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Preparational Uncertainty Relations for N Continuous Variables

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Abstract

A smooth function of the second moments of N continuous variables gives rise to an uncertainty relation if it is bounded from below. We present a method to systematically derive such bounds by generalizing an approach applied previously to a single continuous variable. New uncertainty relations are obtained for multi-partite systems which allow one to distinguish entangled from separable states. We also investigate the geometry of the "uncertainty region" in the $N(2N+1)$-dimensional space of moments. It is shown to be a convex set for any number continuous variables, and the points on its boundary found to be in one-to-one correspondence with pure Gaussian states of minimal uncertainty. For a single degree of freedom, the boundary can be visualized as one sheet of a "Lorentz-invariant" hyperboloid in the three-dimensional space of second moments.

1 Introduction

Uncertainty relations express limitations on the precision with which one can measure specific properties of a quantum system, such as position and momentum of a quantum particle. These relations come in different flavours. They may express the inability to *prepare* a quantum system in a state for which incompatible properties possess exact values. Alternatively, *error-disturbance* uncertainty relations refer to the constraints encountered when attempting to extract precise values through measurements on a single system. Both cases point to the uncertainty inherent in the quantum description of the world.

Heisenberg was the first to realize, in 1927, that uncertainty relations exist for quantum systems [1]. His physical arguments were quickly developed by Kennard [2], Weyl [3], Robertson [4] and Schrödinger [5]. Except for Heisenberg's paper, the focus of these contributions was on preparational uncertainty, not yet clearly distinguished from measurement uncertainty. Only in 1965, Arthurs and Kelly presented a model of joint measurement of position and momentum [6], laying the foundations for interest in error-disturbance uncertainty relations which has grown considerably over the last two de-

cades. Different approaches rely on different concepts of error which has led to lively debates [7, 8].

In recent years, the discussion of uncertainty relations has turned from conceptual aspects to applications, in line with the overall thrust of quantum information. For example, the first protocol of quantum cryptography, known as BB84 [9], is based on pairs of mutual unbiased bases which are known to come with maximal preparational uncertainty. It is also possible to use variance-based uncertainty relations to formulate criteria to detect entangled states of bi-partite systems [10, 11].

This work investigates the structure of preparational uncertainty relations in quantum systems with more than one continuous variable, i.e. $N \geq 2$. Examples are given by a point particle moving in a plane ($N = 2$) or in three-dimensional space ($N = 3$); alternatively, one may consider N particles each moving along a real line, each with configuration space $\mathbb{R}$. Our main goals are (i) to obtain lower bounds for given smooth functions depending on the $N(2N + 1)$ second moments of a system with N continuous variables, (ii) turn these bounds into criteria which enable us to detect entangled states, and (iii) to understand the geometric structure of uncertainty functionals in the space of second moments, spanned by the independent elements of the covariance matrix.

Using a variational technique originally introduced by Jackiw [12], we will generalize an approach which has been carried out successfully for quantum systems with a single particle-type degree of freedom, i.e. $N = 1$ [13]. Encouraged by the new uncertainty relations obtained in this way for a single continuous variable, we are particularly interested in the possibility to create inequalities which are capable to detect entangled states in systems with two or more continuous variables. Tools to detect entanglement are crucial for the implementation of any protocol in quantum information which relies on entangled states. For continuous variables, quantum optical methods are available to reliably check variance-based entanglement criteria, allowing one to verify that a required entangled state has indeed been created [14, 15, 16].

In Sec. 2, we will introduce uncertainty functionals for N continuous variables depending on second moments and describe a method to determine their extrema and, subsequently, their minima. Sec. 3 applies the approach to simple cases, leading to new uncertainty relations some of which may be used to signal the presence of entangled states. A useful geometrical picture of the uncertainty region – i.e. the covariance matrices represented in the space of second moments – is derived in Sec. 4. The final section contains a brief summary.

2 Lower bounds of uncertainty functionals

2.1 Extrema of uncertainty functionals

To describe a quantum system of continuous variables with N spatial degrees of freedom, one associates N pairs of canonical operators obeying the commutation relations

$$[\hat{q}_k, \hat{p}_{k'}] = i\hbar\delta_{kk'}\,, \quad [\hat{q}_k, \hat{q}_{k'}] = [\hat{p}_k, \hat{p}_{k'}] = 0\,, \quad k, k' = 1, \ldots, N\,. \tag{1}$$

We will arrange the momentum and position operators of the k-th degree of freedom, $\hat{p}_k$ and $\hat{q}_k$, respectively, into a column vector $\hat{\mathbf{z}}$,

$$\hat{\mathbf{z}}^\top = (\hat{p}_1, \hat{q}_1, \ldots, \hat{p}_N, \hat{q}_N) \equiv (\hat{z}_1, \hat{z}_2, \ldots, \hat{z}_{2N-1}, \hat{z}_{2N})\,, \tag{2}$$

with $2N$ components $\hat{z}_\mu, \mu = 1, \ldots, 2N$. The pure states of the quantum systems considered here are represented by unit vectors $|\psi\rangle \in \mathscr{H}$, in an infinite-dimensional Hilbert space $\mathscr{H}$. Of the $(2N)^2$ second moments

$$c_{\mu\nu} = \frac{1}{2}\langle\psi|\left(\hat{z}_\mu\hat{z}_\nu + \hat{z}_\mu\hat{z}_\nu\right)|\psi\rangle\,, \quad \mu\,, \nu = 1, \ldots, 2N\,, \tag{3}$$

only $N(2N+1)$ are independent. We assume (without loss of generality) that all first moments vanish, which follows from the invariance of the second moments under rigid phase-space translations. The second moments $c_{\mu\nu}$ form the *covariance matrix* $\mathbf{C}$ associated with the pure state $|\psi\rangle$.

With $k = 1, \ldots, N$, and for $\mu = \nu = 2k-1$ ($\mu = \nu = 2k$) one obtains the variance of momentum (position) of the k-th degree of freedom, while for $\mu = 2k, \nu = 2k-1$ we obtain their covariance; all other values of the indices μ, ν, correspond to moments which mix different degrees of freedom. Occasionally, we will denote the variances of the k-th momentum and position with x_k and y_k, respectively, and their covariance by w_k.

Given a real function of the second moments for N continuous variables, $f : \mathbb{R}^{N(2N+1)} \to \mathbb{R}$, we wish to establish whether it has a non-trivial lower bound b. If it does, the statement $f \geq b$ provides an uncertainty relation.

Following an idea of Jackiw [12] (see also [17, 18, 19]), we define an *uncertainty functional* associated with the function f by

$$\begin{aligned} J[\psi] &= f\left(\Delta^2 p_1, \Delta^2 q_1, C_{p_1q_1}, \ldots C_{p_1p_2}, C_{p_1q_2}, \ldots\right) - \lambda(\langle\psi|\psi\rangle - 1)\,, \\ &= f\left(x_1, y_1, w_1, \ldots, c_{13}, c_{14}, \ldots\right) - \lambda(\langle\psi|\psi\rangle - 1)\,, \end{aligned} \tag{4}$$

where the Lagrange multiplier λ ensures that any solutions will be given by a normalised state. We first list all *local* second moments for each degree of freedom (the two variances and the covariance), followed by the *non-local* moments which involve different degrees of freedom. A variation of such a functional will, in analogy to the one-dimensional case (cf. [13, 20]) , lead to an eigenvalue equation quadratic in position and momentum

operators. Let us briefly spell out the derivation in the more general setting.

