Geometric and algebraic origins of additive uncertainty relations

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Abstract
Constructive techniques to establish state-independent uncertainty relations for the sum of variances of arbitrary two observables are presented. We investigate the range of simultaneously attainable pairs of variances, which can be applied to a wide variety of problems including finding exact bound for the sum of variances of two components of angular momentum operator for any total angular momentum quantum number \(j\) and detection of quantum entanglement. Resulting uncertainty relations are state-independent, semianalytical, bounded-error and can be made arbitrarily tight. The advocated approach, based on the notion of joint numerical range of a number of observables and uncertainty range, allows us to improve earlier numerical works and to derive semianalytical tight bounds for the uncertainty relation for the sum of variances expressed as roots of a polynomial of a single real variable.

Keywords: additive uncertainty relations, numerical range, quantum states, planar squeezing

(Some figures may appear in colour only in the online journal)

1. Introduction

Uncertainty relations form a wide branch of problems with ubiquitous applications: from the tests of quantum theory \cite{1} through quantum cryptography \cite{2} and entanglement detection \cite{3, 4} to direct usage in experiments \cite{5}. There exist various approaches to the problem: the original articles by Heisenberg and Kennard \cite{6, 7} consider the product of variances of two observables, while a recent approach by Maccone and Pati \cite{8} concerns the sum of variances, \textsuperscript{3}Author to whom any correspondence should be addressed.
especially useful for finite-dimensional systems. Entropic uncertainty relation [9] bounds from below the sum of entropies of probability distributions of observed quantities. In the state-independent approach for a selected pair of observables one derives lower bounds for a given quantity valid for any quantum state. These results can be often improved in the state-dependent approach, in which one establishes more precise dedicated bounds, which depend explicitly on the measured quantum state.

Current interest in improving uncertainty relations, both in finite [10–12] and infinite-dimensional case [8, 13–15], is motivated by their numerous applications in mathematical physics and in the theory of quantum information processing. The goal of this work is to provide a novel, geometrical view on the variance-based uncertainty relations, which allows one to establish exact analytical results. The current contribution extends recent works [13, 16], in which approximate uncertainty relations for the sum of variances were obtained with help of numerical techniques.

We provide here semianalytical, bounded-error, state-independent bounds for uncertainty relations involving variances of two operators and analyze properties of an associated geometric object, called uncertainty range. In principle the procedure can be extended also to the case of multiple observables [12, 15]. Furthermore, we propose a procedure, applicable in finite dimensions, determining a tight, state-independent bound for the sum of variances as a root of a certain polynomial. While the roots of the algorithmically generated polynomials always exist, usually the procedure is feasible in low dimensions and leads to exact, explicit analytic bounds. The procedure is exemplified by analytical determination of minimal sum of variances for angular momentum operators, \( \Delta^2 J_x + \Delta^2 J_y \) for several values of the total angular momentum quantum number \( j \), which expands on known numerical results [12, 17, 18].

2. Sum-of-variances uncertainty relations

To characterize uncertainty related to a double quantum measurement one can analyze the sum of variances [8]. For any two operators \( X \) and \( Y \) we wish to provide a state-independent bound \( C(X, Y) \) for the sum of variances:

\[
\Delta^2 X + \Delta^2 Y \geq C(X, Y).
\]  

(1)

One of the possible approaches makes use of the following fact: it is possible to rewrite the sum of variances as a function of the averages,

\[
\Delta^2 X + \Delta^2 Y = \langle X^2 + Y^2 \rangle - \langle X \rangle^2 - \langle Y \rangle^2,
\]  

(2)

so it is sufficient to minimize the function \( v = \langle X^2 + Y^2 \rangle - \langle X \rangle^2 - \langle Y \rangle^2 \) over all states. If one could determine the set of allowed triples of expectation values \( (\langle X \rangle, \langle Y \rangle, \langle X^2 + Y^2 \rangle) \), the function \( g \) could be interpreted as a simple polynomial of three variables, which is minimized over set of triples. This can be done, and numerical methods employing this observation have been recently developed [13, 16], here we present an analytical extension allowing for strict treatment of several interesting classes of observables.

3. Numerical range of observables

In this work on uncertainty relations we will use the notion of numerical range—the set of simultaneously allowed expectation values. In this section the most important properties necessary for discussion of uncertainty relations are presented.
Expectation value of an observable $F$ on a pure state, $\langle F \rangle_\psi = \langle \psi | F | \psi \rangle$, is a key concept of the quantum theory. For any hermitian matrix $F$ of a fixed order $d$ one can pose the question, what is the range of possible expectation values among all normalized pure states: the answer is a segment of the real axis bounded by the extremal eigenvalues of $F_i = [\lambda_{\text{min}}, \lambda_{\text{max}}]$.

