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Uncertainty relations for complementary unitary matrices

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BAKALÁŘSKÁ PRÁCE

Relace neurčitosti pro komplementární unitární matice

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Declaration

I hereby declare that the thesis entitled "Uncertainty relations for complementary unitary matrices " has been composed solely by myself under the guidance of doc. Mgr. Ladislav Mišta Ph.D. by using resources, which are referred to in the list of literature. I agree with the further usage of this document according to the requirements of the Department of Optics.

In Olomouc May 15, 2024

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Abstract	The importance of the uncertainty principle is unquestionable. Not only does it capture the fundamental nature of many quantum systems, but it also presents important limitations relevant to many technical applications, such as quantum cryptography. A primitive for studying the incompatibility of physical quantities and the corresponding uncertainty relations is the pair of complementary unitary matrices. For this pair one can formulate uncertainty relations [1, 2] as well as a quantum-mechanical representation for a general quantum system with finite-dimensional Hilbert state space. Remarkably, the uncertainty in any unitary operator has direct physical meaning, and moreover, by taking a proper limit, one can obtain the standard complementary observables and the respective representations for basic quantum systems with infinite-dimensional Hilbert state space [3]. Given the efforts aimed at developing the formalism based on complementary unitary matrices, it might seem that this topic has been exhausted, but this is not the case. The purpose of this thesis is to explore the uncertainty relation and more general uncertainty principle for a pair of complementary unitary matrices. The objectives include examining an appropriate uncertainty measure for the unitary operators, establishing the corresponding uncertainty relations, and investigating the properties of minimum uncertainty states. Through a systematic analysis, this work aims to improve our understanding of the uncertainty principle and the minimum uncertainty states.
Keywords	complementarity, unitary matrices, uncertainty measure, uncertainty principle, minimum uncertainty states, quantum mechanics
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Abstrakt	Význam principu neurčitosti je nezpochybnitelný. Nejenže vystihuje základní povahu mnoha kvantových systémů, ale představuje také důležitá omezení pro mnoho technických aplikací, jako je například kvantová kryptografie. Základním modelem pro studium nekompatibility fyzikálních veličin a odpovídajících relací neurčitosti je dvojice komplementárních unitárních matic. Pro tuto dvojici lze formulovat relace neurčitosti [1, 2] i kvantově-mechanickou reprezentaci pro obecný kvantový systém s konečně-rozměrným Hilbertovým stavovým prostorem. Neurčitost v libovolném unitárním operátoru má bezprostřední fyzikální význam, a navíc lze po provedení vhodné limity získat standardní komplementární pozorovatelné a příslušné reprezentace pro základní kvantové systémy s nekonečně rozměrným Hilbertovým stavovým prostorem [3]. Účelem této bakalářské práce je prozkoumat relace neurčitosti a obecnější princip neurčitosti pro dvojici komplementárních unitárních matic. To zahrnuje studium správné míry neurčitosti pro unitární operátory a nalezení příslušných relací neurčitosti, jakožto i odpovídajících stavů, které je saturují. Tato práce si prostřednictvím systematické analýzy klade za cíl zlepšit naše chápání principu neurčitosti a odpovídajících stavů neurčitost minimalizujících.
Klíčová slova	komplementarita, unitární matice, míra neurčitosti, princip neurčitosti, stavy minimalizující neurčitost, kvanová mechanika
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Contents

Motivation

A great truth is a truth whose
opposite is also a great truth.

Niels Bohr

It was in September 1927 in Como, Italy, during the International Congress of Physics, that Niels Bohr for the first time introduced in a public lecture his formulation of complementarity [4, 5] - the concept which has no classical analogue and therefore underlies one of the major differences between classical and quantum mechanics. Bohr has pointed out that quantum systems have properties which are equally real but mutually exclusive. The complementary nature of quantum systems is expressed by the uncertainty principle. First formulated by Kennard [6] (and understood by Heisenberg [7]) was the uncertainty relation:

$$\left\langle (\Delta x)^2 \right\rangle \left\langle (\Delta p)^2 \right\rangle \geq \frac{\hbar^2}{4}, \tag{1}$$

which imposes fundamental limitation on variances $\langle(\Delta x)^2\rangle = \langle(x^2\rangle - \langle x\rangle^2$ and $\langle(\Delta p)^2\rangle = \langle p^2\rangle - \langle p\rangle^2$ of position x and momentum p respectively, that any quantum state of a particle can simultaneously have.

In general, uncertainty relations are fundamental principles that are crucial to our understanding of quantum mechanics and have broad relevance to theoretical and practical applications. They highlight the inherently probabilistic nature of quantum mechanics and raise questions about the nature of quantum measurement and the role of observers in quantum systems. They are central to the development of quantum technologies such as quantum cryptography, particularly in quantum key distribution (QKD) protocols [8], where they enable secure communication, and quantum tomography [9], where they provide fundamental constraints on the precision of measurements necessary to reconstruct accurate quantum states from experimental data.

In this work, we investigate complementarity and the associated uncertainty relation using unitary matrices U and V in the finite-dimensional Hilbert space. The advantage of describing quantum systems with unitaries lies in the fact that in the corresponding uncertainty relations, the general eigenvalues (found in Hermitian operators) do not play a role. Thus we get base-dependent relations that are not affected by eigenvalues. In addition, the pair U, V functions as a primitive for studying the incompatibility of physical observables, since any observable can be decomposed into them similarly to the case of the classical phase-space quantities.

However, the use of this non-standard description through complementary unitary matrices gives rise to several questions, such as how one can quantify the uncertainty of the unitary matrix in a given state, how this measure can be interpreted, and whether it has a direct physical meaning. We address these questions and show through mathematical analysis how one can derive the associated uncertainty relations as well as a quantum-mechanical representation for a general quantum system with finite-dimensional Hilbert state space.

This thesis is organized as follows. In Chapter 1, we give a brief introduction to quantum mechanics, the mathematical description of complementary variables and finally introduce the pair of unitary complementary matrices U and V under study. Chapter 2 is devoted to the dispersion as the most commonly used uncertainty measure for unitary operators. We also show how it satisfies the essential properties of a proper uncertainty measure. Chapter 3 presents the main results of this thesis. We first show a mechanical interpretation of the dispersion of a unitary matrix. Then we derive a set of inequalities for the moments of the matrices U and V, which play the role of uncertainty principle in a finite-dimensional Hilbert space. We investigate the simplest nontrivial uncertainty relation and study the properties of the corresponding minimum uncertainty states (MUS)[1]. In Appendix A we show a detailed computation of certain mathematical objects that appeared in the Chapter 3. To conclude, in Appendix B we give a simple example concerning the two-dimensional limit, for which the U, V pair takes the form of the σ_x and σ_z Pauli matrices.

[1]In this thesis, the term 'minimum uncertainty states' refers to states for which the uncertainty inequality is saturated. In the existing literature, however, 'MUS' is often used to refer to states that minimize the uncertainty of one observed quantity relative to the uncertainty of another [3].

Chapter 1

Introduction

The primary objective of this thesis is to investigate an issue rooted in modern physics. Therefore we begin this chapter with Sec. 1.1, briefly introducing the key concepts of quantum mechanics, that will form the basis of our research. Then we focus on the fundamental principle of complementarity. In Sec. 1.2 we examine its mathematical foundations in detail and in Sec. 1.3 we introduce a particular pair of unitary matrices U and V, crucial to our analysis.

1.1 Introduction to quantum mechanics

1.1.1 State vectors, operators and quantum measurement

In quantum mechanics we associate with every physical system a Hilbert space $\mathcal{H}$, which is a complete inner product space. Here we are interested in systems with finite dimension, $\dim \mathcal{H} = N \in \mathbb{N}$, i.e. $\mathcal{H} = \mathbb{C}^N$. State of such a system is represented by a vector. Following Dirac's notation, we denote this vector $|\psi\rangle$ and postulate it to contain maximal accessible information about the quantum-mechanical system. Given that $|\psi\rangle$ and $c\,|\psi\rangle$, with c being any non-zero complex number, represent the same physical state, we are working with rays rather than vectors [10].

There are two important classes of operators in quantum mechanics encompassing Hermitian and unitary operators. Physical observables are represented by Hermitian operators, which are bounded linear operators on the considered Hilbert space $\mathcal{H}$ that are equal to their Hermitian adjoint (A is Hermitian if and only if $A^\dagger = A$). The eigenvalues of such operators are real and their eigenvectors can always be chosen as normalized and mutually orthogonal, in other words othonormal, forming the basis of the Hilbert space $\mathcal{H}$ under consideration. [11].

Unitary operators are used to change from one orthonormal basis to another, to represent symmetries such as rotational symmetry, or to describe a time evolution of a quantum system while preserving the inner product [10]. The eigenvalues of unitary operators are complex numbers of magnitude 1, i.e., they lie on the complex unit circle. Their eigenvectors can be chosen as to form a basis in a similar way to the eigenvectors of Hermitian operators (this is no coincidence, both of these types of operators fall under the class of normal operators that commute with their Hermitian adjoint, and the orthonormality property of their eigenvectors can always be satisfied). We say, that U is unitary if and only if $U^\dagger U = UU^\dagger = \mathbb{1}$, where $\mathbb{1}$ is the identity operator [11].

Once we perform a measurement on a quantum system, we cause the state of the measured system to transition (collapse) into an eigenstate of the operator corresponding to the measured quantity. The measured value is then the eigenvalue of the operator. It turns out that some physical properties cannot be measured silmutaneously, that is, they are not diagonal in the same basis and cannot be both known with an arbitrary accuracy. This issue will be further discussed in Sec. 1.2.

1.1.2 Density matrix

Let us consider an ensemble of quantum systems all in the same state $|\psi\rangle$. We say that the system is then in a pure state. The expectation value of an observable A in the pure state $|\psi\rangle$ is given by

$$\langle A\rangle_{|\psi\rangle} = \langle\psi|A|\psi\rangle\,, \tag{1.1}$$

which can be equivalently written as

$$\langle A\rangle_{|\psi\rangle} = \mathrm{Tr}(A\,|\psi\rangle\langle\psi|), \tag{1.2}$$

where the symbol Tr(.) stands for the trace.

However, pure states are an idealized description not fully characterizing statistical mixtures often found in experiments. In a situation where N_i systems of the ensemble are in a state $|\psi_i\rangle$, such that $\sum_i N_i = N$, the probability p_i of obtaining an individual system described by the state $|\psi_i\rangle$ is then as follows:

$$p_i = \frac{N_i}{N}, \quad \text{where} \quad \sum_i p_i = 1. \tag{1.3}$$

We then say that the system is in the mixed state, which is characterized by the so-called density matrix

$$\rho = \sum_i p_i\,|\psi_i\rangle\langle\psi_i|\,. \tag{1.4}$$

The expectation value of the observable A in the density matrix ρ is then given by

$$\langle A\rangle_\rho = \mathrm{Tr}(\rho A). \tag{1.5}$$

It is essential to point out the following properties of the density matrix ρ:

1. *Hermicity*
$$\rho^\dagger = \rho. \tag{1.6}$$

2. *Positive-semidefiniteness*
$$\rho \geq 0. \tag{1.7}$$

3. *Normalization*
$$\mathrm{Tr}\,\rho = 1. \tag{1.8}$$

Finally, it's worth noting that for pure ensembles, the equality $\rho^2 = \rho$ holds, and the quantity $\mathrm{Tr}(\rho^2)$, known as purity, equals 1. For mixed ensembles, purity is a positive number less than one [12].

1.2 Complementarity

Following the Ref. [10], consider a sequence of measurements of properties A and B on a quantum system. Suppose A is measured first, yielding result a'. Subsequently, B is measured, resulting in b'. Finally, A is measured again. If A and B are compatible observables, the third measurement always yields a' with certainty, meaning the second (B) measurement does not destroy the information obtained in the first (A) measurement. When the eigenvalues of A are non-degenerate, this implies:

$$|\alpha\rangle \xrightarrow{A \text{ measurement}} |a', b'\rangle \xrightarrow{B \text{ measurement}} |a', b'\rangle \xrightarrow{A \text{ measurement}} |a', b'\rangle\,, \tag{1.9}$$

where $|\alpha\rangle$ is the initial state of the system and $|a', b'\rangle$ is a simultaneous eigenket of A and B, i.e., $A\,|a', b'\rangle = a'\,|a', b'\rangle$, $B\,|a', b'\rangle = b'\,|a', b'\rangle$. For compatible observables, the commutator $[A, B]$, defined as

$$[A, B] = AB - BA, \tag{1.10}$$

is equal to zero.

However, if $[A, B] \neq 0$, A and B do not share a common eigenbasis and the third measurement does not result in a'. In this case, we say that the pair A and B is incompatible. Under the formulations by Weyl [13], Schwinger [14], and Durt [15], we refer to this incompatible pair as complementary if

1. their eigenvalues are non-degenerate (allowing for the complete set of N distinct possible measurement outcomes),

2. the sets of normalized vectors $|a_j\rangle$ and $|b_k\rangle$ that describe states with predictable measurement outcomes for A and B, respectively, are mutually unbiased. That is, the transition probabilities from each state in one basis to all states of the other basis are the same irrespective of which pair of states is chosen, [2]

$$|\langle a_j|b_k\rangle|^2 = \frac{1}{N} \quad j, k = 1, 2, \ldots, N. \tag{1.11}$$

To summarize, if the physical system is prepared in a state of the first basis (property A is known), then all outcomes are equally probable when we conduct a measurement that probes for the states of the second basis (property B is completely unknown). This situation is symmetrical, it does not matter from which of the two bases we choose the prepared state and which is the other basis being measured.