First, we compare the value of the functional $J[\psi]$ in the state $|\psi+\varepsilon\rangle = |\psi\rangle + \varepsilon|e\rangle$ with its value in the state $|\psi\rangle$, where $|e\rangle \in \mathscr{H}$ is an arbitrary normalised state. Expanding it up to second order in the small parameter ε, we find

$$J[\psi+\varepsilon] = J[\psi] + \varepsilon D_\varepsilon J[\psi] + O\left(\varepsilon^2\right), \tag{5}$$

where the expression

$$D_\varepsilon = \langle e| \frac{\delta}{\delta\langle\psi|} + \frac{\delta}{\delta|\psi\rangle} |e\rangle, \tag{6}$$

denotes a Gâteaux derivative. The stationary points of the functional are characterised by the vanishing of the first-order term in the expansion (5),

$$D_\varepsilon J[\psi] = \langle e| \left(\frac{\delta}{\delta\langle\psi|} f\left(x_1, y_1, w_1, \ldots, c_{13}, c_{14}, \ldots\right) - \lambda|\psi\rangle \right) + \text{c.c.} = 0\,. \tag{7}$$

More explicitly, this condition reads

$$\langle e| \left(\sum_{\mu\leq\nu} \left(\frac{\partial f}{\partial c_{\mu\nu}} \frac{\delta c_{\mu\nu}}{\delta\langle\psi|} \right) - \lambda|\psi\rangle \right) + \text{c.c.} = 0\,, \tag{8}$$

where the sum runs over the values $1 \leq \mu \leq 2N$ and $\mu \leq \nu \leq 2N$. Since Eq. (8) should hold for arbitrary variations of the ket $|e\rangle$ and its dual $\langle e|$ (which are independent), the expression in round brackets as well as its complex conjugate must vanish identically.

The functional derivatives of the second moments are

$$\frac{\delta c_{\mu\nu}}{\delta\langle\psi|} \equiv \frac{1}{2}\left(\hat{z}_\mu\hat{z}_\nu + \hat{z}_\nu\hat{z}_\mu\right)|\psi\rangle\,, \tag{9}$$

resulting in an *Euler-Lagrange*-type equation,

$$\left(\sum_{\mu\leq\nu} \frac{1}{2}\left(\hat{z}_\mu\hat{z}_\nu + \hat{z}_\nu\hat{z}_\mu\right) \frac{\partial f}{\partial c_{\mu\nu}} - \lambda \right) |\psi\rangle = 0\,. \tag{10}$$

The value of the multiplier λ can be found by multiplying this equation with the bra $\langle\psi|$ from the left and solving for λ. Substituting its value back into Eq. (10), one finds the nonlinear eigenvector-eigenvalue equation,

$$\sum_{\mu\leq\nu} \frac{1}{2}\left(\hat{z}_\mu\hat{z}_\nu + \hat{z}_\nu\hat{z}_\mu\right) \frac{\partial f}{\partial c_{\mu\nu}}|\psi\rangle = \sum_{\mu\leq\nu} c_{\mu\nu} \frac{\partial f}{\partial c_{\mu\nu}}|\psi\rangle\,, \tag{11}$$

or, in matrix notation,

$$\left(\hat{\mathbf{z}}^\top \mathbf{F}\, \hat{\mathbf{z}}\right)|\psi\rangle = \mathrm{Tr}\left(\mathbf{C}\,\mathbf{F}\right)|\psi\rangle\,, \tag{12}$$

where the matrix $\mathbf{F}$ is defined in terms of the first partial derivatives of the function f: its diagonal elements are equal to $f_{c_{\mu\mu}}$, while the off-diagonal ones are given by $f_{c_{\mu\nu}}/2$, using

the standard convention to denote partial derivatives by subscripts. As an example, the eigenvalue equation becomes, for $N = 2$,

$$\left(\sum_{k=1}^{2}\left(f_{x_k}\hat{p}_k^2 + f_{y_k}\hat{q}_k^2 + \frac{f_{w_k}}{2}\left(\hat{q}_k\hat{p}_k + \hat{p}_k\hat{q}_k\right)\right) + f_{c_{13}}\hat{p}_1\hat{p}_2 + \ldots + f_{c_{24}}\hat{q}_1\hat{q}_2\right)|\psi\rangle = \\ = \left(\sum_{k=1}^{2}\left(x_k f_{x_k} + y_k f_{y_k} + w_k f_{z_k}\right) + c_{13}f_{c_{13}} + \ldots + c_{24}f_{c_{24}}\right)|\psi\rangle\,. \tag{13}$$

Note that Eq. (12) is generally non-linear in the state $|\psi\rangle$ since the second moments and the partial derivatives of f are functions of expectation values in the state $|\psi\rangle$. As we will show in next section, one can nevertheless solve Eq. (12), given a number of assumptions.

2.2 Consistency conditions

To solve Eq. (12), we initially assume that the matrix $\mathbf{F}$ of partial derivatives is *constant*, i.e. we suppress its dependence on the state $|\psi\rangle$. If we further require that $\mathbf{F}$ is positive definite, then Williamson's theorem [21, 22] guarantees the existence of a symplectic matrix $\mathbf{\Sigma}$ that puts $\mathbf{F}$ into a diagonal form, i.e.

$$\mathbf{F} = \mathbf{\Sigma}^\top \mathbf{D}\,\mathbf{\Sigma}\,, \tag{14}$$

where the diagonal matrix $\mathbf{D}$ is defined by $\mathbf{D} = \mathrm{diag}(\lambda_1, \lambda_1, \ldots, \lambda_N, \lambda_N)$, and the positive real numbers $\lambda_k > 0$, $k = 1, \ldots, N$, are the *symplectic eigenvalues* of $\mathbf{F}$ [23, 24, 22]. We recall that a symplectic matrix of order $2N$ satisfies $\mathbf{\Sigma}^\top \mathbf{\Omega}\,\mathbf{\Sigma} = \mathbf{\Omega}$, where $\mathbf{\Omega}$ is uniquely determined by the commutation relations, $[\hat{z}_\mu, \hat{z}_\nu] = i\hbar\Omega_{\mu\nu}$, $\mu, \nu = 1, \ldots, 2N$.

Multiplying both sides of Eq. (12) with the metaplectic unitary operator $\hat{S}^\dagger$ from the left, defined by the relation

$$\mathbf{\Sigma}\,\hat{\mathbf{z}} = \hat{S}\,\hat{\mathbf{z}}\,\hat{S}^\dagger\,, \tag{15}$$

we find that its left-hand-side can be expressed as

$$\hat{S}^\dagger\left(\hat{\mathbf{z}}^\top \mathbf{F}\,\hat{\mathbf{z}}\right)\hat{S}\left(\hat{S}^\dagger|\psi\rangle\right) = \left(\hat{S}^\dagger\hat{\mathbf{z}}^\top\hat{S}\right)\mathbf{F}\left(\hat{S}^\dagger\hat{\mathbf{z}}\hat{S}\right)\left(\hat{S}^\dagger|\psi\rangle\right) \\ = \left(\mathbf{\Sigma}^{-1}\hat{\mathbf{z}}\right)^\top\left(\mathbf{\Sigma}^\top\mathbf{D}\,\mathbf{\Sigma}\right)\left(\mathbf{\Sigma}^{-1}\hat{\mathbf{z}}\right)\left(\hat{S}^\dagger|\psi\rangle\right)\,. \tag{16}$$

