_{(p,q),(r,s)})_{(p,q),(r,s)\in\{1,\ldots,n\}^2} (\rho_{(r,s),(t,u)})_{(r,s),(t,u)\in\{1,\ldots,n\}^2} \right) = \\
&tr\left(\left(\sum_{r=1}^{n}\sum_{s=1}^{n} x^{(i,j)}_{(p,q),(r,s)} \rho_{(r,s),(t,u)} \right)_{(p,q),(t,u)\in\{1,\ldots,n\}^2} \right) = \\
&\sum_{p=1}^{n}\sum_{q=1}^{n}\sum_{r=1}^{n}\sum_{s=1}^{n} x^{(i,j)}_{(p,q),(r,s)} \rho_{(r,s),(p,q)} = \\
&\sum_{p=1}^{n}\sum_{q=1}^{n}\sum_{r=1}^{n}\sum_{s=1}^{n} a^{(i)}_{p,r} b^{(j)}_{q,s} \rho_{(r,s),(p,q)}
\end{aligned} \tag{164}$$

and

$$\begin{aligned}
&\beta_{i,j} = tr(C_i \otimes D_j \sigma) = \\
&tr\left((y^{(i,j)}_{(p,q),(r,s)})_{(p,q),(r,s)\in\{1,\ldots,m\}^2} (\sigma_{(r,s),(t,u)})_{(r,s),(t,u)\in\{1,\ldots,m\}^2} \right) = \\
&tr\left(\left(\sum_{r=1}^{m}\sum_{s=1}^{m} y^{(i,j)}_{(p,q),(r,s)} \sigma_{(r,s),(t,u)} \right)_{(p,q),(t,u)\in\{1,\ldots,n\}^2} \right) = \\
&\sum_{p=1}^{m}\sum_{q=1}^{m}\sum_{r=1}^{m}\sum_{s=1}^{m} y^{(i,j)}_{(p,q),(r,s)} \sigma_{(r,s),(p,q)} = \\
&\sum_{p=1}^{m}\sum_{q=1}^{m}\sum_{r=1}^{m}\sum_{s=1}^{m} c^{(i)}_{p,r} d^{(j)}_{q,s} \sigma_{(r,s),(p,q)}.
\end{aligned} \tag{165}$$

We now define, for $i, j \in \{1, \ldots, N\}$, linear operators $E_i, F_j : \mathbb{C}^{n+m} \to \mathbb{C}^{n+m}$ by specifying their matrix representations $(e^{(i)}_{k,l})^{n+m}_{k,l=1}, (f^{(i)}_{k,l})^{n+m}_{k,l=1}$ with respect to the standard basis. The elements of these matrices are given by:

$$e^{(i)}_{k,l} = \begin{cases} a^{(i)}_{k,l} & \text{for } k,l \in \{1,\ldots,n\} \\ c^{(i)}_{k-n,l-n} & \text{for } k,l \in \{n+1,\ldots,n+m\} \\ 0 & \text{otherwise} \end{cases} \tag{166}$$

and

$$f^{(j)}_{k,l} = \begin{cases} b^{(j)}_{k,l} & \text{for } k,l \in \{1,\ldots,n\} \\ d^{(j)}_{k-n,l-n} & \text{for } k,l \in \{n+1,\ldots,n+m\} \\ 0 & \text{otherwise} \end{cases}. \tag{167}$$

We note that

$$(e_{l,k}^{(i)})^* = \begin{cases} (a_{l,k}^{(i)})^* = a_{k,l}^{(i)} & \text{for } k,l \in \{1,\dots,n\} \\ (c_{l-n,k-n}^{(i)})^* = c_{k-n,l-n}^{(i)} & \text{for } k,l \in \{n+1,\dots,n+m\} \\ 0^* = 0 & \text{otherwise} \end{cases} \tag{168}$$

and

$$(f_{l,k}^{(j)})^* = \begin{cases} (b_{l,k}^{(j)})^* = b_{k,l}^{(j)} & \text{for } k,l \in \{1,\dots,n\} \\ (d_{l-n,k-n}^{(j)})^* = d_{k-n,l-n}^{(j)} & \text{for } k,l \in \{n+1,\dots,n+m\} \\ 0^* = 0 & \text{otherwise} \end{cases} \tag{169}$$

where we used the fact that A_i and B_j are self-adjoint and that their matrix representations are therefore Hermitian. We see that $(e_{l,k}^{(i)})^* = e_{k,l}^{(i)}$ and $(f_{l,k}^{(j)})^* = f_{k,l}^{(j)}$ so the matrix representations of E_i and F_j are Hermitian and consequently E_i and F_j are self-adjoint operators. Let $\alpha = (\alpha_l)_{l=1}^{n+m} \in \mathbb{C}^{n+m}$. We note that

$$\begin{aligned}
&\|E_i\alpha\|_2^2 = \left\|(e_{k,l}^{(i)})_{k,l=1}^{n+m}(\alpha_l)_{l=1}^{n+m}\right\|_2^2 = \left\|\left(\sum_{l=1}^{n+m} e_{k,l}^{(i)}\alpha_l\right)_{k=1}^{n+m}\right\|_2^2 = \\
&\sum_{k=1}^{n+m}\left|\sum_{l=1}^{n+m} e_{k,l}^{(i)}\alpha_l\right|^2 = \sum_{k=1}^{n}\left|\sum_{l=1}^{n+m} e_{k,l}^{(i)}\alpha_l\right|^2 + \sum_{k=n+1}^{n+m}\left|\sum_{l=1}^{n+m} e_{k,l}^{(i)}\alpha_l\right|^2 = \\
&\sum_{k=1}^{n}\left|\sum_{l=1}^{n} a_{k,l}^{(i)}\alpha_l\right|^2 + \sum_{k=n+1}^{n+m}\left|\sum_{l=n+1}^{n+m} c_{k-n,l-n}^{(i)}\alpha_l\right|^2 = \\
&\sum_{k=1}^{n}\left|\sum_{l=1}^{n} a_{k,l}^{(i)}\alpha_l\right|^2 + \sum_{k=1}^{m}\left|\sum_{l=1}^{m} c_{k,l}^{(i)}\alpha_{l+n}\right|^2 = \\
&\left\|\left(\sum_{l=1}^{n} a_{k,l}^{(i)}\alpha_l\right)_{k=1}^{n}\right\|_2^2 + \left\|\left(\sum_{l=1}^{m} c_{k,l}^{(i)}\alpha_{l+n}\right)_{k=1}^{m}\right\|_2^2 = \\
&\left\|(a_{k,l}^{(i)})_{k,l=1}^{n}(\alpha_l)_{l=1}^{n}\right\|_2^2 + \left\|(c_{k,l}^{(i)})_{k,l=1}^{m}(\alpha_{l+n})_{l=1}^{m}\right\|_2^2 \leq \\
&\|A_i\|^2\|(\alpha_l)_{l=1}^{n}\|_2^2 + \|C_i\|^2\|(\alpha_{l+n})_{l=1}^{m}\|_2^2 \leq \|(\alpha_l)_{l=1}^{n}\|_2^2 + \|(\alpha_{l+n})_{l=1}^{m}\|_2^2 = \\
&\sum_{l=1}^{n}|\alpha_l|^2 + \sum_{l=1}^{m}|\alpha_{l+n}|^2 = \sum_{l=1}^{n}|\alpha_l|^2 + \sum_{l=n+1}^{n+m}|\alpha_l|^2 = \sum_{l=1}^{n+m}|\alpha_l|^2 = \|\alpha\|_2^2
\end{aligned} \tag{170}$$

and

$$\|F_j\alpha\|_2^2 = \left\|(f_{k,l}^{(j)})_{k,l=1}^{n+m}(\alpha_l)_{l=1}^{n+m}\right\|_2^2 = \left\|\left(\sum_{l=1}^{n+m} f_{k,l}^{(j)}\alpha_l\right)_{k=1}^{n+m}\right\|_2^2 =$$
$$\sum_{k=1}^{n+m}\left|\sum_{l=1}^{n+m} f_{k,l}^{(j)}\alpha_l\right|^2 = \sum_{k=1}^{n}\left|\sum_{l=1}^{n+m} f_{k,l}^{(j)}\alpha_l\right|^2 + \sum_{k=n+1}^{n+m}\left|\sum_{l=1}^{n+m} f_{k,l}^{(j)}\alpha_l\right|^2 =$$
$$\sum_{k=1}^{n}\left|\sum_{l=1}^{n} b_{k,l}^{(j)}\alpha_l\right|^2 + \sum_{k=n+1}^{n+m}\left|\sum_{l=n+1}^{n+m} d_{k-n,l-n}^{(j)}\alpha_l\right|^2 =$$
$$\sum_{k=1}^{n}\left|\sum_{l=1}^{n} b_{k,l}^{(j)}\alpha_l\right|^2 + \sum_{k=1}^{m}\left|\sum_{l=1}^{m} d_{k,l}^{(j)}\alpha_{l+n}\right|^2 = \tag{171}$$
$$\left\|\left(\sum_{l=1}^{n} b_{k,l}^{(j)}\alpha_l\right)_{k=1}^{n}\right\|_2^2 + \left\|\left(\sum_{l=1}^{m} d_{k,l}^{(j)}\alpha_{l+n}\right)_{k=1}^{m}\right\|_2^2 =$$
$$\left\|(b_{k,l}^{(j)})_{k,l=1}^{n}(\alpha_l)_{l=1}^{n}\right\|_2^2 + \left\|(d_{k,l}^{(j)})_{k,l=1}^{m}(\alpha_{l+n})_{l=1}^{m}\right\|_2^2 \leq$$
$$\|B_j\|^2\|(\alpha_l)_{l=1}^{n}\|_2^2 + \|D_j\|^2\|(\alpha_{l+n})_{l=1}^{m}\|_2^2 \leq \|(\alpha_l)_{l=1}^{n}\|_2^2 + \|(\alpha_{l+n})_{l=1}^{m}\|_2^2 =$$
$$\sum_{l=1}^{n}|\alpha_l|^2 + \sum_{l=1}^{m}|\alpha_{l+n}|^2 = \sum_{l=1}^{n}|\alpha_l|^2 + \sum_{l=n+1}^{n+m}|\alpha_l|^2 = \sum_{l=1}^{n+m}|\alpha_l|^2 = \|\alpha\|_2^2.$$

So it follows that $\|E_i\| = \sup_{\alpha\in\mathbb{C}^{n+m},\alpha\neq 0}\frac{\|E_i\alpha\|_2}{\|\alpha\|_2} \leq 1$ and $\|F_j\| = \sup_{\alpha\in\mathbb{C}^{n+m},\alpha\neq 0}\frac{\|F_j\alpha\|_2}{\|\alpha\|_2} \leq 1$ for all $i,j \in \{1,\ldots,N\}$ and we see that $\max\{\|E_1\|,\ldots,\|E_N\|,\|F_1\|,\ldots,\|F_N\|\} \leq 1$. We conclude that the operators E_i, F_j satisfy all requirements in Definition 6.1. We now define the linear operator $\tau : \mathbb{C}^{n+m}\otimes\mathbb{C}^{n+m} \to \mathbb{C}^{n+m}\otimes\mathbb{C}^{n+m}$ by specifying its matrix representation $(\tau_{(p,q),(r,s)})_{(p,q),(r,s)\in\{1,\ldots,n+m\}^2}$ with respect to the standard basis with:

$$\tau_{(p,q),(r,s)} = \begin{cases} (1-t)\rho_{(p,q),(r,s)} & \text{for } p,q,r,s \in \{1,\ldots,n\} \\ t\sigma_{(p-n,q-n),(r-n,s-n)} & \text{for } p,q,r,s \in \{n+1,\ldots,n+m\} \\ 0 & \text{otherwise} \end{cases}. \tag{172}$$

Let $\alpha \in \mathbb{C}^{n+m}\otimes\mathbb{C}^{n+m}$ and $(\alpha_{(r,s)})_{(r,s)\in\{1,\ldots,n+m\}^2}$ its representation with respect to the standard basis. Let $\alpha' \in \mathbb{C}^n\otimes\mathbb{C}^n$ with representation $(\alpha'_{(r,s)})_{(r,s)\in\{1,\ldots,n\}^2}$ with respect to the standard basis with $\alpha'_{(r,s)} = \alpha_{(r,s)}$. Also let $\alpha'' \in \mathbb{C}^m\otimes\mathbb{C}^m$ with representation $(\alpha''_{(r,s)})_{(r,s)\in\{1,\ldots,m\}^2}$ with respect to the standard basis with $\alpha''_{(r,s)} = \alpha_{(r+n,s+n)}$. We note that:

$$
\begin{aligned}
&\langle \alpha, \tau\alpha \rangle = \\
&\left\langle (\alpha_{(p,q)})_{(p,q)\in\{1,\dots,n+m\}^2}, (\tau_{(p,q),(r,s)})_{(p,q),(r,s)\in\{1,\dots,n+m\}^2} (\alpha_{(r,s)})_{(r,s)\in\{1,\dots,n+m\}^2} \right\rangle = \\
&\left\langle (\alpha_{(p,q)})_{(p,q)\in\{1,\dots,n+m\}^2}, \left(\sum_{r=1}^{n+m}\sum_{s=1}^{n+m} \tau_{(p,q),(r,s)}\alpha_{(r,s)} \right)_{(p,q)\in\{1,\dots,n+m\}^2} \right\rangle = \\
&\sum_{p=1}^{n+m}\sum_{q=1}^{n+m} \alpha^*_{(p,q)} \sum_{r=1}^{n+m}\sum_{s=1}^{n+m} \tau_{(p,q),(r,s)}\alpha_{(r,s)} = \sum_{p=1}^{n+m}\sum_{q=1}^{n+m}\sum_{r=1}^{n+m}\sum_{s=1}^{n+m} \tau_{(p,q),(r,s)}\alpha^*_{(p,q)}\alpha_{(r,s)} = \\
&\sum_{p=1}^{n}\sum_{q=1}^{n}\sum_{r=1}^{n}\sum_{s=1}^{n}(1-t)\rho_{(p,q),(r,s)}\alpha^*_{(p,q)}\alpha_{(r,s)} + \\
&\sum_{p=n+1}^{n+m}\sum_{q=n+1}^{n+m}\sum_{r=n+1}^{n+m}\sum_{s=n+1}^{n+m} t\sigma_{(p-n,q-n),(r-n,s-n)}\alpha^*_{(p,q)}\alpha_{(r,s)} = \\
&(1-t)\sum_{p=1}^{n}\sum_{q=1}^{n}\sum_{r=1}^{n}\sum_{s=1}^{n} \rho_{(p,q),(r,s)}\alpha^*_{(p,q)}\alpha_{(r,s)} + \\
&t\sum_{p=1}^{m}\sum_{q=1}^{m}\sum_{r=1}^{m}\sum_{s=1}^{m} \sigma_{(p,q),(r,s)}\alpha^*_{(p+n,q+n)}\alpha_{(r+n,s+n)} = \\
&(1-t)\sum_{p=1}^{n}\sum_{q=1}^{n}\sum_{r=1}^{n}\sum_{s=1}^{n} \rho_{(p,q),(r,s)}(\alpha'_{(p,q)})^*\alpha'_{(r,s)} + \\
&t\sum_{p=1}^{m}\sum_{q=1}^{m}\sum_{r=1}^{m}\sum_{s=1}^{m} \sigma_{(p,q),(r,s)}(\alpha''_{(p,q)})^*\alpha''_{(r,s)} = \\
&(1-t)\sum_{p=1}^{n}\sum_{q=1}^{n}(\alpha'_{(p,q)})^* \sum_{r=1}^{n}\sum_{s=1}^{n} \rho_{(p,q),(r,s)}\alpha'_{(r,s)} + \\
&t\sum_{p=1}^{m}\sum_{q=1}^{m}(\alpha''_{(p,q)})^* \sum_{r=1}^{m}\sum_{s=1}^{m} \sigma_{(p,q),(r,s)}\alpha''_{(r,s)} = \\
&(1-t)\left\langle (\alpha'_{(p,q)})_{(p,q)\in\{1,\dots,n\}^2}, \left(\sum_{r=1}^{n}\sum_{s=1}^{n} \rho_{(p,q),(r,s)}\alpha'_{(r,s)} \right)_{(p,q)\in\{1,\dots,n\}^2} \right\rangle + \\
&t\left\langle (\alpha''_{(p,q)})_{(p,q)\in\{1,\dots,m\}^2}, \left(\sum_{r=1}^{m}\sum_{s=1}^{m} \sigma_{(p,q),(r,s)}\alpha''_{(r,s)} \right)_{(p,q)\in\{1,\dots,m\}^2} \right\rangle = \\
&(1-t)\left\langle (\alpha'_{(p,q)})_{(p,q)\in\{1,\dots,n\}^2}, (\rho_{(p,q),(r,s)})_{(p,q),(r,s)\in\{1,\dots,n\}^2} (\alpha'_{(r,s)})_{(r,s)\in\{1,\dots,n\}^2} \right\rangle + \\
&t\left\langle (\alpha''_{(p,q)})_{(p,q)\in\{1,\dots,m\}^2}, (\sigma_{(p,q),(r,s)})_{(p,q),(r,s)\in\{1,\dots,m\}^2} (\alpha''_{(r,s)})_{(r,s)\in\{1,\dots,m\}^2} \right\rangle = \\
&(1-t)\langle \alpha', \rho\alpha' \rangle + t\langle \alpha'', \sigma\alpha'' \rangle \geq 0
\end{aligned}
\tag{173}
$$

where we used that $(1-t), t, \langle \alpha', \rho\alpha' \rangle, \langle \alpha'', \sigma\alpha'' \rangle \geq 0$ because $t \in [0,1]$ and ρ, σ are positive. So we see that τ is a positive operator. We also have:

$$\begin{aligned} &tr(\tau) = tr\left((\tau_{(p,q),(r,s)})_{(p,q),(r,s)\in\{1,\ldots,n+m\}^2} \right) = \sum_{p=1}^{n+m}\sum_{q=1}^{n+m} \tau_{(p,q),(p,q)} = \\ &\sum_{p=1}^{n}\sum_{q=1}^{n}(1-t)\rho_{(p,q),(p,q)} + \sum_{p=n+1}^{n+m}\sum_{q=n+1}^{n+m} t\sigma_{(p-n,q-n),(p-n,q-n)} = \\ &(1-t)\sum_{p=1}^{n}\sum_{q=1}^{n}\rho_{(p,q),(p,q)} + t\sum_{p=1}^{m}\sum_{q=1}^{m}\sigma_{(p,q),(p,q)} = \\ &(1-t)tr(\rho) + ttr(\sigma) = (1-t) + t = 1. \end{aligned} \tag{174}$$