A similar problem was earlier analyzed by mathematicians, who studied an algebraic notion of numerical range of an (not necessarily hermitian) operator $X$—a subset of the complex plane defined by

$$W(X) = \{ z \in \mathbb{C} : z = \langle \psi | X | \psi \rangle, \langle \psi | \psi \rangle = 1 \}. \quad (3)$$

Numerical range $W(X)$ may be interpreted as a set of allowed expectation values of a single operator $X$. A classical theorem of Toeplitz and Hausdorff, obtained nearly a century ago [19, 20], states that for any matrix $X$ the set $W(X)$ is convex. If the matrix $X$ is normal then the set $W(X)$ forms the convex hull of the spectrum of $X$. For a hermitian observable $F$ the corresponding set $W(F)$ reduces to an interval belonging to the real axis [21]. For operators of dimension $d \leq 3$ the possible shapes of numerical ranges are classified [22, 23].

Expectation value of single operator may not capture the whole complexity of some problems. Furthermore, in the definition in equation (3), only pure states are taken into account, while the set of mixed states is potentially much more intricate. A natural generalization to sequence of $k$ averages of fixed operators $(F_i)_{i=1}^k$ taken over all mixed states is used instead. The set of $k$ expectation values which can be obtained by measuring $k$ Hermitian observables $(F_i)_{i=1}^k$ over a common quantum state $\rho$ is called joint numerical range (JNR) [24] and defined by

$$W(F_1, F_2, \ldots, F_k) = \{ x \in \mathbb{R}^k : x_j = \langle F_j | \rho \rangle, j = 1, \ldots, k; \rho \in \mathcal{M}_d \}, \quad (4)$$

where $\langle F \rangle_\rho = \text{Tr} F \rho$. Here $\mathcal{M}_d = \{ \rho : \rho^\dagger = \rho \succeq 0; \text{Tr} \rho = 1 \}$ denotes the set of all normalized mixed states of size $d$. The additional motivation for taking mixed states into account is to ensure convexity of the resulting set: evidently, the set of expectation values of three Pauli matrices among pure states forms the hollow Bloch sphere. As any operator can be decomposed into its hermitian and antihermitian part, $X = F_H + i F_A$, the set $W(X)$ can be considered as a JNR of two hermitian observables, $W(F_H, F_A)$. This is the set of simultaneously attainable expectation values of these two observables obtained in a double quantum measurement performed on two copies of the same state.

A classification of 3D numerical ranges of a triple of operators of size $d = 3$ was given in [25]. JNR and its extensions find diverse applications, the notion allows for visualization of phase transitions [26–28], construction of nonlinear entanglement witnesses or to improve our understanding of the geometry of the set of quantum states, as JNR describes its projection onto lower dimensional subspaces (up to affine transformations) [25].

4. Reformulated definition of variance

The methods used in this paper strongly rely on an equivalent definition of variance, which allows for efficient analytical treatment and—if necessary—is easy to approximate. This is achieved by defining the variance over the specific state $\Delta^2 X_\rho$ by minimal expectation value taken over the set of linear functions of $\langle X^2 \rangle$ and $\langle X \rangle$. This equivalent definition of variance reads

$$\Delta^2 X_\rho := \min_{x \in \mathbb{R}} \langle (X - x 1)^2 \rangle_\rho = \min_{x \in \mathbb{R}} \langle X^2 - 2 x X + x^2 1 \rangle_\rho, \quad (5)$$
that is, the minimum taken over the set of linear functions of operators \( X^2 \) and \( X \) parametrized by \( x \in \mathbb{R} \). In order to calculate, for instance, a lower bound for the sum of variances, both terms can be simultaneously optimized,

\[
\min_{\rho} \Delta^2 X_\rho + \Delta^2 Y_\rho = \min_{\rho} \min_{x,y \in \mathbb{R}} (X^2 + Y^2 - 2(xX + yY) + (x^2 + y^2)\mathbb{1})_\rho. \tag{6}
\]

Analytical treatment of this formulation is demonstrated in the next section.

Efficient approximations are made possible by selecting other (finite) set \( S \) of operators which are linear in \( X \) and \( X^2 \). This method is discussed in details after the next section.

5. Application to uncertainty relations

Exchanging the order of minimisation in equation (6) does not change the value of this expression, as we are looking for global minima. Then the expression reads,

\[
\min_{\rho} \Delta^2 X_\rho + \Delta^2 Y_\rho = \min_{x,y \in \mathbb{R}} (X^2 + Y^2 - 2(xX + yY) + (x^2 + y^2)\mathbb{1})_\rho, \tag{7}
\]

with the notation that the operator proportional to identity \((x^2 + y^2)\mathbb{1}\) is denoted by the proportionality factor only, \((x^2 + y^2)\); this notation is going to be used in the following text.