Thus, Eq. (12) simplifies to

$$\left(\hat{\mathbf{z}}^\top\mathbf{D}\,\hat{\mathbf{z}}\right)\left(\hat{S}^\dagger|\psi\rangle\right) = \mathrm{Tr}\left(\mathbf{C}\,\mathbf{F}\right)\left(\hat{S}^\dagger|\psi\rangle\right)\,, \tag{17}$$

which can be written as

$$\sum_{k=1}^{N}\lambda_k\left(\frac{\hat{p}_k^2 + \hat{q}_k^2}{2}\right)\left(\hat{S}^\dagger|\psi\rangle\right) = \frac{1}{2}\,\mathrm{Tr}\left(\mathbf{C}\,\mathbf{F}\right)\left(\hat{S}^\dagger|\psi\rangle\right)\,. \tag{18}$$

Thus, we have transformed the quadratic operator on the left-hand-side of Eq. (12) into a Hamiltonian operator given by a sum of N decoupled harmonic oscillators. The solutions of Eq. (18) are given by tensor products of number states for each degree of freedom,

$$|\psi\rangle = \hat{S}\left(|n_1\rangle \otimes \ldots \otimes |n_N\rangle\right) \equiv \hat{S}\left(\bigotimes_{k=1}^{N} |n_k\rangle\right). \tag{19}$$

Note that the constraint

$$\frac{1}{2}\,\mathrm{Tr}\left(\mathbf{C}\,\mathbf{F}\right) = \sum_{k=1}^{N} \lambda_k \left(n_k + \frac{1}{2}\right)\hbar\,, \tag{20}$$

must be satisfied by all potential extremal states.

Recall that we have treated the matrix elements of the matrix $\mathbf{F}$ introduced in Eq. (12) as constants, on which the unitary transformation $\hat{S}$ and hence the states $|\psi\rangle$ in Eq. (19) now depend. To achieve consistency, we determine the expectation value of the covariance matrix in the solution $|\psi\rangle$. A set of coupled equations in matrix form results for the extremal second moments, which we will call the *consistency conditions*. Explicitly, we find

$$\begin{aligned}\mathbf{C} = \langle\psi|\hat{\mathbf{C}}|\psi\rangle &\equiv \frac{1}{2}\langle\psi|\left(\hat{\mathbf{z}}\otimes\hat{\mathbf{z}}^\top + \left(\hat{\mathbf{z}}\otimes\hat{\mathbf{z}}^\top\right)^\top\right)|\psi\rangle \\ &= \frac{1}{2}\left(\bigotimes_{k=1}^{N}\langle n_k|\right)\hat{S}^\dagger\left(\hat{\mathbf{z}}\otimes\hat{\mathbf{z}}^\top + \left(\hat{\mathbf{z}}\otimes\hat{\mathbf{z}}^\top\right)^\top\right)\hat{S}\left(\bigotimes_{k'=1}^{N}|n_{k'}\rangle\right),\end{aligned} \tag{21}$$

where $\hat{\mathbf{z}}\otimes\hat{\mathbf{z}}^\top$ denotes the Kronecker product of the column vector $\hat{\mathbf{z}}$ with its transpose, $\hat{\mathbf{z}}^\top$. Using the identity (15) in the form $\boldsymbol{\Sigma}^{-1}\,\hat{\mathbf{z}} = \hat{S}^\dagger\,\hat{\mathbf{z}}\,\hat{S}$, we can express the covariance matrix in the form

$$\mathbf{C} = \boldsymbol{\Sigma}^{-1}\frac{1}{2}\left(\mathbf{N} + \mathbf{N}^\top\right)(\boldsymbol{\Sigma}^{-1})^\top, \tag{22}$$

with the matrix

$$\mathbf{N} = \left(\bigotimes_{k=1}^{N}\langle n_k|\right)\hat{\mathbf{z}}\otimes\hat{\mathbf{z}}^\top\left(\bigotimes_{k'=1}^{N}|n_{k'}\rangle\right), \tag{23}$$

having elements

$$N_{\mu\nu} = \langle n_1,\ldots,n_N|\,\hat{z}_\mu\hat{z}_\nu\,|n_1,\ldots,n_N\rangle\,,\quad \mu,\nu = 1,\ldots,2N\,. \tag{24}$$

Recalling that the components of the vector $\hat{\mathbf{z}}$ are position and momentum operators, it is not difficult to see that the only non-zero matrix elements of $\mathbf{N}$ are on its diagonal, i.e.

$$\mathbf{N} = \hbar\,\mathrm{diag}\left(n_1+\frac{1}{2}, n_1+\frac{1}{2}, \ldots, n_N+\frac{1}{2}, n_N+\frac{1}{2}\right) \tag{25}$$

Using the property $\mathbf{N}^\top = \mathbf{N}$, which holds for any diagonal matrix, we finally obtain the

consistency conditions for N continuous variables,

$$\mathbf{C} = \mathbf{\Sigma}^{-1}\mathbf{N}\left(\mathbf{\Sigma}^{-1}\right)^{\top}. \tag{26}$$

These conditions select the extrema that are compatible with the specific function of the second moments considered. The constraint given in (20) can be rewritten as

$$\mathrm{Tr}(\mathbf{C}\,\mathbf{F}) = \mathrm{Tr}(\mathbf{D}\,\mathbf{N})\,, \tag{27}$$

and it is easy to check that this condition is trivially satisfied if the consistency conditions (26) hold.

The take-away message from the conditions (26) can be summarised as follows: *a function f of the second moments of N positions and momenta has an extremum in a pure state $|\psi\rangle$ if there exists a symplectic matrix $\mathbf{\Sigma}$ that diagonalises the covariance matrix $\mathbf{C}$ and, at the same time, the transpose of its inverse, $\left(\mathbf{\Sigma}^{-1}\right)^{\top}$, diagonalises the matrix $\mathbf{F}$ of the partial derivatives of the function f.*

According to (26), the determinant of the covariance matrix for extremal states of the uncertainty functional $J[\psi]$ takes the value

$$\det\mathbf{C} = \prod_{k=1}^{N}\left(n_k + \frac{1}{2}\right)^2\hbar^2\,. \tag{28}$$

Clearly, the minimum is achieved when each oscillator resides in its ground state,

$$\det\mathbf{C} \geq \left(\frac{\hbar}{2}\right)^{2N}, \tag{29}$$

corresponding to $n_1 = \ldots = n_N = 0$ in Eq. (28).

No pure N-particle state can give rise to a covariance matrix $\mathbf{C}$ violating the inequality (29). This universally valid constraint generalizes the single-particle inequality derived by Robertson and Schrödinger to N particles, expressing it elegantly as a condition on the determinant of the covariance matrix of a state. Supplying (28) with the lower-dimensional Robertson-Schrödinger-type inequalities that need to be obeyed in by each subsystem of dimension 2 to $N-1$, we get the general uncertainty statement for more than one degrees of freedom, usually expressed in the form,

$$\mathbf{C} + i\frac{\hbar}{2}\mathbf{\Omega} \geq 0\,. \tag{30}$$

Alternatively, this requirement can be expressed in terms of inequalities for the symplectic eigenvalues of the covariance matrix [22, 24].