We conclude that τ is a density operator and therefore satisfies all requirements in Definition 6.1. Since the linear operators E_i, B_j, τ meet all the necessary requirements, we conclude that $(tr(E_i \otimes F_j \tau))_{i,j=1}^{N} \in \mathscr{Q}_N$. Let $(z^{(i,j)}_{(p,q),(r,s)})_{(p,q),(r,s)\in\{1,\ldots,n+m\}^2}$ be the matrix representation of $E_i \otimes F_j$ with respect to the standard basis. Then by Theorem 2.9:

$$z^{(i,j)}_{(p,q),(r,s)} = e^{(i)}_{p,r} f^{(j)}_{q,s}. \tag{175}$$

Now we have:

$$
\begin{aligned}
&tr(E_i \otimes F_j \tau) = \\
&tr\left((z^{(i,j)}_{(p,q),(r,s)})_{(p,q),(r,s)\in\{1,\ldots,n+m\}^2} (\tau_{(r,s),(t,u)})_{(r,s),(t,u)\in\{1,\ldots,n+m\}^2} \right) = \\
&tr\left(\left(\sum_{r=1}^{n+m} \sum_{s=1}^{n+m} z^{(i,j)}_{(p,q),(r,s)} \tau_{(r,s),(t,u)} \right)_{(p,q),(t,u)\in\{1,\ldots,n+m\}^2} \right) = \\
&\sum_{p=1}^{n+m} \sum_{q=1}^{n+m} \sum_{r=1}^{n+m} \sum_{s=1}^{n+m} z^{(i,j)}_{(p,q),(r,s)} \tau_{(r,s),(p,q)} = \sum_{p=1}^{n+m} \sum_{q=1}^{n+m} \sum_{r=1}^{n+m} \sum_{s=1}^{n+m} e^{(i)}_{p,r} f^{(j)}_{q,s} \tau_{(r,s),(p,q)} = \\
&\sum_{p=1}^{n} \sum_{q=1}^{n} \sum_{r=1}^{n} \sum_{s=1}^{n} e^{(i)}_{p,r} f^{(j)}_{q,s} (1-t) \rho_{(r,s),(p,q)} + \\
&\sum_{p=n+1}^{n+m} \sum_{q=n+1}^{n+m} \sum_{r=n+1}^{n+m} \sum_{s=n+1}^{n+m} e^{(i)}_{p,r} f^{(j)}_{q,s} t \sigma_{(r-n,s-n),(p-n,q-n)} = \\
&(1-t) \sum_{p=1}^{n} \sum_{q=1}^{n} \sum_{r=1}^{n} \sum_{s=1}^{n} a^{(i)}_{p,r} b^{(j)}_{q,s} \rho_{(r,s),(p,q)} + \\
&t \sum_{p=n+1}^{n+m} \sum_{q=n+1}^{n+m} \sum_{r=n+1}^{n+m} \sum_{s=n+1}^{n+m} c^{(i)}_{p-n,r-n} d^{(j)}_{q-n,s-n} \sigma_{(r-n,s-n),(p-n,q-n)} = \\
&(1-t) \sum_{p=1}^{n} \sum_{q=1}^{n} \sum_{r=1}^{n} \sum_{s=1}^{n} a^{(i)}_{p,r} b^{(j)}_{q,s} \rho_{(r,s),(p,q)} + \\
&t \sum_{p=1}^{m} \sum_{q=1}^{m} \sum_{r=1}^{m} \sum_{s=1}^{m} c^{(i)}_{p,r} d^{(j)}_{q,s} \sigma_{(r,s),(p,q)} = (1-t)\gamma_{i,j} + t\beta_{i,j}.
\end{aligned}
\tag{176}
$$

So $(1-t)\gamma + t\beta = (tr(E_i \otimes F_j \tau))_{i,j=1}^{N} \in \mathscr{Q}_N$ and we conclude that $\mathscr{Q}_N$ is a convex set.

□

7 Grothendieck's theorem

Now that we have introduced classical correlation matrices and quantum correlation matrices and proved some results regarding them we are ready to look at Bell inequalities and try to find out to what extent they can be violated. This chapter is also based on chapter 5 of [2]. For $N \in \mathbb{N}$ we consider an $N \times N$ matrix $\gamma = (\gamma_{i,j})_{i,j=1}^N$, an $N \times N$ matrix $M = (M_{i,j})_{i,j=1}^N$ with real elements $M_{i,j}$ and a constant $C \geq 0$. Using these matrices and constant we can construct the following inequality:

$$\left| \sum_{i,j=1}^{N} M_{i,j}\gamma_{i,j} \right| \leq C \tag{177}$$

which might or might not hold depending on γ, M and C. For a fixed M (of size $N \times N$) and C we might ask whether the above inequality holds for all $\gamma \in \mathscr{L}_N$ and whether it holds for all $\gamma \in \mathscr{Q}_N$. If M and C are such that the associated inequality holds for all $\gamma \in \mathscr{L}_N$ we will call this a Bell inequality. In fact we will use this as our definition of a Bell inequality.

Definition 7.1. Bell inequality. If $N \in \mathbb{N}$, M is an $N \times N$ matrix with real elements $M_{i,j}$ and $C \geq 0$ is a constant, then the inequality:

$$\left| \sum_{i,j=1}^{N} M_{i,j}\gamma_{i,j} \right| \leq C \tag{178}$$

where $\gamma_{i,j}$ are the elements of an $N \times N$ matrix is a Bell-inequality if it holds for all classical correlation matrices $\gamma = (\gamma_{i,j})_{i,j=1}^N$.

We will consider the Bell inequality to be violated in quantum mechanics if there is some $\gamma \in \mathscr{Q}_N$ for which the inequality does not hold. In order to find out to what extent a Bell inequality can be violated we want to choose the constant C, for a given M, as small as possible such that the associated inequality will hold for all $\gamma \in \mathscr{L}_N$. We will call this smallest C the classical value of M and it is defined as follows just as in chapter 5 of [2].

Definition 7.2. Classical value. Given a real matrix $M = (M_{i,j})_{i,j=1}^N$, the classical value of M is defined as:

$$\omega(M) = \sup \left\{ \left| \sum_{i,j=1}^{N} M_{i,j}\gamma_{i,j} \right| : (\gamma_{i,j})_{i,j=1}^N \in \mathscr{L}_N \right\}. \tag{179}$$

It makes sense to choose the constant as small as possible if we want to consider large violations of Bell inequalities, because if we find some $\gamma \in \mathscr{Q}_N$ that violates a given Bell inequality, the violation will only become worse if we make the constant smaller (while making sure the inequality stays a Bell inequality). Similarly, if we want to find the largest violation of a given Bell inequality, we

want to consider $\gamma \in \mathscr{Q}_N$ for which $\left|\sum_{i,j=1}^N M_{i,j}\gamma_{i,j}\right|$ is large. If we want the largest violation, we need the find the quantum value of M which is defined as in chapter 5 of [2].

Definition 7.3. Quantum value. Given a real matrix $M = (M_{i,j})_{i,j=1}^N$, the quantum value of M is defined as:

$$\omega^*(M) = \sup\left\{\left|\sum_{i,j=1}^N M_{i,j}\gamma_{i,j}\right| : (\gamma_{i,j})_{i,j=1}^N \in \mathscr{Q}_N\right\}. \tag{180}$$

So far we have only considered the extent to which a Bell inequality is violated in a qualitative manner, without providing a way to quantify the extent of a violation. The extent to which a Bell inequality is violated can be quantified as follows. If M and C are such that the associated inequality is a Bell inequality and $\gamma \in \mathscr{Q}_N$, then the violation of this Bell inequality by γ can be quantified by the fraction

$$\frac{\left|\sum_{i,j=1}^N M_{i,j}\gamma_{i,j}\right|}{C}. \tag{181}$$

If this fraction is less than or equal to 1, there is no violation since the associated inequality holds. If the fraction is larger than 1, the associated Bell inequality is violated by γ. This fraction increases when $\left|\sum_{i,j=1}^N M_{i,j}\gamma_{i,j}\right|$ increases with respect to C and is therefore a reasonable way to quantify the violation of a Bell inequality. Since we wish to find out how large the violation of a Bell inequality can get, and therefore how large the above fraction can get we will consider, for fixed M, the supremum of the above fraction. This supremum is taken over all constants C such that the associated inequality is a Bell inequality and over all $\gamma \in \mathscr{Q}_N$. This supremum is obtained by taking the supremum of the numerator and the infimum of the denominator and results in a quantity called the largest violation of M which is defined as in chapter 5 of [2].

Definition 7.4. Largest violation of M. For an $N \times N$ (non-zero) matrix M with real elements, the largest violation of M is defined as:

$$LV(M) = \frac{\omega^*(M)}{\omega(M)}. \tag{182}$$

We note that both $\omega(M)$ and $\omega^*(M)$ are defined as the supremum of a set of non-negative numbers. This means that the classical and quantum values of a matrix M might be equal to 0 or ∞ which could lead to some issues in the definition of the largest violation. For the classical value we have the following theorem which is also stated in chapter 5 of [2].

Theorem 7.1. *Let $N \in \mathbb{N}$ and M an $N \times N$ matrix with real elements, then:*

$$\omega(M) = \sup\left\{\left|\sum_{i,j=1}^N M_{i,j}t_i s_j\right| : (t_1,\ldots,t_N,s_1,\ldots,s_N) \in \{1,-1\}^{2N}\right\}. \tag{183}$$

Proof.

$$\sup\left\{\left|\sum_{i,j=1}^{N} M_{i,j}t_i s_j\right| : (t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}\right\}\leq \omega(M) \quad (184)$$

follows from the fact that each deterministic correlation matrix is also a classical correlation matrix. To prove the opposite inequality, let $\gamma=(\gamma_{i,j})_{i,j=1}^{N}\in \mathscr{L}_N$. As we proved before, γ is a linear combination of deterministic correlation matrices, so there exist $a_{(t_1,\ldots,t_N,s_1,\ldots,s_N)}$ with $a_{(t_1,\ldots,t_N,s_1,\ldots,s_N)}\geq 0$ and $\sum_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} a_{(t_1,\ldots,t_N,s_1,\ldots,s_N)}=1$ such that equation (129) holds. Then we have

$$\begin{aligned}
&\left|\sum_{i,j=1}^{N} M_{i,j}\gamma_{i,j}\right| = \\
&\left|\sum_{i,j=1}^{N} M_{i,j}\sum_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} a_{(t_1,\ldots,t_N,s_1,\ldots,s_N)}t_i s_j\right| = \\
&\left|\sum_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} a_{(t_1,\ldots,t_N,s_1,\ldots,s_N)}\sum_{i,j=1}^{N} M_{i,j}t_i s_j\right| \leq \\
&\sum_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}}\left|a_{(t_1,\ldots,t_N,s_1,\ldots,s_N)}\sum_{i,j=1}^{N} M_{i,j}t_i s_j\right| = \\
&\sum_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}}\left|a_{(t_1,\ldots,t_N,s_1,\ldots,s_N)}\right|\left|\sum_{i,j=1}^{N} M_{i,j}t_i s_j\right| = \\
&\sum_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} a_{(t_1,\ldots,t_N,s_1,\ldots,s_N)}\left|\sum_{i,j=1}^{N} M_{i,j}t_i s_j\right| \leq \\
&\sup\left\{\left|\sum_{i,j=1}^{N} M_{i,j}t_i s_j\right| : (t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}\right\} \\
&\sum_{(t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}} a_{(t_1,\ldots,t_N,s_1,\ldots,s_N)} = \\
&\sup\left\{\left|\sum_{i,j=1}^{N} M_{i,j}t_i s_j\right| : (t_1,\ldots,t_N,s_1,\ldots,s_N)\in\{1,-1\}^{2N}\right\}
\end{aligned} \quad (185)$$

and since this holds for any $\gamma\in\mathscr{L}_N$, we have

$$\omega(M) \leq \sup\left\{\left|\sum_{i,j=1}^{N} M_{i,j}t_i s_j\right| : (t_1,\ldots,t_N,s_1,\ldots,s_N) \in \{1,-1\}^{2N})\right\} \quad (186)$$

which completes the proof. □

From this theorem it follows that $\omega(M)$ is the supremum of a finite set and therefore it must be finite, so this excludes the possibility that $\omega(M) = \infty$.

Corollary 7.1.1. *Let $N \in \mathbb{N}$ and M an $N \times N$ matrix with real elements, then $\omega(M) < \infty$.*

This assures us that no division by ∞ occurs in the definition of the largest violation. Moreover, $\omega(M)$ can be calculated for each fixed M by considering a finite number of cases. In case M is the $(N \times N)$ zero-matrix, we have $\left|\sum_{i,j=1}^{N} M_{i,j}\gamma_{i,j}\right| = 0$ for any $N \times N$ matrix γ, so $\omega(M) = \omega^*(M) = 0$ if M is the zero-matrix. This would lead to division by 0 in the definition of the largest violation and for this reason the zero-matrix is excluded. If $\omega(M) = 0$ for some other matrix this would again lead to the issue of having to divide by 0 in the definition of the largest violation of M. Fortunately the following theorem ensures us that this only occurs if M is the zero-matrix.

Theorem 7.2. *Let $N \in \mathbb{N}$ and M an $N \times N$ matrix with real elements such that $\omega(M) = 0$, then M is the zero-matrix.*

Proof. Let $N \in \mathbb{N}$ and M an $N \times N$ matrix with real elements such that $\omega(M) = 0$. This means that:

$$\sup\left\{\left|\sum_{i,j=1}^{N} M_{i,j}t_i s_j\right| : (t_1,\ldots,t_N,s_1,\ldots,s_N) \in \{1,-1\}^{2N}\right\} = 0. \quad (187)$$

So we must have

$$\sum_{i,j=1}^{N} M_{i,j}t_i s_j = 0 \quad (188)$$

for all $(t_1,\ldots,t_N,s_1,\ldots,s_N) \in \{1,-1\}^{2N}$. This means that for arbitrary $t_i \in \{1,-1\}$ and $k \in \{1,\ldots,N\}$ we have

$$\begin{aligned}
&\sum_{i=1}^{N} M_{i,k}t_i = \frac{1}{2}\left(\sum_{i=1}^{N} M_{i,k}t_i + \sum_{i=1}^{N} M_{i,k}t_i\right) = \\
&\frac{1}{2}\left(\sum_{i=1}^{N} M_{i,k}t_i + \sum_{i=1}^{N} M_{i,k}t_i + \sum_{i,j=1,j\neq k}^{N} M_{i,j}t_i - \sum_{i,j=1,j\neq k}^{N} M_{i,j}t_i\right) = \\
&\frac{1}{2}\left(\sum_{i,j=1}^{N} M_{i,j}t_i - \left(\sum_{i,j=1,j\neq k}^{N} M_{i,j}t_i - \sum_{i=1}^{N} M_{i,k}t_i\right)\right) = \\
&\frac{1}{2}\left(\sum_{i,j=1}^{N} M_{i,j}t_i - \sum_{i,j=1}^{N} M_{i,j}t_i(1-2\delta_{j,k})\right) = \frac{1}{2}(0-0) = 0
\end{aligned} \tag{189}$$

where we used $\sum_{i,j=1}^{N} M_{i,j}t_i s_j = 0$ with $s_j = 1$ and with $s_j = 1 - 2\delta_{j,k}$. Now we have that for any $k, l \in \{1, \ldots, N\}$

$$\begin{aligned}
&M_{l,k} = \frac{1}{2}\left(M_{l,k} + M_{l,k}\right) = \frac{1}{2}\left(M_{l,k} + M_{l,k} + \sum_{i=1,i\neq l}^{N} M_{i,k} - \sum_{i=1,i\neq l}^{N} M_{i,k}\right) = \\
&\frac{1}{2}\left(\sum_{i=1}^{N} M_{i,k} - \left(\sum_{i=1,i\neq l}^{N} M_{i,k} - M_{l,k}\right)\right) = \\
&\frac{1}{2}\left(\sum_{i=1}^{N} M_{i,k} - \sum_{i=1}^{N} M_{i,k}(1-2\delta_{i,l})\right) = \frac{1}{2}(0+0) = 0
\end{aligned} \tag{190}$$

where we used $\sum_{i=1}^{N} M_{i,k}t_i = 0$ with $t_i = 1$ and with $t_i = 1 - 2\delta_{i,l}$. So we see that $M_{l,k} = 0$ for all $k, l \in \{1, \ldots, N\}$, which means M is the $N \times N$ zero-matrix. □

So we see that requiring that M is not the zero-matrix is sufficient to ensure that $\omega(M)$ is finite and larger than 0. $\omega^*(M)$ is also always finite for any M, as ensured by the following theorem which given an upper bound on $\omega^*(M)$.