For a fixed operator \( Z \) it is known that the minimal value of the expectation value \( \min_{\rho} \langle Z \rangle_\rho \) is equal to the minimal eigenvalue of \( Z \). Let us denote it by \( \lambda_{\min}(Z) \) and write

\[
\min_{\rho} \Delta^2 X_\rho + \Delta^2 Y_\rho = \min_{x,y \in \mathbb{R}} \lambda_{\min} (X^2 + Y^2 - 2(xX + yY) + x^2 + y^2). \tag{8}
\]

We are now looking for a minimal eigenvalue of a certain family of operators. This is a problem well suited for treatment with the theory of solving a system of polynomial equations: the conditions for minima in \( x, y \) in equation (8) can be written as derivatives of characteristic polynomial (i.e. the minima are smooth and not cusp-like, see appendix A). As a result the set of three polynomial equations in three real variables: \( \lambda, x, y \) is obtained,

\[
\begin{aligned}
D := \det (X^2 + Y^2 - 2(xX + yY) + (x^2 + y^2 - \lambda)) &= 0, \\
\partial_\lambda D &= 0, \\
\partial_x D &= 0.
\end{aligned} \tag{9}
\]

These three equations always have a common solution, but not for arbitrary \( \lambda \); the set of values of \( \lambda \) for which real solutions to equation (9) exist is discrete. This set can be deduced from above equations by systematic reduction of polynomials, in the end leading to single polynomial of \( \lambda \) only—see appendix B for the details. Let us denote this final polynomial by \( R(\lambda) \). This means that a polynomial \( R(\lambda) \), which minimal real root (with corresponding \( x, y \) being real as well) is the lower bound of the additive uncertainty relation,

\[
\min_{\rho} \Delta^2 X_\rho + \Delta^2 Y_\rho = \min \{ c : R(c) = 0 \; \text{corresponding} \; x, y \; \text{are real} \}. \tag{10}
\]

Geometric interpretation of this method reveals a close relation to the 3D JNR \( W(X, Y, X^2 + Y^2) \). If a triple \( (\langle X \rangle, \langle Y \rangle, \langle X^2 + Y^2 \rangle) \) belongs to the set \( W(X, Y, X^2 + Y^2) \), the sum of variances, denoted by \( v \), can be rewritten as

\[
v(\langle X \rangle, \langle Y \rangle, \langle X^2 + Y^2 \rangle) = \langle X^2 \rangle + \langle Y^2 \rangle - \langle X \rangle^2 - \langle Y \rangle^2. \tag{11}
\]

Is it clear that the surfaces of equal variance are paraboloids of revolution. If we now introduce one of the functions \( w_{x,y} \) we are minimizing over in equation (6),
\[ w_{x,y}(X, Y, \langle X^2 + Y^2 \rangle) = \langle X^2 + Y^2 \rangle - 2(\langle X \rangle + \langle Y \rangle) + x^2 + y^2, \]  
(12)

it can be easily concluded that the condition \( w_{x,y}(X, Y, \langle X^2 + Y^2 \rangle) = v(X, Y, \langle X^2 + Y^2 \rangle) \) is equivalent to \( x = \langle X \rangle, y = \langle Y \rangle \) with no restrictions on \( \langle X^2 + Y^2 \rangle \). Hence, the function \( w_{x,y} \) calculates true sum of variances if restricted to the straight vertical line; elsewhere it is a strictly upper bound.

Using this property we conclude that if a global minimum of \( w_{x,y} \) is attained for certain \( x = x_0, y = y_0 \) with triple of arguments \( (\langle X \rangle, \langle Y \rangle, \langle X^2 + Y^2 \rangle) \), then the triple corresponds to minimal global sum of variances.

5.1. Examples

(A) **Bounds for angular momentum operators.** The method described above allow us to obtain new analytical bounds for sum of variances of angular momentum, known as planar uncertainty relations useful in quantum metrology \([12, 17, 18, 29]\). This particular problem enjoys additional symmetry, which greatly reduces the computational load: since \( W(JX, JY, J^2) \) has rotational symmetry (see figure 1), we can set either of the variables \( x, y \) in equation (9) to 0 and we are left with the set of two polynomial equations with two variables (see appendix D for the explicit form of polynomials for \( j \leq 4 \)). Making use of the techniques described above we obtained new, tight and analytical bounds for a pair of angular momentum operators \( X = JX \) and \( Y = JY \) for arbitrary value of total angular momentum quantum number \( j \). The data presented in table 1 corresponding to tight and exact values of additive uncertainty relation bounds constitute a key result of this work.