We conclude this section by explicitly working out the consistency conditions for one degree of freedom, $N = 1$. In this case, we obtain the matrices $\mathbf{N} = \hbar(n + 1/2)\mathbf{I}$ and

$\mathbf{\Sigma} = \mathbf{S}_\gamma \mathbf{G}_b$, with symplectic matrices $\mathbf{G}_b$ and $\mathbf{S}_\gamma$ given by

$$\mathbf{G}_b = \begin{pmatrix} 1 & 0 \\ b & 1 \end{pmatrix}, \quad \text{and} \quad \mathbf{S}_\gamma = \begin{pmatrix} e^{-\gamma} & 0 \\ 0 & e^{\gamma} \end{pmatrix}, \tag{31}$$

respectively, and real parameters

$$b = \frac{f_w}{2f_y} \in \mathbb{R} \quad \text{and} \quad \gamma = \frac{1}{2} \ln \left(\frac{f_y}{\sqrt{\det \mathbf{F}}} \right) \in \mathbb{R}\,. \tag{32}$$

The consistency conditions now take the simple form

$$\mathbf{C} = \mathbf{\Sigma}^{-1} \mathbf{N} (\mathbf{\Sigma}^{-1})^\top = \mathbf{G}_b^{-1} \mathbf{S}_\gamma^{-1} (\mathbf{S}_\gamma^{-1})^\top (\mathbf{G}_b^{-1})^\top \hbar \left(n + \frac{1}{2} \right) = \mathbf{F}^{-1} \hbar \left(n + \frac{1}{2} \right) \sqrt{\det \mathbf{F}} \tag{33}$$

or finally,

$$\frac{\mathbf{F}\,\mathbf{C}}{\sqrt{\det \mathbf{F}}} = \hbar \left(n + \frac{1}{2} \right) \mathbf{I}\,, \qquad n \in \mathbb{N}_0\,. \tag{34}$$

Therefore, the formalism developed here correctly reproduces the findings of [13].

3 Inequalities for two or more continuous variables

3.1 Inequalities without correlation terms

Let us now examine the consistency conditions for more than one degree of freedom while allowing only product states. Correlations between the degrees of freedom being absent, the functional will only depend on the *local* second moments, that is, $f \equiv f(x_1, y_1, w_1, \ldots, x_N, y_N, w_N)$; the $2N(N-1)$ moments mixing the degrees of freedom are always zero in a separable state. For simplicity, we only consider $N = 2$ in some detail, the generalisation to $N > 2$ being straightforward.

Using matrices $\mathbf{G}_b$ and $\mathbf{S}_\gamma$ defined in (31), we construct two symplectic matrices $\mathbf{S}_1$ and $\mathbf{S}_2$ as follows,

$$\mathbf{\Sigma}_1 = \begin{pmatrix} \mathbf{S}_{\gamma_1} \mathbf{G}_{b_1} & 0 \\ 0 & \mathbf{I} \end{pmatrix} \quad \text{and} \quad \mathbf{\Sigma}_2 = \begin{pmatrix} \mathbf{I} & 0 \\ 0 & \mathbf{S}_{\gamma_2} \mathbf{G}_{b_2} \end{pmatrix}. \tag{35}$$

Their product, $\mathbf{\Sigma} = \mathbf{\Sigma}_1 \mathbf{\Sigma}_2$ describes the action of the factorised unitary operator

$$\hat{S} = \hat{S}_1 \otimes \hat{S}_2\,, \tag{36}$$

when solving the eigenvalue equation (12). The consistency conditions become

$$\mathbf{C} = \mathbf{\Sigma}^{-1} \mathbf{N} (\mathbf{\Sigma}^{-1})^\top = \mathbf{\Sigma}^{-1} (\mathbf{\Sigma}^{-1})^\top \mathbf{N} = \mathbf{F}_{pr}^{-1} \mathbf{N}\,, \tag{37}$$

with

$$\mathbf{F}_{pr} = \begin{pmatrix} \mathbf{F}_1/\sqrt{\det \mathbf{F}_1} & 0 \\ 0 & \mathbf{F}_2/\sqrt{\det \mathbf{F}_2} \end{pmatrix}, \tag{38}$$

so that we finally obtain

$$\mathbf{F}_{pr}\mathbf{C} = \mathbf{N}\,; \tag{39}$$

in Eq. (38), the 2×2 matrices $\mathbf{F}_k, k = 1, 2$, denote the collection of partial derivatives of the function f with respect to the moments of the k-th degree of freedom. Therefore, the consistency conditions for functionals of product states reduce to a pair of one-dimensional ones which must be solved simultaneously.

The generalisation to N degrees of freedom is straightforward: for each extra degree of freedom, a matrix $\mathbf{F}_k/\sqrt{\det \mathbf{F}_k}$ must be added to the diagonal of the block matrix $\mathbf{F}_{pr}$. After introducing the suitably generalized matrices $\mathbf{C}$ and $\mathbf{N}$, Eqs. (39) describe the consistency conditions for separable quantum states. It is often useful to express Eq. (39) as

$$x_k f_{x_k} = y_k f_{y_k}\,, \quad 2w_k f_{y_k} = -x_k f_{w_k}\,, \quad x_k y_k - w_k^2 = \hbar^2 \left(n_k + \frac{1}{2}\right), \tag{40}$$

with $k = 1, \ldots, N$.

The simplest example of a factorized uncertainty relation is given by the product of two one-dimensional Robertson-Schrödinger inequalities, following from the functional

$$f(x_1, y_1, w_1, x_2, y_2, w_2) = (x_1 y_1 - w_1^2)(x_2 y_2 - w_2^2)\,, \tag{41}$$

The resulting inequality,

$$\left(\Delta^2 p_1\, \Delta^2 q_1 - C^2_{p_1 q_1}\right)\left(\Delta^2 p_2\, \Delta^2 q_2 - C^2_{p_2 q_2}\right) \geq \left(\frac{\hbar}{2}\right)^4, \tag{42}$$

corresponds to the boundary described by Eq. (29) in the absence of correlations, to be discussed in more detail in Sec. 4. Note that this inequality is only invariant under $\mathrm{Sp}(2, \mathbb{R}) \otimes \mathrm{Sp}(2, \mathbb{R})$ transformations instead of the those of $\mathrm{Sp}(4, \mathbb{R})$ group that leave invariant the Robertson-Schrödinger-type inequality for two degrees of freedom. However, the matrix inequality $\mathbf{C} + i\mathbf{\Omega}\hbar/2 \geq 0$ is invariant under any symplectic transformation and serves as the required generalisation.

Starting from the functional

$$f(x_1, y_1, w_1, x_2, y_2, w_2) = x_1\, y_1 x_2\, y_2 - w_1^2\, w_2^2 \tag{43}$$

and after solving (39), we arrive at the inequality

$$\Delta^2 p_1 \, \Delta^2 q_1 \Delta^2 p_2 \, \Delta^2 q_2 \geq \left(\frac{\hbar}{2}\right)^4 + C^2_{p_1 q_1} C^2_{p_2 q_2} \,, \tag{44}$$

which cannot be obtained by a combination of inequalities for $N = 1$. It is *stronger* than the (factorized) "Heisenberg"-type inequality for more than two observables,

$$\Delta p_1 \, \Delta q_1 \, \Delta p_2 \, \Delta q_2 \geq \left(\frac{\hbar}{2}\right)^2 , \tag{45}$$

first mentioned in a paper by Robertson [25], but *weaker* than (42). An inequality I_1 is said to be weaker than the inequality I_2 if less states saturate I_1 than I_2.

Mixing products of variances related to different degrees of freedom also leads to non-trivial inequalities such as

$$a \left(\Delta^2 p_1 \Delta^2 q_2\right)^n + b \left(\Delta^2 p_2 \Delta^2 q_1\right)^n \geq 2\sqrt{ab} \left(\frac{\hbar}{2}\right)^{2n} , \quad a, b > 0 \,. \tag{46}$$

For $a = b = 1$ and $n = 1$, one obtains

$$\Delta p_1 \Delta q_2 + \Delta p_2 \Delta q_1 \geq \hbar \,,$$

which resembles the inequality for the sum of two one-dimensional Heisenberg inequalities,

$$\Delta p_1 \Delta q_1 + \Delta p_2 \Delta q_2 \geq \hbar \,, \tag{47}$$

but differs fundamentally from it.