Theorem 7.3. *Let M be an $N \times N$ matrix with real elements, then $\omega^*(M) \leq \sum_{i,j=1}^{N} |M_{i,j}|$.*

Proof. Let M be an $N \times N$ matrix with real elements and $\gamma \in \mathscr{Q}_N$. We note that $|\gamma_{i,j}| \leq 1$ for all $i, j \in \{1, \ldots, N\}$ and it follows that:

$$\left|\sum_{i,j=1}^{N} M_{i,j}\gamma_{i,j}\right| \leq \sum_{i,j=1}^{N} |M_{i,j}||\gamma_{i,j}| \leq \sum_{i,j=1}^{N} |M_{i,j}|. \tag{191}$$

This holds for every $\gamma \in \mathscr{Q}_N$, so $\sum_{i,j=1}^N |M_{i,j}|$ is an upper bound for $\left\{\left|\sum_{i,j=1}^N M_{i,j}\gamma_{i,j}\right| : (\gamma_{i,j})_{i,j=1}^N \in \mathscr{Q}_N\right\}$. This means $\omega^*(M)$ exists as a real number and $\omega^*(M) \leq \sum_{i,j=1}^N |M_{i,j}|$. □

We've seen that as long as M is not the zero-matrix, $LV(M)$ is a finite positive number. Now since $\mathscr{L}_N \subseteq \mathscr{Q}_N$ according to Theorem 6.2, we note that $\omega^*(M) \geq \omega(M)$, so $LV(M) \geq 1$ for any non-zero M. In case M is a 1×1 matrix, $LV(M) = 1$ since $\mathscr{L}_1 = \mathscr{Q}_1$ according to Theorem 6.3. $LV(M)$ gives the largest violation possible for all Bell inequalities associated with the matrix M, so the question of how large the violation of a Bell inequality can be in general comes down to the question of how large $LV(M)$ can become. This can be considered either for matrices M of a fixed size N or allowing all sizes. For M a non-zero matrix of size 1 we have shown that $LV(M) = 1$. For larger matrices M it is more difficult to determine $LV(M)$. Because of Theorem 7.1 $\omega(M)$ can be determined in a straightforward way by considering all $N \times N$ deterministic correlation matrices, although this process takes more time the larger N is since the number of deterministic correlation matrices is increasing in N. The real problem however, lies in determining $\omega^*(M)$ since we cannot in general determine it by considering a finite number of quantum correlation matrices. Our next theorem, known as Tsirelson's theorem, gives an alternative description of Q_N and an alternative expression for $\omega^*(M)$ which in some cases is more convenient than our current definitions. This theorem can also be found in chapter 5 of [2] along with a proof on which our proof is based. Before we state and prove Tsirelson's theorem we will first prove the following lemma:

Lemma 7.4. *Given $N \in \mathbb{N}$ with $N \geq 2$ and a complex Hilbert space H of dimension $2^{\lfloor \frac{N}{2} \rfloor}$ there exist self-adjoint operators $X_i : H \to H$ for $i \in \{1, \ldots, N\}$ satisfying:*

$$X_i X_j + X_j X_i = 2\delta_{i,j} id_H. \tag{192}$$

Proof. Let $N \in \mathbb{N}$ with $N \geq 2$. We note that it is sufficient to consider only a single Hilbert space H of dimension $2^{\lfloor \frac{N}{2} \rfloor}$ and prove the existence of operators X_i with the required properties. Suppose H and G are complex Hilbert spaces of dimension $2^{\lfloor \frac{N}{2} \rfloor}$ and $X_i : H \to H$ are self-adjoint operators for $i \in \{1, \ldots, N\}$ satisfying for all $i, j \in \{1, \ldots, N\}$:

$$X_i X_j + X_j X_i = 2\delta_{i,j} id_H. \tag{193}$$

Since H and G have the same finite dimension, we can find orthonormal bases for H and G with the same cardinality. By Theorem 2.23 we can find an isomorphism $F : H \to G$. By Corollary 2.18.1 the operators $FX_iF^{-1} : G \to G$ are self-adjoint and for all $i, j \in \{1, \ldots, N\}$ we have:

$$FX_iF^{-1}FX_jF^{-1} + FX_jF^{-1}FX_iF^{-1} = FX_iX_jF^{-1} + FX_jX_iF^{-1} = F(X_iX_j + X_jX_i)F^{-1} = F(2\delta_{i,j}id_H)F^{-1} = 2\delta_{i,j}Fid_HF^{-1} = 2\delta_{i,j}FF^{-1} = 2\delta_{i,j}id_G. \tag{194}$$

So we see that if the lemma holds for H it holds for G as well and therefore it suffices to prove it for one specific Hilbert space of dimension $2^{\lfloor \frac{N}{2} \rfloor}$. We will prove the lemma for the complex Hilbert space $H = \bigotimes_{\lfloor \frac{N}{2} \rfloor} \mathbb{C}^2$, where if G is a Hilbert space and $n \in \mathbb{N}$, $\bigotimes_n G$ is the Hilbert space obtained by repeatedly taking the tensor product of n copies of G. Since $\mathbb{C}^2$ has dimension 2, it follows by repeatedly applying Theorem 2.9 that H has dimension $2^{\lfloor \frac{N}{2} \rfloor}$. Let $k = \lfloor \frac{N}{2} \rfloor$, then $N = 2k$ or $N = 2k + 1$. We define linear operators X_i for $i \in \{1, \ldots, N\}$ on H by letting:

$$X_i = \bigotimes_{l=1}^{k} X_{i,l} \tag{195}$$

where $\bigotimes_{l=1}^{k} X_{i,l}$ is the linear operator obtained by repeatedly taking the tensor product of the still to be specified operators $X_{i,l}$ on $\mathbb{C}^2$ for $l \in \{1, \ldots, k\}$. We will be choosing each $X_{i,l}$ equal to the identity id on $\mathbb{C}^2$ or one of the Pauli-matrices X,Y or Z. These are all self-adjoint operators so each $X_{i,l}$ will be self-adjoint. It follows from repeated applications of Theorem 2.7 that X_i will be a self-adjoint operator for each $i \in \{1, \ldots, N\}$. We choose the $X_{i,l}$ as follows:

$$X_{2m-1,l} = \begin{cases} Z, & \text{if} \quad l < m \\ X, & \text{if} \quad l = m \\ id, & \text{if} \quad l > m \end{cases} \tag{196}$$

with $m \in \{1, \ldots, k\}$ if $N = 2k$ or $m \in \{1, \ldots, k+1\}$ if $N = 2k + 1$ and

$$X_{2m,l} = \begin{cases} Z, & \text{if} \quad l < m \\ Y, & \text{if} \quad l = m \\ id, & \text{if} \quad l > m \end{cases} \tag{197}$$

with $m \in \{1, \ldots, k\}$. We note that by repeated application of Theorem 2.5:

$$X_iX_j = \bigotimes_{l=1}^{k} X_{i,l}X_{j,l}. \tag{198}$$

Since all the $X_{i,l}$ satisfy $X_{i,l}^2 = id$ it follows that:

$$2X_i^2 = 2\bigotimes_{l=1}^{k} X_{i,l}^2 = 2\bigotimes_{l=1}^{k} id = 2id_H. \tag{199}$$

If $i = 2m-1$ and $j = 2n-1$ with $m > n$ we find that:

$$X_{2m-1,l}X_{2n-1,l} = \begin{cases} Z^2 = X_{2n-1,l}X_{2m-1,l}, & \text{if} \quad l < n \\ ZX = -XZ = -X_{2n-1,l}X_{2m-1,l}, & \text{if} \quad l = n \\ Z = X_{2n-1,l}X_{2m-1,l}, & \text{if} \quad n < l < m \\ X = X_{2n-1,l}X_{2m-1,l}, & \text{if} \quad l = m \\ id = X_{2n-1,l}X_{2m-1,l}, & \text{if} \quad l > m \end{cases} . \tag{200}$$

If $i = 2m$ and $j = 2n$ with $m > n$ we find that:

$$X_{2m,l}X_{2n,l} = \begin{cases} Z^2 = X_{2n,l}X_{2m,l}, & \text{if} \quad l < n \\ ZY = -YZ = -X_{2n,l}X_{2m,l}, & \text{if} \quad l = n \\ Z = X_{2n,l}X_{2m,l}, & \text{if} \quad n < l < m \\ Y = X_{2n,l}X_{2m,l}, & \text{if} \quad l = m \\ id = X_{2n,l}X_{2m,l}, & \text{if} \quad l > m \end{cases} . \tag{201}$$

If $i = 2m-1$ and $j = 2m$ we find that:

$$X_{2m-1,l}X_{2m,l} = \begin{cases} Z^2 = X_{2m,l}X_{2m-1,l}, & \text{if} \quad l < m \\ XY = -YX = -X_{2m,l}X_{2m-1,l}, & \text{if} \quad l = m \\ id = X_{2m,l}X_{2m-1,l}, & \text{if} \quad l > m \end{cases} . \tag{202}$$

If $i = 2m-1$ and $j = 2n$ with $m > n$ we find that:

$$X_{2m-1,l}X_{2n,l} = \begin{cases} Z^2 = X_{2n,l}X_{2m-1,l}, & \text{if} \quad l < n \\ ZY = -YZ = -X_{2n,l}X_{2m-1,l}, & \text{if} \quad l = n \\ Z = X_{2n,l}X_{2m-1,l}, & \text{if} \quad n < l < m \\ X = X_{2n,l}X_{2m-1,l}, & \text{if} \quad l = m \\ id = X_{2n,l}X_{2m-1,l}, & \text{if} \quad l > m \end{cases} . \tag{203}$$

If $i = 2m$ and $j = 2n-1$ with $m > n$ we find that:

$$X_{2m,l}X_{2n-1,l} = \begin{cases} Z^2 = X_{2n-1,l}X_{2m,l}, & \text{if} \quad l < n \\ ZX = -XZ = -X_{2n-1,l}X_{2m,l}, & \text{if} \quad l = n \\ Z = X_{2n-1,l}X_{2m,l}, & \text{if} \quad n < l < m \\ Y = X_{2n-1,l}X_{2m,l}, & \text{if} \quad l = m \\ id = X_{2n-1,l}X_{2m,l}, & \text{if} \quad l > m \end{cases} . \tag{204}$$

We see that in each case where $i \neq j$ we have some $l_0 \in \{1, \ldots, k\}$ such that $X_{i,l}X_{j,l} = X_{j,l}X_{i,l}$ for $l \neq l_0$ and $X_{i,l_0}X_{j,l_0} = -X_{j,l_0}X_{i,l_0}$. From this it follows that for $i \neq j$, $X_iX_j = -X_jX_i$ and therefore:

$$X_iX_j + X_jX_i = 0_H. \tag{205}$$

We can now conclude that the operators X_i satisfy:

$$X_iX_j + X_jX_i = 2\delta_{i,j}id_H \tag{206}$$

which concludes the proof. □

A collection of operators X_i on a Hilbert space H satisfying the conditions in Lemma 7.4 is called a CAR-algebra on H. We will now state and prove Tsirelson's theorem in two parts.

Theorem 7.5. *Tsirelson's theorem (part 1). If $\gamma = (\gamma_{i,j})_{i,j=1}^N \in \mathscr{Q}_N$, then there exists a real Hilbert space H of finite dimension and $x_i, y_i \in H$ with $\|x_i\|_2 = \|y_i\|_2 = 1$ for $i \in \{1, \ldots, N\}$ such that:*

$$\gamma_{i,j} = \langle x_i, y_j \rangle \tag{207}$$

for all $i, j \in \{1, \ldots, N\}$.

Proof. Suppose $\gamma = (\gamma_{i,j})_{i,j=1}^N \in \mathscr{Q}_N$. Then there exists an $n \in \mathbb{N}$, self-adjoint operators A_i, B_j on $\mathbb{C}^n$ for $i, j \in \{1, \ldots, n\}$ with $\|A_i\|, \|B_j\| \leq 1$ and a density operator ρ on $\mathbb{C}^n \otimes \mathbb{C}^n$ such that $\gamma_{i,j} = tr((A_i \otimes B_j)\rho)$ for all $i, j \in \{1, \ldots, n\}$. Let H_1 be the set of all self-adjoint operators acting on $\mathbb{C}^n \otimes \mathbb{C}^n$. The set of all linear operators acting on $\mathbb{C}^n \otimes \mathbb{C}^n$ is a real vector space under the standard definitions for addition and scalar multiplication of linear operators. The conjugate-linearity of the adjoint ensures that H_1 is closed under addition and multiplication with real scalars, so H_1 is a subspace of this vector space and therefore is itself a real vector space. We define on H_1 an operation $\langle \cdot, \cdot \rangle : H_1 \times H_1 \to \mathbb{R}$ by letting:

$$\langle A, B \rangle = \mathrm{Re}(tr(AB\rho)) \in \mathbb{R}. \tag{208}$$

Let $A, B \in H_1$. Since A, B, ρ are all self-adjoint (ρ by Theorem 2.11), it follows by Theorem 2.31 that:

$$\langle A, B \rangle = \mathrm{Re}(tr(AB\rho)) = \mathrm{Re}((tr(BA\rho))^*) = \mathrm{Re}(tr(BA\rho)) = \langle B, A \rangle . \tag{209}$$

By the linearity of the trace it follows that for all $A, B, C \in H_1$ and $a \in \mathbb{R}$:

$$\langle A, aB \rangle = \mathrm{Re}(tr(aAB\rho)) = \mathrm{Re}(atr(AB\rho)) = a\mathrm{Re}(tr(AB\rho)) = a \langle A, B \rangle \tag{210}$$

and

$$\begin{aligned} &\langle A, B + C \rangle = \mathrm{Re}(tr(A(B + C)\rho)) = \mathrm{Re}(tr(AB\rho + AC\rho)) = \\ &\mathrm{Re}(tr(AB\rho) + tr(AC\rho)) = \mathrm{Re}(tr(AB\rho)) + \mathrm{Re}(tr(AC\rho)) = \langle A, B \rangle + \langle A, C \rangle . \end{aligned} \tag{211}$$

Let $A \in H_1$. Since A is self-adjoint and ρ is positive, it follows from Theorem 2.32 that:

$$\langle A, A \rangle = \mathrm{Re}(tr(A^2\rho)) \geq 0. \tag{212}$$

We can now conclude that the operation we defined is a (possibly degenerate) inner product. We define $G = \{A \in H_1 : \langle A, A \rangle = 0\}$. By Theorem 2.34 this is a subspace of H_1. We consider the real vector space $H_2 = H_1/G$ and define on it an operation $\langle \cdot, \cdot \rangle : H_2 \times H_2 \to \mathbb{R}$ by letting:

$$\left\langle \overline{A}, \overline{B} \right\rangle = \langle A, B \rangle . \tag{213}$$

This operation is, again by Theorem 2.34, a well-defined non-degenerate inner product on H_2, so H_2 is an inner product space. We now define for $i, j \in \{1, \ldots, N\}$:

$$x_i = \overline{A_i \otimes id_{\mathbb{C}^n}} \tag{214}$$

and

$$y_j = \overline{id_{\mathbb{C}^n} \otimes B_j}. \tag{215}$$

$A_i, B_j, id_{\mathbb{C}^n}$ are all self-adjoint operators on $\mathbb{C}^n$ so by Theorem 2.7, $A_i \otimes id_{\mathbb{C}^n}$ and $id_{\mathbb{C}^n} \otimes B_j$ are self-adjoint operators on $\mathbb{C}^n \otimes \mathbb{C}^n$ and therefore elements of H_1. It follows that $x_i, y_j \in H_2$ for all $i, j \in \{1, \ldots, N\}$. We note that the elements of H_2 are equivalence classes of operators. To avoid confusion we stress that for $A \in H_1$ we use the notation $\|A\|$ for the operator norm of A and $\left\|\overline{A}\right\|_2 = \sqrt{\left\langle \overline{A}, \overline{A} \right\rangle} = \sqrt{\langle A, A \rangle}$ for the norm of $\overline{A}$ associated with the inner product we defined on H_2. By Theorem 2.14 we note that for all $i, j \in \{1, \ldots, N\}$:

$$\|A_i \otimes id_{\mathbb{C}^n}\| = \|A_i\| \|id_{\mathbb{C}^n}\| = \|A_i\| \leq 1 \tag{216}$$

and

$$\|id_{\mathbb{C}^n} \otimes B_j\| = \|id_{\mathbb{C}^n}\| \|B_j\| = \|B_j\| \leq 1. \tag{217}$$

Then by Theorem 2.28 we have for all $i, j \in \{1, \ldots, N\}$:

$$\left\|(A_i \otimes id_{\mathbb{C}^n})^2\right\| = \|A_i \otimes id_{\mathbb{C}^n}\|^2 \leq 1 \tag{218}$$

and

$$\left\|(id_{\mathbb{C}^n} \otimes B_j)^2\right\| = \|id_{\mathbb{C}^n} \otimes B_j\|^2 \leq 1. \tag{219}$$

It now follows by Theorems 2.32 and 2.17 that for all $i, j \in \{1, \ldots, N\}$:

$$\begin{aligned} &tr((A_i \otimes id_{\mathbb{C}^n})^2\rho) = \left|tr((A_i \otimes id_{\mathbb{C}^n})^2\rho)\right| \leq \left\|(A_i \otimes id_{\mathbb{C}^n})^2\right\| tr(\rho) = \\ &\left\|(A_i \otimes id_{\mathbb{C}^n})^2\right\| \leq 1 \end{aligned} \tag{220}$$

and

$$tr((id_{\mathbb{C}^n} \otimes B_j)^2\rho) = \left|tr((id_{\mathbb{C}^n} \otimes B_j)^2\rho)\right| \leq \left\|(id_{\mathbb{C}^n} \otimes B_j)^2\right\| tr(\rho) = \left\|(id_{\mathbb{C}^n} \otimes B_j)^2\right\| \leq 1. \tag{221}$$

This means that for all $i, j \in \{1, \ldots, N\}$ we have:

$$\|x_i\|_2 = \sqrt{\langle x_i, x_i\rangle} = \sqrt{\langle A_i \otimes id_{\mathbb{C}^n}, A_i \otimes id_{\mathbb{C}^n}\rangle} = \sqrt{\text{Re}(tr((A_i \otimes id_{\mathbb{C}^n})^2\rho))} = \sqrt{tr((A_i \otimes id_{\mathbb{C}^n})^2\rho)} \leq 1 \tag{222}$$

and

$$\|y_j\|_2 = \sqrt{\langle y_j, y_j\rangle} = \sqrt{\langle id_{\mathbb{C}^n} \otimes B_j, id_{\mathbb{C}^n} \otimes B_j\rangle} = \sqrt{\text{Re}(tr((id_{\mathbb{C}^n} \otimes B_j)^2\rho))} = \sqrt{tr((id_{\mathbb{C}^n} \otimes B_j)^2\rho)} \leq 1. \tag{223}$$

So $x_i, y_j \in H_2$ all have norm no larger than 1. Now for all $i, j \in \{1, \ldots, N\}$ we note that A_i and B_j are self-adjoint so $A_i \otimes B_j$ is self-adjoint by Theorem 2.7 and therefore by Theorem 2.17 we have:

$$\langle x_i, y_j\rangle = \langle A_i \otimes id_{\mathbb{C}^n}, id_{\mathbb{C}^n} \otimes B_j\rangle = \text{Re}(tr((A_i \otimes id_{\mathbb{C}^n})(id_{\mathbb{C}^n} \otimes B_j)\rho)) = \text{Re}(tr((A_i \otimes B_j)\rho)) = tr((A_i \otimes B_j)\rho) = \gamma_{i,j}. \tag{224}$$