(B) **Family of uncertainty relations.** Consider a family of uncertainty relations derived from angular momentum operators for \( j = 1 \):

\[ \Delta^2 J_X + \alpha \Delta^2 J_Y \geq C(\alpha). \]  
(13)

The bound for weighted sum of variances can be determined in the same way as previously — there is no conceptual change in the calculations apart from the fact that the number of variables is higher—leading to a piecewise function,

\[ C(\alpha) = \begin{cases} \frac{1}{2} - \frac{1}{32\alpha^2} : & \alpha \geq 1 \\ \frac{\alpha^2}{2} - \frac{\alpha}{16} : & \alpha \leq 1 \end{cases} . \]  
(14)

(C) **Arbitrary operators.** The method described above is not limited to angular momentum operators only. Using the same technique we can determine, for instance, the minimal sum of variances for operators

\[ X = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad Y = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & i \\ 0 & -i & 0 \end{pmatrix}. \]  
(15)

The polynomial arising from solving equation (9) leads to strict bound for sum of variances \( \Delta^2 X + \Delta^2 Y \geq C = 15/32 \). The 3D numerical range corresponding to this pair of operators is presented in figure A2 in appendix A.
6. Uncertainty range

In analogy to numerical range \( W(X, Y) \) defined in (4), the set of possible expectation values, one can introduce a geometric object containing information about simultaneously possible variances of two operators,

\[
U(X, Y) := \left\{ (\Delta^2_{\rho}X, \Delta^2_{\rho}Y) \in \mathbb{R}^2 : \rho \in \mathcal{M}_d \right\},
\]

which will be called uncertainty range—see [12, 13] for examples of application.

Uncertainty range is a nonlinear transformation of the 4-dimensional numerical range \( W(X, X^2, Y, Y^2) \) and in general it is not a convex set—see figure 3. Note that uncertainty range contains information about all additive uncertainty relations \( \Delta^2(aX) + \Delta^2(bY) \geq C(a, b) \).
The bound $C(a, b)$ is determined by the line with normal $(-b, a)$ tangent to the uncertainty range.

6.1. **Sector decomposition**

In this section we are going to present the procedure of approximate variance; it is able to generate a set of operators $S$ defining approximation to variance through the relation

$$\Delta^2 X_\rho \approx \min_{V \in S} \langle V \rangle_{\rho}. \quad (17)$$

It enjoys several favorable characteristics: the approximation is a lower bound; its error is bounded and easily controlled.

We are going to use the spectral structure of the arbitrary analyzed observables $X$ and $Y$. Observe that the numerical range $W(X, X^2)$ is determined by the spectrum of $X$: since operators $X$ and $X^2$ do commute, the range $W(X, X^2)$ is a polygon formed by the convex hull of points $(\lambda_i, \lambda_i^2)$, where $\lambda_i$ denote eigenvalues of $X$—see figure 2. The aim is to provide a linear approximation $f((X), (X^2)) = \alpha \langle X \rangle + \beta \langle X^2 \rangle + \gamma$ to the true variance $\nu((X), (X^2)) = \langle X^2 \rangle - \langle X \rangle^2$ valid in some subset of $W(X, X^2)$ in the sense: $f$ approximates $\nu$ nontrivially from below, $0 \leq f((X), (X^2)) \leq \nu((X), (X^2))$.

No single choice of linear function is valid in the entire set $W(X, X^2)$. To obtain meaningful results this set has to be covered with validity regions of finite numbers of approximations. Natural choice is to split the whole region into vertical bands $a \leq \langle X \rangle \leq b$, such that the approximation is exact on $\langle X \rangle = a$ and $\langle X \rangle = b$—see figure 2. By minimizing the maximal possible error, $|a - f|$, we are left with equation $f((X), (X^2)) = -(a + b) \langle X \rangle + \langle X^2 \rangle + ab$.

The minimal choice of the bands corresponds to an approximation of the variance with $d - 1$ linear functions between adjacent eigenvalues: for ordering $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_d$, parameters of $i$th function are: $a_i = \lambda_i$ and $b_i = \lambda_{i+1}$. Denoting the maximum spacing between adjacent eigenvalues by $s_{\text{max}} = \max_i(\lambda_i - \lambda_{i+1})$, we find that the maximum error of variance approximation for $X$ reads $\delta_X = (s_{\text{max}})^2/4$. Let us denote the sector decomposition of two operators $X, Y$ by $\{X_i, \{Y_i\}$, where each $X_i$ is defined as

$$X_i = X^2 - (\lambda_i + \lambda_{i+1})X + \lambda_i \lambda_{i+1}, \quad (18)$$

with $\lambda_i$ being $i$th eigenvalue of $X$. The sequence of operators $\{Y_i\}$ is defined analogously with eigenvalues of $Y$.

Then we can provide ‘a lower approximation’ to the uncertainty range $V(X, Y)$ by

$$\hat{V} = \bigcup_{i,j} W(X_i, Y_j), \quad i,j = 1, \ldots, d - 1, \quad (19)$$

where the ‘lower approximation’ is to be understood in the following way: if at each point $(x, y) \in \hat{V}$ we attach a rectangle $[x, x + \delta_x] \times [y, y + \delta_y]$ (the maximun error of the variance approximation), the uncertainty range is contained in the resulting set, Minkowski sum [31] of $\hat{V}$ and $E := [0, \delta_x] \times [0, \delta_y]$ (see figure 3):

$$V(X, Y) \subset \hat{V} \oplus E = \{v + e : v \in \hat{V}, e \in E\}. \quad (20)$$