3.2 Inequalities with correlation terms

Dropping the limitation to product states, we now turn to functionals that involve terms to which different degrees of freedom contribute. To begin, let us consider a linear combination of second moments,

$$f\left(\Delta^2 p_1, \ldots, C_{q_1 q_2}\right) = a \left(\Delta^2 p_1 + \Delta^2 q_1\right) + b \left(\Delta^2 p_2 + \Delta^2 q_2\right) + c \left(C_{p_1 p_2} - C_{q_1 q_2}\right) ,$$

for which the matrix $\mathbf{F}$ takes the form

$$\mathbf{F} = \begin{pmatrix} a & 0 & c/2 & 0 \\ 0 & a & 0 & -c/2 \\ c/2 & 0 & b & 0 \\ 0 & -c/2 & 0 & b \end{pmatrix} . \tag{48}$$

It is positive definite whenever the coefficients a, b, c obey the conditions $a, b > 0$ and $4ab > c^2$, which we assume from now on. The symplectic matrix $\mathbf{S}$ that brings $\mathbf{F}$ to

diagonal form is given by (cf. [26]):

$$\mathbf{\Sigma} = \begin{pmatrix} \sigma_+ & 0 & \sigma_- & 0 \\ 0 & \sigma_+ & 0 & -\sigma_- \\ \sigma_- & 0 & \sigma_+ & 0 \\ 0 & -\sigma_- & 0 & \sigma_+ \end{pmatrix}, \tag{49}$$

where

$$\sigma_\pm = \sqrt{\frac{a+b\pm\sqrt{y}}{2\sqrt{y}}}, \quad \text{and} \quad y = (a+b)^2 - c^2\,. \tag{50}$$

The consistency conditions (26) can be solved in closed form, leading to the covariance matrix at the extrema

$$\mathbf{C} = \begin{pmatrix} \Delta^2 p_1^{(e)} & 0 & C^{(e)}_{p_1p_2} & 0 \\ 0 & \Delta^2 q_1^{(e)} & 0 & C^{(e)}_{q_1q_2} \\ C^{(e)}_{p_1p_2} & 0 & \Delta^2 p_2^{(e)} & 0 \\ 0 & C^{(e)}_{q_1q_2} & 0 & \Delta^2 q_2^{(e)} \end{pmatrix}, \tag{51}$$

with elements explicitly given by

$$\Delta^2 p_1^{(e)} = \Delta^2 q_1^{(e)} = \frac{(n_1-n_2)\hbar}{2} + \frac{(a+b)(n_1+n_2+1)\hbar}{2\sqrt{(a+b)^2-c^2}}\,, \tag{52}$$

$$\Delta^2 p_2^{(e)} = \Delta^2 q_2^{(e)} = \frac{(n_2-n_1)\hbar}{2} + \frac{(a+b)(n_1+n_2+1)\hbar}{2\sqrt{(a+b)^2-c^2}}\,, \tag{53}$$

and

$$C^{(e)}_{p_1p_2} = -C^{(e)}_{q_1q_2} = -\frac{c(n_1+n_2+1)\hbar}{2\sqrt{(a+b)^2-c^2}}\,. \tag{54}$$

One can check that the expressions on the right-hand side of Eqs. (52) and (53) are positive, while

$$\left(C^{(e)}_{p_1p_2}\right)^2 \leq \Delta^2 p_1^{(e)}\,\Delta^2 p_2^{(e)} \quad \text{and} \quad \left(C^{(e)}_{q_1q_2}\right)^2 \leq \Delta^2 q_1^{(e)}\,\Delta^2 q_2^{(e)} \tag{55}$$

also hold, as required. In fact, these two inequalities are never saturated by the extremal states although one can get arbitrarily close if n_1 is zero while n_2 tends to infinity (or *vice versa).*

Substituting the extremal values of the second moments back into the functional, we find

$$f^{(e)}_{a,b,c}(n_1,n_2) = (a-b)(n_1-n_2)\hbar + \sqrt{(a+b)^2-c^2}(n_1+n_2+1)\hbar \geq f_{a,b,c}(0,0) \tag{56}$$

implying the following inequality, satisfied by any quantum state:

$$a\left(\Delta^2 p_1 + \Delta^2 q_1\right) + b\left(\Delta^2 p_2 + \Delta^2 q_2\right) + c\left(C_{p_1p_2} - C_{q_1q_2}\right) \geq \hbar\sqrt{(a+b)^2-c^2}\,. \tag{57}$$

Pure separable states are known to satisfy the relation

$$a\left(\Delta^2 p_1 + \Delta^2 q_1\right) + b\left(\Delta^2 p_2 + \Delta^2 q_2\right) \geq (a+b)\hbar\,. \tag{58}$$

Now consider the limit $c \to \pm 2\sqrt{ab}$ in (57) which, however, breaks the positive definiteness of **F**: its right-hand-side tends to zero and the terms on the left are just the sum of the variances of the EPR-type operators $\hat{u}_1 = \sqrt{a}\,\hat{p}_1 + \sqrt{b}\,\hat{p}_2$ and $\hat{u}_2 = \sqrt{a}\,\hat{q}_1 - \sqrt{b}\,\hat{q}_2$ [10, 11]. In this case, the pair of inequalities (57) and (58) form the prototypical example of using uncertainty relations for entanglement detection. More specifically, whenever the sum of the variances of $\hat{u}_1$ and $\hat{u}_2$ in a given state $|\psi\rangle$ violates the bound of (58), then the state is entangled. Although inequality (58) provides only a sufficient condition for inseparability of an arbitrary state, it can become a sufficient and necessary condition for pure Gaussian states, if recast in an appropriate form [10].

Returning to inequality (57) in the case of arbitrary a, b, c, it is not immediately obvious whether it can be used to detect entangled states. However, let us define four EPR-type operators,

$$\begin{aligned} \hat{u}_1 &= \alpha_1\hat{p}_1 + \beta_1\hat{p}_2\,, \quad \hat{v}_1 = \gamma_1\hat{q}_1 - \delta_1\hat{q}_2 \\ \hat{u}_2 &= \alpha_2\hat{p}_1 + \beta_2\hat{p}_2\,, \quad \hat{v}_2 = \gamma_2\hat{q}_1 - \delta_2\hat{q}_2\,, \end{aligned} \tag{59}$$

with eight real parameters $\alpha_1, \ldots \delta_2$, which are constrained by the relations

$$\begin{gathered} \alpha_1^2 + \alpha_2^2 = \gamma_1^2 + \gamma_2^2 = a\,, \quad \beta_1^2 + \beta_2^2 = \delta_1^2 + \delta_2^2 = b\,, \\ \alpha_1\beta_1 + \alpha_2\beta_2 = \gamma_1\delta_1 + \gamma_2\delta_2 = c/2\,. \end{gathered} \tag{60}$$

Now we can write Eq. (57) as

$$\Delta^2 u_1 + \Delta^2 v_1 + \Delta^2 u_2 + \Delta^2 v_2 \geq \hbar\sqrt{(a+b)^2 - c^2}\,, \tag{61}$$

reducing to the inequality

$$\Delta^2 u_1 + \Delta^2 v_1 + \Delta^2 u_2 + \Delta^2 v_2 \geq \hbar(a+b), \tag{62}$$

if the the system resides in a separable state. Since its right-hand-side is always greater than or equal to the bound in (61), the violation of (62) indicates the presence of an entangled state.

Clearly, inequality (61) is more general than the corresponding one for the pair of operators $\hat{u}_1 = \sqrt{a}\,\hat{p}_1 + \sqrt{b}\,\hat{p}_2$ and $\hat{u}_2 = \sqrt{a}\,\hat{q}_1 - \sqrt{b}\,\hat{q}_2$, as the former reduces to the latter in the limit $c \to \pm 2\sqrt{ab}$ and thus extends a known result [10].