We now define the subspace $H_3 = span(\{x_1, \ldots, x_N, y_1, \ldots, y_N\}) \subseteq H_2$ of H_2. This subspace contains the elements x_i, y_j for $i, j \in \{1, \ldots, N\}$ and inherits the inner product we defined on H_2. H_3 is therefore also an inner product space. Since H_3 is spanned by the finite set $\{x_1, \ldots, x_N, y_1, \ldots, y_N\}$ of at most $2N$ elements, there exists a basis for H_3 which is a subset of this set and is therefore finite. So H_3 is a real finite-dimensional inner product space and therefore also a real finite-dimensional Hilbert space. Let $k \in \mathbb{N}$ be the dimension of H_3. We define the real inner product space $H_4 = H_3 \oplus \mathbb{R} \oplus \mathbb{R}$. H_4 is the direct sum of real inner product spaces and is therefore also a real inner product space itself. The dimension of H_4 is equal to $k + 2$ so H_4 is also of finite dimension and therefore a finite-dimensional real Hilbert space. On H_4 we define for $i, j \in \{1, \ldots, N\}$ the elements:

$$\hat{x}_i = x_i \oplus \sqrt{1 - \|x_i\|_2^2} \oplus 0 \tag{225}$$

and

$$\hat{y}_j = y_j \oplus 0 \oplus \sqrt{1 - \|y_j\|_2^2}. \tag{226}$$

Now for all $i, j \in \{1, \ldots, N\}$ we have:

$$\|\hat{x}_i\|_2 = \sqrt{\langle \hat{x}_i, \hat{x}_i \rangle} = \sqrt{\langle x_i, x_i \rangle + \left\langle \sqrt{1 - \|x_i\|_2^2}, \sqrt{1 - \|x_i\|_2^2} \right\rangle + \langle 0, 0 \rangle} = \sqrt{\|x_i\|_2^2 + \left(\sqrt{1 - \|x_i\|_2^2} \right)^2 + 0^2} = \sqrt{\|x_i\|_2^2 + 1 - \|x_i\|_2^2} = \sqrt{1} = 1 \tag{227}$$

and

$$\|\hat{y}_j\|_2 = \sqrt{\langle \hat{y}_j, \hat{y}_j \rangle} = \sqrt{\langle y_j, y_j \rangle + \langle 0, 0 \rangle + \left\langle \sqrt{1 - \|y_j\|_2^2}, \sqrt{1 - \|y_j\|_2^2} \right\rangle} = \sqrt{\|y_j\|_2^2 + 0^2 + \left(\sqrt{1 - \|y_j\|_2^2} \right)^2} = \sqrt{\|y_j\|_2^2 + 1 - \|y_j\|_2^2} = \sqrt{1} = 1. \tag{228}$$

Furthermore we have for all $i, j \in \{1, \ldots, N\}$:

$$\langle \hat{x}_i, \hat{y}_j \rangle = \langle x_i, y_j \rangle + \left\langle \sqrt{1 - \|x_i\|_2^2}, 0 \right\rangle + \left\langle 0, \sqrt{1 - \|y_j\|_2^2} \right\rangle = \gamma_{i,j} + 0 + 0 = \gamma_{i,j}. \tag{229}$$

So H_4 is a real finite-dimensional Hilbert space, $\hat{x}_i, \hat{y}_j \in H_4$ for $i, j \in \{1, \ldots, N\}$ have norm equal to 1 and $\gamma_{i,j} = \langle \hat{x}_i, \hat{y}_j \rangle$. □

Theorem 7.6. *Tsirelson's theorem (part 2). If $\gamma = (\gamma_{i,j})_{i,j=1}^N$ is a matrix such that there exists a real Hilbert space H of finite dimension and $x_i, y_i \in H$ with $\|x_i\|_2 = \|y_i\|_2 = 1$ for $i \in \{1, \ldots, N\}$ such that:*

$$\gamma_{i,j} = \langle x_i, y_j \rangle \tag{230}$$

for all $i, j \in \{1, \ldots, N\}$, then $\gamma \in \mathcal{Q}_N$.

Proof. Suppose that H is a real Hilbert space of finite dimension M, $x_i, y_j \in H$ for $i, j \in \{1, \ldots, N\}$ have norm equal to 1 and $\gamma = (\gamma_{i,j})_{i,j=1}^N$ with $\gamma_{i,j} = \langle x_i, y_j \rangle$. We fix an orthonormal basis for H and let $(x_{i,k})_{k=1}^M \in \mathbb{R}^M$, $(y_{j,k})_{k=1}^M \in \mathbb{R}^M$ for $i, j \in \{1, \ldots, N\}$ be the representations of x_i and y_j with respect to this basis. We note that for all $i, j \in \{1, \ldots, N\}$ we have:

$$1 = \|x_i\|_2 = \left\| (x_{i,k})_{k=1}^M \right\|_2 = \sqrt{\sum_{k=1}^M x_{i,k}^2}, \tag{231}$$

$$1 = \|y_j\|_2 = \left\| (y_{j,k})_{k=1}^M \right\|_2 = \sqrt{\sum_{k=1}^M y_{j,k}^2} \tag{232}$$

and

$$\gamma_{i,j} = \langle x_i, y_j \rangle = \left\langle (x_{i,k})_{k=1}^M, (y_{j,k})_{k=1}^M \right\rangle = \sum_{k=1}^M x_{i,k} y_{j,k}. \tag{233}$$

In case $M = 1$ this reduces to $|x_{i,1}| = 1$, $|y_{j,1}| = 1$ and $\gamma_{i,j} = x_{i,1} y_{j,1}$. Since $x_{i,1}, y_{j,1} \in \mathbb{R}$ we have $x_{i,1}, y_{j,1} \in \{1, -1\}$ for all $i, j \in \{1, \ldots, N\}$. This means that γ is a deterministic correlation matrix so $\gamma \in \mathscr{L}_N \subseteq \mathscr{Q}_N$. If $M \geq 2$, let $n = 2^{\lfloor \frac{M}{2} \rfloor}$, then by Lemma 7.4 there exist self-adjoint operators X_k for $k \in \{1, \ldots, M\}$ on $\mathbb{C}^n$ such that:

$$X_k X_l + X_l X_k = 2\delta_{k,l} id_{\mathbb{C}^n}. \tag{234}$$

We now define for $i, j \in \{1, \ldots, N\}$ the following operators on $\mathbb{C}^n$:

$$A_i = \sum_{k=1}^M x_{i,k} X_k \tag{235}$$

and

$$B_j = \sum_{k=1}^M y_{j,k} X_k. \tag{236}$$

The X_k are self-adjoint and $x_{i,k}, y_{j,k}$ are real, so by the conjugate-linearity of the adjoint it follows that A_i, B_j are self-adjoint for all $i, j \in \{1, \ldots, N\}$. For all $i, j \in \{1, \ldots, N\}$ we have:

$$\begin{aligned}
&A_i^2 = \left(\sum_{k=1}^M x_{i,k} X_k \right)^2 = \sum_{k=1}^M \sum_{l=1}^M x_{i,k} x_{i,l} X_k X_l = \\
&\sum_{k=1}^M x_{i,k}^2 X_k^2 + \sum_{k=1}^M \sum_{l=1}^{k-1} x_{i,k} x_{i,l} X_k X_l + \sum_{k=1}^M \sum_{l=k+1}^M x_{i,k} x_{i,l} X_k X_l = \\
&\sum_{k=1}^M x_{i,k}^2 X_k^2 + \sum_{k=1}^M \sum_{l=1}^{k-1} x_{i,k} x_{i,l} X_k X_l + \sum_{l=1}^M \sum_{k=1}^{l-1} x_{i,k} x_{i,l} X_k X_l = \\
&\sum_{k=1}^M x_{i,k}^2 X_k^2 + \sum_{k=1}^M \sum_{l=1}^{k-1} x_{i,k} x_{i,l} X_k X_l + \sum_{k=1}^M \sum_{l=1}^{k-1} x_{i,l} x_{i,k} X_l X_k = \\
&\sum_{k=1}^M x_{i,k}^2 X_k^2 + \sum_{k=1}^M \sum_{l=1}^{k-1} x_{i,k} x_{i,l} (X_k X_l + X_l X_k) = \\
&\sum_{k=1}^M x_{i,k}^2 X_k^2 = \sum_{k=1}^M x_{i,k}^2 id_{\mathbb{C}^n} = \left(\sum_{k=1}^M x_{i,k}^2 \right) id_{\mathbb{C}^n} = id_{\mathbb{C}^n}
\end{aligned} \tag{237}$$

and

$$
\begin{aligned}
&B_j^2 = \left(\sum_{k=1}^{M} y_{j,k} X_k\right)^2 = \sum_{k=1}^{M}\sum_{l=1}^{M} y_{j,k} y_{j,l} X_k X_l = \\
&\sum_{k=1}^{M} y_{j,k}^2 X_k^2 + \sum_{k=1}^{M}\sum_{l=1}^{k-1} y_{j,k} y_{j,l} X_k X_l + \sum_{k=1}^{M}\sum_{l=k+1}^{M} y_{j,k} y_{j,l} X_k X_l = \\
&\sum_{k=1}^{M} y_{j,k}^2 X_k^2 + \sum_{k=1}^{M}\sum_{l=1}^{k-1} y_{j,k} y_{j,l} X_k X_l + \sum_{l=1}^{M}\sum_{k=1}^{l-1} y_{j,k} y_{j,l} X_k X_l = \\
&\sum_{k=1}^{M} y_{j,k}^2 X_k^2 + \sum_{k=1}^{M}\sum_{l=1}^{k-1} y_{j,k} y_{j,l} X_k X_l + \sum_{k=1}^{M}\sum_{l=1}^{k-1} y_{j,l} y_{j,k} X_l X_k = \\
&\sum_{k=1}^{M} y_{j,k}^2 X_k^2 + \sum_{k=1}^{M}\sum_{l=1}^{k-1} y_{j,k} y_{j,l} (X_k X_l + X_l X_k) = \\
&\sum_{k=1}^{M} y_{j,k}^2 X_k^2 = \sum_{k=1}^{M} y_{j,k}^2 id_{\mathbb{C}^n} = \left(\sum_{k=1}^{M} y_{j,k}^2\right) id_{\mathbb{C}^n} = id_{\mathbb{C}^n}.
\end{aligned}
\tag{238}
$$

Now by Theorem 2.28 for all $i, j \in \{1, \ldots, N\}$ we have:

$$
\|A_i\|^2 = \left\|A_i^2\right\| = \|id_{\mathbb{C}^n}\| = 1 \tag{239}
$$

and

$$
\|B_j\|^2 = \left\|B_j^2\right\| = \|id_{\mathbb{C}^n}\| = 1. \tag{240}
$$

So we find that $\|A_i\| = \|B_j\| = 1$ for all $i, j \in \{1, \ldots, N\}$. We also have by Theorem 2.29 that for all $i, j \in \{1, \ldots, N\}$:

$$\frac{1}{n}tr(A_iB_j) = \frac{1}{2n}\cdot 2tr(A_iB_j) = \frac{1}{2n}(tr(A_iB_j)+tr(B_jA_i)) =$$
$$\frac{1}{2n}tr(A_iB_j+B_jA_i) =$$
$$\frac{1}{2n}tr\left(\left(\sum_{k=1}^{M}x_{i,k}X_k\right)\left(\sum_{l=1}^{M}y_{j,l}X_l\right)+\left(\sum_{k=1}^{M}y_{j,k}X_k\right)\left(\sum_{l=1}^{M}x_{i,l}X_l\right)\right) =$$
$$\frac{1}{2n}tr\left(\sum_{k=1}^{M}\sum_{l=1}^{M}x_{i,k}y_{j,l}X_kX_l+\sum_{k=1}^{M}\sum_{l=1}^{M}y_{j,k}x_{i,l}X_kX_l\right) =$$
$$\frac{1}{2n}tr\left(\sum_{k=1}^{M}\sum_{l=1}^{M}x_{i,k}y_{j,l}X_kX_l+\sum_{l=1}^{M}\sum_{k=1}^{M}x_{i,l}y_{j,k}X_kX_l\right) =$$
$$\frac{1}{2n}tr\left(\sum_{k=1}^{M}\sum_{l=1}^{M}x_{i,k}y_{j,l}X_kX_l+\sum_{k=1}^{M}\sum_{l=1}^{M}x_{i,k}y_{j,l}X_lX_k\right) = \tag{241}$$
$$\frac{1}{2n}tr\left(\sum_{k=1}^{M}\sum_{l=1}^{M}x_{i,k}y_{j,l}(X_kX_l+X_lX_k)\right) =$$
$$\frac{1}{2n}tr\left(\sum_{k=1}^{M}\sum_{l=1}^{M}x_{i,k}y_{j,l}2\delta_{k,l}id_{\mathbb{C}^n}\right) = \frac{1}{2n}tr\left(\sum_{k=1}^{M}x_{i,k}y_{j,k}2id_{\mathbb{C}^n}\right) =$$
$$\frac{1}{n}tr\left(\left(\sum_{k=1}^{M}x_{i,k}y_{j,k}\right)id_{\mathbb{C}^n}\right) = \frac{1}{n}\sum_{k=1}^{M}x_{i,k}y_{j,k}tr\left(id_{\mathbb{C}^n}\right) =$$
$$\frac{1}{n}\sum_{k=1}^{M}x_{i,k}y_{j,k}n = \sum_{k=1}^{M}x_{i,k}y_{j,k} = \left\langle (x_{i,k})_{k=1}^{M},(y_{j,k})_{k=1}^{M}\right\rangle = \langle x_i,y_j\rangle .$$

Let $(a_{k,l}^{(i)})_{k,l=1}^{n}$ and $(b_{k,l}^{(j)})_{k,l=1}^{n}$ be the matrix representations of A_i and B_j with respect to the standard basis $\{e_k=(\delta_{k,l})_{l=1}^{n}:k\in\{1,\ldots,n\}\}$ of $\mathbb{C}^n$. Since A_i and B_j are self-adjoint, their matrix representations are Hermitian, so $(a_{k,l}^{(i)})^* = a_{l,k}^{(i)}$ and $(b_{k,l}^{(j)})^* = b_{l,k}^{(j)}$. We define for $j\in\{1,\ldots,n\}$ the linear operators $\hat{B}_j$ by specifying their matrix representation with respect to the standard basis. We choose these matrix representations to be $((b_{k,l}^{(j)})^*)_{k,l=1}^{n}$. Since $((b_{k,l}^{(j)})^*)^* = b_{k,l}^{(j)} = (b_{l,k}^{(j)})^*$ we see that the matrix representations of the operators $\hat{B}_j$ are Hermitian, so these operators are self-adjoint. Now the matrix representation of $\hat{B}_j^2$ is given by:

$$((b_{k,m}^{(j)})^*)_{k,m=1}^{n}((b_{m,l}^{(j)})^*)_{m,l=1}^{n} = \left(\sum_{m=1}^{n}(b_{k,m}^{(j)})^*(b_{m,l}^{(j)})^*\right)_{k,l=1}^{n} =$$
$$\left(\left(\sum_{m=1}^{n}b_{k,m}^{(j)}b_{m,l}^{(j)}\right)^*\right)_{k,l=1}^{n}. \tag{242}$$

This is the matrix obtained by conjugating all elements of the matrix representation of $B_j^2 = id_{\mathbb{C}^n}$. The matrix representation of B_j^2 is equal to $(\delta_{k,l})_{k,l=1}^n$ and we see that it has only real elements. So the matrix representations of B_j^2 and $\hat{B}_j^2$ are the same and therefore by Theorem 2.28 we have:

$$\left\|\hat{B}_j\right\|^2 = \left\|\hat{B}_j^2\right\| = \left\|B_j^2\right\| = 1 \tag{243}$$

so $\left\|\hat{B}_j\right\| = 1$. We see that the operators A_i and $\hat{B}_j$ satisfy all the necessary requirements in the definition of $\mathscr{Q}_N$. By Theorem 2.9, the operators $A_i \otimes \hat{B}_j$ have matrix representations $(a_{p,r}^{(i)}(b_{q,s}^{(j)})^*)_{(p,q),(r,s)\in\{1,\ldots,n\}^2}$ with respect to the basis $\{e_k \otimes e_l : k,l \in \{1,\ldots,n\}\}$ of $\mathbb{C}^n \otimes \mathbb{C}^n$. We now define the operator ρ on $\mathbb{C}^n \otimes \mathbb{C}^n$ by letting $\left(\frac{1}{n}\delta_{p,q}\delta_{r,s}\right)_{(p,q),(r,s)\in\{1,\ldots,n\}^2}$ be its matrix representation with respect to the same basis. For any $c \in \mathbb{C}^n \otimes \mathbb{C}^n$ with representation $(c_{(p,q)})_{(p,q)\in\{1,\ldots,n\}^2}$ we have:

$$\begin{aligned}
&\langle c, \rho c\rangle = \\
&\left\langle (c_{(p,q)})_{(p,q)\in\{1,\ldots,n\}^2}, \left(\frac{1}{n}\delta_{p,q}\delta_{r,s}\right)_{(p,q),(r,s)\in\{1,\ldots,n\}^2} (c_{(r,s)})_{(r,s)\in\{1,\ldots,n\}^2} \right\rangle = \\
&\left\langle (c_{(p,q)})_{(p,q)\in\{1,\ldots,n\}^2}, \left(\sum_{r=1}^n\sum_{s=1}^n \frac{1}{n}\delta_{p,q}\delta_{r,s}c_{(r,s)}\right)_{(p,q)\in\{1,\ldots,n\}^2} \right\rangle = \\
&\sum_{p=1}^n\sum_{q=1}^n\sum_{r=1}^n\sum_{s=1}^n \frac{1}{n}\delta_{p,q}\delta_{r,s}c_{(p,q)}^* c_{(r,s)} = \frac{1}{n}\sum_{p=1}^n\sum_{r=1}^n c_{(p,p)}^* c_{(r,r)} = \\
&\frac{1}{n}\left(\sum_{p=1}^n c_{(p,p)}^*\right)\left(\sum_{r=1}^n c_{(r,r)}\right) = \frac{1}{n}\left(\sum_{p=1}^n c_{(p,p)}^*\right)\left(\sum_{p=1}^n c_{(p,p)}\right) = \\
&\frac{1}{n}\left(\sum_{p=1}^n c_{(p,p)}\right)^*\left(\sum_{p=1}^n c_{(p,p)}\right) = \frac{1}{n}\left|\sum_{p=1}^n c_{(p,p)}\right|^2 \geq 0.
\end{aligned} \tag{244}$$

So we see that ρ is a positive operator. We also have that:

$$tr(\rho) = tr\left(\left(\frac{1}{n}\delta_{p,q}\delta_{r,s}\right)_{(p,q),(r,s)\in\{1,\ldots,n\}^2}\right) = \sum_{p=1}^n\sum_{q=1}^n \frac{1}{n}\delta_{p,q}\delta_{p,q} = \sum_{p=1}^n \frac{1}{n} = 1. \tag{245}$$

From this we conclude that ρ is a density operator. Now for all $i,j \in \{1,\ldots,N\}$ we have that:

$$
\begin{aligned}
&tr((A_i \otimes \hat{B}_j)\rho) = \\
&tr\left(\left(a_{p,r}^{(i)}\left(b_{q,s}^{(j)}\right)^*\right)_{(p,q),(r,s)\in\{1,\ldots,n\}^2}\left(\frac{1}{n}\delta_{r,s}\delta_{t,u}\right)_{(r,s),(t,u)\in\{1,\ldots,n\}^2}\right) = \\
&tr\left(\left(\sum_{r=1}^{n}\sum_{s=1}^{n}a_{p,r}^{(i)}\left(b_{q,s}^{(j)}\right)^*\frac{1}{n}\delta_{r,s}\delta_{t,u}\right)_{(p,q),(t,u)\in\{1,\ldots,n\}^2}\right) = \\
&\sum_{p=1}^{n}\sum_{q=1}^{n}\sum_{r=1}^{n}\sum_{s=1}^{n}a_{p,r}^{(i)}\left(b_{q,s}^{(j)}\right)^*\frac{1}{n}\delta_{r,s}\delta_{p,q} = \frac{1}{n}\sum_{p=1}^{n}\sum_{r=1}^{n}a_{p,r}^{(i)}\left(b_{p,r}^{(j)}\right)^* = \\
&\frac{1}{n}\sum_{p=1}^{n}\sum_{r=1}^{n}a_{p,r}^{(i)}b_{r,p}^{(j)} = \frac{1}{n}tr\left(\left(\sum_{r=1}^{n}a_{p,r}^{(i)}b_{r,q}^{(j)}\right)_{p,q=1}^{n}\right) = \\
&\frac{1}{n}tr((a_{p,r}^{(i)})_{p,r=1}^{n}(b_{r,q}^{(j)})_{r,q=1}^{n}) = \frac{1}{n}tr(A_iB_j) = \langle x_i, y_j\rangle = \gamma_{i,j}.
\end{aligned}
\tag{246}
$$

From this we see that $\gamma \in \mathscr{Q}_N$. □

These last two results combined give us Tsirelson's theorem.