This construction is compatible with a nonconvex structure of the uncertainty range $V(X, Y)$—see figure 3. Such a procedure provides simple bounds for the sum-of-variances uncertainty relation: a state-independent bound reads
Additionally, the error of approximation is at most the sum of sector decomposition errors of $X$ and $Y$, so in case of the minimal selection the difference of approximation and real bound is
\[ \left| \left( \min_{ij} \Delta^2 X + \Delta^2 Y \right) - \min_{ij} \lambda_{\text{min}} (X_i + Y_j) \right| \leq \delta_X + \delta_Y. \tag{22} \]

The above reasoning allows us to formulate the following statement, which provides new analytical bounds with controlled errors:

**Proposition 1.** For arbitrary two Hermitian operators $X$ and $Y$, let $\Lambda(X)$ and $\Lambda(Y)$ denote the set of eigenvalues of the respective operators. Then, for the increasing finite sequences $(x) = (x_1, \ldots, x_n)$, $(y) = (y_1, \ldots, y_m)$ such that the eigenvalues are contained in corresponding sequences, $\Lambda(X) \subset (x)$ and $\Lambda(Y) \subset (y)$, the following holds:
\[ \Delta^2 X + \Delta^2 Y \geq \min_{ij} \lambda_{\text{min}} (X_i + Y_j), \]  

where
\[ X_i = X^2 - (x_i + x_{i+1})X + \|x_i x_{i+1}\|, \]
\[ Y_j = Y^2 - (y_j + y_{j+1})Y + \|y_j y_{j+1}\|. \tag{24} \]

The maximal error of approximation is bounded:
\[ \Delta^2 X + \Delta^2 Y - \min_{ij} \lambda_{\text{min}} (X_i + Y_j) \leq \delta_X + \delta_Y, \]  

where
\[ \delta_X = \left( \frac{\max_i (x_{i+1} - x_i)}{2} \right)^2 \] and \[ \delta_Y = \left( \frac{\max_j (y_{j+1} - y_j)}{2} \right)^2. \tag{26} \]
This proposition and general idea about approximating uncertainty ranges generalizes naturally to higher number of observables: union of numerical ranges of sector decompositions is still the main object of interest.

7. Concluding remarks

In this work we advocated a geometric approach to uncertainty relations, obtained state-independent tight analytical bounds applicable in low dimensions and semianalytical approximations for which maximal error can be controlled. On one hand we presented a direct link between the algebraic notion of numerical range of an operator [19–21] and uncertainty relations for the sum of variances [8]. Furthermore, as numerical range of a matrix of order $d$ can be interpreted as a projection of the set $\mathcal{M}_d$ of mixed quantum states of size $d$ on a plane, we have shown that uncertainty relations can be considered as a direct consequence of the highly non-trivial geometry of the set of quantum states.

In particular, we applied the techniques described above to obtain exact analytical bounds for the sum of variances (1) of angular momentum operators for arbitrary total angular momentum quantum number $j$. Furthermore, in proposition 1 we provide an efficient method to generate arbitrarily precise approximations to uncertainty relations, applicable if exact calculations are too computationally expensive.

Our approach relies on geometric properties of the uncertainty region, the set of simultaneously attainable variances, which is generically not convex. The method can be applied in entanglement detection schemes, analysis of security of quantum cryptographic protocols and diagnostics of quantum states. Further generalization to state-dependent uncertainty relations is also possible with only minor modifications: along with calculation of the uncertainty range, averages of the observables of interest need to be determined.
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Appendix A. Complementary approach using dual sets

To proceed with an analytical approach it is convenient to work in the dual space. This alternative description of the JNR $W(X)$ is given by its dual set. Dual of an convex set $X$ can be defined as a set of linear functions $v$, for which the maximal over $X$ is equal to 1, that is to say, $\sup_{x \in X} v(x) = 1$. All these function may be viewed as calculating scalar products with some vectors, therefore we need to find vectors $\vec{v}$ such that $\sup_{x \in X} \vec{v} \cdot \vec{x} = 1$. This is the set $X^0$, dual to $X$:

$$X^0 = \left\{ \vec{v} : \sup_{x \in X} \vec{v} \cdot \vec{x} = 1 \right\}.$$  \hfill (A.1)

Dual sets of numerical ranges admit an especially simple description as a set of roots of appropriately parametrized characteristic polynomial. This is a consequence of the relation between boundary of the numerical range $W(F_1, \ldots, F_n)$ and eigenvectors of mixed operators $\sum a_i F_i$.