In technical terms, A and B are normal operators, that is, they are continuous linear operators that commute with their Hermitian adjoints, i.e. $AA^\dagger = A^\dagger A$ and $BB^\dagger = B^\dagger B$ [16]. Their eigenvectors $|a_j\rangle$ and $|b_k\rangle$ make up two bases which are orthonormal and complete,

$$\langle a_j|a_k\rangle = \delta_{j,k} = \langle b_j|b_k\rangle\,, \quad \sum_{j=1}^{N} |a_j\rangle\langle a_j| = \mathbb{1} = \sum_{k=1}^{N} |b_k\rangle\langle b_k|\,, \tag{1.12}$$

where $\mathbb{1}$ is the identity operator and $\delta_{j,k}$ is the Kronecker symbol, that is $\delta_{j,k} = 1$ for $j = k$, otherwise $\delta_{j,k} = 0$.

[2] Familiar examples of mutually unbiased bases are the ones of position and momentum for a particle moving along a line, and of the spin-$\frac{1}{2}$ particle for two perpendicular directions [15].

It can be shown [15] that for each quantum degree of freedom, there is a pair of complementary observables and that this pair parameterizes the degree of freedom completely, in other words, all other operators are functions of this pair.

1.3 Complementary unitary matrices

Following the formalism developed in [15], we represent complementary quantities by unitary operators U and V. These are non-degenerate cyclic $N \times N$ matrices [3] with period N, that is, they have non-degenerate spectra and satisfy the cyclicity conditions,

$$U^N = \mathbb{1}, \quad V^N = \mathbb{1}, \tag{1.13}$$

with products of fewer than N factors not equaling the identity. The eigenvalues of U and V are then the N different Nth roots of unity:

$$U\,|u_j\rangle = \gamma_N^j\,|u_j\rangle\,, \quad V\,|v_k\rangle = \gamma_N^k\,|v_k\rangle\,, \tag{1.14}$$

where $\gamma_N = e^{i\frac{2\pi}{N}}$. Further we assume that the matrices U and V are such that the bases formed by their eigenvectors $|u_j\rangle$ and $|v_k\rangle$ are related by a discrete quantum Fourier transform:

$$|u_j\rangle = \frac{1}{\sqrt{N}}\sum_{k=1}^{N} \gamma_N^{-jk}\,|v_k\rangle\,, \tag{1.15}$$

so that

$$\langle u_j|v_k\rangle = \frac{1}{\sqrt{N}}\gamma_N^{jk} \quad \text{for } j,k = 1,2,\ldots,N. \tag{1.16}$$

As anticipated, these two bases are mutually unbiased. Thus the cyclic matrices U and V as introduced above serve as unitary shift operators that permute vectors of the respective other basis cyclically (cf. Fig. 1.1):

$$U\,|v_k\rangle = |v_{k+1}\rangle \quad \text{for } k = 1,2,\ldots,N-1, \quad U\,|v_N\rangle = |v_1\rangle\,, \tag{1.17}$$

as well as

$$V\,|u_j\rangle = |u_{j-1}\rangle \quad \text{for } j = 2,3\ldots,N, \quad V\,|u_1\rangle = |u_N\rangle\,. \tag{1.18}$$

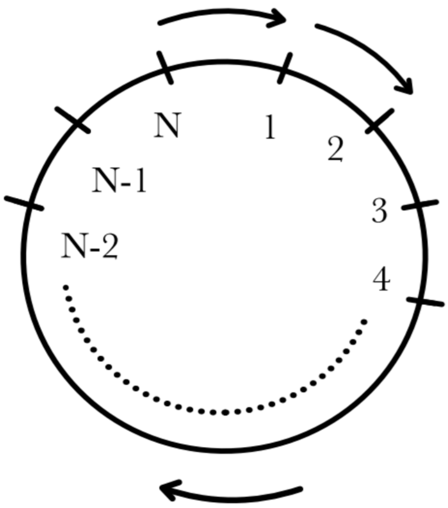


Figure 1.1: Permutation of the V-basis vectors by the matrix U, inspired by [14].

[3]Here N is the dimension of the Hilbert space $\mathcal{H}$ under consideration

The commutation relation is determined by the Weyl commutator $VU = \gamma_N UV$. However, it is more generally stated as

$$V^m U^n = \gamma_N^{mn} U^n V^m, \tag{1.19}$$

valid for all positive and negative integers m and n. Following the fact that all operators are functions of a complementary pair (U and V comprise an operator basis on $\mathcal{H}$), we state that one can express an arbitrary $N \times N$ matrix F as [17]

$$F = \sum_{k,l=1}^{N} f_{kl} V^k U^l, \tag{1.20}$$

where the coefficients f_{kl} are given by

$$f_{kl} = \frac{1}{N} \mathrm{Tr}(V^{-k} F U^{-l}). \tag{1.21}$$

Chapter 2

Uncertainty measures

In this chapter, we introduce the dispersion, the measure of uncertainty for unitary operators, as our tool, to investigate uncertainty relations for unitary complementary matrices. We justify this choice by showing that the dispersion satisfies the essential properties of a proper uncertainty measure and also by giving its direct physical meaning. In Chapter 3 we further show that the dispersion allows a mechanical interpretation as the moment of inertia of equidistantly distributed point masses on a unit ring.

2.1 Dispersion

The dispersion ΔU^2 of a unitary matrix U is defined as [18]

$$\Delta U^2 := \langle U^\dagger U\rangle - \langle U^\dagger\rangle\langle U\rangle = 1 - |\langle U\rangle|^2, \quad \Delta U^2 \in \mathbb{R}. \tag{2.1}$$

It is worth mentioning that this definition is a straightforward generalisation of the variance, which, for unitary operators, can generally yield complex values. Also, note, that the dispersion is bounded as $0 \leq \Delta U^2 \leq 1$, since $|\langle U\rangle|^2 \geq 0$ holds and by the Cauchy-Schwarz inequality and Eq (1.1):

$$|\langle U\rangle|^2 = |\langle\psi|U|\psi\rangle|^2 \leq \||\psi\rangle\|^2 \|U|\psi\rangle\|^2 = \||\psi\rangle\|^2 \langle\psi|U^\dagger U|\psi\rangle = 1, \tag{2.2}$$

where we considered the expectation value of the operator U in the normalized state vector $|\psi\rangle$.

While there is no unique way of quantifying uncertainty, all proper uncertainty measures have the following properties [3]:

U.1 They are well-defined and assign a nonnegative number to every distribution of the random variable,

U.2 they acquire the minimal value (usually = 0) in all limits of a sharp distribution (only one value of the random variable occurs) and only then,

U.3 they should reach their largest value (finite or infinite) in the limit of a uniform distribution,

U.4 they are concave: a convex sum of distributions cannot have an uncertainty measure less than the corresponding average of the uncertainty measures for the ingredient distributions.

As the property **U.1** has already been discussed, let us examine the properties **U.2** and **U.3**. Consider the matrices U and V as introduced in the Section 1.3. The modulus of the average value of U in the eigenstate $|u_j\rangle$, where $j = 1, 2, \ldots, N$, is given by:

$$|\langle U\rangle_{|u_j\rangle}| = |\langle u_j|U|u_j\rangle| = |e^{i\frac{2\pi}{N}j}| = 1 \tag{2.3}$$

and so $\Delta U^2_{|u_j\rangle} = 0$ (minimal value). However, taking the average value of U in the eigenstate $|v_j\rangle$ of the matrix V results in

$$\langle U\rangle_{|v_j\rangle} = \langle v_j|U|v_j\rangle = \frac{1}{N}\sum_{k,l=1}^{N} e^{i\frac{2\pi}{N}j(l-k)}\langle u_k|U|u_l\rangle = \frac{1}{N}\sum_{k=1}^{N} e^{i\frac{2\pi}{N}k} = \frac{1}{N}e^{i\frac{2\pi}{N}}\frac{1-e^{i2\pi}}{1-e^{i\frac{2\pi}{N}}} = 0, \tag{2.4}$$

where we have used the Eq (1.15) to express $|v_j\rangle$ in the $\{|u_j\rangle\}$ basis. We can see that the dispersion of U in the state $|v_j\rangle$ leads to $\Delta U^2_{|v_j\rangle} = 1$ (maximal value).

The property **U.4** simply says, that if the uncertainty relation holds for pure states, then it also holds for mixed states. It can be stated in the following equation:

$$|\langle U\rangle_{\sum_i p_i\rho_i}|^2 \leq \sum_i p_i |\langle U\rangle_{\rho_i}|^2 \tag{2.5}$$

For detailed computation of the latter inequality see Appendix A.1.

2.2 Physical meaning of uncertainty in a unitary operator

Following the References [1, 19], we show that the uncertainty in any unitary operator has a clear physical meaning. It is related to the Fubini-Study metric [20, 21] on the projective Hilbert space $\mathcal{P}(\mathcal{H})$, which is defined as the set of rays of the Hilbert space $\mathcal{H}$, of the quantum system. The Fubini-Study metric for two quantum states $|\psi_1\rangle$ and $|\psi_2\rangle$ is defined as [22, 23]

$$S(\psi_1, \psi_2)^2 = 4(1 - |\langle\psi_1|\psi_2\rangle|^2). \tag{2.6}$$

If we assume $|\psi_1\rangle = U|\psi\rangle$ and $|\psi_2\rangle = V|\psi\rangle$, then the uncertainty in any unitary operator is the distance between the original and the unitarily evolved quantum state (up to a constant factor). The uncertainty relation for two complementary unitary operators then limits how well we can distinguish two different unitary evolutions of a state from the original one.

As a simple application of this result, consider a qubit. In this case the corresponding Hilbert space is a two-dimensional vector space over the complex numbers $\mathcal{H} = \mathbb{C}^2$ and the projective Hilbert space $\mathcal{P}(\mathcal{H}) = \mathcal{P}_1(\mathbb{C})$ is the Bloch sphere. In this instance, an arbitrary state can be expressed as a linear combination of the Pauli matrices σ_x, σ_y and σ_z, together with the identity matrix $\mathbb{1}$. Therefore, we can write:

$$\begin{aligned} \rho_1 = |\psi_1\rangle\langle\psi_1| &= \frac{1}{2}\left(\mathbb{1} + \overrightarrow{\xi_1}\cdot\overrightarrow{\sigma}\right), \\ \rho_2 = |\psi_2\rangle\langle\psi_2| &= \frac{1}{2}\left(\mathbb{1} + \overrightarrow{\xi_2}\cdot\overrightarrow{\sigma}\right), \end{aligned} \tag{2.7}$$

where $\overrightarrow{\xi_1}, \overrightarrow{\xi_2} \in \mathbb{R}^3$ are the Bloch vectors specifying a point on the unit Bloch sphere. Next, considering only the pure states, that is, $\|\overrightarrow{\xi_1}\| = 1$ and $\|\overrightarrow{\xi_2}\| = 1$, we see that

$$\mathrm{Tr}(\rho_1\rho_2) = |\langle\psi_1|\psi_2\rangle|^2 = \frac{1 + \overrightarrow{\xi_1} \cdot \overrightarrow{\xi_2}}{2} = \frac{1 + \cos(\upsilon)}{2}, \tag{2.8}$$

where υ is the angle between $\overrightarrow{\xi_1}$ and $\overrightarrow{\xi_2}$. The Fubini-Study metric defined above then yields

$$S(\psi_1, \psi_2)^2 = 4(1 - |\langle\psi_1|\psi_2\rangle|^2) = 2[1 - \cos(\upsilon)] = \|\overrightarrow{\xi_1} - \overrightarrow{\xi_2}\|^2 \tag{2.9}$$

and so is the Euclidean distance between two points on the unit sphere.

Note, that the dispersion of a unitary matrix U is related to the Fubini-Study metric as $\Delta U^2 = S(|\psi\rangle), U|\psi\rangle)/4$. For a graphical visualisation we refer to Fig. 2.1.

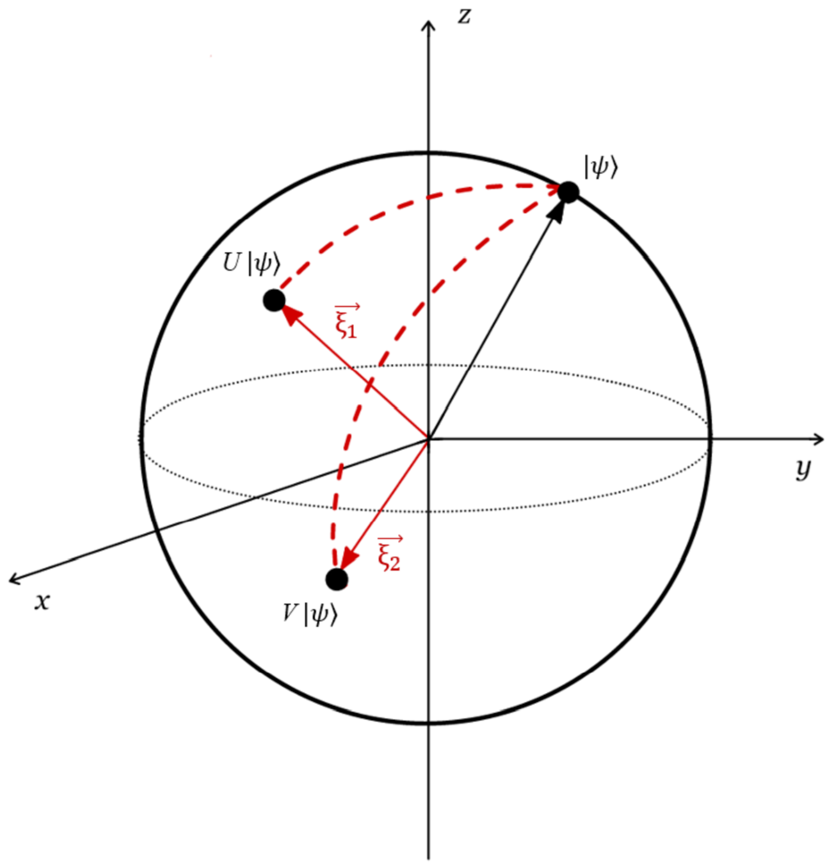


Figure 2.1: Graphical visualisation of unitarily evolved states $U|\psi\rangle$ and $V|\psi\rangle$ from an inital state $|\psi\rangle$ on a Bloch sphere, where $\overrightarrow{\xi_1}, \overrightarrow{\xi_2} \in \mathbb{R}^3$ are their Bloch vectors.