As a final example, consider the sum of the variances of the EPR-type operators for *three* degrees of freedom, $\hat{u}_1 = \hat{q}_1 + \hat{p}_2 + \hat{q}_3$, $\hat{u}_2 = \hat{q}_2 + \hat{p}_3 + \hat{q}_1$, $\hat{u}_3 = \hat{q}_3 + \hat{p}_1 + \hat{q}_2$, which is in general only bounded by zero. However, the lower possible value achievable in a

separable state is given by the inequality

$$\Delta^2 u_1 + \Delta^2 u_2 + \Delta^2 u_3 \geq 3\sqrt{2}\,\hbar\,, \tag{63}$$

readily obtained from the solution of Eq. (39). Again, violations of (63) detect the presence of entangled degrees of freedom.

It is, of course, possible to minimise other functions than the sum of the variances, leading to different entanglement-detecting inequalities which we will discuss elsewhere.

4 The uncertainty region

In this section, we will develop a geometric view of quantum uncertainty for a system with N continuous variables. To do so, we associate a direction of the space $\mathbb{R}^d$ with each of the second moments $C_{\mu\nu}, \mu, \nu = 1, \ldots, 2N$. Then, any quantum state gives rise to a point in the *space of second moments*, $\mathscr{S}$, which has dimension $d = N(2N+1)$.

Some points in the space $\mathscr{S} = \mathbb{R}^d$ will represent moments of quantum states while others will not. The accessible part of the space is called the *uncertainty region*, as the points it contains are in one-to-one correspondence with admissible covariance matrices $\mathbf{C} \in \mathbb{R}^{2N\times 2N}$. This region is bounded by a $(d-1)$-dimensional surface given by the relation

$$\det\left(\mathbf{C} + i\frac{\hbar}{2}\mathbf{\Omega}\right) = 0\,, \tag{64}$$

where $\mathbf{\Omega}$ is the standard symplectic matrix of order $2N \times 2N$.

4.1 More than one continuous variable: $N > 1$

We will show now that the uncertainty region in the space $\mathscr{S}$ is a *convex* set, by affirming (i) that its *boundary* (64) is convex and (ii) that all points of the uncertainty region emerge as expectations taken in *pure* states. In other words, the uncertainty region has no "pure-state holes." This property justifies our initial decision to search for extrema of uncertainty functionals among pure states only: no other extrema would result had we included mixed states. On the boundary of the uncertainty region, the relation between quantum states and their moments is unique (up to rigid translations) while (iii) points inside the uncertainty region can also be obtained from infinitely many different convex combinations of pure (or mixed) states.

The uncertainty region has a convex boundary The region defined by Eq. (29) is a *convex* set in the $N(2N+1)$-dimensional space of second moments. To see this, we consider two covariance matrices $\mathbf{C}_1$ and $\mathbf{C}_2$ which are located on its boundary given by (64), i.e. they

satisfy

$$\det \mathbf{C}_1 = \det \mathbf{C}_2 = \left(\frac{\hbar}{2}\right)^{2N} . \tag{65}$$

We recall that covariance matrices are positive definite, $\mathbf{C}_1, \mathbf{C}_2 > 0$, and that they must have sufficiently large symplectic eigenvalues in order to stem from quantum states. Convexity holds if the (positive definite) convex combination of two covariance matrices,

$$\mathbf{C}(t) = t\mathbf{C}_1 + (1-t)\mathbf{C}_2 , \qquad t \in [0,1] , \tag{66}$$

either lies on the boundary of the uncertainty region or in its interior. This property follows from the fact that the matrix function

$$g(\mathbf{A}) = -\ln \det \mathbf{A} \tag{67}$$

is convex [27], i.e. the inequality

$$g(t\mathbf{A} + (1-t)\mathbf{A}') \leq tg(\mathbf{A}) + (1-t)g(\mathbf{A}') \tag{68}$$

holds for any pair of strictly positive definite matrices, $\mathbf{A}, \mathbf{A}' > 0$. Rewriting (65) in the form

$$-\ln \det (\mathbf{C}_1/\hbar) = -\ln \det (\mathbf{C}_2/\hbar) = 2N \ln 2 , \tag{69}$$

one immediately finds that

$$-\ln \det \left[(t\mathbf{C}_1 + (1-t)\mathbf{C}_2)/\hbar \right] \leq -t \ln \det (\mathbf{C}_1/\hbar) - (1-t) \ln \det (\mathbf{C}_2/\hbar) = 2N \ln 2 . \tag{70}$$

Since

$$\det (t\mathbf{C}_1 + (1-t)\mathbf{C}_2) \geq \left(\frac{\hbar}{2}\right)^{2N} , \quad t \in [0,1] , \tag{71}$$

follows, we have shown that the convex combination of two covariance matrices on the boundary of the uncertainty region cannot produce a point outside of it. Equality holds in (71) only if $t = 0$ or $t = 1$. Therefore, states on the boundary cannot be written as mixtures which means that the states on the boundary must be pure states.

Clearly, the argument just given extends to convex combinations of covariance matrices located *inside* the uncertainty region: no such combination will produce a covariance matrix on its boundary or outside of it.

The uncertainty region has no pure-state holes We determined the conditions for uncertainty functionals to have extrema by evaluating them on all *pure* states of N quantum particles. We now show that the inclusion of mixed states as potential extrema does

not change our findings. It is sufficient to show that all points of the uncertainty region defined by the inequality (29) correspond to covariance matrices which stem from pure states.

Recall that any admissible covariance matrix can be diagonalised according to Williamson's theorem [21, 23] using a suitable symplectic transformation. Let us order its N finite symplectic eigenvalues s_1 to s_N from smallest to largest and choose an integer $M \geq 2$ such that $s_N \leq M + 1/2$ holds. Suppose now that the k-th subsystem resides in the pure state

$$|\psi_k\rangle = \sqrt{t_k}|n_k = 0\rangle + \sqrt{1-t_k}|n_k = M\rangle\,, \quad k \in \{1,\ldots,N\}\,, \quad t_k \in [0,1]\,. \tag{72}$$

The variances of position and momentum take the values

$$\Delta^2 p_k\big|_{\psi_k} = \Delta^2 q_k\big|_{\psi_k} = (1-t_k)\left(M + \frac{1}{2}\right)\hbar\,, \quad k \in \{1,\ldots,N\}\,, \quad t_k \in [0,1]\,, \tag{73}$$

where we use that the expectations of the operators $\hat{p}_k$ and $\hat{q}_k$ vanish. Thus, a suitable value of the parameter t_k leads to the desired entries s_k on the diagonal of the covariance matrix, and the covariance of position and momentum $\hat{p}_k$ and $\hat{q}_k$ equals zero. In addition, the remaining off-diagonal matrix elements – associated with the bilinear operators $\hat{p}_k\hat{q}_{k'}$ for $k \neq k'$ – also vanish in the product state

$$|\Psi\rangle = |\psi_1\rangle \otimes \ldots \otimes |\psi_N\rangle\,. \tag{74}$$

Consequently, there is a pure product state, namely $|\Psi\rangle$, to generate any desired *diagonal* covariance matrix – which is sufficient to create any admissible *non-diagonal* covariance matrix, simply by undoing the symplectic transformation used to diagonalize the initially given covariance matrix.

The map from the set of pure states to the interior of the space of moments is, of course, many-to-one. This can be seen directly by recalling that each admissible covariance matrix $\mathbf{C}$ can also be obtained from a Gaussian state characterized by a quadratic form determined by the matrix $\mathbf{C}$.