As an example let us consider the numerical range of two operators $W(X, Y)$—we wish to calculate its dual set using the definition in equation (A.1). One may ask: which vectors $\vec{v}$ proportional to $(\cos \theta, \sin \theta)$ belong to $W^0$? The defining criterion becomes then

$$\sup_{\rho} |v|(\cos \theta, \sin \theta) \cdot (\langle X \rangle, \langle Y \rangle)_\rho = 1,$$

where the supremum is taken over all density matrices $\rho$. This is of course the same as asking that

$$\sup_{\rho} (X \cos \theta + Y \sin \theta)_\rho = \frac{1}{|v|},$$

that is to say, maximum eigenvalue of $X \cos \theta + Y \sin \theta$ is $|v|^{-1}$. Therefore, for every $\theta \in [0, 2\pi)$, the point $(\cos \theta, \sin \theta)[\max \lambda(X \cos \theta + Y \sin \theta)]^{-1}$ belongs to $W^0$. This implies the following constraint

$$\vec{v} \in W^0 \rightarrow \det (X_{\nu_x} + Y_{\nu_y} - 1) = 0.$$  \hfill (A.4)

The reverse implication is not true: $|v|$ may be inverse of any eigenvalue, including these which do not contribute to the boundary at all (i.e. not the extreme ones). There exists however unique way of determining which part of the curve defined by $\det (X_{\nu_x} + Y_{\nu_y} - 1) = 0$ belongs to $W^0$.

If the origin (zero vector) lies in the interior of $W(F_1, \ldots, F_n)$, the subset of the affine variety forming $W^0$ can be easily identified—since the boundary of JNR is defined by maximal eigenvalues, if we choose any direction $\vec{n} \in S^{k-1}$ and take all solutions of the right side in (A.4) of the form $\vec{v} = \lambda \vec{n} (\lambda > 0)$, the boundary $\partial W$ of JNR is described by the one with minimal $\lambda$. The set $W^0$ is therefore a kind of a ‘cell’ around the origin of the dual space, see figure A.1.
In previous sections the function
\[ v = \langle X^2 + Y^2 \rangle - \langle X \rangle^2 - \langle Y \rangle^2 \]
and a method to generate the set of all triples of expectation values
\[ (\langle X \rangle, \langle Y \rangle, \langle X^2 + Y^2 \rangle) \]
have been introduced. Here we demonstrate how to leverage the algebraic structure of numerical range \( W(X, Y, X^2 + Y^2) \) in the dual space to determine the tight, analytical bounds for the sum of variances (equation (1)).

As a starting point we can assume that without loss of generality \( \text{Tr} X = \text{Tr} Y = 0 \)—constant shift does not change the variances. Furthermore, let us introduce a traceless operator \( Z \) related to the sum of squares,
\[ Z = X^2 + Y^2 - \frac{\text{Tr}(X^2 + Y^2)}{d} \mathbb{1}, \quad (A.5) \]

**Figure A1.** Visualization of the process of finding the set \( W^\circ \) (right panel), dual of the numerical range \( W \) (left panel). The maximum of a scalar product is attained on an image of an eigenvector to the maximal eigenvalue, as shown on left panel.

**Figure A2.** 3D numerical range \( W(X, Y, X^2 + Y^2) \) for \( X \) and \( Y \) defined in equation (15), shaded according to sum of variances \( \Delta^2 X + \Delta^2 Y \). Paraboloid of a minimal uncertainty (sum of variances) is shown, as well as the minimizing point (yellow dot and dashed guiding lines).
The problem can also be rephrased in terms of geometry: for a given convex set \( W(X, Y, Z) \subset \mathbb{R}^3 \) calculate the minimal shift \( t \) of the paraboloid of a constant uncertainty, \( P_r = \{ (x, y, z) \in \mathbb{R}^3 : z = x^2 + y^2 = \tau \} \), such that the paraboloid \( P_r \) is tangent to the numerical range \( W \)—see figure 1.

The theory of numerical range implies [32] that the dual set \( W^c \) is contained in the set of roots of the polynomial in real variables \( u, v \) and \( w \):

\[
Q(u, v, w) := \det (uX + vY + wZ - 1) = 0. \tag{A.6}
\]

Tracelessness of all operators come in handy during the analysis of this set: we exactly know what subset of solutions of this equation forms \( W^c \). From the definition involving dual space it is also apparent why to minimize equation (8) we can assume smooth behavior of the function, as in equation (9): the cusps in dual the space correspond to flat surfaces in real space: variance, being a strictly convex function, does not attain minimum on a flat part of numerical range.

The paraboloid is not a numerical range, however, its dual can be defined analogously by relation (A.1). It admits the same analytical treatment at determination of the defining polynomial in dual space: the dual of the paraboloid \( P_r \) for a fixed parameter \( \tau \), denoted by \( P_r^\circ \), is determined by equation

### Table D1. Table of polynomials defining strict minimal values of sum of variances for angular momentum operators. The polynomials are minimal: there exist no lower order polynomials with integer coefficients for which \( \min \Delta^2 J_X + \Delta^2 J_Y = 0 \) is one of the roots.