Further, it was noticed, that the interference fringe visibility can be linked to the uncertainty of the unitary operators. If we send a particle in a pure state $|\psi\rangle$ through a Mach-Zehnder interferometer and apply a unitary operator in one arm of the interferometer, then the visibility $\mathcal{V}$ is governed by $\mathcal{V} = |\langle\psi|U|\psi\rangle|$. Thus, we have the relation $\mathcal{V}^2 + \Delta U^2 = 1$ [1, 24, 25]. This illustrates a strong complementarity between the interference visibility and the uncertainty of the unitary operator U.

Chapter 3

Results

This thesis aims to investigate the formalism based on complementary unitary matrices U and V and explore the uncertainty principle for this pair in a more general sense than what is found in the existing literature.

This chapter is divided into the following sections. In Section 3.1 we show a mechanical interpretation of the dispersion of a unitary matrix. In Section 3.2, building upon the conceptual framework outlined in Chapters 1 and 2, we derive a set of inequalities for moments of unitary matrices U and V which comprise a necessary and sufficient condition for a Hermitian trace-one matrix to be a legitimate density matrix of a quantum state. As one of the inequalities, we obtain an uncertainty relation for the sum of dispersions ΔU^2 and ΔV^2, a result that has already been established in [1].[4] In Section 3.2 we shift our focus to the simplest nontrivial case of the uncertainty relation and demonstrate a method for identifying pure states saturating the inequality, i.e. minimum uncertainty states. In Sections 3.4 and 3.5 we analyze the situation for which the corresponding MUS yield equal dispersions $\Delta U^2 = \Delta V^2$. In Section 3.6 we summarize the key findings and explain, why there is a need for further research (while analyzing the special case where $\Delta U^2 = \Delta V^2$ is straightforward, having both operators reach their maximum uncertainty is not ideal). Therefore, in Section 3.7, we explore a general three-dimensional system where we closely examine the dependence of MUS on the parameter characterizing the ratio between ΔU^2 and ΔV^2. Analytical methods are limited, so we provide a graphical visualization illustrating the parameter dependence of the MUS properties as well as the corresponding dispersions.

3.1 Mechanical analogy

As commonly understood, the mechanical analogue of the mean value is the centre of mass. Inspired by the approach [28], we show in this section how the mechanical analogue of the dispersion of a unitary matrix (introduced in Section 2.1), is the moment of inertia.

Consider a system of N point masses in a plane. Each of them has mass m_i, where $i = 1, \ldots, N$, and the total mass is one, $\sum_{i=1}^{N} m_i = 1$ (in the corresponding units). These points are equidistantly distributed around a unit ring of negligible thickness. Assume that the ring rotates about an axis Z passing through its centre of mass G with a moment of inertia I_G with respect to this axis. If the ring rotates about a new

[4] Our derivation is inspired by the derivation of inseparability criteria for two modes based on moments of annihilation and creation operators [26, 27]

axis Z' which is parallel to the original axis but displaced by a distance d and passes through the ring's centre O, then the moment of inertia I with respect to the axis Z' can be determined using the parallel axes theorem [29] as

$$I = I_G + d^2 = 1 \tag{3.1}$$

where we have used the fact that $\sum_j^N m_i r_i^2 = 1$. Let us now consider the unitary matrix U (as introduced in the Section 1.3),

$$U = \sum_j^N e^{i\frac{2\pi}{N}j} |u_j\rangle \langle u_j| .$$

If we consider the following pair of commuting Hermitian matrices:

$$C = \frac{U + U^\dagger}{2}, \quad S = \frac{U - U^\dagger}{2i}, \quad [C, S] = 0. \tag{3.2}$$

we are allowed to decompose the unitary matrix U into its real and imaginary parts:

$$U = C + iS. \tag{3.3}$$

Let us now look at the average value of the matrix U with respect to some state vector $|\psi\rangle$ of the considered system,

$$\langle U\rangle_{|\psi\rangle} = \langle C\rangle_{|\psi\rangle} + i\langle S\rangle_{|\psi\rangle} = \sum_{j=1}^N p_j \overrightarrow{r_j}, \tag{3.4}$$

where the last term on the right-hand side (RHS) is a straightforward consequence of the form of the matrix U, while $p_j = |\langle u_j|\psi\rangle|^2$ is the probability of obtaining the state $|u_j\rangle$ for given $|\psi\rangle$, and the position vector $\overrightarrow{r_j}$ is defined as

$$\overrightarrow{r_j} = \left[\sum_j^N \cos\left(\frac{2\pi}{N}j\right), \sum_j^N \sin\left(\frac{2\pi}{N}j\right) \right]. \tag{3.5}$$

Substituting the term $\sum_{j=1}^N p_j \overrightarrow{r_j}$ in Eq. (3.4) with $\overrightarrow{r_T} = (\mathrm{Re}\langle U\rangle, \mathrm{Im}\langle U\rangle)$ we arrive at the following relation:

$$|\langle U\rangle_{|\psi\rangle}|^2 = \|\overrightarrow{r_T}\|. \tag{3.6}$$

We see that similarly to how the mass points are equidistantly placed on the unit radius ring, the eigenvalues of the matrix U are equidistantly distributed on the complex unit circle. And just as the total mass of the ring is 1, the summation of the probabilities p_j over all j equals 1. These observations prompt us to formulate the following analogy between the moment of inertia of the considered ring I_G with respect to the axis z passing through its centre of mass G and the dispersion ΔU^2:

$$I_G = 1 - |\langle U\rangle_{|\psi\rangle}|^2 = \Delta U^2. \tag{3.7}$$

To better illustrate the idea behind the analogy, we provide a visualisation in Fig. 3.1.

This analogy between the dispersion and the moment of inertia is not only a classical mechanical motivation for the use of dispersion but also a method for potentially introducing additional measures of uncertainty for unitary matrices based on moments of inertia about axes not parallel to the plane of the ring.

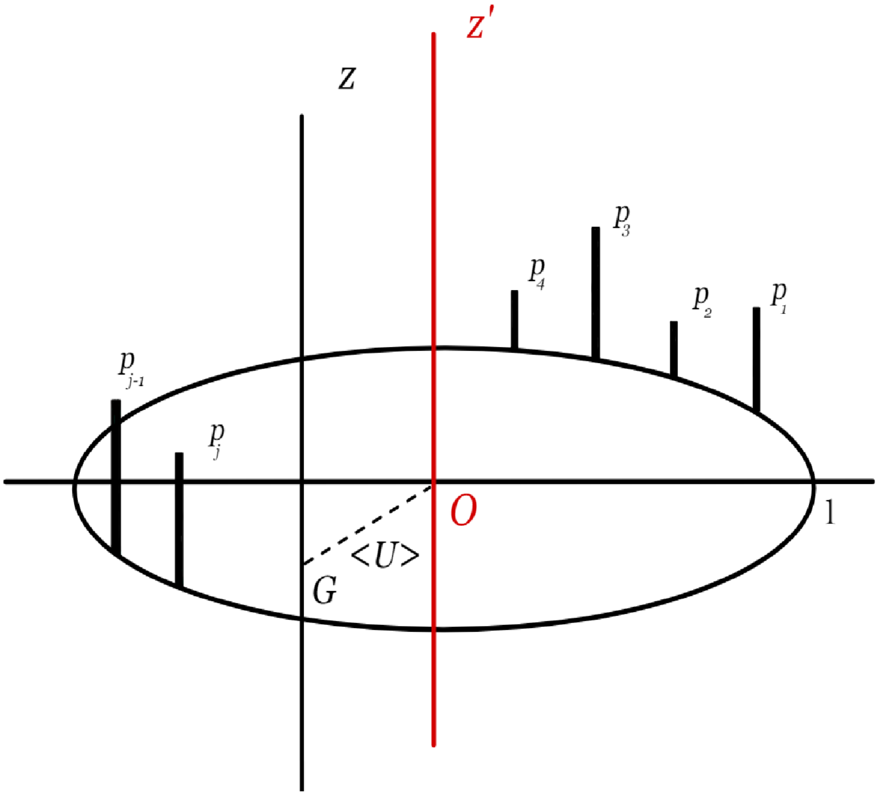


Figure 3.1: Graphical representation of the mechanical analogy between the dispersion $1-|\langle U\rangle_{|\psi\rangle}|^2 = \Delta U^2$ and the moment of inertia I_G with respect to an axis Z passing through the centre of mass G and parallel to the plane of the ring.

3.2 Uncertainty relations for complementary unitary matrices

In Chapter 1, Section 1.1.2 we have shown that a generic quantum state can be described by a density matrix ρ being an $N \times N$ Hermitian, positive-semidefinite trace-one matrix. A Hermitian matrix ρ is positive semi-definite if and only if

$$\langle\psi|\,\rho\,|\psi\rangle \geq 0, \quad \forall\,|\psi\rangle \in \mathcal{H}. \tag{3.8}$$

This condition can be expressed by an equivalent statement saying that a Hermitian matrix ρ is positive-semidefinite if and only if [26]

$$\langle X^\dagger X\rangle = \mathrm{Tr}(\rho X^\dagger X) \geq 0 \tag{3.9}$$

for any $N \times N$ matrix X. Next, making use of the Eqs. (1.20) and (1.21), we express the matrix X in the form

$$X = \sum_{k,l=1}^{N} c_{kl} V^k U^l, \tag{3.10}$$

where

$$c_{kl} = \frac{1}{N}\mathrm{Tr}(V^{-k} X U^{-l}). \tag{3.11}$$

Now we return to the condition of semi-definiteness (3.9) and express the inequality as

$$\langle X^\dagger X\rangle = \sum_{k,l,m,n=1}^{N} c_{kl}^* M_{kl,mn} c_{mn} \geq 0, \tag{3.12}$$

which has to be valid for any vector c, and where

$$M_{kl,mn} = \langle (V^k U^l)^\dagger V^m U^n\rangle = \langle U^{-l} V^{m-k} U^n\rangle = e^{-i\frac{2\pi}{N}l(m-k)}\langle V^{m-k}U^{n-l}\rangle \tag{3.13}$$

is a matrix of moments of U and V.

Given the dependency on four indices in the expression above, we aim to simplify the situation by introducing a unique single number to represent each multi-index (j,k), where $j,k = 1,\dots,N$. Inspired by the approach of Ref. [26] we order the set of multi-indices (j,k), and then replace each multi-index with its ordinal number. More precisely, we use the following rule:

$$(j,k) < (j',k') \iff \begin{cases} j+k < j'+k' & \text{or} \\ j+k = j'+k' & \text{and} \quad j<j', \end{cases} \tag{3.14}$$

which orders the multi-indeces (j,k) as follows

$$\underbrace{(1,1)}_{1} < \underbrace{(1,2)}_{2} < \underbrace{(2,1)}_{3} < \underbrace{(1,3)}_{4} < \underbrace{(2,2)}_{5} < \underbrace{(3,1)}_{6} < \dots \tag{3.15}$$

As a result, we can rewrite the formula (3.12) as

$$\langle X^\dagger X\rangle = \sum_{j,k=1}^{N^2} c_j^* M_{jk} c_k = c^\dagger M c \geq 0, \quad \forall c. \tag{3.16}$$

Therefore, the $N^2\times N^2$ matrix M takes on the following structure (for detailed computation of some of the matrix elements, see Appendix A.2)

$$M = \begin{pmatrix} 1 & \langle U\rangle & \gamma_N\langle V\rangle & \langle U^2\rangle & \dots & \langle U^\dagger V^\dagger\rangle \\ \langle U^\dagger\rangle & 1 & \gamma_N\langle U^\dagger V\rangle & \langle U\rangle & \dots & \langle (U^2)^\dagger V^\dagger\rangle \\ \gamma_N{}^*\langle V^\dagger\rangle & \gamma_N{}^*\langle V^\dagger U\rangle & 1 & (\gamma_N^3)^*\langle U^2 V^\dagger\rangle & \dots & \langle U^\dagger (V^2)^\dagger\rangle \\ \langle (U^2)^\dagger\rangle & \langle U^\dagger\rangle & \gamma_N^3\langle V(U^2)^\dagger\rangle & 1 & \dots & \langle (U^3)^\dagger V^\dagger\rangle \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \langle VU\rangle & \langle VU^2\rangle & \langle V^2 U\rangle & \langle VU^3\rangle & \dots & 1 \end{pmatrix}, \tag{3.17}$$

where $\gamma_N = e^{i\frac{2\pi}{N}}$ as defined in Eq. (1.14).