Theorem 7.7. *Tsirelson's theorem. If $\gamma = (\gamma_{i,j})_{i,j=1}^{N}$ is a matrix with real elements, then $\gamma \in \mathscr{Q}_N$ if and only if there exists a real Hilbert space H of finite dimension and $x_i, y_i \in H$ with $\|x_i\|_2 = \|y_i\|_2 = 1$ for $i \in \{1,\ldots,N\}$ such that:*

$$\gamma_{i,j} = \langle x_i, y_j\rangle \tag{247}$$

for all $i,j \in \{1,\ldots,N\}$. Furthermore:

$$\omega^*(M) = \sup\left|\sum_{i,j=1}^{N}M_{i,j}\langle x_i, y_j\rangle\right| \tag{248}$$

with the supremum taken over all real Hilbert spaces H of finite dimension and $x_i, y_i \in H$ with $\|x_i\|_2 = \|y_i\|_2 = 1$ for $i \in \{1,\ldots,N\}$.

Proof. Theorems 7.5 and 7.6 combined, imply that if $\gamma = (\gamma_{i,j})_{i,j=1}^{N}$ is a matrix with real elements, then $\gamma \in \mathscr{Q}_N$ if and only if there exists a real Hilbert space H of finite dimension and $x_i, y_i \in H$ with $\|x_i\|_2 = \|y_i\|_2 = 1$ for $i \in \{1,\ldots,N\}$ such that:

$$\gamma_{i,j} = \langle x_i, y_j\rangle \tag{249}$$

for all $i,j \in \{1,\ldots,N\}$. Now it follows from the definition of the quantum value that for any $N \times N$ matrix M with real elements:

$$\omega^*(M) = \sup\left\{\left|\sum_{i,j=1}^{N} M_{i,j}\gamma_{i,j}\right| : (\gamma_{i,j})_{i,j=1}^{N} \in \mathscr{Q}_N\right\} = \sup\left\{\left|\sum_{i,j=1}^{N} M_{i,j}\left\langle x_i, y_j\right\rangle\right|\right\} \tag{250}$$

with the last supremum taken over all real Hilbert spaces H of finite dimension and $x_i, y_i \in H$ with $\|x_i\|_2 = \|y_i\|_2 = 1$ for $i \in \{1, \ldots, N\}$. This completes the proof of Tsirelson's theorem. □

Remark. The requirement that the Hilbert space H must be finite-dimensional in Tsirelson's theorem can be omitted. This is because if $x_i, y_j \in H$ for $i, j \in \{1, \ldots, N\}$ with H an arbitrary real Hilbert space, then $x_i, y_j \in \hat{H}$ for all $i, j \in \{1, \ldots, N\}$ with $\hat{H} = span(\{x_1, \ldots, x_N, y_1, \ldots, y_N\}) \subseteq H$ a real finite-dimensional Hilbert space.

Now that we have formally defined Bell inequalities and have a way to quantify the violation of a Bell-inequality, we will take another look at the first Bell inequality we have seen, the CHSH-inequality. We recall that the quantum mechanical context we considered was that of the composite system of two physical systems in some state and measurements Q and R that can be performed on the first system and S and T that can be performed on the second system all with outcomes in $\{1, -1\}$. The associated inequality that should hold under the assumption of a local hidden variable model was:

$$|\mathbb{E}(QS) + \mathbb{E}(RS) + \mathbb{E}(RT) - \mathbb{E}(QT)| \leq 2 \tag{251}$$

which we derived in general for $\{1, -1\}$-valued random variables Q, R, S, T on some probability space. In the more general setting we have developed, the CHSH-inequality can be rephrased as the inequality:

$$\left|\sum_{i,j=1}^{N} M_{i,j}\gamma_{i,j}\right| \leq C \tag{252}$$

with $N = 2$, $C = 2$ and

$$M = M_{CHSH} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{253}$$

and since it holds for all 2×2 classical correlation matrices γ, it is indeed a Bell inequality. Suppose $t_1, t_2, s_1, s_2 \in \{1, -1\}$. Then we have:

$$\begin{aligned} &\left|\sum_{i,j=1}^{2} (M_{CHSH})_{i,j} t_i s_j\right| = |t_1 s_1 + t_1 s_2 + t_2 s_1 - t_2 s_2| = \\ &|t_1(s_1 + s_2) + t_2(s_1 - s_2)| = 2. \end{aligned} \tag{254}$$

The last equality holds because either $s_1 = s_2$ in which case $t_2(s_1 - s_2) = 0$ and $s_1 + s_2 \in \{2, -2\}$, $t_1 \in \{1, -1\}$ so $t_1(s_1 + s_2) \in \{2, -2\}$ or $s_1 = -s_2$ in which case $t_1(s_1 + s_2) = 0$ and $s_1 - s_2 \in \{2, -2\}$, $t_2 \in \{1, -1\}$ so $t_2(s_1 - s_2) \in \{2, -2\}$. By Theorem 7.1 it follows that $\omega(M_{CHSH}) = 2$ so it turns out that the constant $C = 2$ in the CHSH-inequality is the smallest constant such that the associated inequality is a Bell inequality. We managed to violate the CHSH-inequality by finding a composite quantum system, a quantum state and measurements P, Q, R, S such that:

$$|\mathbb{E}(QS) + \mathbb{E}(RS) + \mathbb{E}(RT) - \mathbb{E}(QT)| = 2\sqrt{2}. \tag{255}$$

In other words we found a quantum correlation matrix $\gamma \in \mathscr{Q}_2$ such that:

$$\left| \sum_{i,j=1}^{N} (M_{CHSH})_{i,j} \gamma_{i,j} \right| = 2\sqrt{2}. \tag{256}$$

Earlier we used the state vector ψ and observables to violate the CHSH-inequality, but the same quantum correlation matrix can be obtained from the definition we gave by letting the component systems be described by $\mathbb{C}^2$, letting $\rho = \rho_\psi$ with:

$$\rho_\psi(v) = \langle \psi, v \rangle \, \psi \tag{257}$$

and choosing $A_1 = Z$, $A_2 = X$, $B_1 = \frac{-Z-X}{\sqrt{2}}$ and $B_2 = \frac{Z-X}{\sqrt{2}}$. We omit the calculations needed to derive that for this choice of operators

$$\gamma = \begin{pmatrix} \frac{1}{2}\sqrt{2} & \frac{1}{2}\sqrt{2} \\ \frac{1}{2}\sqrt{2} & -\frac{1}{2}\sqrt{2} \end{pmatrix} \tag{258}$$

as they are very similar to the calculations of $\mathbb{E}(QS)$, $\mathbb{E}(RS)$, $\mathbb{E}(RT)$ and $\mathbb{E}(QT)$ we've done before. This specific quantum correlation matrix shows that $\omega^*(M_{CHSH}) \geq 2\sqrt{2}$. Our next theorem shows that in fact $\omega^*(M_{CHSH}) = 2\sqrt{2}$.

Theorem 7.8. $\omega^*(M_{CHSH}) = 2\sqrt{2}$.

Proof. We have found a $\gamma \in \mathscr{Q}_2$ for which

$$\left| \sum_{i,j=1}^{N} (M_{CHSH})_{i,j} \gamma_{i,j} \right| = 2\sqrt{2} \tag{259}$$

so $\omega^*(M_{CHSH}) \geq 2\sqrt{2}$. To show that $\omega^*(M_{CHSH}) \leq 2\sqrt{2}$, let $\gamma \in \mathscr{Q}_2$. By Theorem 7.7 there exists a real Hilbert space H and $x_1, x_2, y_1, y_2 \in H$ with

$$\|x_1\|_2 = \|x_2\|_2 = \|y_1\|_2 = \|y_2\|_2 = 1 \tag{260}$$

such that

$$\gamma_{i,j} = \langle x_i, y_j \rangle \, . \tag{261}$$

Using the triangle inequality and the Cauchy-Schwarz inequality we find that:

$$\begin{aligned}
&\left|\sum_{i,j=1}^{2}(M_{CHSH})_{i,j}\gamma_{i,j}\right| = |\langle x_1,y_1\rangle + \langle x_1,y_2\rangle + \langle x_2,y_1\rangle - \langle x_2,y_2\rangle| = \\
&|\langle x_1,y_1+y_2\rangle + \langle x_2,y_1-y_2\rangle| \leq |\langle x_1,y_1+y_2\rangle| + |\langle x_2,y_1-y_2\rangle| \leq \\
&\|x_1\|_2\|y_1+y_2\|_2 + \|x_2\|_2\|y_1-y_2\|_2 = \|y_1+y_2\|_2 + \|y_1-y_2\|_2 = \\
&\sqrt{\langle y_1+y_2,y_1+y_2\rangle} + \sqrt{\langle y_1-y_2,y_1-y_2\rangle} = \\
&\sqrt{\langle y_1,y_1\rangle + \langle y_1,y_2\rangle + \langle y_2,y_1\rangle + \langle y_2,y_2\rangle} + \\
&\sqrt{\langle y_1,y_1\rangle - \langle y_1,y_2\rangle - \langle y_2,y_1\rangle + \langle y_2,y_2\rangle} = \\
&\sqrt{\|y_1\|_2 + \|y_2\|_2 + 2\langle y_1,y_2\rangle} + \sqrt{\|y_1\|_2 + \|y_2\|_2 - 2\langle y_1,y_2\rangle} = \\
&\sqrt{2+2\langle y_1,y_2\rangle} + \sqrt{2-2\langle y_1,y_2\rangle} = \\
&\sqrt{2}\left(\sqrt{1+\langle y_1,y_2\rangle} + \sqrt{1-\langle y_1,y_2\rangle}\right).
\end{aligned} \tag{262}$$

Since H is a real Hilbert space, $\langle y_1,y_2\rangle$ is real and by the Cauchy-Schwarz inequality we have:

$$\langle y_1,y_2\rangle \leq \|y_1\|_2\|y_2\|_2 = 1. \tag{263}$$

For $z \in [-1,1]$ we note that

$$\sqrt{1+z} + \sqrt{1-z} \geq 0 \tag{264}$$

and

$$(\sqrt{1+z}+\sqrt{1-z})^2 = 1+z+1-z+2\sqrt{(1+z)(1-z)} = 2+2\sqrt{1-z^2} \leq 2+2 = 4. \tag{265}$$

Therefore we have:

$$\sqrt{1+z} + \sqrt{1-z} \leq 2. \tag{266}$$

Because $\langle y_1,y_2\rangle \in [-1,1]$ it follows that:

$$\left|\sum_{i,j=1}^{2}(M_{CHSH})_{i,j}\gamma_{i,j}\right| \leq \sqrt{2}\left(\sqrt{1+\langle y_1,y_2\rangle} + \sqrt{1-\langle y_1,y_2\rangle}\right) \leq 2\sqrt{2}. \tag{267}$$

Since this holds for all $\gamma \in \mathscr{Q}_2$ it follows that $\omega^*(M_{CHSH}) = 2\sqrt{2}$ which completes the proof. □

So we see that the violation we had obtained for the CHSH-inequality was already maximal and we have $LV(M_{CHSH}) = \frac{2\sqrt{2}}{2} = \sqrt{2}$. This shows that $LV(M)$ can become at least as large as $\sqrt{2}$. It turns out that there exists an upper bound on the value of $LV(M)$ even when allowing the size of the matrices M to vary. Moreover, $LV(M_{CHSH}) = \sqrt{2}$ is fairly close to this upper bound. These results follow from a theorem known as Grothendieck's theorem which we will state without proof. This theorem can also be found (without proof) in chapter 5 of [2].

Theorem 7.9. *Grothendieck's theorem. There exists a positive constant K_G such that for every $N \in \mathbb{N}$ and every non-zero $N \times N$ matrix M with real elements the following inequality holds:*

$$\begin{aligned} &\sup \left| \sum_{i,j=1}^{N} M_{i,j} \langle x_i, y_j \rangle \right| \leq \\ &K_G \sup \left\{ \left| \sum_{i,j=1}^{N} M_{i,j} t_i s_j \right| : (t_1, \ldots, t_N, s_1, \ldots, s_N) \in \{1, -1\}^{2N} \right\}. \end{aligned} \tag{268}$$

with the first supremum taken over all real Hilbert spaces H and $x_i, y_i \in H$ with $\|x_i\|_2 = \|y_i\|_2 = 1$ for $i \in \{1, \ldots, N\}$.

Using Tsirelson's theorem (without the condition that H is finite-dimensional) and Theorem 7.1 we can reformulate Grothendieck's theorem as follows:

Theorem 7.10. *Grothendieck's theorem. There exists a positive constant K_G such that for every $N \in \mathbb{N}$ and every non-zero $N \times N$ matrix M with real elements the following inequality holds:*

$$\omega^*(M) \leq K_G \cdot \omega(M) \tag{269}$$

or equivalently

$$LV(M) \leq K_G. \tag{270}$$

The constant K_G is known as the real Grothendieck's constant. The exact value of K_G is unknown but it is known that (see chapter 5 of [2]):

$$1.67696\cdots \leq K_G \leq \frac{\pi}{2\log\left(1+\sqrt{2}\right)} \approx 1.7822139781. \tag{271}$$

The remainder of this thesis will revolve around approximating Grothendieck's constant. In particular we will attempt to calculate or approximate the largest violation of matrices and optimize the largest violation for a fixed matrix size.

8 Calculating classical and quantum values

As a first step in attempting to optimize the largest value of matrices, we need to be able to calculate or approximate the classical and quantum value of a given matrix M with real entries. Theorem 7.1 ensures that we can calculate the classical value of an $N \times N$ matrix exactly by taking the supremum (or maximum) of a finite set. This set consists of the numbers $\left|\sum_{i,j=1}^{N} M_{i,j} t_i s_j\right|$ for all possible combinations of $t_i, s_j \in \{1, -1\}^{2N}$. Since there are $2^{2N} = 4^N$ possible combinations of the t_i and s_j, the calculation $\left|\sum_{i,j=1}^{N} M_{i,j} t_i s_j\right|$ needs to be performed 4^N times. This means that while $\omega(M)$ can be calculated exactly in a straightforward way, we expect the time it takes to calculate $\omega(M)$ to increase exponentially in the matrix size N. The number of times $\left|\sum_{i,j=1}^{N} M_{i,j} t_i s_j\right|$ has to be calculated can be reduced by noting that we can fix $t_1 = s_1 = 1$ without omitting any elements from the set $\left\{\left|\sum_{i,j=1}^{N} M_{i,j} t_i s_j\right| : t_i, s_j \in \{1, -1\}\right\}$.

Theorem 8.1. *Let M be an $N \times N$ matrix with real elements and $t_i, s_j \in \{1, -1\}$ for all $i, j \in \{1, \ldots, N\}$. Then there exist $t'_i, s'_j \in \{1, -1\}$ for all $i, j \in \{1, \ldots, N\}$ with $t'_1 = s'_1 = 1$ such that $\left|\sum_{i,j=1}^{N} M_{i,j} t_i s_j\right| = \left|\sum_{i,j=1}^{N} M_{i,j} t'_i s'_j\right|$.*

Proof. Let M be an $N \times N$ matrix with real elements and $t_i, s_j \in \{1, -1\}$ for all $i, j \in \{1, \ldots, N\}$. Let $t'_i = t_1 t_i$ and $s'_j = s_1 s_j$ for all $i, j \in \{1, \ldots, N\}$. Clearly $t'_i, s'_j \in \{1, -1\}$, $t'_1 = t_1^2 = 1$ and $s'_1 = s_1^2 = 1$. We also have

$$\begin{aligned} &\left|\sum_{i,j=1}^{N} M_{i,j} t'_i s'_j\right| = \left|\sum_{i,j=1}^{N} M_{i,j} t_i t_1 s_j s_1\right| = \left|t_1 s_1 \sum_{i,j=1}^{N} M_{i,j} t_i s_j\right| = \\ &|t_1||s_1|\left|\sum_{i,j=1}^{N} M_{i,j} t_i s_j\right| = \left|\sum_{i,j=1}^{N} M_{i,j} t_i s_j\right| \end{aligned} \tag{272}$$

which concludes the proof. □

Theorem 8.1 allows us to fix $t_1 = s_1 = 1$, so we only have to calculate $\left|\sum_{i,j=1}^{N} M_{i,j} t_i s_j\right|$ $2^{2N-2} = 4^{N-1}$ times. For calculation of $\omega^*(M)$ we will rely on Tsirelson's theorem (Theorem 7.7). So we need to find the supremum of $\left|\sum_{i,j=1}^{N} M_{i,j} \langle x_i, y_j \rangle\right|$ taken over all possible unit vectors x_i and y_j in all finite-dimensional real Hilbert spaces. We now define:

Definition 8.1. $\omega_n^*(M) = \sup\left|\sum_{i,j=1}^{N} M_{i,j} \langle x_i, y_j \rangle\right|$ with the supremum taken over all unit vectors x_i, y_j in real Hilbert spaces of dimension n.