| Total angular momentum \( j \) | Polynomial \( P(\lambda) \) for which \( P(\min \Delta^2 J_X + \Delta^2 J_Y) = 0 \) |
|---------------------------------|--------------------------------------------------|
| 1/2                            | \( 4\lambda - 1 \)                               |
| 1                              | \( 16\lambda - 7 \)                              |
| 3/2                            | \( 64\lambda^3 - 336\lambda^2 + 480\lambda - 181 \) |
| 2                              | \( 1024\lambda^3 - 7104\lambda^2 + 13404\lambda - 6487 \) |
| 5/2                            | \( 4194 304\lambda^7 - 117 440 512\lambda^6 + 1323 466 752\lambda^5 - 7743 660 032\lambda^4 + 2530 187 0144\lambda^3 + 42 609 045 676\lambda - 15 158 613 241 \) |
| 3                              | \( 262 144\lambda^9 - 8159 232\lambda^8 + 98 042 880\lambda^7 - 574 842 880\lambda^6 + 1709 341 632\lambda^5 \) |
|                                | \( -2397 898 539\lambda + 1179 352 998 \)       |
| 7/2                            | \( 8589 934 592\lambda^{13} - 807 453 851 648\lambda^{12} + 33 979 291 585 024 \lambda^{11} - 846 111 845 646 336\lambda^{10} + 13 886 438 674 268 160 \lambda^{9} - 158 338 610 153 127 936 \lambda^{8} + 1288 197 712 964 943 872\lambda^7 - 7558 113 438 967 267 328\lambda^6 + 31 923 050 400 995 246 592\lambda^5 - 95 672 589 723 220 763 904\lambda^4 + 197 231 954 550 318 498 240\lambda^3 - 263 781 099 083 569 171 968\lambda^2 + 203 719 751 641 654 010 210\lambda - 67 745 907 126 251 250 695 \) |
| 4                              | \( 268 435 456\lambda^{10} - 24 326 963 200\lambda^9 + 952 177 262 592\lambda^8 - 21 110 360 768 512\lambda^7 + 292 217 512 296 448\lambda^6 - 2624 974 965 550 080\lambda^5 + 15 404 738 985 045 728\lambda^4 - 57 914 832 267 046 937\lambda^3 + 132 277 607 024 648 928\lambda^2 - 163 205 035 294 297 553\lambda + 79 926 677 043 771 116 \) |

where \( d \) denotes the dimension of the Hilbert space. Minimizing the function \( v' = (Z) - (X)^2 - (Y)^2 + \text{Tr}(X^2 + Y^2)/d \) is equivalent to the original problem: the result \( v_{\text{min}} \) yields the desired bound for sum of variances. Working with traceless operators later proves to be convenient.
\[ D(\tau) := u^2 + v^2 + 4w - 4w^2\tau = 0. \]  

(A.7)

For a negative \( \tau \), the set of roots of (A.7) becomes a hollow ellipsoid. We are going to seek the roots in this region, since the operator \( Z \) is \( X^2 + Y^2 \) shifted by identity matrix times \(-\text{Tr}(X^2 + Y^2)/d\); let us denote this value by \( \lambda_0 \) for further usage.

The bound \( C \) for the sum of variances, is thus determined by two conditions: the two sets must intersect and have common normal vector. In the dual space approach these properties correspond to opposite ones in real space:

(i) The manifolds must intersect, \( D(\lambda - \lambda_0) = Q = 0 \) for particular real \( \lambda, u, v, w \). In real space this corresponds to numerical range \( W(X, Y, Z) \) and parabola of constant uncertainty \( P_\tau \) having the same supporting plane.

(ii) At the point of intersection the sets must have colinear normal vectors, which amounts to \( \nabla Q(\lambda) \propto \nabla D \). In real space this requirement alone means that the numerical range and parabola of constant uncertainty intersect.

These conditions are equivalent to solving the following set of polynomial equations for real variables \( u, v, w, \lambda \) and the multiplier \( \alpha \),

\[
\begin{align*}
D(\lambda - \lambda_0) & = 0, \\
Q(u, v, w) & = 0, \\
\partial_i (Q(u, v, w) - \alpha D(\lambda - \lambda_0)) & = 0 \text{ for } i = u, v, w.
\end{align*}
\]

(A.8)

The reasoning behind solving this set of equations is analogous to this presented in equation (9): the set of values of \( \lambda \) for which equation (A.8) has a solution is discrete (each corresponding to local extremum of variance on \( W(X, Y, Z) \)); this set can be deduced from above equations by systematic reduction of polynomials, in the end leading to single polynomial of \( \lambda \) only, denoted by \( R(\lambda) \)—see appendix B for the details.

The bound corresponds to the minimal real root of the polynomial equation \( R(\lambda) = 0 \), denoted by \( \lambda_{\min} \), equivalent to the above set of five equations, for which real solutions to \( u, v, w, \alpha \) exist (in general they may be complex regardless of real \( \lambda \)). Then the tight bound for \( \Delta^2 X + \Delta^2 Y \) reads

\[ \Delta^2 X + \Delta^2 Y \geq C(X, Y) = \lambda_{\min}. \]  

(A.9)

It is possible to determine the state saturating the uncertainty relation by solving the polynomial system described in (A.8) with variable \( \lambda \) set to the calculated constant \( \lambda_{\min} \).