Let us now discuss some properties of the matrix M. First note, that since $M_{mn,kl}{}^* = M_{kl,mn}$ applies, M is Hermitian, as is also visible from Eq. (3.17). Second, due to the unitary and cyclic nature of U and V, one can express any power of $U^\dagger$ (resp.$V^\dagger$), in terms of a positive power of U (resp. V). Hence, the entire matrix can be described in moments of the form $\langle U^k V^l\rangle$, where $k,l = 1,2,\dots,N$.

Coming back to the Eq. (3.16), we can see that the positive-semidefiniteness condition of the density matrix ρ, Eq. (3.8), can be equivalently expressed as positive-semidefiniteness of the $N^2\times N^2$ Hermitian matrix M, i.e.

$$M \geq 0. \tag{3.18}$$

In what follows, we use the formalism employed in Ref. [27] for a principal minor test to establish a set of inequalities serving as both necessary and sufficient condition for a matrix to be positive semidefinite. These inequalities have the role of an uncertainty principle expressed in terms of a pair of complementary unitary matrices.

Let $M^{\mathbf{r}}$, where $\mathbf{r} = (r_1, r_2, \ldots, r_k)$, with $1 \leq r_1 < r_2 < \ldots < r_k$ and $k = 1, 2, \ldots, N^2$, be a matrix obtained from M by deleting all rows and columns except the ones labelled by $r_1, r_2, \ldots, r_k$. According to Sylvester's criterion [30], a necessary and sufficient condition for the matrix M to be positive-semidefinite is that all possible principal minors are nonnegative, meaning $\det M^{\mathbf{r}} \geq 0$ for any $\mathbf{r}$ introduced above.

Note, that for an $N^2 \times N^2$ matrix M and fixed k, there are $\binom{N^2}{k}$ different kth principle minors. If we sum over all k's, we find that the matrix M possesses altogether $2^{N^2} - 1$ principal minors [31]. The count of principle minors grows rapidly, as for a 4×4 matrix ($N = 2$) it is 15, for a 9×9 matrix ($N = 3$) it is 511 and so on.

To summarize, by applying Sylvester's criterion to the matrix M in Eq. (3.17), the matrix inequality (3.18) extends to a set of $2^{N^2} - 1$ inequalities $\det M^{\mathbf{r}} \geq 0$. Thus, we can formulate a condition that is both necessary and sufficient for a Hermitian $N \times N$ trace-one matrix to qualify as a density matrix of a quantum state in the following manner:

$$\rho \text{ is a density matrix} \iff \det M^{\mathbf{r}} \geq 0 \ \forall \mathbf{r}. \tag{3.19}$$

The set on the RHS represents a complete set of constraints which moments of a pair of complementary unitaries U and V have to obey in order for ρ to be a physical density matrix. For fixed $k = 2$ (principal minors of the second order) the constraints are trivial. For instance, $\det M^{(1,2)} \geq 0$ is equivalent with $1 \geq |\langle U \rangle|^2$ and analogously $\det M^{(1,3)} \geq 0$ with $1 \geq |\langle V \rangle|^2$. Inequalities obtained from the higher-order principal minors may represent true uncertainty relations involving both U and V.

As an illustration, we demonstrate the third-order case. The submatrix under consideration is

$$M^{(1,2,3)} = \begin{pmatrix} 1 & \langle U \rangle & e^{i\frac{2\pi}{N}} \langle V \rangle \\ \langle U^\dagger \rangle & 1 & e^{i\frac{2\pi}{N}} \langle U^\dagger V \rangle \\ e^{-i\frac{2\pi}{N}} \langle V^\dagger \rangle & e^{-i\frac{2\pi}{N}} \langle V^\dagger U \rangle & 1 \end{pmatrix}. \tag{3.20}$$

It is an easy exercise to show that the inequality $\det M^{(1,2,3)} \geq 0$ gives the sum uncertainty relation

$$\Delta U^2 + \Delta V^2 \geq 1 + |\langle U^\dagger V \rangle|^2 - 2\,\mathrm{Re} \langle U \rangle \langle V^\dagger \rangle \langle U^\dagger V \rangle \tag{3.21}$$

which aligns with the uncertainty relation established by [1] through the conventional method employing the Cauchy-Schwarz inequality. In the next section, we examine this simplest nontrivial inequality from the point of view of the states saturating it.

3.3 Minimum uncertainty states

The inequality (3.21) can be equivalently expressed as

$$\Delta U^2 \Delta V^2 \geq |\langle U^\dagger V \rangle - \langle U^\dagger \rangle \langle V \rangle|^2, \tag{3.22}$$

where the details of the derivation can be found in Appendix A.3. To find the pure states saturating the latter inequality we consider the following vectors [1]

$$\begin{aligned} |\psi_U\rangle &= (U - \langle U\rangle)\,|\psi\rangle \\ |\psi_V\rangle &= (V - \langle V\rangle)\,|\psi\rangle\,. \end{aligned} \tag{3.23}$$

As $\|\psi_U\|^2 = \Delta U^2$, $\|\psi_V\|^2 = \Delta V^2$ and $|\langle\psi_U|\,\psi_V\rangle|^2 = |\langle U^\dagger V\rangle - \langle U^\dagger\rangle\langle V\rangle|^2$, we can further write the uncertainty relation as follows:

$$\|\psi_U\|^2\,\|\psi_V\|^2 \geq |\langle\psi_U|\,\psi_V\rangle|^2, \tag{3.24}$$

by using the Cauchy-Schwarz inequality. Note, that equality holds if and only if the vectors $|\psi_U\rangle$ and $|\psi_V\rangle$ are linearly dependent, that is, one is a scalar multiple of the other:

$$|\psi_U\rangle = \lambda\,|\psi_V\rangle\,, \tag{3.25}$$

which yields

$$(U - \lambda V)\,|\psi\rangle = \mu\,|\psi\rangle\,, \quad \lambda \in \mathbb{C}, \tag{3.26}$$

where $\mu = \langle U\rangle - \lambda\langle V\rangle$.

It appears that λ is not only a constant denoting linear dependence, instead, it also reveals a direct connection between the square of its modulus and the ratio of dispersions ΔU^2 and ΔV^2 [5]:

$$|\lambda|^2 = \frac{\Delta U^2}{\Delta V^2}. \tag{3.27}$$

Consequently, if we find MUS satisfying the Eq. (3.26), their dispersions automatically obey the latter equation, whereas the argument of λ is determined as [6]

$$\arg\lambda = 2m\pi - \arg(\langle U^\dagger V\rangle - \langle U^\dagger\rangle\langle V\rangle), \quad m \in \mathbb{Z}. \tag{3.28}$$

It evidently follows that if the vector $|\mu,\lambda\rangle$ satisfies Eq. (3.26), then the vectors of the form $\left|\mu\gamma^{-l}, \lambda\gamma^{-(l+k)}\right\rangle$ also satisfy this equation, whereby:

$$\left|\mu\gamma^{-l}, \lambda\gamma^{-(l+k)}\right\rangle = U^k V^l\,|\mu,\lambda\rangle\,, \quad \text{where} \quad k, l = 1, 2, \ldots, N. \tag{3.29}$$

The expectation values of unitary operators in states $\left|\mu\gamma^{-l}, \lambda\gamma^{-(l+k)}\right\rangle$ (for computation see Appendix A.5) are given by

$$\begin{aligned} \langle U\rangle_{\left|\mu\gamma^{-l},\lambda\gamma^{-(l+k)}\right\rangle} &= \gamma^{-l}\langle U\rangle_{|\mu,\lambda\rangle}, \\ \langle V\rangle_{\left|\mu\gamma^{-l},\lambda\gamma^{-(l+k)}\right\rangle} &= \gamma^{k}\langle V\rangle_{|\mu,\lambda\rangle}, \\ \langle U^\dagger V\rangle_{\left|\mu\gamma^{-l},\lambda\gamma^{-(l+k)}\right\rangle} &= \gamma^{(l+k)}\langle U^\dagger V\rangle_{|\mu,\lambda\rangle}, \end{aligned} \tag{3.30}$$

implying that these states exhibit the same dispersions ΔU^2, ΔV^2, as well as the square modulus $|\langle U^\dagger V\rangle - \langle U^\dagger\rangle\langle V\rangle|^2$, as the original state $|\mu,\lambda\rangle$. Additionally, the latter equation also holds for the replaced values $l \to -l$ and/or $k \to -k$. Hence, upon finding a single MUS for the uncertainty relation (3.22), we inherently ascertain a set of N^2 MUS by using the formula (3.29). What is more, equations (3.30) reveal that

[5] For derivation of relation (3.27) see Appendix A.4.

[6] The reasoning for this is shortly described in Appendix A.4.

the transformation $|\mu,\lambda\rangle \to U^k V^l |\mu,\lambda\rangle$ preserves the absolute value of λ but shifts the argument by $-\frac{2\pi}{N}(l+k)$.

It is evident from the Eq. (3.26) that the MUS $|\mu,\lambda\rangle$ is an eigenvector of the matrix $(U-\lambda V)$ corresponding to the eigenvalue μ, which is dependent on the parameter λ. Note, that the matrix $(U-\lambda V)$ is not normal in general, thus no restrictions are imposed on its eigenvectors. The eigenvalues are found by solving the characteristic equation

$$\det[U-(\lambda V+\mu\mathbb{1})]=0. \tag{3.31}$$

Working in the V-representation:

$$U=\sum_{j=1}^{N}|v_{j+1}\rangle\langle v_j|, \quad V=\sum_{j=1}^{N}e^{i\frac{2\pi}{N}j}|v_j\rangle\langle v_j|, \tag{3.32}$$

we find the characteristic polynomial to be [7]

$$\det\left[U-(\lambda V+\mu\mathbb{1})\right]=(-1)^N\left[\mu^N-(-\lambda)^N-1\right]. \tag{3.33}$$

The latter equation indicates, that μ is an eigenvalue of the matrix $(U-\lambda V)$ if and only if it is a solution of the following equation

$$\mu^N=1+(-\lambda)^N=1+|\lambda|^N e^{iN(\phi+\pi)}. \tag{3.34}$$

In the next two sections, we analyze a special case, in which $|\lambda|=1$. In this instance, the corresponding MUS possess equal dispersions, and as we will demonstrate, both reach their maximal value, i.e. $\Delta U^2=\Delta V^2=1$. To maintain clarity, we study odd and even dimensions separately.

3.4 MUS for even dimensions

For even dimensions, where $N=2l$ and $l=1,2,\ldots$, the Eq. (3.34) simplifies to the following [8]:

$$\mu^{2l}=2\cos(l\phi)e^{il\phi}. \tag{3.35}$$

Assuming $\phi\in[0,2\pi)$ and distinguishing the cases when the RHS of the Eq. (3.35) is zero, positive or negative, we can further rewrite the latter equation as

$$\mu^{2l}=\begin{cases}0 & \text{for } \phi=(2k+1)\frac{\pi}{2l},\ \ k=0,1,\ldots,2l-1,\\ 2\cos(l\phi)e^{il\phi} & \text{for } \phi\in\left[0,\frac{\pi}{2l}\right)\cup\left(\frac{3\pi}{2l},\frac{5\pi}{2l}\right)\cup\ldots\cup\left(2\pi-\frac{\pi}{2l},2\pi\right),\\ 2|\cos(l\phi)|e^{il\phi+i\pi} & \text{for } \phi\in\left(\frac{\pi}{2l},\frac{3\pi}{2l}\right)\cup\left(\frac{5\pi}{2l},\frac{7\pi}{2l}\right)\cup\ldots\cup\left(2\pi-\frac{3\pi}{2l},2\pi-\frac{\pi}{2l}\right),\end{cases} \tag{3.36}$$

and the $2l$th roots of μ^{2l} are

[7] The computation procedure is further elaborated in Appendix A.6.

[8] For detailed computation see Appendix A.7

$$\mu_n = \begin{cases} 0 & \text{for } \phi = (2k+1)\frac{\pi}{2l}, \; k = 0, 1, \ldots, 2l-1, \\ \sqrt[2l]{2\cos(l\phi)} e^{i\frac{\phi}{2}} e^{i\frac{\pi}{l}n} & \text{for } \phi \in \left[0, \frac{\pi}{2l}\right) \cup \left(\frac{3\pi}{2l}, \frac{5\pi}{2l}\right) \cup \ldots \cup \left(2\pi - \frac{\pi}{2l}, 2\pi\right), \\ \sqrt[2l]{2|\cos(l\phi)|} e^{i(\frac{\phi}{2}+\frac{\pi}{2l})} e^{i\frac{\pi}{l}n} & \text{for } \phi \in \left(\frac{\pi}{2l}, \frac{3\pi}{2l}\right) \cup \left(\frac{5\pi}{2l}, \frac{7\pi}{2l}\right) \cup \ldots \cup \left(2\pi - \frac{3\pi}{2l}, 2\pi - \frac{\pi}{2l}\right), \end{cases} \tag{3.37}$$

where $n = 0, 1, \ldots, 2l-1$.