We note that $\omega^*(M) = \sup_{n \in \mathbb{N}} \omega_n^*(M)$. We also note that given a real Hilbert space H of dimension n and unit vectors $x_i, y_j \in H$, we can take an arbitrary

orthonormal basis of H. If we consider the representations of the vectors x_i and y_j in $\mathbb{R}^n$ with respect to the chosen basis, then we can replace x_i and y_j by their representations without changing the inner products $\langle x_i, y_j \rangle$. Consequently $\left|\sum_{i,j=1}^N M_{i,j} \langle x_i, y_j \rangle\right|$ will remain unchanged if we replace the vectors by their representations in $\mathbb{R}^n$. In other words it is sufficient to only consider unit vectors in $\mathbb{R}^n$ when calculating $\omega_n^*(M)$.

Theorem 8.2. *$\omega_n^*(M) = \sup\left|\sum_{i,j=1}^N M_{i,j} \langle x_i, y_j \rangle\right|$ with the supremum taken over all unit vectors $x_i, y_j \in \mathbb{R}^n$.*

Our next theorem shows that $\omega_n^*(M)$ is increasing in n.

Theorem 8.3. *Let M be an $N \times N$ matrix with real entries and $n \in \mathbb{N}$, then $\omega_{n+1}^*(M) \geq \omega_n^*(M)$.*

Proof. Let M be an $N \times N$ matrix with real entries and $n \in \mathbb{N}$. Let $x_i, y_j \in \mathbb{R}^n$ be unit vectors. We consider the vectors $x_i \oplus 0$ and $y_j \oplus 0$. These are vectors in a vector space of dimension $n+1$ which can easily be identified with $\mathbb{R}^{n+1}$. In other words we consider vectors $x_i', y_j' \in \mathbb{R}^{n+1}$ whose first entries match those of x_i and y_j and whose last entry is equal to 0. These are clearly unit vectors in $\mathbb{R}^{n+1}$ with $\langle x_i, y_j \rangle = \langle x_i', y_j' \rangle$. It follows that

$$\left|\sum_{i,j=1}^N M_{i,j} \langle x_i, y_j \rangle\right| = \left|\sum_{i,j=1}^N M_{i,j} \langle x_i', y_j' \rangle\right|. \tag{273}$$

This shows that

$$\begin{aligned}&\left\{\left|\sum_{i,j=1}^N M_{i,j} \langle x_i, y_j \rangle\right| : x_i, y_j \in \mathbb{R}^n, \|x_i\|_2 = \|y_j\|_2 = 1\right\} \subseteq \\ &\left\{\left|\sum_{i,j=1}^N M_{i,j} \langle x_i, y_j \rangle\right| : x_i, y_j \in \mathbb{R}^{n+1}, \|x_i\|_2 = \|y_j\|_2 = 1\right\}\end{aligned} \tag{274}$$

and it follows that $\omega_{n+1}^*(M) \geq \omega_n^*(M)$. □

In addition, the following theorem shows that $\omega_n^*(M)$ is eventually constant in n.

Theorem 8.4. *Let M be an $N \times N$ matrix with real entries and $n \geq N+1$, then $\omega_n^* = \omega_{N+1}^*$.*

Proof. Let M be an $N \times N$ matrix with real entries and $n \geq N+1$. $\omega_n^* \geq \omega_{N+1}^*$ is clear from Theorem 8.3. For the reverse inequality note that given unit vectors x_i, y_j for $i, j \in \{1, \ldots, N\}$ in $H = \mathbb{R}^n$, we can consider the real Hilbert space H' spanned by the vectors $x_1, \ldots, x_N$. This Hilbert space has dimension

at most N and contains the vectors $x_1, \ldots, x_N$. We define the vectors y'_j for $j \in \{1, \ldots, N\}$ as the projection of y_j on H'. This gives us vectors $y'_j \in H'$ with $\|y'_j\| \leq \|y_j\| = 1$ and $\langle x_i, y'_j \rangle = \langle x_i, y_j \rangle$. Similarly to what we did in the proof of Tsirelson's theorem we consider the real Hilbert space $H'' = H' \oplus \mathbb{R}$ and the vectors $x''_i = x_i \oplus 0$ and $y''_j = y'_j \oplus \sqrt{1 - \|y'_j\|^2}$ in H''. These are unit vectors in H'' with $\langle x''_i, y''_j \rangle = \langle x_i, y'_j \rangle = \langle x_i, y_j \rangle$. We note that the dimension k of H'' is one larger than the dimension of H' and therefore $k \leq N + 1$. So

$$\left| \sum_{i,j=1}^{N} M_{i,j} \langle x''_i, y''_j \rangle \right| = \left| \sum_{i,j=1}^{N} M_{i,j} \langle x_i, y_j \rangle \right| \tag{275}$$

with $x''_i, y''_j \in H''$ unit vectors and H'' of dimension $k \leq N + 1$. We can replace x''_i and y''_j by their representations x'''_i and y'''_j in $\mathbb{R}^k$ with respect to an orthonormal basis of H''. We subsequently replace x'''_i and y'''_j by vectors x''''_i and y''''_j in $\mathbb{R}^{N+1}$ by adding $N + 1 - k$ zeros as the last entries. These replacements do not change the inner products between the vectors or the fact that they are unit vectors. Therefore

$$\left| \sum_{i,j=1}^{N} M_{i,j} \langle x''''_i, y''''_j \rangle \right| = \left| \sum_{i,j=1}^{N} M_{i,j} \langle x_i, y_j \rangle \right| \tag{276}$$

with x''''_i and y''''_j unit vectors in $\mathbb{R}^{N+1}$. This shows that

$$\begin{aligned} &\left\{ \left| \sum_{i,j=1}^{N} M_{i,j} \langle x_i, y_j \rangle \right| : x_i, y_j \in \mathbb{R}^n, \|x_i\|_2 = \|y_j\|_2 = 1 \right\} \subseteq \\ &\left\{ \left| \sum_{i,j=1}^{N} M_{i,j} \langle x_i, y_j \rangle \right| : x_i, y_j \in \mathbb{R}^{N+1}, \|x_i\|_2 = \|y_j\|_2 = 1 \right\} \end{aligned} \tag{277}$$

and it follows that $\omega_n^*(M) \leq \omega_{N+1}^*(M)$. We conclude that $\omega_n^* = \omega_{N+1}^*$. □

Since $\omega_n^*(M)$ is increasing in n and constant for $n \geq N+1$ we have the following corollary.

Corollary 8.4.1. *Let M be an $N \times N$ matrix with real entries, then $\omega^*(M) = \omega_{N+1}^*(M)$.*

Corollary 8.4.1 allows us to only consider unit vectors in $\mathbb{R}^{N+1}$ when calculating the quantum value of a matrix. We will not be calculating the quantum value of matrices M exactly and will instead use an optimization algorithm in python to approximate the quantum value, giving us lower bounds. This optimization becomes easier if we can omit the absolute value in $\left| \sum_{i,j=1}^{N} M_{i,j} \langle x_i, y_j \rangle \right|$, which the following theorem allows us to do.

Theorem 8.5. *Let M be an $N \times N$ matrix with real entries and $n \in \mathbb{N}$, then:*

$$\omega_n^*(M) = \sup \sum_{i,j=1}^{N} M_{i,j} \langle x_i, y_j \rangle = -\inf \sum_{i,j=1}^{N} M_{i,j} \langle x_i, y_j \rangle . \tag{278}$$

Proof. Let M be an $N \times N$ matrix with real entries and $n \in \mathbb{N}$. We note that given unit vectors $x_i, y_j \in \mathbb{R}^n$ for $i, j \in \{1, \ldots, N\}$, $-x_i \in \mathbb{R}^n$ are also unit vectors and

$$\sum_{i,j=1}^{N} M_{i,j} \langle -x_i, y_j \rangle = -\sum_{i,j=1}^{N} M_{i,j} \langle x_i, y_j \rangle . \tag{279}$$

This means that the set $\{\sum_{i,j=1}^{N} M_{i,j} \langle x_i, y_j \rangle : x_i, y_j \in \mathbb{R}^n, \|x_i\|_2 = \|y_j\|_2 = 1\}$ is symmetric around 0 in the sense that if it contains a it also contains $-a$ and $|a|$. For a set A of real numbers having this property we have $\sup A = -\inf A$ and $\sup A = \sup\{|a| : a \in A\}$. This directly implies the statement from the theorem completing the proof. □

The optimization algorithm we will use is a minimization algorithm. We will use it to minimize $\sum_{i,j=1}^{N} M_{i,j} \langle x_i, y_j \rangle$ for a given matrix M over all unit vectors $x_i, y_j \in \mathbb{R}^n$. This should give us an upper bound on $-\omega^*(M)$ which, if the optimization is successful, should be quite accurate if we choose $n = N + 1$. If we write $x_i = (x_{i,k})_{k=1}^n$ and $y_j = (y_{j,k})_{k=1}^n$ we can write, for an arbitrary $N \times N$ matrix with real entries M:

$$f_M = \sum_{i,j=1}^{N} M_{i,j} \langle x_i, y_j \rangle = \sum_{i,j=1}^{N} M_{i,j} \sum_{k=1}^{n} x_{i,k} y_{j,k} \tag{280}$$

and minimize f_M as function of the real variables $x_{i,k}, y_{j,k}$ (with $i, j \in \{1, \ldots, N\}$, $k \in \{1, \ldots, n\}$) under the condition that $\sum_{k=1}^{n} x_{i,k}^2 = \sum_{k=1}^{n} y_{j,k}^2 = 1$. The function f_M is differentiable with partial derivatives given by:

$$\frac{\partial f_M}{\partial x_{i_0,k_0}} = \sum_{j=1}^{N} M_{i_0,j} y_{j,k_0} \tag{281}$$

and

$$\frac{\partial f_M}{\partial y_{j_0,k_0}} = \sum_{i=1}^{N} M_{i,j_0} x_{i,k_0}. \tag{282}$$

To enforce the condition that $\sum_{k=1}^{n} x_{i,k}^2 = \sum_{k=1}^{n} y_{j,k}^2 = 1$ (the vectors must be unit vectors) we will not optimize using the variables $x_{i,k}$ and $y_{j,k}$ directly. Instead we will express the vectors x_i and y_j using (higher dimensional) spherical coordinates fixing the radius at 1 and optimizing using the angles as variables. A point $z \in \mathbb{R}^n$ with $\|z\|_2 = 1$ can be represented using $n-1$ angles ϕ_1 through

ϕ_{n-1}. The function $g : \mathbb{R}^{n-1} \to \mathbb{R}^n$ mapping $\phi = (\phi_m)_{m=1}^{n-1}$ to $z = (z_k)_{k=1}^{n}$ has components g_k ($k \in \{1, \ldots, n\}$) given by:

$$g_k(\phi) = \begin{cases} \cos(\phi_k) \prod_{m=1}^{k-1} \sin(\phi_m), & k \leq n-1 \\ \prod_{m=1}^{n-1} \sin(\phi_m), & k = n \end{cases} \tag{283}$$

and it can be verified that the range of g consists of all unit vectors in $\mathbb{R}^n$. For our optimization we use the real variables $\phi_{i,m}$ and $\psi_{j,m}$ for $i, j \in \{1, \ldots, N\}$ and $m \in \{1, \ldots, n-1\}$ and substitute $x_{i,k}$ by $g_k((\phi_{i,m})_{m=1}^{n-1})$ and $y_{j,k}$ by $g_k((\psi_{j,m})_{m=1}^{n-1})$ in the objective function f_M. So the function to be optimized becomes:

$$f_M = \sum_{i,j=1}^{N} M_{i,j} \sum_{k=1}^{n} g_k((\phi_{i,m})_{m=1}^{n-1}) g_k((\psi_{j,m})_{m=1}^{n-1}) \tag{284}$$

with no restrictions necessary on the variables $\phi_{i,m}$ and $\psi_{j,m}$ (although the periodicity of sine and cosine makes it possible to restrict the domain if we want). We want to provide the optimization algorithm with the partial derivatives of the objective function f_M. Using the chain rule for partial derivatives we find that:

$$\frac{\partial f_M}{\partial \phi_{i_0,m_0}} = \sum_{k_0=1}^{n} \sum_{j=1}^{N} M_{i_0,j} g_{k_0}((\psi_{j,m})_{m=1}^{n-1}) \frac{\partial g_{k_0}}{\partial \phi_{i_0,m_0}}((\phi_{i_0,m})_{m=1}^{n-1}) \tag{285}$$

and

$$\frac{\partial f_M}{\partial \psi_{j_0,m_0}} = \sum_{k_0=1}^{n} \sum_{i=1}^{N} M_{i,j_0} g_{k_0}((\phi_{i,m})_{m=1}^{n-1}) \frac{\partial g_{k_0}}{\partial \psi_{j_0,m_0}}((\psi_{j_0,m})_{m=1}^{n-1}). \tag{286}$$

It remains to calculate the partial derivatives of the g_k which are given by:

$$\frac{\partial g_k}{\partial \phi_{m_0}} = \begin{cases} 0, & m_0 > k \\ \cos(\phi_k) \cos(\phi_{m_0}) \prod_{m=1, m \neq m_0}^{k-1} \sin(\phi_m), & m_0 < k < n \\ -\prod_{m=1}^{k} \sin(\phi_m), & m_0 = k \\ \cos(\phi_{m_0}) \prod_{m=1, m \neq m_0}^{n-1} \sin(\phi_m), & k = n \end{cases}. \tag{287}$$

Substituting the explicit form of the g_k and their partial derivatives into the partial derivatives of f_M would give an explicit expression of the partial derivatives of f_M as a function of the $\phi_{i,m}$ and $\psi_{j,m}$. The algorithm we use to approximate the quantum value of a matrix M is the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm which is part of the scipy.optimize.minimize function in python. We use f_M as the objective function with $\phi_{i,m}$ and $\psi_{j,m}$ as the variables. We also provide the algorithm with a function calculating the gradient

of f_M, using the expressions for the partial derivatives we have found. We will usually choose $n = N + 1$, unless we wish to save on run-time in which case we can choose $n < N + 1$ to reduce the number of variables. Combined with the calculation of the exact value of the classical value we can calculate lower bounds for the largest violation of a matrix M. The lower bounds obtained (when using $n = N + 1$) seem to accurately approximate the exact value of the largest violation at least in cases where the exact value is known. Using the BFGS algorithm on the CHSH-matrix, we find a largest violation of 1.4142135623710677, which agrees with the exact value to 11 decimal places.

9 Approximating Grothenieck's constant

Now that we can calculate the largest violation of a matrix M, we want to optimize this largest violation to approximate Grothendieck's constant. We will first lay out our method for approximating Grothendieck's constant and then discuss the results we have obtained.

9.1 Method for approximating Grothendieck's constant

We first introduce a variation on Grothendieck's constant.

Definition 9.1. Grothendieck's constant for $N \times N$ matrices is given by $K_N = \sup_{M \in \mathrm{Mat}_{N\times N}(\mathbb{R})\setminus\{0\}} LV(M)$, where $\mathrm{Mat}_{N\times N}(\mathbb{R})$ is the set of all $N \times N$ matrices with real entries and 0 denotes the zero-matrix.

We note that K_G can be defined in a similar way, by taking the supremum over all non-zero square matrices of arbitrary size with real entries. This means that $K_G = \sup_{N\in\mathbb{N}} K_N$. The next theorem shows that K_N is increasing in N.

Theorem 9.1. *Let $N \in \mathbb{N}$, then $K_{N+1} \geq K_N$.*

Proof. Let $N \in \mathbb{N}$. Let $M = (M_{i,j})_{i,j=1}^{N}$ be an arbitrary non-zero $N \times N$ matrix with real entries. we consider the matrix $M' = (M'_{i,j})_{i,j=1}^{N+1}$ with $M'_{i,j} = M_{i,j}$ for $i, j \in \{1, \ldots, N\}$ and $M'_{i,j} = 0$ if $i = N+1$ or $j = N+1$. Given $t_i, s_j \in \{1, -1\}$ for $i, j \in \{1, \ldots, N+1\}$ we note that:

$$\left|\sum_{i,j=1}^{N+1} M'_{i,j} t_i s_j\right| = \left|\sum_{i,j=1}^{N} M'_{i,j} t_i s_j\right| = \left|\sum_{i,j=1}^{N} M_{i,j} t_i s_j\right|. \tag{288}$$

This shows that:

$$\left\{\left|\sum_{i,j=1}^{N+1} M'_{i,j} t_i s_j\right| : t_i, s_j \in \{1,1\}\right\} = \left\{\left|\sum_{i,j=1}^{N} M_{i,j} t_i s_j\right| : t_i, s_j \in \{1,1\}\right\} \tag{289}$$

and therefore $\omega(M') = \omega(M)$. Similarly, given $x_i, y_j \in \mathbb{R}^{N+2}$ with $\|x_i\|_2 = \|y_j\|_2 = 1$ we have:

$$\left|\sum_{i,j=1}^{N+1} M'_{i,j} \langle x_i, y_j\rangle\right| = \left|\sum_{i,j=1}^{N} M'_{i,j} \langle x_i, y_j\rangle\right| = \left|\sum_{i,j=1}^{N} M_{i,j} \langle x_i, y_j\rangle\right|. \tag{290}$$

It follows that:

$$\left\{\left|\sum_{i,j=1}^{N+1} M'_{i,j}\left\langle x_i, y_j\right\rangle\right| : x_i, y_j \in \mathbb{R}^{N+2}, \left\|x_i\right\|_2 = \left\|y_j\right\|_2 = 1\right\} = \left\{\left|\sum_{i,j=1}^{N} M_{i,j}\left\langle x_i, y_j\right\rangle\right| : x_i, y_j \in \mathbb{R}^{N+2}, \left\|x_i\right\|_2 = \left\|y_j\right\|_2 = 1\right\}. \tag{291}$$

This means that:

$$\omega^*(M') = \omega^*_{N+2}(M') = \omega^*_{N+2}(M) = \omega^*_{N+1}(M) = \omega^*(M). \tag{292}$$

Since $\omega(M') = \omega(M)$ and $\omega^*(M') = \omega^*(M)$ we have:

$$LV(M') = LV(M). \tag{293}$$

So we have:

$$\{LV(M) : M \in \mathrm{Mat}_{N\times N}(\mathbb{R})\backslash\{0\}\} \subseteq \{LV(M) : M \in \mathrm{Mat}_{N+1\times N+1}(\mathbb{R})\backslash\{0\}\} \tag{294}$$

and consequently $K_N \leq K_{N+1}$. □

We see that the K_N form an increasing sequence increasing to K_G. If we can find a lower bound for K_N for some $N \in \mathbb{N}$, then this is also a lower bound on K_G. Furthermore by increasing N we can hope to find increasingly better lower bounds on K_G. We note without proof that $K_2 = K_3 = \sqrt{2}$ (see [4]). In other words there are no 2×2 or 3×3 matrices M with $LV(M) > \sqrt{2} = LV(M_{CHSH})$. To find lower bounds on K_N we have used Powell's method. This is a minimization algorithm, which is also part of the scipy.minimize.optimize function in python, and does not require the objective function to be differentiable. The objective function we used is given by $-LV(M)$, where we calculate $LV(M)$ by calculating $\omega(M)$ exactly and approximating $\omega^*(M)$ using the BFGS algorithm. So the objective function is actually an upper bound on $-LV(M)$. The variables are the N^2 entries of the matrix M. Powell's method should find a (local) minimum of the objective function, which will give an upper bound on $-K_N$. The reason we have used an algorithm that does not require the objective function to be differentiable is the following. Even though the expression

$$\frac{\sum_{i,j=1}^{N} M_{i,j}\left\langle x_i, y_j\right\rangle}{\sum_{i,j=1}^{N} t_i s_j M_{i,j}} \tag{295}$$

is differentiable with respect to the matrix entries $M_{i,j}$ when we take t_i, s_j, x_i, y_j fixed, the values of t_i and s_j for which $\sum_{i,j=1}^{N} t_i s_j M_{i,j} = \omega(M)$ depend on the matrix M and similarly for x_i and y_j. Without knowing the exact dependence it is unclear if $LV(M)$ is differentiable as a function of the matrix entries of M. For this reason we have chosen to use a different optimization algorithm.