A general solution of the problem in the simplest case \( d = 2 \) is provided in appendix C, while for higher dimensions, calculations performed for individual cases yield analytical results determined by roots of a particular polynomial.

**Appendix B. Solving the equations leading to uncertainty relation**

The simplification of the set of equation (A.8) or (9) may be found in an algebraic way, which presents the result in an explicitly analytical way. This is the method of Gröbner basis, described below.

Consider arbitrary set of polynomial equations of finite number of variables:

\[
\begin{align*}
P_1(x_1, \ldots, x_k) & = 0, \\
P_2(x_1, \ldots, x_k) & = 0, \\
\ldots \\
P_n(x_1, \ldots, x_k) & = 0.
\end{align*}
\]

(B.1)
Our goal is to calculate the realization of variables \((x_1, \ldots, x_k)\) with minimal \(x_1\) among all real solutions to this system of equations. Let us assume that the set of all solutions—which may be complex—is discrete. It is the generic case if number of equations \(n\) is equal to number of variables \(k\)—a result reminiscent to the linear algebra in which a matrix equation \(Ax = \vec{y}\) has a single solution if matrix \(A\) is nondegenerate.

The algorithm used to determine set of common solutions to (B.1) has some resemblance to Gaussian elimination known from linear algebra. To solve the system of linear equations we

(i) choose an order of variables, i.e. any permutation of \((x_1, \ldots, x_k)\) interpreted as sequence of symbols,
(ii) recursively reduce system of equations by multiplication and addition, such that at the end a single equation for the last variable in the chosen order is obtained (e.g. for a natural order \((x_1, \ldots, x_k)\) we get a linear equation for \(x_k\)),
(iii) recursively solve the equations for remaining variables by back substitution.

Conceptually, the Buchberger algorithm [33] which solves the system of polynomial equation (B.1) does not differ much:

(i) a choice of order of monomials—expressions of form \(x_1^{\alpha_1}x_2^{\alpha_2}\cdots x_k^{\alpha_k}\)—is needed. This order will determine the last remaining equation to solve, just as in the case of variables in Gaussian elimination. Since exponents \(\alpha_1, \ldots, \alpha_k\) in monomials may potentially become very large, a consistent and simple to calculate order choice is needed. A natural choice is such that the last elements of order are powers of \(x_k\) only.
(ii) The system of polynomial equations is recursively reduced by multiplication by polynomials and addition, such that in each step a leading term (defined by chosen order) of polynomials involved is decreasing. If we choose the order described above, the last polynomial equation consists of monomials in \(x_k\) only.
(iii) The last equation—a polynomial in \(x_k\) only—is solved; remaining equations are recursively solved by back substitution.

In our case we wish to set \(\lambda\) of appearing in equation (A.8) or (9) as the last variable, so that all others (\(x, y\) in equation (A.8), \(u, v, w, \alpha\) in equation (9)) do not appear in the final solution. The minimal real root of the resulting polynomial in \(\lambda\) for which all the other corresponding variables also have real values is exactly what we are looking for in the first place.

Appendix C. Numerical range and bounds for \(d = 2\)

In the case of qubit observable \(X\), the squared operator \(X^2\) may always be written as combination of identity and \(X\): \(X^2 = \frac{1}{2}\text{Tr}X^2 + \frac{1}{4}X\text{Tr}X\). Additionally, the JNR of two operators of size \(d = 2\) is an ellipse, hence the JNR of three operators \(W(X, Y, X^2 + Y^2)\) is a flat object—linear transformation of ellipse. The variance is thus minimized on the curve bounding the JNR. This is already known [34]; here we reconstruct the result using the analytical method of solving the equation (A.8).

Arbitrary qubit observables \(X\) and \(Y\) can always be rescaled to form

\[
X = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad Y = \begin{pmatrix} a & b \\ b^* & -a \end{pmatrix}.
\]  

(C.1)

The resulting polynomial reads

\[
a^2t + |b|^2t + |b|^2 + t^2 + t.
\]  

(C.2)
and implies bound $C$ for the sum of variances

$$C = \frac{1}{2} \left( a^2 + |b|^2 + 1 - \sqrt{(a^2 + |b|^2 + 1)^2 - 4|b|^2} \right). \quad (C.3)$$

**Appendix D. Resulting polynomials**

In table D1 we present some of the resulting polynomials defining the minimal sums of variances presented in table 1. The polynomials for higher total angular momenta ($j > 4$) are omitted due to their length. The only discernible pattern we have observed is in the order of polynomials—the online catalogue OEIS recognizes this sequence as part of A243099, with general term (for $n \geq 1$)

$$a(n) = \frac{1}{16} \left( 6 + n(3n + 2) - (-1)^n(n - 2) + 6 \right). \quad (D.1)$$

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