Let us now turn our attention to the simplest case where $\phi = \frac{\pi}{2l}$, and determine the corresponding MUS $\left|0, e^{i\frac{\pi}{2l}}\right\rangle$. Once more, we will initiate our analysis with the equation (3.26), which, when λ and μ are substituted, yields the following form:

$$(U - e^{i\frac{\pi}{2l}} V) \left|0, e^{i\frac{\pi}{2l}}\right\rangle = 0. \tag{3.38}$$

Next, we express matrices U and V by means of Eq. (3.32) and expand the eigenvector $\left|0, e^{i\frac{\pi}{2l}}\right\rangle$ as

$$\left|0, e^{i\frac{\pi}{2l}}\right\rangle = \sum_{j=1}^{2l} c_j \left|v_j\right\rangle \tag{3.39}$$

Through employing the linear independence of the base vectors $\{|v_j\rangle\}$, we derive expressions for the c_j and c_{2l} coefficients

$$\begin{aligned} c_j &= c_{j+1} e^{i\left[\frac{\pi}{l}(j+1)+\frac{\pi}{2l}\right]}, \; j = 1, 2, \ldots, 2l-1, \\ c_{2l} &= c_1 e^{i\left(\frac{\pi}{l}+\frac{\pi}{2l}\right)}, \end{aligned} \tag{3.40}$$

allowing us to determine the c_j coefficient with relation to c_{2l} as

$$c_j = e^{-i\frac{\pi}{2l}j(j+2)}. \tag{3.41}$$

Therefore, we obtain MUS, normalized when $c_{2l} = \frac{1}{\sqrt{2l}}$, for the uncertainty relation (3.22) in even dimensions, corresponding to the parameter $\lambda = e^{i\frac{\pi}{2l}}$ in the following form:

$$\left|0, e^{i\frac{\pi}{2l}}\right\rangle = \frac{1}{\sqrt{2l}} \sum_{j=1}^{2l} e^{-i\frac{\pi}{2l}j(j+2)} \left|v_j\right\rangle \tag{3.42}$$

Now, following the relation (3.29), we aim to find MUS corresponding to different values of λ. If we multiply the Eq. (3.38) with $(U^\dagger)^k$ from the left and use the commutation rule (1.19), we arrive at

$$(U - e^{i\frac{\pi}{2l}(2k+1)} V)(U^\dagger)^k \left|0, e^{i\frac{\pi}{2l}}\right\rangle = 0. \tag{3.43}$$

To ensure consistency in notation, we write the state $(U^\dagger)^k \left|0, e^{i\frac{\pi}{2l}}\right\rangle$ as $\left|0, e^{i\frac{\pi}{2l}(2k+1)}\right\rangle$. Applying $(U^\dagger)^k$ to both sides of Eq. (3.42) then yields

$$\left|0, e^{i\frac{\pi}{2l}(2k+1)}\right\rangle = \frac{1}{\sqrt{2l}} \sum_{j=1}^{2l} e^{-i\frac{\pi}{2l}(j+k)(j+k+2)} \left|v_j\right\rangle. \tag{3.44}$$

Hence,

$$\left\langle 0, e^{i\frac{\pi}{2l}(2m+1)} \middle| 0, e^{i\frac{\pi}{2l}(2n+1)}\right\rangle = \delta_{mn}. \tag{3.45}$$

The eigenvectors $\left|0, e^{i\frac{\pi}{2l}(2k+1)}\right\rangle$, where $k = 0, 1, \ldots, 2l-1$, form an orthonormal basis in the $2l$-dimensional Hilbert state space $\mathcal{H}$ of the considered system. Making use of the complementary nature of U and V along with the Eq. (3.38), it is straightforward to demonstrate that the expectation values in the state $\left|0, e^{i\frac{\pi}{2l}}\right\rangle$ are

$$\begin{aligned} \langle U \rangle_{\left|e^{i\frac{\pi}{2l}}\right\rangle} &= \langle V \rangle_{\left|e^{i\frac{\pi}{2l}}\right\rangle} = 0, \\ \langle U^\dagger V \rangle_{\left|e^{i\frac{\pi}{2l}}\right\rangle} &= e^{-i\frac{\pi}{2l}}. \end{aligned} \tag{3.46}$$

By Eq. (3.44), we observe that the expectation values in states $\left|0, e^{i\frac{\pi}{2l}(2k+1)}\right\rangle$ are given by

$$\begin{aligned} \langle U \rangle_{\left|e^{i\frac{\pi}{2l}(2k+1)}\right\rangle} &= \langle V \rangle_{\left|e^{i\frac{\pi}{2l}(2k+1)}\right\rangle} = 0, \\ \langle U^\dagger V \rangle_{\left|e^{i\frac{\pi}{2l}(2k+1)}\right\rangle} &= e^{-i\frac{\pi}{2l}(2k+1)}, \end{aligned} \tag{3.47}$$

thus we see an alignment with the relations (3.30).

Let us present another intriguing interpretation of MUS (3.44). Firstly, recall that MUS of this form satisfy the following equation:

$$\left(U - e^{i\frac{\pi}{2l}(2k+1)} V\right) \left|0, e^{i\frac{\pi}{2l}(2k+1)}\right\rangle = 0. \tag{3.48}$$

Multiplication of the latter equation by $U^\dagger$ from the left then allows us to write

$$U^\dagger V \left|0, e^{i\frac{\pi}{2l}(2k+1)}\right\rangle = e^{-i\frac{\pi}{2l}(2k+1)} \left|0, e^{i\frac{\pi}{2l}(2k+1)}\right\rangle, \tag{3.49}$$

which reveals that the pure states characterized by the form $\left|e^{i\frac{\pi}{2l}(2k+1)}\right\rangle$, where $k = 0, 1, \ldots, 2l-1$, are also eigenvectors of the unitary matrix $U^\dagger V$ and they thus have to comprise an orthonormal basis.

3.5 MUS for odd dimensions

Let us now consider systems with odd dimensions $N = 2l+1$, where $l = 1, 2, \ldots$, for which the Eq. (3.34) reads

$$\mu^{2l+1} = 2 \sin\left[\left(\frac{2l+1}{2}\right)\phi\right] e^{\left(\frac{2l+1}{2}\right)\phi} e^{i\frac{3}{2}\pi}. \tag{3.50}$$

We adopt the same procedure as in the case of even dimensions and determine the $(2l+1)$th roots of μ^{2l+1} as

$$\mu_n = \begin{cases} 0 & \text{for } \phi = \frac{2k\pi}{2l+1},\ k = 0, 1, \ldots, 2l; \\ \sqrt[2l+1]{2\sin\left[\left(\frac{2l+1}{2}\right)\phi\right]} e^{i\frac{\phi}{2}} e^{i\frac{3\pi}{2(2l+1)}} e^{i\frac{2\pi n}{2l+1}} & \text{for } \phi \in \left[0, \frac{\pi}{2l+1}\right) \cup \ldots \cup \left(2\pi - \frac{4\pi}{2l+1}, 2\pi - \frac{2\pi}{2l+1}\right); \\ \sqrt[2l+1]{2\left|\sin\left[\left(\frac{2l+1}{2}\right)\phi\right]\right|} e^{i\frac{\phi}{2}} e^{i\frac{3\pi}{2(2l+1)}} e^{i\frac{2\pi n}{2l+1}} & \text{for } \phi \in \left(\frac{2\pi}{2l+1}, \frac{4\pi}{2l+1}\right) \cup \ldots \cup \left(2\pi - \frac{2\pi}{2l+1}, 2\pi\right), \end{cases} \tag{3.51}$$

where $n = 0, 1, \ldots, 2l$.

This time we aim to find eigenvectors corresponding to the values $\phi = 0$, $\mu = 0$ and $\lambda = 1$. Substituting λ and μ to the Eq. 3.26 gives

$$(U - V)\left|0, 1\right\rangle = 0. \tag{3.52}$$

We are looking for MUS of the form

$$|0,1\rangle = \sum_{j=1}^{2l} c_j |v_j\rangle \tag{3.53}$$

We find the c_j and c_{2l+1} coefficients expressed as

$$\begin{aligned} c_j &= c_{j+1} e^{i\left[\frac{2\pi}{2l+1}(j+1)\right]}, \ j = 1, 2, \ldots, 2l, \\ c_{2l+1} &= c_1 e^{i\left(\frac{2\pi}{2l+1}\right)}, \end{aligned} \tag{3.54}$$

which yields

$$c_j = e^{-i\frac{\pi}{2l+1}j(j+1)}, \ j = 1, 2, \ldots, 2l \tag{3.55}$$

for the relation between c_j and c_{2l+1} coefficients. By setting $c_{2l+1} = \frac{1}{\sqrt{2l+1}}$ we obtain MUS corresponding to the parameter $\lambda = 1$ for the uncertainty relation (3.22) in odd dimensions in the following form:

$$|0,1\rangle = \frac{1}{\sqrt{2l+1}} \sum_{j=1}^{2l+1} e^{-i\frac{\pi}{2l+1}j(j+1)} |v_j\rangle \tag{3.56}$$

Next, our attention turns to determining MUS corresponding to different values of λ. Employing the same method as in the case of even dimensions, we begin by multiplying the Eq. (3.52) with $(U^\dagger)^k$ from the left and use the commutation rule (1.19):

$$(U - e^{i\frac{2\pi}{2l+1}k} V)(U^\dagger)^k |0,1\rangle = 0. \tag{3.57}$$

The state $(U^\dagger)^k |0,1\rangle$ corresponds to the MUS with $\lambda = e^{i\frac{2\pi}{2l+1}k}$. By applying $(U^\dagger)^k$ to both sides of Eq. (3.56), we arrive at the state $\left|0, e^{i\frac{2\pi}{2l+1}k}\right\rangle$ written in the V-representation:

$$\left|0, e^{i\frac{2\pi}{2l+1}k}\right\rangle = \frac{1}{\sqrt{2l+1}} \sum_{j=1}^{2l+1} e^{-i\frac{\pi}{2l+1}(j+k)(j+k+1)} |v_j\rangle . \tag{3.58}$$

Hence,

$$\left\langle 0, e^{i\frac{2\pi}{2l+1}m} \middle| 0, e^{i\frac{2\pi}{2l+1}n} \right\rangle = \delta_{mn} \tag{3.59}$$

and the vectors $\left|0, e^{i\frac{2\pi}{2l+1}k}\right\rangle$, where $k = 0, 1, \ldots, 2l$, also form an orthonormal basis. Employing the scalar product (3.59) and Eq. (3.57), it is evident that the expectation values associated with the state $\left|0, e^{i\frac{2\pi}{2l+1}k}\right\rangle$ are

$$\begin{aligned} \langle U \rangle_{\left|0, e^{i\frac{2\pi}{2l+1}k}\right\rangle} &= \langle V \rangle_{\left|0, e^{i\frac{2\pi}{2l+1}k}\right\rangle} = 0, \\ \langle U^\dagger V \rangle_{\left|0, e^{i\frac{2\pi}{2l+1}k}\right\rangle} &= e^{-i\frac{2\pi}{2l+1}k}. \end{aligned} \tag{3.60}$$

3.6 Recapitulation and Motivation

In this section, we offer a brief summary of the main findings and explain, why there is a need for further research.

We started by deriving a complete set of constraints which must the moments of a pair of complementary unitary matrices U and V obey in order for ρ to be a physical density matrix. Some of these constraints have the role of uncertainty relations for U and V. We examined one of these inequalities in detail, specifically (3.22):

$$\Delta U^2 \Delta V^2 \geq |\langle U^\dagger V\rangle - \langle U^\dagger\rangle\langle V\rangle|^2,$$

which had been already derived in the literature [1] but using different approaches. Our goal was to identify the MUS that saturate the latter inequality. Remarkably, we found that these states are parameterized by $\lambda \in \mathbb{C}$, and discovering a single MUS corresponding to a fixed λ automatically yields a set of N^2 MUS, each corresponding to a different value of λ. Given that this set comprises N^2 vectors in an N-dimensional space, it is evident that they cannot all be linearly independent. Consequently, our objective was to identify a set of vectors corresponding to a specific value of the parameter λ, capable of spanning the given space while remaining linearly independent, thereby forming the basis of the considered Hilbert space. This task was successfully resolved for the case of $\mu = 0$, resulting in distinct outcomes for even and odd dimensions, respectively:

$$\left|0, e^{i\frac{\pi}{2l}(2k+1)}\right\rangle = \frac{1}{\sqrt{2l}} \sum_{j=1}^{2l} e^{-i\frac{\pi}{2l}(j+k)(j+k+2)} \left|v_j\right\rangle, \;\; k = 0, 1, \ldots, 2l-1,$$

$$\left|0, e^{i\frac{2\pi}{2l+1}k}\right\rangle = \frac{1}{\sqrt{2l+1}} \sum_{j=1}^{2l+1} e^{-i\frac{\pi}{2l+1}(j+k)(j+k+1)} \left|v_j\right\rangle, \;\; k = 0, 1, \ldots, 2l.$$

It is no coincidence that for a system with $\lambda = e^{i\frac{\pi}{2l}(2k+1)}$, where $k = 0, 1, \ldots, 2l-1$ and $\lambda = e^{i\frac{2\pi}{2l+1}k}$ with $k = 0, 1, \ldots, 2l$, for even and odd dimensions respectively, the MUS are orthonormal and generate the whole N-dimensional space, i.e. they form a basis of the corresponding Hilbert space $\mathcal{H}$. Indeed, for these parameter values, $\mu = 0$ which, after a slight modification of Eq. (3.26), gives

$$UV^\dagger(V\left|\psi\right\rangle) = \lambda(V\left|\psi\right\rangle) \tag{3.61}$$

and consequently, $\left|\psi\right\rangle$ is a solution of $(U - \lambda V)\left|\psi\right\rangle = 0$ if and only if $V\left|\psi\right\rangle$ is an eigenvector of the unitary matrix $UV^\dagger$ corresponding to an eigenvalue λ.