We have observed that the bound found using this algorithm can significantly depend on the chosen starting values, which is not too surprising since the minima found are local. To increase the likelyhood of finding the global minimum (or at least a good local minimum) using the algorithm, we can repeat the algorithm several times using different starting values. We have chosen to run the algorithm using random starting values, choosing each matrix entry uniformly in $[-1, 1]$ independent from each other. We note that it is sufficient to only choose starting values in $[-1, 1]$. This is because multiplying a given matrix M by a constant $a \in \mathbb{R}$ will change both the classical and quantum value of the matrix by a factor $|a|$, leaving the largest violation unchanged. Therefore a given non-zero $N \times N$ matrix M with real entries can be multiplied by $\frac{1}{\max |M_{i,j}|}$. The resulting matrix will have the same largest violation and all its entries will be in the interval $[-1, 1]$. Therefore when minimizing $-LV(M)$ it is not necessary (but possible) to consider matrices with large entries (larger than 1 in absolute value). This justifies only using starting values in $[-1, 1]$ for the minimization algorithm. Below we have included the Python code containing the functions we used with comments to explain what each function does. The last function constructs matrices according to the procedure described in [4]. We will also give a brief description of the construction method in the next chapter.

```
import numpy as np
import itertools
import scipy.optimize
import time

'''Takes a vector of angles phi as the spherical coordinates of a
    point x on the surface of an n-dimensional sphere and returns
    the associated point x.'''
def sphertocart(phi):
    '''Calculates n as the number of angles plus one.'''
    n = len(phi) + 1
    '''x is iniated as a vector of length n and each entry is
    calculated using the function g as defined in Equation (283).
    '''
    x = np.zeros(n)
    for i in range(0,n-1):
        x[i] = np.prod(np.sin(phi[0:i]))*np.cos(phi[i])
    x[n-1] = np.prod(np.sin(phi))
    return x

'''Takes a vector of angles theta and two positive integers N and n
    .
The vector theta is treated as a vector containing the spherical
    coordinates of N points on the surface of an n-dimensional
    sphere and must have length equal to N(n-1).
The first n-1 entries are the spherical coordinates of the first
    point etc.
The output is a vector x of length Nn whose first n entries
    represent the coordinates of the first point, etc.'''
def sphertocart2(theta,N,n):
    '''x is iniated as a vector of length Nn.'''
    x = np.zeros(2*N*n)
    for i in range(0,2*N):
```

```
        '''The first n entries of x are calculated using sphertocart, with the input given by the first n-1 entries of theta.
        This process is repeated for the next n entries of x etc.'''
        x[i*n:(i+1)*n] = sphertocart(theta[i*(n-1):(i+1)*(n-1)])
    return x

'''The input is a vector of angles phi, to be interpreted as the spherical coordinates of a point x on the surface of an n-dimensional sphere.
The output is the matrix deriv containing the partial derivatives of the transformation from spherical to cartesian coordinates (the function g in Equation (283)).'''
def sphertocartderiv(phi):
    '''Calculates n as the number of angles plus one.'''
    n = len(phi) + 1
    '''Initiates deriv as an n by n-1 matrix.'''
    deriv = np.zeros([n,n-1])
    '''The entries of deriv, which are the partial derivatives of g, are calculated as in Equation (287).
    The entries which are always equal to 0 (m > k) are unchanged.'''
    for k in range(0,n-1):
        for m in range(0,k):
            deriv[k,m] = np.cos(phi[k])*np.cos(phi[m])* \
            np.prod(np.sin(phi[0:k][np.array(range(0,k)) != m]))
        deriv[k,k] = -np.prod(np.sin(phi[0:k+1]))
    for m in range(0,n-1):
        deriv[n-1,m] = np.cos(phi[m])* \
        np.prod(np.sin(phi[np.array(range(0,n-1)) != m]))
    return deriv

'''The input is a square matrix of real entries M.
The output is the classical value of M.
It is calculated using Theorem 6.1 by considering all combinations of ti and sj in {1,-1}.
t1 and s1 are kept fixed at 1, which is justified by Theorem 7.1.'''
def classicalvalue(M):
    '''Determines the matrix size N.'''
    N = np.size(M,1)
    '''Defines TS as the cartesian product of 2(N-1) copies of {1,-1}.
    TS represents all different choices for the ti and sj (for i,j > 1).'''
    TS = itertools.product([1,-1], repeat=2*(N-1))
    '''Initiates Mcorrmat as an empty set.
    Mcorrmat will contain the value to be maximized for the different choices of ti and sj.'''
    Mcorrmat = set()
    for ts in TS:
        '''For each elements in the cartesian product TS, t and s are defined as the vectors containing the associated ti and sj.'''
        t = np.mat([1]+list(ts[0:N-1]))
        s = np.mat([1]+list(ts[N-1:(2*(N-1))]))
```

```
        '''The deterministic correlation matrix gamma is calculated from t and s (gammaij = ti*sj).'''
        gamma = np.array(np.transpose(t)*s)
        '''M and gamma are multiplicated entrywise, the entries of the resulting matrix are summed and the absolute value is taken.
        The resulting number is added to the set Mcorrmat.'''
        Mcorrmat.add(abs(np.sum(M*gamma)))
        '''The classical value omega of M is calculated by taking the maximum of all numbers in Mcorrmat.'''
    omega = max(Mcorrmat)
    return omega

'''The input should be a square N by N matrix of real entries M and two N by n matrices X and Y.
The rows of the matrices X and Y are to be interpreted as the n-dimensional unit vectors xi and yj from Equation (280).
The output qprod is equal to fM from Equation (280).'''
def quantumprod(M,X,Y):
    '''N and n are determined from the input matrices.'''
    N = np.size(M,1)
    n = np.size(X,1)
    '''Inner products between the rows of X and Y are taken to construct the associated quatum correlation matrix inprod.'''
    inprod = np.mat(X)*np.transpose(np.mat(Y))
    '''qprod is calculated by taking the entrywise product between M and inprod and summing the entries.'''
    qprod = np.sum(M*np.array(inprod))
    return qprod

'''A reformulation of quantumprod to allow for the input to be presented in a different form.
M is the same as in quantumprod, and x must be a vector containing all entries from X and Y.
The entries of x should start with those of X row by row and then those of Y also row by row.'''
def funqprod(x,M):
    '''N and n are determined from the input.'''
    N = np.size(M,1)
    n = np.size(x)/(2*N)
    '''x is reshaped into a 2*N by n matrix Z, whose top half is the matrix X and its bottom half is the matrix Y.'''
    Z = np.reshape(x,(2*N,n))
    '''Z is split into the matrices X and Y, which are used to call quantumprod.'''
    X = Z[0:N,0:n]
    Y = Z[N:2*N,0:n]
    return quantumprod(M,X,Y)

'''Using the same input as funqprod, returns jacob, the Jacobian (or gradient) of funqprod (fM), as function of the components of x, or in other words the components of the vectors xi and yj.
    '''
def jacobfunqprod(x,M):
    '''N and n are determined from the input.'''
    N = np.size(M,1)
    n = np.size(x)/(2*N)
```

```
    '''x is reshaped into a 2*N by n matrix Z, whose top half is
    the matrix X and its bottom half is the matrix Y.'''
    Z = np.reshape(x,(2*N,n))
    '''Z is split into the matrices X and Y.'''
    X = Z[0:N,0:n]
    Y = Z[N:2*N,0:n]
    '''The Jacobian (gradient) jacob is calculated using the
    partial derivatives of fM (Equations (281) and (282)).'''
    jacob = list()
    for i in range(0,N):
        for k in range(0,n):
            jacob = jacob + [sum(M[i,:]*Y[:,k])]
    for j in range(0,N):
        for k in range(0,n):
            jacob = jacob + [sum(M[:,j]*X[:,k])]
    jacob = np.array(jacob)
    return jacob

'''The input is a square N by N matrix M with real entries and a
    vector of angles theta of length 2*N*(n-1).
Each n-1 consecutive components of theta represent the vectors phii
     and psij from Equation (284).
The output is the value of the function fM (as a function of the
    spherical coordinates phii and psij) as in Equation (284).'''
def spherefunqprod(theta,M):
    '''N and n are determined from the input.'''
    N = np.size(M,1)
    n = 1+np.size(theta)/(2*N)
    '''theta is converted to a vector x containing the components
    of the vectors xi and yj using sphertocart2.
    x is then used as the input for qprod to calculate fM.'''
    x = sphertocart2(theta,N,n)
    return funqprod(x,M)

'''Using the same input as spherefunqprod, returns jacob, the
    jacobian (or gradient) of spherefunqprod (fM), as a function of
     the components of theta, or in other words the components of
    the vectors phii and psij.'''
def jacobspherefunqprod(theta,M):
    '''N and n are determined from the input.'''
    N = np.size(M,1)
    n = 1+np.size(theta)/(2*N)
    '''theta is converted to a vector x containing the components
    of the vectors xi and yj using sphertocart2.'''
    x = sphertocart2(theta,N,n)
    '''The Jacobian (gradient) jacob is calculated according to
    Equations (285) and (286).
    jacobfunqprod (gradient of fM with respect to the components of
     xi and yj) and sphertocartderiv (partial derivatives of g) are
     used for this according to the chain rule.'''
    jacob = list()
    for i in range(0,2*N):
        for m in  range(0,n-1):
            jacob = jacob + [np.sum(jacobfunqprod(x,M)[i*n:(i+1)*n
    ]*
            sphertocartderiv(theta[i*(n-1):(i+1)*(n-1)])[:,m])]
    jacob = np.array(jacob)
```

```
    return jacob

'''The input should be a square N by N matrix M with real entries and a positive integer n.
Uses the BFGS algorithm to minimize spherefunqprod as a function of theta.
Returns the minimization results containing the point where the minimum was found, the value at this point and other information regarding the outcome.
The value found approximates -omega n star(M) from above.'''
def quantumvaluespher(M,n):
    '''Determines the matrix size N.'''
    N = np.size(M,1)
    '''Chooses starting values theta0 for theta.'''
    theta0 = np.array(range(2*N*(n-1)))
    '''Calls the optimization algorithm.
    spherefunqprod is the objective function with theta as the variables.
    theta0 gives the starting values of theta.
    M is given as a parameter to the objective function.
    jacobspherfunqprod is used as the Jacobian in the minimization process.'''
    result = scipy.optimize.minimize(spherefunqprod,theta0,args=M,
    jac=jacobspherefunqprod)
    return result

'''Using the same input calls quantumvaluespher and returns the value found by the minimization algorithm multiplied by -1.
The returned value approximates omega n star(M) from below.'''
def quantvalue(M,n):
    return -quantumvaluespher(M,n)['fun']

'''Using the same input calls quantumvaluespher, takes the value of theta where the minimum was found and returns the associated vectors xi and yj.
The output is an 2*N by n matrix Z, whose first N rows contain the components of the xi and the last N rows contain the components of the yj.'''
def quantvaluepoint(M,n):
    '''Determines the matrix size N.'''
    N = np.size(M,1)
    '''Calls quantumvaluespher and takes the optimal value of theta.'''
    theta = quantumvaluespher(M,n)['x']
    '''Uses sphertocart2 to convert the spherical coordinates theta to cartesian coordinates x.'''
    x = sphertocart2(theta,N,n)
    '''Reshapes x to obtain the matrix Z contain the xi and yj.'''
    Z = np.reshape(x,(2*N,n))
    return Z

'''Using the same input calls quantvaluepoint and calculates the associated quantum correlation matrix.'''
def quantvaluegamma(M,n):
    '''Calls quantvaluepoint.'''
    Z = quantvaluepoint(M,n)
    '''Determines the matrix size N.'''
```

```
193     N = np.size(M,1)
194     '''Splits Z into matrices X and Y containing as rows the xi and
         yj respectively.'''
195     X = Z[0:N,:]
196     Y = Z[N:2*N,:]
197     '''Takes inner products between the rows of X and Y to
        calculate the associated quantum correlation matrix gamma.'''
198     gamma = np.array(np.mat(X)*np.transpose(np.mat(Y)))
199     return gamma
200 
201 '''The input should be a square N by N matrix M with real entries
        and a positive integer n.
202 Returns the fraction of quantvalue(M,n) and classicalvalue(M),
        which approximates the largest violation of M from below.'''
203 def LV(M,n):
204     result = quantvalue(M,n)/classicalvalue(M)
205     return result
206 
207 '''Using the same input returns -LV(M,n).'''
208 def negLV(M,n):
209     return -LV(M,n)
210 
211 '''Calculates negLV(M,n) with the input in a different form.
212 x should be the same as M, but reshaped into an N^2 by 1 matrix.'''
213 def negLVfunq(x,n):
214     '''Determines N from the input.'''
215     N = int(len(x)**0.5)
216     '''Determines M by reshaping x.'''
217     M = np.reshape(x,(N,N))
218     return negLV(M,n)
219 
220 '''The input should consist of two positive integers N and n, and a
         vector x0 of length N^2 with real entries.
221 Uses the Powell algorithm to minimize negLVfunq as a function of x
        (with fixed length N^2 for x) using x0 as starting value.
222 Returns the minimization results containing the point where the
        minimum was found, the value at this point and other
        information regarding the outcome.
223 The value found approximates -KN from above.'''
224 def LVopt(N,n,x0):
225     '''Calls the optimization algorithm.
226     negLVfunq is the objective function with x as the variables.
227     x0 gives the starting values of x.
228     n is given as a parameter to the objective function.'''
229     result = scipy.optimize.minimize(negLVfunq,x0,args=n,method='
        Powell')
230     return result
231 
232 '''The input should consist of two positive integers N and n, and a
         negative real number bound.
233 Repeatedly calls LVopt(N,n,x0) for randomly generated x0 untill a
        value smaller than bound is found.'''
234 def LVoptloop(N,n,bound):
235     '''Initiates lastresult at 0.'''
236     lastresult = 0
237     '''Checks if lastresult is >= bound.
238     If it is, randomly generates x0 and calculates LVopt(N,n,x0).
```

```
    '''
    while lastresult >= bound:
        '''Randomly generates each entry of x0 using the uniform
    distribution on [-1,1].'''
        x0 = np.zeros(N**2)
        for i in range(0,N**2):
            x0[i] = np.random.uniform(-1,1)
        '''Calls LVopt(N,n,x0) and sets lastresult equal to the
    value found.'''
        result = LVopt(N,n,x0)
        lastresult = result['fun']
    '''When a value < bound is found, the loop ends.
    The value found (multiplied by -1) is printed as well as the
    associated matrix M.'''
    print -lastresult
    print np.reshape(result['x'],(N,N))

'''The input should consist of an integer k >= 2 and a real number
    lam.
Calculates the k*(k-1) by k*(k-1) matrix M with entries given by
    Equation (308).
Returns M - lam*I with I the k*(k-1) by k*(k-1) identity matrix.'''
def Mfishburn(k,lam):
    '''Creates an empty list F and fills it with all different k-
    dimensional vectors with all but two entries equal to 0, with
    the first of these equal to 1 and the second equal to 1 or -1.
    '''
    F = []
    for i in range(0,k-1):
        for j in range(i+1,k):
            f = np.zeros(k)
            f[i] = 1
            f[j] = 1
            F = F + [f]
    for i in range(0,k-1):
        for j in range(i+1,k):
            f = np.zeros(k)
            f[i] = 1
            f[j] = -1
            F = F + [f]
    '''Constructs the k*(k-1) by k*(k-1) matrix M whose entries are
     all inner products between pairs of vectors in F.'''
    M = np.zeros([k*(k-1),k*(k-1)])
    for i in range(0,k*(k-1)):
        for j in range(0,k*(k-1)):
            M[i,j] = np.sum(F[i]*F[j])
    '''Subtracts lam*I from M.'''
    M = M - lam*np.eye(k*(k-1))
    return M
```

To illustrate the performance of the algorithm and the results it produced we will provide several examples of input and output. The input will each time consist of a starting matrix M_0, which also fixes the size N of the matrices over which we optimize, and the dimension n of the vectors used to approximate quantum values. In these examples we have chosen $n = N + 1$ and the starting matrices M_0 were randomly generated using the described procedure.

9.2 Results for 2×2 matrices

If we optimize $LV(M)$ over 2×2 matrices using vectors in $\mathbb{R}^3$ for approximating $\omega^*(M)$ and use the following matrix as starting value:

$$M_0 = \begin{pmatrix} 0.86886844 & 0.86173587 \\ 0.4383951 & 0.07197179 \end{pmatrix}, \tag{296}$$

the algorithm returns -1.4142133636010936 as its approximation of $-K_2$. This value agrees with $-\sqrt{2}$, the real value of $-K_2$, to 6 decimal places. The algorithm finds this minimum as $-LV(M)$, where M is given by:

$$M = \begin{pmatrix} 0.43897087 & 0.43897095 \\ 0.43897087 & -0.43897103 \end{pmatrix}. \tag{297}$$

We note that M is almost equal to a rescaled version of M_{CHSH}, explaining why $-LV(M)$ is almost equal to $-\sqrt{2}$. The algorithm took 7.7389042 seconds to perform this particular optimization.