All moments arise as convex combinations of two pure states Given any point inside the uncertainty region, one can find infinitely many convex combinations of two pure Gaussian states on the boundary which produce the desired $N(2N+1)$ moments. Here is one way to construct such pairs. Consider any two-dimensional Euclidean plane which passes through the origin of the space of moments, $\mathbb{R}^{N(2N+1)}$, and the given point inside the uncertainty region. The intersection of its boundary with the plane is a one-dimensional set of points which divides the plane into two regions corresponding to acceptable covariance matrices (forming the uncertainty region) and the rest. This line inherits convexity from the boundary in the space $\mathscr{S}$ since any two points on the curve are, of course, also located on the high-dimensional boundary.

To conclude the argument, we only need to identify two points on the boundary such

that the line connecting them goes through the point representing the desired set of moments. It is geometrically obvious that there exist infinitely many pairs of points on the boundary which satisfy this requirement. This situation is illustrated in Fig. 1 in Sec. 4.2, for a single continuous variable where the boundary of the uncertainty region is known to be a hyperbola.

4.2 One continuous variable: $N = 1$

It is instructive to study the properties of the uncertainty region for a single continuous variable since the space of moments has only three dimensions. Even in the absence of entangled states, the uncertainty region has a number of interesting features as it resembles the Bloch ball used to visualize the states of a qubit. For one continuous variable, each point inside the uncertainty region is characterized uniquely by a triple of numbers, the states on the convex boundary are the only pure states, and the decomposition of mixed states into pairs of pure states is clearly not unique. The group of $\mathrm{Sp}(2,\mathbb{R}) \simeq \mathrm{SO}(2,1)$ transformations which leave the uncertainty region invariant play the role of the $\mathrm{SU}(2)$ transformations mapping the Bloch ball to itself.

We simplify the notation to discuss the case $N = 1$. Renaming the elements of the 2×2 covariance matrix according to

$$\mathbf{C} = \begin{pmatrix} \Delta^2 p & C_{pq} \\ C_{pq} & \Delta^2 q \end{pmatrix} \equiv \begin{pmatrix} x & w \\ w & y \end{pmatrix}, \tag{75}$$

the consistency conditions (34) take the form

$$x f_x = y f_y\,, \qquad x f_w = -2w f_y\,, \tag{76}$$

and

$$xy - w^2 = \left(n + \frac{1}{2}\right)^2 \hbar^2\,, \qquad n \in \mathbb{N}_0\,, \tag{77}$$

The third constraint is *universal* since it does not depend on the function $f(x,y,w)$ which characterizes an uncertainty functional $J[\psi]$. It will be convenient to use the variables

$$u = \frac{1}{2}(x+y) > 0\,, \quad v = \frac{1}{2}(x-y) \in \mathbb{R}\,, \tag{78}$$

to parametrize the points in the *three*-dimensional space of second moments, with coordinates $(u,v,w)^\top \in \mathbb{R}^3$. For each non-negative integer, the third condition

$$u^2 - v^2 - w^2 = e_n^2\,, \qquad e_n = \left(n + \frac{1}{2}\right)\hbar\,, \quad n \in \mathbb{N}_0\,, \tag{79}$$

determines one sheet of a two-sheeted hyperboloid, located in the "upper" half of the space of moments, i.e. $u > 0$ and $v, w \in \mathbb{R}$. The n-th sheet – which we call $\mathscr{E}_n$, $n \in \mathbb{N}_0$ – intersects the u-axis at $u = +e_n$, and it is in one-to-one correspondence with the squeezed

states originating from the number state $|n\rangle$ (cf. [13]).

The states which satisfy Eq. (79) for $n = 0$ *saturate* the standard Robertson-Schrödinger inequality. Consequently, not all points in the space of moments can arise as moment triples. The accessible part of the space is bounded by the hyperboloid $\mathscr{E}_0$ defined in Eq. (79), suggesting us to visualize the uncertainty region as a solid body with boundary $\mathscr{E}_0$.

We follow the presentation of the multidimensional case in Sec. 4.1, giving at times alternative proofs of the general results, by appealing to intuition available in the space of second moments due to its low dimension.

The uncertainty region has a convex boundary Given two mixed quantum states described by density matrices $\hat{\rho}_1$ and $\hat{\rho}_2$, their convex combinations $\hat{\rho}_t = t\hat{\rho}_1 + (1-t)\hat{\rho}_2$, $t \in [0,1]$, are also quantum states. We now show that the uncertainty region in the space $\mathbb{R}^3$ inherits convexity from the body of density matrices: any convex combination of the states $\hat{\rho}_1$ and $\hat{\rho}_2$ with moment triples $\vec{\mu}_k = (x_k, y_k, w_k)$, $k = 1,2$, inside the uncertainty region produces another state with a moment triple also in that region. The boundary of an analogously defined uncertainty region for a quantum spin s [28] is not convex. This approach does not use the convexity of the logarithm of positive definite matrices in (68).

The moments $x_k = \mathrm{Tr}(\hat{x}^2\hat{\rho}_k)$, $k = 1,2$, etc., satisfy the Robertson-Schrödinger inequality,

$$x_k y_k - w_k^2 \geq \frac{\hbar^2}{4} \equiv e_0^2\,, \quad k = 1,2\,, \tag{80}$$

and the moments of the mixture are given by

$$\sigma_t = t\sigma_1 + (1-t)\sigma_2\,, \qquad \sigma = x, y, w\,. \tag{81}$$

Writing $\bar{t} = 1 - t$, the variances of the convex combination satisfy

$$x_t y_t - w_t^2 \geq \left(t^2 + \bar{t}^2\right) e_0^2 + t\bar{t}\,(x_1 y_2 + x_2 y_1 - 2w_1 w_2) \tag{82}$$

using (80). Since

$$\begin{aligned} x_1 y_2 + x_2 y_1 - 2w_1 w_2 &\geq e_0^2 \left(\frac{y_2}{y_1} + \frac{y_1}{y_2}\right) + \left(w_1\sqrt{\frac{y_2}{y_1}} - w_2\sqrt{\frac{y_1}{y_2}}\right)^2 \\ &\geq 2e_0^2 \end{aligned}$$

holds, the moment triple of the convex combination $\hat{\rho}_t$ must also be contained in the uncertainty region, i.e.

$$x_t y_t - w_t^2 \geq \frac{\hbar^2}{4}\,. \tag{83}$$

The minimum is obtained only if either $t = 0$ or $t = 1$, so that the resulting density matrix must describe a state on the boundary of the uncertainty region, i.e. a Gaussian state with

minimal uncertainty.

The uncertainty region has no pure-state holes Each mixed state $\hat{\rho}$ generates a moment triple $\vec{\mu}$ with components $x = \mathrm{Tr}\left(\hat{\rho}\hat{x}^2\right)$, etc., satisfying the Robertson-Schrödinger inequality [29]. Thus, the uncertainty region necessarily contains all potential mixed-state minima $\vec{\mu}$ of a given functional. We want to show that all moment triples inside the uncertainty region can be obtained through *pure* states. Two cases occur.

If the triple $\vec{\mu}$ is located on one of the hyperboloids $\mathscr{E}_n$, $n \in \mathbb{N}_0$, then there exists a squeezed number state – i.e. a pure state – which gives rise to the same three expectations. Hence, the point $\vec{\mu}$ has already been included in the search for extrema.