We conclude this section by mentioning the trends observed so far regarding the dispersions ΔU^2 and ΔV^2:

1. For $\lambda = 0$,
$$\langle U\rangle_{|\mu_j,\lambda\rangle} = \langle U\rangle_{|u_j\rangle} = 1 \implies \Delta U^2 = 0,$$
$$\langle V\rangle_{|\mu_j,\lambda\rangle} = \langle V\rangle_{|u_j\rangle} = 0 \implies \Delta V^2 = 1.$$

2. For $\lambda = e^{i\frac{\pi}{2l}(2k+1)}$, where $k = 0, 1, \ldots, 2l-1$,
$$\langle V\rangle_{\left|0,e^{i\frac{\pi}{2l}(2k+1)}\right\rangle} = \langle U\rangle_{\left|0,e^{i\frac{\pi}{2l}(2k+1)}\right\rangle} = 0 \implies \Delta U^2 = \Delta V^2 = 1.$$

3. For $\lambda = e^{i\frac{2\pi}{2l+1}k}$, where $k = 0, 1, \ldots, 2l$,
$$\langle V\rangle_{\left|0,e^{i\frac{2\pi}{2l+1}k}\right\rangle} = \langle U\rangle_{\left|0,e^{i\frac{2\pi}{2l+1}k}\right\rangle} = 0 \implies \Delta U^2 = \Delta V^2 = 1.$$

4. For $\lambda \to \infty$,
$$\langle U\rangle_{|\mu_j,\lambda\rangle} = \langle U\rangle_{|v_j\rangle} = 0 \implies \Delta U^2 = 1,$$
$$\langle V\rangle_{|\mu_j,\lambda\rangle} = \langle V\rangle_{|v_j\rangle} = 1 \implies \Delta V^2 = 0.$$

For the parameter values studied until now, we obtain equal dispersions of U and V, in particular $\Delta U^2 = \Delta U^2 = 1$, which thus reach their maximum value. However, this situation is only an extreme case, leading us to study the system in a three-dimensional context and with the general parameter λ, where we will investigate the dependence of the MUS on this parameter in more detail.

3.7 MUS for generic parameter in three dimensions

Let us revisit the Eq. (3.26) once more:

$$(U - \lambda V)\,|\psi\rangle = \mu\,|\psi\rangle\,.$$

Therefore, μ is an eigenvalue of the matrix $(U - \lambda V)$ in the context of the three-dimensional system if and only if it satisfies the following characteristic equation:

$$\mu^3 = 1 - \lambda^3 = z. \tag{3.62}$$

Again we consider the general form $\lambda = |\lambda|e^{i\phi}$, where $\phi \in [0, 2\pi)$. Then, we can express $z = x + iy$ in a polar form as

$$z = |z|e^{i\arg(z)}, \tag{3.63}$$

where

$$\begin{aligned} x &= 1 + |\lambda|^3\cos[3(\phi+\pi)] = 1 - |\lambda|^3\cos(3\phi), \\ y &= |\lambda|^3\sin[3(\phi+\pi)] = -|\lambda|^3\sin(3\phi). \end{aligned} \tag{3.64}$$

Additionally, for the modulus of z, we have:

$$|z| = \sqrt{x^2 + y^2} = \sqrt{1 - 2|\lambda|^3\cos(3\phi) + |\lambda|^6}, \tag{3.65}$$

and the argument of z, $\arg z \in [0, 2\pi)$, is given by

$$\arg z = \begin{cases} \arctan\left(\frac{y}{x}\right) & \text{for } x > 0 \wedge y \geq 0, \\ \frac{\pi}{2} & \text{for } x = 0 \wedge y > 0, \\ \arctan\left(\frac{y}{x}\right) + \pi & \text{for } x < 0, \\ \frac{3}{2}\pi & \text{for } x = 0 \wedge y < 0, \\ \arctan\left(\frac{y}{x}\right) + 2\pi & \text{for } x > 0 \wedge y < 0. \end{cases} \tag{3.66}$$

The eigenvalue μ, except in the case of $\lambda = 1$, is obtained as the third root of z according to Eq. (3.63), expressed as:

$$\mu_k = \sqrt[3]{|z|}e^{\frac{i}{3}(\arg z + 2\pi k)}, \quad k = 1, 2, 3, \tag{3.67}$$

where $|z|$ is defined in Eq. (3.65) and $\arg z$ can be determined from Eq. (3.66). Thus, we observe that for each λ, there exist a total of 3 distinct eigenvalues μ_k.

Next, we proceed to determine MUS. Applying the same algorithm as previously, we return to Eq. (3.26) and represent the matrices U and V in the V-representation.

Subsequently, the eigenvector corresponding to the eigenvalue μ_k, with k fixed for a given $\lambda \neq 1$, is determined as:

$$|\mu, \lambda\rangle = \sum_{j=1}^{3} c_j \, |v_j\rangle \, , \tag{3.68}$$

where the coefficients are given by

$$\begin{aligned} c_1 &= (\lambda e^{-i\frac{2}{3}\pi} + \mu_k)c_2, \\ c_2 &= (\lambda + \mu_k)c_3, \\ c_3 &= (\lambda e^{i\frac{2}{3}\pi} + \mu_k)c_1. \end{aligned} \tag{3.69}$$

The second coefficient can be also expressed as dependent on the first:

$$c_2 = (\lambda + \mu_k)(\lambda e^{i\frac{2}{3}\pi} + \mu_k)c_1, \tag{3.70}$$

and c_1 serves as a normalization constant. Hence, for each eigenvalue μ_k, where $k = 1, 2, 3$, we obtain the corresponding eigenvector $|\mu_k, \lambda\rangle$ dependent solely on the parameter λ.

It turns out that even for this low-dimensional system, performing analytical computations for quantities like eigenvector overlaps $|\,\langle\mu_i, \lambda|\, \mu_j, \lambda\rangle|$, for $i \neq j = 1, 2, 3$, and expectation values of U, V matrices, is a complex task. Therefore, we now focus on the investigation of this system by means of numerical calculations and subsequent graphical visualization.

3.8 Visualization

Since $|\langle\mu_i,\lambda|\,\mu_j,\lambda\rangle| = \text{const.}$, for $i \neq j = 1,2,3$, it is sufficient to plot only the dependence of the overlap between arbitrary two eigenvectors, say $|\langle\mu_1,\lambda|\,\mu_2,\lambda\rangle|$, on the parameter λ, see Fig.3.2.

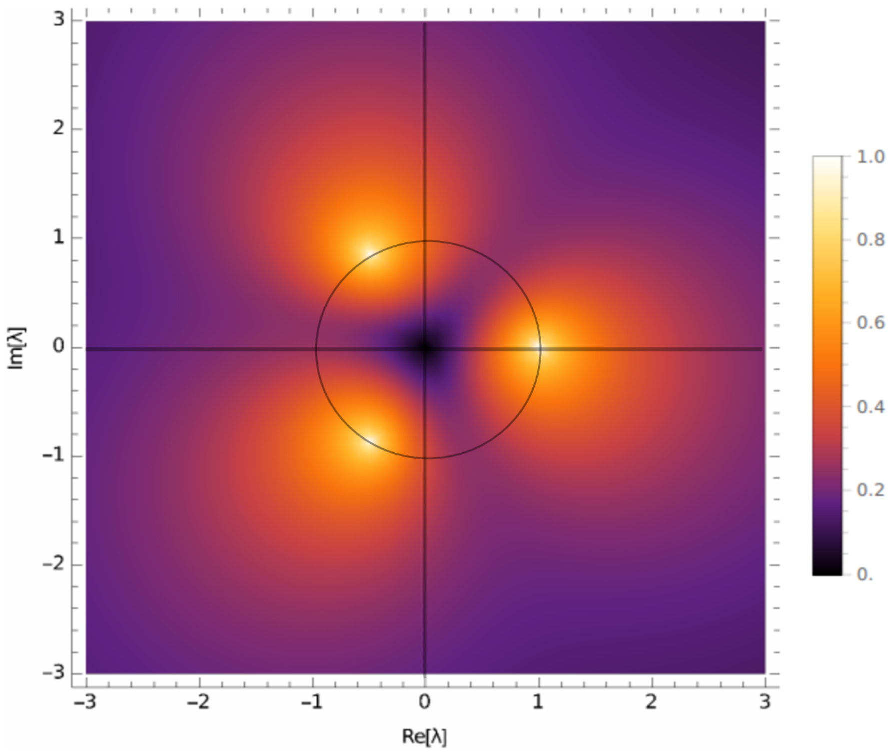
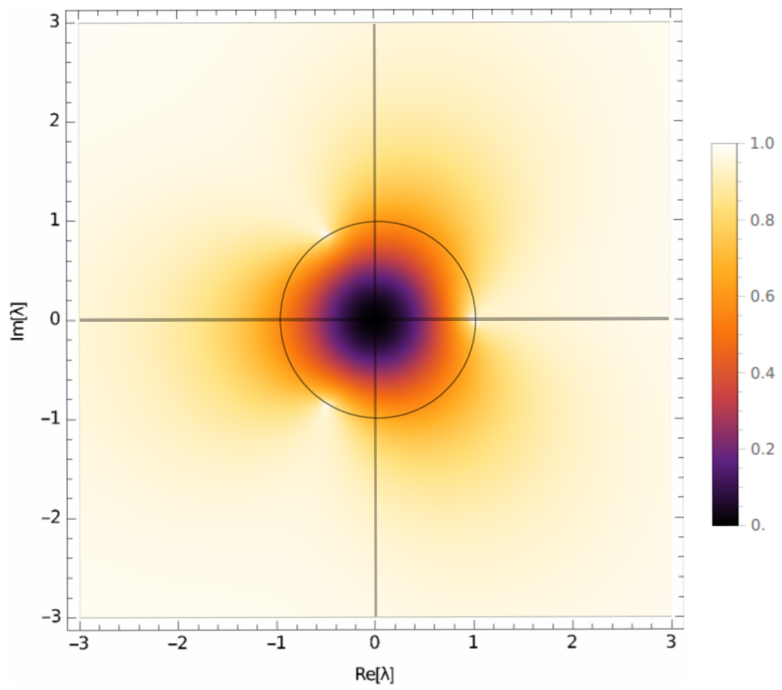


Figure 3.2: Dependence of the absolute value of the overlap of two MUS $|\langle\mu_1,\lambda|\,\mu_2,\lambda\rangle|$ on the parameter λ. The horizontal axis represents the real part of λ, while the vertical axis corresponds to the imaginary part, with $\mathrm{Re}(\lambda), \mathrm{Im}(\lambda) \in \langle -3, 3\rangle$. The color scale on the right side of the graph indicates the numerical value of the overlap $|\langle\mu_1,\lambda|\,\mu_2,\lambda\rangle|$.

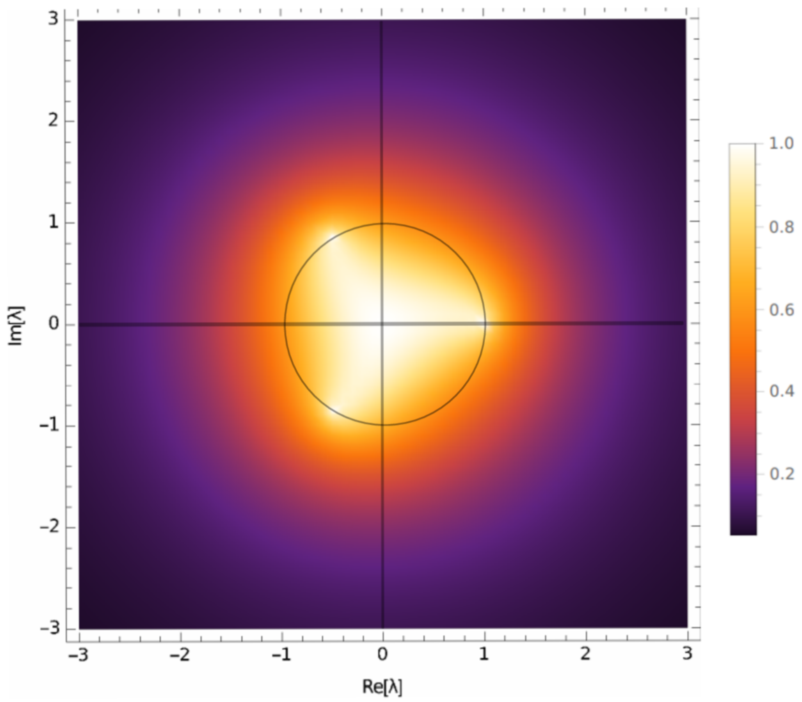
Let us now examine the extreme cases of λ. As $\lambda \to 0$, Eq. (3.26) reduces to $U|\psi\rangle = \mu|\psi\rangle$ and the vectors $|\mu_1,\lambda\rangle$ and $|\mu_2,\lambda\rangle$ become two eigenvectors of the matrix U. Analogously, for the opposite limit $\lambda \to \infty$ we obtain the eigenvectors of the matrix V. In both these cases $|\langle\mu_1,\lambda|\,\mu_2,\lambda\rangle| = 0$ as eigenvectors of the unitary matrices U and V are orthogonal.