9.3 Results for 3×3 matrices

As an another example we run the algorithm with 3×3 matrices and vectors in $\mathbb{R}^4$ with starting matrix:

$$M_0 = \begin{pmatrix} -0.21644749 & -0.83806447 & -0.08462567 \\ -0.87560947 & -0.06566203 & -0.89925771 \\ -0.1488139 & 0.5072271 & 0.39554632 \end{pmatrix}. \tag{298}$$

The algorithm returns -1.3127534836781058, which is $-LV(M)$ where

$$M = \begin{pmatrix} 0.40158651 & -0.3123819 & -0.08920489 \\ -0.55040048 & -0.06564923 & -0.48475118 \\ -0.1488139 & 0.24673272 & 0.39554629 \end{pmatrix}, \tag{299}$$

as an approximation of $-K_3$. This differs significantly from $-\sqrt{2}$, the real value of $-K_3$. This run took 152.3407607 seconds and the algorithm unfortunately failed to find a global minimum. We ran the algorithm again, this time with starting matrix:

$$M_0 = \begin{pmatrix} -0.45874146 & -0.88363231 & 0.11597403 \\ -0.21065968 & -0.77907307 & 0.06008189 \\ 0.92943898 & -0.96576616 & 0.17289409 \end{pmatrix}. \tag{300}$$

This time the algorithm takes 142.3457634 seconds to find the value -1.4142135355751462 as $-LV(M)$ with

$$M = \begin{pmatrix} -0.71870584 & -0.60331727 & 0.11538856 \\ -0.21041449 & -0.15290799 & 0.0575065 \\ 0.92912032 & -0.75622526 & 0.17289506 \end{pmatrix}. \tag{301}$$

The value found agrees with $-K_3 = -\sqrt{2}$ to 7 decimals, so the algorithm seems to have succeeded in finding a global minimum this time. This illustrates that the algorithm is able to find a global minimum, but is not guaranteed to always do so. Therefore we stress that the algorithm's output should be viewed as an upper bound of $-K_N$ and not necessarily (a good approximation to) $-K_N$ itself. We also advise to let the algorithm run multiple times to be more likely to find a good bound on K_N. This run also gives a 3×3 matrix with a largest violation close to $\sqrt{2}$ that does not resemble M_{CHSH} with added zeros. We also note that increasing the matrix size and the dimension of the vectors significantly increases the typical runtime of the algorithm.

9.4 Results for 4×4 matrices

As an example of a run with 4×4 matrices and vectors in $\mathbb{R}^5$ we started with the matrix:

$$M_0 = \begin{pmatrix} -0.71001942 & 0.22106513 & -0.30260331 & 0.43747759 \\ 0.60207936 & 0.1379811 & 0.29031476 & 0.6619015 \\ 0.4777203 & 0.20907129 & 0.58707658 & -0.58041805 \\ -0.04101268 & -0.1157671 & 0.31224929 & 0.25799558 \end{pmatrix}. \quad (302)$$

For this run the algorithm took 1957.2352031 seconds to find the value -1.2804075280622145 as $-LV(M)$ with

$$M = \begin{pmatrix} -0.1612881 & 0.22692921 & -0.30259406 & 0.23888188 \\ 0.53871803 & 0.13171277 & 0.25480289 & 0.6619015 \\ 0.47589537 & 0.20905196 & 0.31357465 & -0.58041805 \\ -0.04101533 & -0.11576446 & 0.31224929 & 0.15749178 \end{pmatrix}. \quad (303)$$

Since $K_4 \geq \sqrt{2}$ the algorithm failed to find a global minimum. To summarize we have let the optimization algorithm run multiple times for different values of the matrix size N and the vector dimension n. We have first done this for $n = N + 1$. Because the runtime increases drastically when increasing matrix size and vector dimensions, we have only been able to do this for $n = N+1$ when $N \leq 5$. While during some of the runs the algorithm was able to find a value close to $-\sqrt{2}$, no matrices with largest violation greater than $\sqrt{2}$ were found. We have also tried runs with a fixed low vector dimension and a somewhat larger matrix size. Keeping the vector dimension small improved the runtime and we were able to consider slightly larger matrices. Even when fixing $n = 3$ we were only able to run the algorithm within reasonable time for matrices of size up to $N = 10$. Unfortunately no matrices with largest violation greater than $\sqrt{2}$ were found in these runs either.

10 Further research regarding Grothendieck's constant

With our initial attempts to find a matrix M with $LV(M) > \sqrt{2}$ being unsuccessful, we decided to look at earlier research regarding Grothendieck's constant. We would hope to find an explicit matrix M with known largest violation $LV(M) > \sqrt{2}$. Given such a matrix M we could approximate its largest violation using our algorithm and see if the algorithm gives a good approximation. We could also attempt to make small changes to the matrix M and approximate the largest violation of the resulting matrix, possibly finding a matrix with largest violation greater than that of M. Alternatively, if we were unable to explicitly find such a matrix M, we might at least find out for what matrix size N we might be able to find a matrix with largest violation greater than $\sqrt{2}$. We have looked at two articles that seemed relevant for our purposes. We will briefly summarize the contents of these articles and how they relate to our research.

10.1 A Generalized Grothendieck Inequality and Nonlocal Correlations that Require High Entanglement

We first looked at [5]. This article introduces a variation on Grothendieck's constant and proves a lower bound for it. Using our own notation, this variation on Grothendieck's constant is defined as:

Definition 10.1. For $n, m \in \mathbb{N}$ with $m < n$, let:

$$K_G(n \mapsto m) = \sup \frac{\omega_n^*(M)}{\omega_m^*(M)} \tag{304}$$

with the supremum taken over all non-zero square matrices of arbitrary size with real entries.

We note that $\omega_1^*(M) = \omega(M)$ for any $N \times N$ matrix M. Combining this with the fact that $\omega_n^*(M) \leq \omega^*(M)$, it follows that for all $n \in \mathbb{N}$:

$$K_G(n \mapsto 1) \leq K_G. \tag{305}$$

This means that any lower bound on $K_G(n \mapsto 1)$ is also a lower bound on K_G. In [5] the following lower bound on $K_G(n \mapsto m)$ is stated and proved:

Theorem 10.1.

$$K_G(n \mapsto m) \geq \frac{m}{n} \left(\frac{\Gamma\left(\frac{m}{2}\right)}{\Gamma\left(\frac{m+1}{2}\right)} \frac{\Gamma\left(\frac{n+1}{2}\right)}{\Gamma\left(\frac{n}{2}\right)} \right)^2, \tag{306}$$

where Γ is the gamma function. We hoped to find, somewhere in this proof, a way to explicitly construct a matrix M that would satisfy the inequality in Theorem 10.1 or at least come arbitrarily close to satisfying it. These matrices

appear in the proof of Lemma 2 of [5]. Unfortunately the matrices used in the proof seem difficult to calculate explicitly for use in our algorithm. There are several reasons for this:

1. The construction of the matrices in Lemma 2 relies on the existence of an ϵ-net E_n^ϵ for the surface of an n-dimensional unit sphere S_{n-1}. This is a finite subset of S_{n-1}, such that for each point $x \in S_{n-1}$, there exists a $y \in E_n^\epsilon$ such that $\|x - y\|_2 \leq \epsilon$. The existence of such an ϵ-net is proved in Lemma 3 of [5], but the proof makes use of Zorn's Lemma. This makes the proof of the existence of the ϵ-net non-constructive. Since the matrices used in the proof of Lemma 2 are constructed using the ϵ-net from Lemma 3, this makes the proof of the existence of these matrices non-constructive as well. This means we do not have a way to explicitly construct the matrices we are interested in.

2. It might be possible to alter the proof of Lemma 3 to make it constructive. This would in theory make it possible to explicitly construct the matrices in the proof of Lemma 2. However, these matrices would still be difficult to calculate. To illustrate this we will state how these matrices are defined. Given an ϵ-net $E_n^\epsilon = \{w_1, \ldots, w_k\}$ for S_{n-1}, the sets R_w for $w \in E_n^\epsilon$ are defined as follows. R_w consists of all points in S_{n-1} that are closer to w than to any other $v \in E_n^\epsilon$ with points equidistant to two or more $w \in E_n^\epsilon$ arbitrarily assigned to one of these w. Next for $M' : S_{n-1} \times S_{n-1} \to \mathbb{R}$ a measurable function, the entries of matrices M used in the proof of Lemma 2 are defined as:

$$M_{i,j} = \int_{a \in R_{w_i}} \int_{b \in R_{w_j}} M'(a,b) da db. \tag{307}$$

   These matrix entries are defined as integrals over complicated subsets of spherical surfaces. To use these matrices in our algorithm we would need to approximate these integrals numerically, which would be difficult.

3. Even if we manage to accurately approximate these matrices, they might still not be of much use for us. This is because these matrices might be too large for our algorithm to handle. As part of Lemma 3 of [5], the number of elements in the ϵ-net E_n^ϵ is proved to bounded from above by $\left(\frac{3}{\epsilon}\right)^n$. We note that the n here is the dimension of the vectors used in calculating $\omega_n^*(M)$. Also, for appropriate choice of M', ϵ is related to how close the matrix M (constructed from the measurable function M') comes to satisfying the inequality in Theorem 10.1. The smaller the choice of ϵ, the closer M comes to satisfying this inequality. We see that even for small n and relatively large ϵ, the upper bound $\left(\frac{3}{\epsilon}\right)^n$ allows for matrices that might be larger than our algorithm can handle. Furthermore, we note that this upper bound is proved to hold for the ϵ-net constructed using Zorn's Lemma. Since we would need to alter Lemma 3 to construct an ϵ-net without using Zorn's Lemma, this upper bound might not hold if we construct our ϵ-net in a different way.

Because of the above reasons, we conclude that the matrices used in [5] cannot be used for our research.

10.2 Bell Inequalities, Grothendieck's Constant, and root two

We have also looked at [4]. This article addresses the problem of finding specific $N \times N$ matrices M for which $LV(M) > \sqrt{2}$, indicating that $K_N > \sqrt{2}$. The article mentions that finding these specific examples is surprisingly difficult, which agrees with our own inability to find these specific examples. The article presents a method for constructing specific matrices M and calculates $LV(M)$ for these matrices. For some of these matrices $LV(M) > \sqrt{2}$. We will outline the construction of these matrices and state their largest violations. For the calculation of the largest violations we refer to [4]. For any integer $k \geq 2$, a $k(k-1) \times k(k-1)$ matrix can be constructed using the following procedure. We consider all vectors in $\mathbb{R}^k$ whose entries are all equal to 0 except for two entries. These two entries will either both be equal to 1 or the first will be equal to 1 and the second to -1. There are $k(k-1)$ vectors that meet these requirements. For example for $k = 3$ these vectors are given by $\begin{pmatrix}1\\1\\0\end{pmatrix}$, $\begin{pmatrix}1\\0\\1\end{pmatrix}$, $\begin{pmatrix}0\\1\\1\end{pmatrix}$, $\begin{pmatrix}1\\-1\\0\end{pmatrix}$, $\begin{pmatrix}1\\0\\-1\end{pmatrix}$ and $\begin{pmatrix}0\\1\\-1\end{pmatrix}$. We number these vectors f_1 through $f_{k(k-1)}$ and define a $k(k-1) \times k(k-1)$ matrix M with entries given by:

$$M_{i,j} = \langle f_i, f_j \rangle . \tag{308}$$

The largest violation of a matrix constructed in this way is given by $\frac{3k-3}{2k-1}$ as proved in [4]. The fraction $\frac{3k-3}{2k-1}$ is increasing in k and its limit as $k \to \infty$ is equal to $1.5 > \sqrt{2}$. $k = 10$ is the smallest k for which $\frac{3k-3}{2k-1} > \sqrt{2}$. This gives a way to explicitly construct a 90×90 matrix with largest violation exceeding $\sqrt{2}$. [4] also provides a way to modify the matrices obtained in the procedure described earlier to increase their largest violation. This is done by taking such a matrix M and replacing it with $M - \lambda I$ for a constant λ and I the identity matrix. It is shown in [4] that for $k \in \{3, 4, 5\}$ the optimal choice for λ is given by $\lambda = \frac{4}{3}$. This is equivalent to replacing each diagonal entry of M, which are all equal to 2, by $\frac{2}{3}$. The largest violation of the modified matrix is given by $\frac{3k-5}{2k-3}$ for $k \in \{3, 4, 5\}$. For $k \in \{3, 4\}$ this fraction is still smaller than $\sqrt{2}$, but for $k = 5$ this fraction equals $\frac{10}{7} > \sqrt{2}$. This gives a 20×20 matrix with largest violation greater than $\sqrt{2}$, showing that $K_{20} > \sqrt{2}$. This matrix can be found explicitly in [4] as Figure 1. This 20×20 matrix would serve as a good starting point to search for more matrices with larger violation greater than $\sqrt{2}$, possibly even exceeding $\frac{10}{7}$. Unfortunately we have found that 20×20 matrices are too large to handle for our algorithm. The largest violation of the matrices in [4]

could be calculated by relying on the specific way in which these matrices were constructed. However, if we start making changes to these matrices we can no longer rely on this. We have found that the time it takes for us to calculate the classical value of an arbitrary $N \times N$ matrix M increases exponentially in N. Increasing N by 1, increases the time it takes to calculate the classical value by approximately a factor 4. Using this to extrapolate the runtimes for smaller matrices we estimate that it would take about 75 days to calculate the classical value of a 20×20 matrix. Approximating the quantum value would probably take even longer, so unfortunately it does not seem feasible to calculate the largest violation of 20×20 matrices using our methods. We were able to calculate the largest violations of the matrices constructed in [4] for $k \leq 4$ with our algorithm and our results agreed with [4]. We note that 20×20 matrices have associated Bell inequalities with up to 400 terms. The violation of these Bell inequalities would probably involve much more complicated experimental setup than the CHSH-inequality and would therefore not be very suitable for practical experiments.

11 Conclusion

As stated in Grothendieck's theorem, $LV(M)$ is bounded when considering square matrices M of arbitrary size with real entries. The smallest upper bound for $LV(M)$ is given by the Grothendieck's constant K_G. It is known that

$$1.67696\cdots \leq K_G \leq \frac{\pi}{2\log\left(1+\sqrt{2}\right)} \approx 1.7822139781. \tag{309}$$

$M_{CHSH} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ is a matrix with $LV(M_{CHSH}) = \sqrt{2}$. Even though it is easy to find a matrix with largest violation equal to $\sqrt{2}$, finding an explicit matrix M with $LV(M) > \sqrt{2}$ has proven to be a difficult problem.

We have attempted to find such a matrix using optimization algorithms. We are, in theory, able to calculate exactly the classical value of any matrix M. The time this takes increases exponentially in the matrix size N, with the calculation time increasing by a factor 4 when increasing N by 1. This makes it impractical to calculate classical values for large matrices using our method. We are also able to approximate the quantum value of a matrix M from below, using an optimization algorithm. For matrices with an exactly known quantum value, such as the CHSH-matrix and the matrices constructed in [4], the approximations provided by this algorithm seem accurate (up to 11 decimal places for M_{CHSH}). Approximating the quantum value generally seems to take at least as long as calculation the classical value and is therefore alo impractical for large matrices.

Combining these two procedures allows us to (presumably accurately) approximate the largest violation of a matrix from below. Subsequently we can optimize the largest violation of matrices of a fixed size, giving us a lower bound on Grothendieck's constant. This process can take a long time depending on the matrix size N and on the dimension n of the vectors used to approximate quantum values. This process can be completed within a reasonable amount of time (at most about 1 day) when $N \leq 5$ and $n = N+1$. If n is fixed, N can be taken a bit larger. For $n = 3$, the process can be completed within a reasonable time for $N \leq 10$. The lower bounds found for Grothendieck's constant depend strongly on the matrix used as starting point for the optimization algorithm. Therefore the lower bound found when running the algorithm once, is not guaranteed to be accurate for that matrix size. It is therefore advised to run the algorithm multiple times with different starting matrices. Using our optimization algorithms, we were unable to find any matrix M with $LV(M) > \sqrt{2}$.

[4] provides a method for constructing matrices with known largest violations. For sufficiently large matrices this includes matrices with largest violation exceeding $\sqrt{2}$. The smallest matrix provided in [4] with largest violation exceeding $\sqrt{2}$ is of size 20×20. These matrices are too large for us to calculate largest violations, so we have not been able to calculate the largest violation of other

20×20 matrices in an attempt to improve on the results in [4].

The calculation of largest violations of matrices as we have done it seems sufficiently accurate, but not fast enough to find matrices with largest violation exceeding $\sqrt{2}$. If a significantly faster implementation of a similar process is realized, or a faster computer is used, it might be possible to use this process to more success. If the optimization process for largest violations is to be used in further research, it should ideally be improved in a way to not depend so strongly on the starting matrix. If sufficient improvements can be made to the optimization processes to significantly decrease the running time of the algorithms, we suggest to look into 20×20 matrices for further research. As it is not clear if the matrix presented in [4] attains the greatest largest violation for 20×20 matrices, it might be possible to find a 20×20 matrix with even greater largest violation. A good starting point might be to consider matrices obtained by slightly modifying the matrix in [4], to see if this matrix is a (local) maximum for the largest violation or not.

References

[1] Michael A. Nielsen and Isaac L. Chuang (2010). *Quantum Computation and Information*. Cambridge University Press.

[2] Carlos Palazuelos (2013). *Introduction to Quantum Information Theory*. Instituto de Ciencias Matemáticas.

[3] Martijn Caspers (2019). *14 lectures on operator algebras, dilation theory and quantum information*.

[4] P. C. Fishburn and J. A. Reeds (1994). Bell Inequalities, Grothendieck's Constant, and root two. *SIAM J. Discrete Math. 7 (1994), no. 1*, 48–56.

[5] Jop Briët, Harry Buhrman and Ben Toner (2011), A Generalized Grothendieck Inequality and Nonlocal Correlations that Require High Entanglement. *Comm. Math. Phys. 305 (2011), no. 3*, 827–843

[6] A.P. Aspect, G. Grangier, G. Roger (1982), Experimental Realization of Einstein-Podolsky-Rosen-Bohm Gedankenexperiment: A New Violation of Bell's Inequalities. *Phys. Rev. Lett. 49 (2),* 91-94.

[7] B. Hensen, H. Bernien, A.E. Dréau, A. Reiserer, N. Kalb, M.S. Blok, J. Ruitenberg, R.F.L. Vermeulen, R.N. Schouten, C. Abellán, W. Amaya, V. Pruneri, M. W. Mitchell, M. Markham, D.J. Twitchen, D. Elkouss, S. Wehner, T.H. Taminiau, R. Hanson (2015) Loophole-free Bell inequality violation using electron spins separated by 1.3 kilometres. *Nature 526 (7575)*, 682–686, published online October 21, 2015.