Alternatively, the point $\vec{\mu}$ is located between two hyperboloids, $\mathscr{E}_n$ and $\mathscr{E}_{n+1}$, say, with $n \in \mathbb{N}_0$. Again, there is a pure state with moments given by $\vec{\mu}$. To see this, we first consider only the line segment with end points $(u_n, 0, 0)$ and $(u_{n+1}, 0, 0)$, which are associated with the number states $|n\rangle$ and $|n+1\rangle$, respectively. The moments of the superposition

$$|n\rangle_t = \sqrt{t}|n\rangle + \sqrt{1-t}|n+1\rangle, \quad t \in [0,1]\,, \tag{84}$$

indeed lead to all moment triples located on the line segment,

$$\vec{n}_t = \left(u_{n+1} + t\left(u_n - u_{n+1}\right), 0, 0\right)\,, \quad t \in [0,1]\,, \tag{85}$$

since the matrix elements of the second moments between states of different parity vanish.

Finally, any moment triple $\vec{\mu}$ off the u-axis will lie on a hyperboloid with a specific value of $t = t_0$, say. This moment triple can be obtained, however, from the state $\hat{S}(\xi)|n\rangle_{t_0}$, with a suitable value ξ. Using relativistic terminology, the operator $\hat{S}(\xi)$ must induce a Lorentz transformation which maps the given point on the u-axis to the desired point $\vec{\mu}$ on the same hyperboloid.

In conclusion, each triple $\vec{\mu}$ of the uncertainty region can be obtained from a suitable pure state. Thus, mixed states do not give rise to candidates for minima different from those associated with pure states.

All moments arise as convex combinations of two pure states Consider a state $|\xi\rangle$ giving rise to the moment vector $\vec{\xi} = (u_\xi, v_\xi, w_\xi)$ *inside* the uncertainty region. It is possible to identify infinitely many pairs of Gaussian states on the boundary such that their mixture reproduces the given triple $\vec{\xi}$.

On the level of moments, it is geometrically obvious that any moment triple $\vec{\xi}$ can be reached as a convex combination of two points located on the boundary (cf. Fig. 1). It is sufficient to consider states with vanishing covariance, $w = 0$. This choice is equivalent to selecting a particular two-dimensional plane in the space of moments which passes through the origin and the given moment triple $\vec{\xi}$ (cf. Sec. 4.1). Picking any point $\vec{\varphi}$

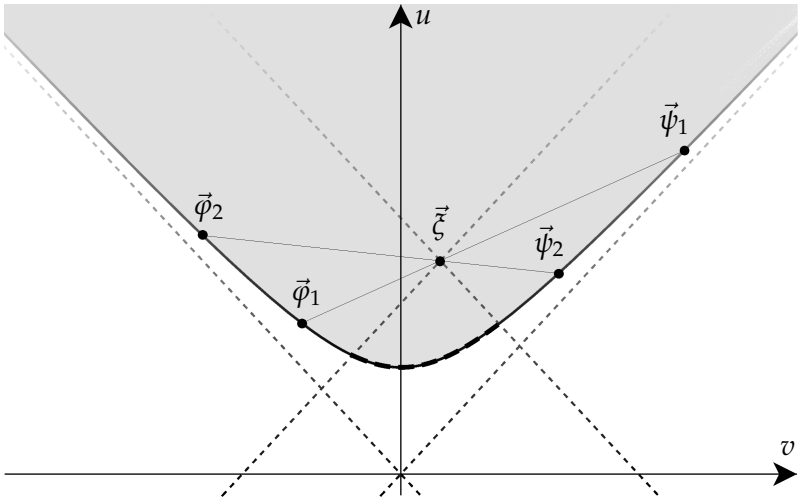

Figure 1: Cross-section ($w = 0$) of the uncertainty region (shaded) illustrating the convexity of its boundary $u^2 - v^2 - w^2 = \hbar^2/4$; convex combinations of moment triples located on the hyperboloid (associated with pure Gaussian states with minimal uncertainty) reproduce any given moment vector $\vec{\xi}$ inside the uncertainty region (the points must be outside of the "back-ward light-cone" of the point $\vec{\xi}$, indicated by the dashed segment of the hyperbola).

"space-like" relative to $\vec{\xi}$ and located on the hyperboloid, the pair determines a line intersecting the boundary in a unique point $\vec{\psi}$. Then, the desired point $\vec{\xi}$ must lie on the line segment $\vec{\xi}(t) = \vec{\varphi} + t(\vec{\psi} - \vec{\varphi})$, $t \in [0, 1]$, connecting the points $\vec{\varphi}$ and $\vec{\psi}$; it will pass through the point $\vec{\xi}$ if

$$t_0 = \frac{u_\xi - u_\varphi}{u_\psi - u_\varphi} \equiv \frac{v_\xi - v_\varphi}{v_\psi - v_\varphi} \in [0, 1]\,. \tag{86}$$

When writing the line segment in the form $\vec{\xi}(t) = t\vec{\psi} + (1-t)\vec{\varphi}$, it becomes obvious that the reasoning valid in the space of moments extends to quantum states. In other words, the mixture

$$\hat{\rho}_{t_0} = t_0 \hat{P}_\psi + (1 - t_0)\hat{P}_\varphi \tag{87}$$

of the rank-1 projectors $\hat{P}_\psi = |\psi\rangle\langle\psi|$ and $\hat{P}_\varphi = |\varphi\rangle\langle\varphi|$ onto Gaussian states on the boundary defines a mixed quantum state with the desired moment triple $\vec{\xi}$. Clearly, continuously many other convex combinations of pure states exist which lead to the same moment triple.

The relation between quantum states and points inside of the uncertainty region is, of course, many-to-one. For example, the state $|1\rangle$ with moment vector $\vec{\xi}_1 = (9\hbar^2/4, 0, 0)$, i.e. the first excited state of a harmonic oscillator with unit mass and frequency, being a pure state, cannot be written as a mixture of two Gaussian states. Nevertheless, suitable mixtures of Gaussian states will produce its moment vector $\vec{\xi}_1$. The only moment vectors $\vec{\xi}$ which cannot be obtained from mixtures are those on the boundary of the uncertainty region. Here, the relation between states and moment vectors is one-to-one, in agreement

with the fact that these Gaussian states are determined uniquely by their covariance matrix **C**.

5 Summary

We have presented a method to systematically determine lower bounds of uncertainty functionals, defined in terms of second moments of quantum systems with two or more continuous variables. In analogy to the one-dimensional case discussed in [13], we find that the states which extremize an uncertainty functional of N degrees of freedom must satisfy a (non-standard) eigenvalue equation which is quadratic in the $2N$ position and momentum operators. If the quadratic form associated with this operator is positive (or negative) definite, Williamson's theorem ensures that it can be diagonalised by a symplectic transformation. In general, the matrix describing the quadratic form depends on the unknown state which suggests to solve it in a self-consistent way. The solutions of the resulting *consistency conditions* determine the set of states which minimise a given functional. We also introduced the $N(2N+1)$-dimensional uncertainty region for a system with N continuous variables. We show that this region is a convex subset of the space of second moments, and the points located on the boundary correspond to Gaussian states with minimal uncertainty.

Applying this method to specific functionals associated with quantum systems described by two continuous variables, we both re-derived existing uncertainty relations and previously unknown ones. We are not aware of other methods to obtain these inequalities.

One of the new inequalities generalizes an existing inequality which is capable of detecting entanglement in states of bi-partite particle systems. This example hints at the possibility to systematically construct inequalities that can be used for entanglement detection: take an arbitrary number of EPR-type operators that pairwise commute, and define a monotonically increasing function of their variances that is finite at the origin. Typically, the lower bound given by the value of the functional at the origin will be achieved by an *entangled* state, and it will be smaller than the value of the functional which it can take in any separable state. This bound can be obtained by solving the consistency conditions (39) for product states as described in Sec. 3.1. Clearly, a violation of the pure-state bound will detect the presence of an entangled state. The details of this construction will be left to a future publication.

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