Next, we focus on the case of $|\lambda| = 1$. The three brightest points located on the unit circle are associated with the parameter values $\lambda \in \{1, e^{i\frac{2}{3}\pi}, e^{-i\frac{2}{3}\pi}\}$ which we already investigated. It is important to note that these overlaps do not correspond to those of the eigenvectors of the matrix $UV^\dagger$, because there the parameter λ plays the role of an eigenvalue, whereas in Fig.3.2 each point corresponds to a fixed value of λ. In this case, we consider the overlaps of the eigenvectors of the matrix $(U - \lambda V)$, which is for $\lambda \in \{1, e^{i\frac{2}{3}\pi}, e^{-i\frac{2}{3}\pi}\}$ nondiagonalisable - it has only one non-zero eigenvector, and the overlap only confirms its normality as it shows its square magnitude.

The dependency of dispersions ΔU^2 and ΔV^2 on λ is shown in Fig. 3.3(a) and Fig. 3.3(b). Since $\Delta U^2_{|\mu_j,\lambda\rangle} = \text{const.}$, resp. $\Delta V^2_{|\mu_j,\lambda\rangle} = \text{const.}$ for $j = 1,2,3$, we show here only the case of $|\mu_1,\lambda\rangle$. By assumption, these graphs look partially like negatives of each other, thus highlighting the complementary nature of the pair U, V. One can also observe the trends of dispersions mentioned in Sec.3.6.



(a) Dispersion $\Delta U^2_{|\mu_1,\lambda\rangle}$



(b) Dispersion $\Delta V^2_{|\mu_1,\lambda\rangle}$

Figure 3.3: Dependence of $\Delta U^2_{|\mu_1,\lambda\rangle}$ **(a)** and $\Delta V^2_{|\mu_1,\lambda\rangle}$ **(b)** in the MUS $|\mu_1, \lambda\rangle$ on the parameter λ, where $\mathrm{Re}(\lambda), \mathrm{Im}(\lambda) \in \langle -3, 3\rangle$.

Finally, we present a graphical visualization depicted in Fig. 3.4 showcasing the relationship between the product of dispersions $\Delta U^2 \Delta V^2$ and the parameter λ. This graph corresponds to the LHS (left hand side) of the uncertainty relation (3.22)

$$\Delta U^2 \Delta V^2 \geq |\langle U^\dagger V\rangle - \langle U^\dagger\rangle\langle V\rangle|^2$$

Same visualization is obtained for the RHS, which confirms the saturation of the uncertainty inequality.

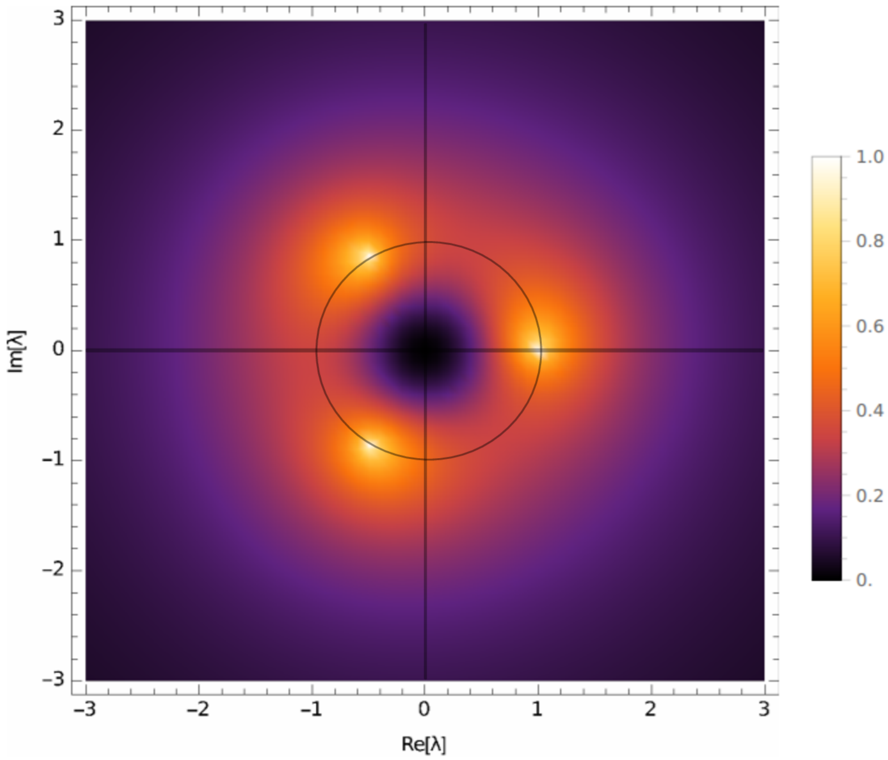


Figure 3.4: Dependence of $\Delta U^2_{|\mu_1,\lambda\rangle} \cdot \Delta V^2_{|\mu_1,\lambda\rangle}$ on the parameter λ, with $\mathrm{Re}(\lambda), \mathrm{Im}(\lambda) \in\langle -3, 3\rangle$.

Looking back at all the above graphs, one can notice three points on the circle $|\lambda| = 1$ corresponding to $\lambda \in \{e^{i\frac{\pi}{3}}, -1, e^{-i\frac{\pi}{3}\pi}\}$. From Fig. 3.2 it is evident that the absolute values of their overlaps are close to zero. From Fig. 3.3(a) and Fig. 3.3(b) it becomes apparent that the dispersions ΔU^2 and ΔV^2 are equal at these points and reach the smallest possible value at the same time, as well as both sides of the uncertainty relation (3.22) (cf. Fig. 3.4). The specific values are summarised in Tab. 3.1.

Table 3.1: Absolute value of overlaps $|\langle\mu_j, \lambda|\, \mu_j, \lambda\rangle|$, dispersions $\Delta U^2_{|\mu_j,\lambda\rangle}$, $\Delta V^2_{|\mu_j,\lambda\rangle}$ and saturated inequality $\Delta U^2_{|\mu_1,\lambda\rangle} \cdot \Delta V^2_{|\mu_1,\lambda\rangle}$ for $\lambda \in \{e^{i\frac{\pi}{3}}, -1, e^{-i\frac{\pi}{3}}\}$, where $i \neq j = 1, 2, 3$, rounded to four decimal places.

Overlaps	$|\langle\mu_j, \lambda|\, \mu_j, \lambda\rangle|$, $i \neq j = 1, 2, 3$	0.2599
Dispersions	$\Delta U^2_{|\mu_j,\lambda\rangle} = \Delta V^2_{|\mu_j,\lambda\rangle}$, $i = 1, 2, 3$	0.5874
Dispersion product (LHS)	$\Delta U^2_{|\mu_j,\lambda\rangle} \cdot \Delta V^2_{|\mu_j,\lambda\rangle}$, $i = 1, 2, 3$	0.3450

To illustrate the different special cases of λ and the respective MUS, we refer to Fig. 3.5, where eigenvectors corresponding to values $\lambda = \infty$, $|\lambda| = 1$ and $\lambda = 0$ are shown on the Riemann sphere. The generalization of this result would hold for a generic dimension N of a Hilbert space $\mathcal{H}$ (in higher dimensions it is no longer a sphere but a structure with a more complicated topology.).

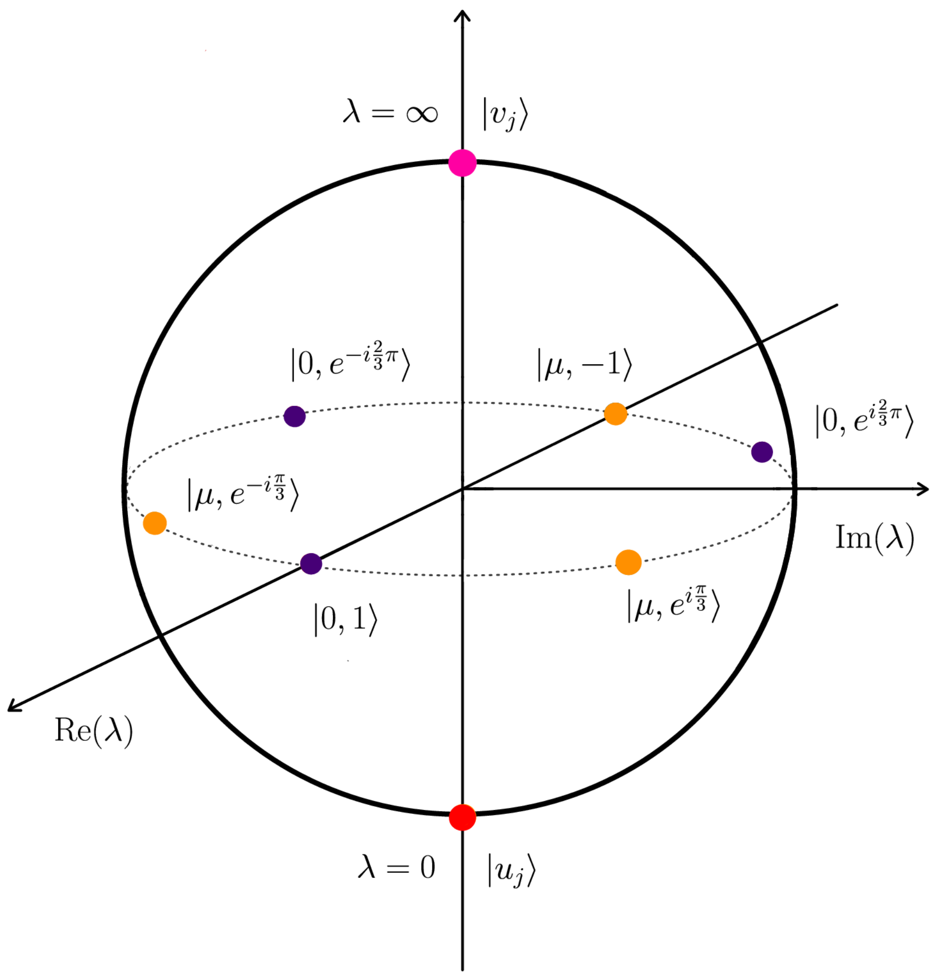


Figure 3.5: Riemann sphere with highlighted MUS corresponding to special cases $\lambda = \infty$, $|\lambda| = 1$ and $\lambda = 0$, where $\mu \in \{\sqrt[3]{2}, \sqrt[3]{2}e^{i\frac{2\pi}{3}}, \sqrt[3]{2}e^{-i\frac{2\pi}{3}}\}$

The MUS associated with $\lambda \in \{e^{i\frac{\pi}{3}}, -1, e^{-i\frac{\pi}{3}}\}$ comprise a set of linearly independent vectors $\left|\sqrt[3]{2}, \lambda\right\rangle$, $\left|\sqrt[3]{2}e^{i\frac{2\pi}{3}}, \lambda\right\rangle$, $\left|\sqrt[3]{2}e^{-i\frac{2\pi}{3}}, \lambda\right\rangle$, which, however, do not resolve the identity matrix and therefore cannot be used as basis vectors. The question of the existence of a complete set of MUS which would be analogous to the set of coherent states is left for future research.

Conclusion

This thesis explores a fundamental feature of quantum mechanics - the principle of complementarity. We investigate the unitary operators U and V, which satisfy the Weyl commutator, in a finite-dimensional Hilbert space. These operators are non-degenerate cyclic matrices, whose bases are mutually unbiased and related by a discrete quantum Fourier transform.

While Hermitian operators, possessing real spectra, are commonly used to represent physical quantities, their eigenvalues complicate computations when studying uncertainty relations. However, the spectrum of a unitary operator lies on the complex unit circle, leading to base-dependent relations unaffected by eigenvalues.

The investigated pair interpolates between the two-dimensional limit, where the U and V unitaries take the form of the σ_x and σ_z Pauli matrices, and the $N \to \infty$ limit, where one can express U and V as complex exponentials of their Hermitian generators u and v. The uncertainties ΔU^2 and ΔV^2 then become proportional to those of u and v and for a specific class of states, the operators u and v are analogous to position x and momentum p variables.

We used the dispersion as a measure of uncertainty for unitary operators and verified that it satisfies the essential properties of a proper uncertainty measure. Further, we have also presented some direct connections between the uncertainty of a unitary operator and the Fubini-Study metric and between the visibility of the interference fringe. Also, inspired by the literature, we were able to derive a straightforward mechanical analogy between dispersion and moment of inertia.

Building upon on the work of S. Massar and P. Spindel [2], S. Bagchi and A.K. Pati [1] and others, we investigated a set of inequalities for moments of unitary matrices U and V, providing a necessary and sufficient condition for a Hermitian trace-one matrix to be a legitimate density matrix of a quantum state. We explored the simplest nontrivial uncertainty relation and demonstrated a method for identifying the MUS saturating the inequality.

We have shown that saturation of the uncertainty relation does not necessarily imply minimum values of the corresponding dispersions, since there is a strong dependence on the parameter characterizing the mutual relationship of the individual dispersions. We have studied in detail the situation for which the corresponding MUS yield equal dispersions. When they both reach their maximum value, one can find a set of MUS forming an orthonormal basis of a given finite-dimensional Hilbert space. However, for the situation where both dispersions reach their smallest possible value simultaneously, MUS (though linearly independent) do not form a basis.

In summary, this thesis contributes to the ongoing research efforts aimed at examining the fundamental principles of quantum mechanics and their implications for quantum technologies. By advancing our understanding of complementarity and uncertainty relations, we pave the way for future developments in quantum information processing, quantum cryptography, and quantum computing. Additionally, we hope that our findings will inspire further research and investigation of the fundamental unitary pair, especially with respect to the question of simultaneous measurement.

Appendix A

Computation of certain mathematical objects

A.1 Computation of the property of concavity

To compute the inequality (2.5), we first show that:

$$|\langle U\rangle_{\sum_i p_i\rho_i}| = |\sum_i p_i \langle U\rangle_{\rho_i}| \leq \sum_i |p_i \langle U\rangle_{\rho_i}| = \sum_i p_i|\langle U\rangle_{\rho_i}|. \tag{A.1}$$

Next, we use the latter equation and proceed as follows:

$$\begin{aligned}
|\langle U\rangle_{\sum_i p_i\rho_i}|^2 &\leq \sum_i p_i|\langle U\rangle_{\rho_i}|\sum_j p_j|\langle U\rangle_{\rho_j}| = \sum_{i,j} p_ip_j|\langle U\rangle_{\rho_i}||\langle U\rangle_{\rho_j}|+ \\
&-\frac{1}{2}\sum_i p_i\sum_j p_j|\langle U\rangle_{\rho_j}|^2 - \frac{1}{2}\sum_j p_j\sum_i p_i|\langle U\rangle_{\rho_i}|^2 + \sum_i p_i|\langle U\rangle_{\rho_i}|^2 = \\
&= \sum_i p_i|\langle U\rangle_{\rho_i}|^2 - \frac{1}{2}\sum_{i,j} p_ip_j\left(|\langle U\rangle_{\rho_i}|^2 + |\langle U\rangle_{\rho_j}|^2 - 2|\langle U\rangle_{\rho_i}||\langle U\rangle_{\rho_j}|\right) = \\
&= \sum_i p_i|\langle U\rangle_{\rho_i}|^2 - \frac{1}{2}\sum_{i,j} p_ip_j\left(|\langle U\rangle_{\rho_i}| - |\langle U\rangle_{\rho_j}|\right)^2 \leq \sum_i p_i|\langle U\rangle_{\rho_i}|^2.
\end{aligned} \tag{A.2}$$

A.2 Computation of the matrix M elements

For illustration, we offer a computation of some of the matrix M elements, Eq. (3.13) of the main text, with the help of Eq. (1.19).

$$
\begin{aligned}
&M_{1,1} = M_{1,1;1,1} = M_{2,2} = M_{1,2;1,2} = \ldots = M_{N^2,N^2} = M_{N,N;N,N} = 1,\\
&M_{1,2} = M_{1,1;1,2} = M_{2,4} = M_{1,2;1,3} = M_{3,5} = M_{2,1;1,1} = \langle U\rangle,\\
&M_{1,3} = M_{1,1;2,1} = e^{i\frac{2\pi}{N}}\langle V\rangle,\\
&M_{2,3} = M_{1,2;2,1} = e^{i\frac{2\pi}{N}}\langle e^{i\frac{2\pi}{N}} VU^\dagger\rangle = e^{i\frac{2\pi}{N}}\langle U^\dagger V\rangle,\\
&M_{1,4} = M_{1,1;1,3} = \langle U^2\rangle,\\
&M_{1,5} = M_{1,1;2,2} = e^{i\frac{2\pi}{N}2}\langle UV\rangle,\\
&M_{2,5} = M_{1,2;2,2} = e^{i\frac{2\pi}{N}2}\langle V\rangle,\\
&M_{3,4} = M_{2,1;1,3} = e^{-i\frac{2\pi}{N}}\langle V^\dagger U^2\rangle = e^{-i\frac{2\pi}{N}3}\langle U^2 V^\dagger\rangle,\\
&M_{4,5} = M_{1,3;2,2} = e^{i\frac{2\pi}{N}3}\langle VU^{-1}\rangle = e^{i\frac{2\pi}{N}2}\langle U^\dagger V\rangle,\\
&M_{1,N^2} = M_{1,1;N,N} = e^{i\frac{2\pi}{N}(N-1)}\langle V^{N-1}U^{N-1}\rangle = \langle e^{i\frac{2\pi}{N}(N-1)}V^{N-1}U^{-1}U^N\rangle = \langle U^\dagger V^N V^\dagger U^N\rangle,\\
&\vdots
\end{aligned}
$$

By employing the fact that $U^N = \mathbb{1}$, $V^N = \mathbb{1}$ and $\gamma_N = e^{i\frac{2\pi}{N}}$, the elements correspond identically to those in the matrix in Eq. (3.17).

A.3 Sum into Product Uncertainty relation

Consider a submatrix in Eq. (3.20)

$$
M^{(1,2,3)} = \begin{pmatrix} 1 & \langle U\rangle & e^{i\frac{2\pi}{N}}\langle V\rangle \\ \langle U^\dagger\rangle & 1 & e^{i\frac{2\pi}{N}}\langle U^\dagger V\rangle \\ e^{-i\frac{2\pi}{N}}\langle V^\dagger\rangle & e^{-i\frac{2\pi}{N}}\langle V^\dagger U\rangle & 1 \end{pmatrix}.
$$

By making use of the condition $\det M^{(1,2,3)} \geq 0$ we get

$$
\det M^{(1,2,3)} = 1+\langle U^\dagger\rangle\langle V^\dagger U\rangle\langle V\rangle+\langle V^\dagger\rangle\langle U\rangle\langle U^\dagger V\rangle-|\langle V\rangle|^2-|\langle U^\dagger V\rangle|^2-|\langle U\rangle|^2 \geq 0. \tag{A.3}
$$

Next, we rewrite the inequality as

$$
\Delta U^2 + \Delta V^2 \geq 1 + |\langle U^\dagger V\rangle|^2 - 2\,\mathrm{Re}(\langle U\rangle\langle V^\dagger\rangle\langle U^\dagger V\rangle),
$$

where $\Delta U^2 = 1 - |\langle U\rangle|^2$ is the dispersion of U and $\Delta V^2 = 1 - |\langle V\rangle|^2$ the dispersion of V. Since

$$
\begin{aligned}
\Delta U^2\Delta V^2 &= (1 - |\langle U\rangle|^2)(1 - |\langle V\rangle|^2)\\
&= 1 - |\langle U\rangle|^2 - |\langle V\rangle|^2 + |\langle U\rangle|^2|\langle V\rangle|^2\\
&= \Delta U^2 + \Delta V^2 - 1 + |\langle U\rangle|^2|\langle V\rangle|^2
\end{aligned} \tag{A.4}
$$

holds, by substituting into the sum inequality (3.21) we get the relation

$$
\Delta U^2\Delta V^2 \geq |\langle U^\dagger V\rangle - \langle U^\dagger\rangle\langle V\rangle|^2. \tag{A.5}
$$

A.4 Computation of the relation between $|\lambda|^2$ and $\Delta U^2, \Delta V^2$

To derive the formula (3.27), we first consider the relation (A.4)

$$(U - \lambda V) |\psi\rangle = (\langle U\rangle - \lambda\langle V\rangle) |\psi\rangle \,,$$

Multiplying the latter equation from the left with $V^\dagger$, followed by multiplication with $\langle\psi|$, and subsequent complex conjugation yields

$$\lambda^* \Delta V^2 = \langle U^\dagger V\rangle - \langle U^\dagger\rangle\langle V\rangle. \tag{A.6}$$

Returning to the Eq. (A.4), multiplication with $U^\dagger$ from the left and subsequently with $\langle\psi|$ results in:

$$\Delta U^2 = \lambda(\langle U^\dagger V\rangle - \langle U^\dagger\rangle\langle V\rangle). \tag{A.7}$$

Comparison of Eqs. (A.6) and (A.7) then implies the relation (3.27)

$$|\lambda|^2 = \frac{\Delta U^2}{\Delta V^2}.$$

Coming back to the Eq. (A.7), one can see that the argument of λ satisfies the formula (3.28), by $\Delta U^2 \in \mathbb{R}$.

A.5 Computation of the expectation values taken with respect to MUS of the form $\left|\mu\gamma^{-l}, \lambda\gamma^{-(l+k)}\right\rangle$

In the following we offer a short calculation of the expectation values in Eq. (3.30):

$$\begin{aligned}
\langle U\rangle_{\left|\mu\gamma^{-l},\lambda\gamma^{-(l+k)}\right\rangle} &= \langle\lambda| V^{-l}U^{-k}UU^kV^l |\lambda\rangle = e^{-i\frac{2\pi}{N}l} \langle\lambda| UV^{-l}V^l |\lambda\rangle = e^{-i\frac{2\pi}{N}l}\langle U\rangle_{|\mu,\lambda\rangle}, \\
\langle V\rangle_{\left|\mu\gamma^{-l},\lambda\gamma^{-(l+k)}\right\rangle} &= \langle\lambda| V^{-l}U^{-k}VU^kV^l |\lambda\rangle = \langle\lambda| U^{-k}V^{-l}VV^lU^k |\lambda\rangle = e^{i\frac{2\pi}{N}k}\langle V\rangle_{|\mu,\lambda\rangle}, \\
\langle U^\dagger V\rangle_{\left|\mu\gamma^{-l},\lambda\gamma^{-(l+k)}\right\rangle} &= e^{i\frac{2\pi}{N}k} \langle\lambda| V^{-l}U^{-1}VV^l |\lambda\rangle = e^{i\frac{2\pi}{N}(k+l)}\langle U\rangle_{|\mu,\lambda\rangle},
\end{aligned}$$

where we have used the commutation rule (1.19).

A.6 Computation of the determinant in Eq. (3.31)

For clarity, we express the term $U - (\lambda V + \mu\mathbb{1})$ in a matrix format:

$$\begin{pmatrix}
-(\lambda e^{i\frac{2\pi}{N}} + \mu) & 0 & 0 & \cdots & 1 \\
1 & -(\lambda e^{i\frac{2\pi}{N}2} + \mu) & 0 & \cdots & 0 \\
0 & 1 & -(\lambda e^{i\frac{2\pi}{N}3} + \mu) & \cdots & 0 \\
\vdots & \vdots & & \ddots & \vdots \\
0 & 0 & \cdots & 1 & -(\lambda e^{i\frac{2\pi}{N}N} + \mu)
\end{pmatrix},$$

The determinant of this matrix can be computed by using the Laplace expansion along any one of its rows or columns. We perform an expansion along the last column as follows:

$$\begin{aligned}
\det[U-(\lambda V+\mu\mathbb{1})] &= (-1)^{N+1}+(-1)^{2N}(-1)^{N}\prod_{j=1}^{N}(\lambda e^{i\frac{2\pi}{N}j}+\mu)\\
&= (-1)^{N+1}+(-1)^{N}(-\lambda)^{N}\prod_{j=1}^{N}\left[\left(-\frac{\mu}{\lambda}\right)-e^{i\frac{2\pi}{N}}j\right]\\
&= (-1)^{N+1}+(-1)^{N}(-\lambda)^{N}\left[\left(-\frac{\mu}{\lambda}\right)^{N}-1\right]\\
&= (-1)^{N+1}+(-1)^{N}[\mu^{N}-(-\lambda)^{N}],
\end{aligned} \tag{A.8}$$

where we have used the fact that $\prod_{j=1}^{N}\left(z-e^{i\frac{2\pi}{N}}j\right)=z^{N}-1$ for $z\in\mathbb{C}$.

A.7 Eigenvalue equation for even dimensions

Here we present a straightforward computation of the Eq. (3.34) for even dimensions ($N=2l$, where $l=1,2,\ldots$) resulting in Eq. (3.35):

$$\begin{aligned}
\mu^{2l} &= 1+e^{i2l\phi}\\
&= 1+\cos(2l\phi)+i\sin(2l\phi)\\
&= 1+\cos^{2}(l\phi)-\sin^{2}(l\phi)+2i\sin(l\phi)\cos(l\phi)\\
&= 2\cos(l\phi)\left[\cos(l\phi)+i\sin(l\phi)\right]\\
&= 2\cos(l\phi)e^{il\phi}.
\end{aligned}$$

Appendix B

Limit cases

Here we present a special cases of the complementary pair of unitary matrices U and V as introduced in the section 1.3 concerning the well-known $N = 2$ example of a qubit. One can also show the $N \to \infty$ limit, where the uncertainties ΔU^2 and ΔV^2 become proportional to those of Hermitian operators u and v, while $U = \exp(iu2\pi/N)$ and $V = \exp(-iv2\pi/N)$, and one can find a special class of states for which the operators u and v are analogous to the position x and momentum p variables, for detailed derivation we recommend [2].

B.1 Two-dimensional case

For a quantum system possessing two-dimensional Hilbert space $\mathcal{H}$, the matrices U and V take the form

$$U = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad V = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{B.1}$$

and we arrive at the familiar example of a complementary pair - the σ_x and σ_z Pauli matrices. The Weyl commutator is then (according to the Eq. (1.19))

$$VU = e^{i\frac{2\pi}{2}} UV = -UV, \tag{B.2}$$

which gives $[U, V] = 2UV = -2i\sigma_y$ and is thus consistent with the well-known formula $[\sigma_x, \sigma_z] = -2i\sigma_y$ [10].

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