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Universality in Uncertainty Relations for a Quantum Particle

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Abstract

A general theory of preparational uncertainty relations for a quantum particle in one spatial dimension is developed. We derive conditions which determine whether a given smooth function of the particle's variances and its covariance is bounded from below. Whenever a global minimum exists, an uncertainty relation has been obtained. The squeezed number states of a harmonic oscillator are found to be *universal*: no other pure or mixed states will saturate any such relation. Geometrically, we identify a *convex uncertainty region* in the space of second moments which is bounded by the inequality derived by Robertson and Schrödinger. Our approach provides a unified perspective on existing uncertainty relations for a single continuous variable, and it leads to new inequalities for second moments which can be checked experimentally.

1 Introduction and main result

Inspired by Heisenberg's analysis [1] of Compton scattering, Kennard [2] proved the preparational uncertainty relation

$$\Delta p \, \Delta q \geq \frac{\hbar}{2} \,, \tag{1}$$

for the standard deviations Δp and Δq of momentum and position of a quantum particle with a single spatial degree of freedom. Experimentally, they are determined by measurements performed on an ensemble of systems prepared in a specific state $|\psi\rangle$. The only states which saturate the bound (1) are *squeezed states* with a *real* squeezing parameter [3, 4, 5] (we follow the review [6] regarding the naming of squeezed states). Squeezed states are conceptually important since they achieve the best possible localization of a quantum particle in phase-space, and they are easily visualized by "ellipses of uncertainty". Each squeezed state may be displaced rigidly in phase space without affecting the value of the variances, resulting in a three-parameter family of states saturating the lower bound (1).

Not many other uncertainty relations are known. The *sum* of the position and momentum variances is bounded [7, 8] according to the relation

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$$\Delta^2 p + \Delta^2 q \geq \hbar \,, \tag{2}$$

which holds in a system of units where the physical dimensions of both position and momentum equal $\sqrt{\hbar}$. Only the ground state of a harmonic oscillator with unit mass and frequency saturates this inequality (ignoring rigid displacements in phase-space). The Robertson-Schrödinger (RS) inequality [9, 10],

$$\Delta^2 p \, \Delta^2 q - C_{pq}^2 \geq \frac{\hbar^2}{4} \,, \tag{3}$$

sharpens Heisenberg's inequality (1) by including the covariance C_{pq} defined in Eq. (8). Eq. (3) is saturated by the two-parameter family of *squeezed states* with a *complex* squeezing parameter [6], again ignoring phase-space displacements. The additional free parameter describes the phase-space orientation of the uncertainty ellipse which, in the previous case, was aligned with the position and momentum axes.

By introducing the observable $\hat{r} = -\hat{p} - \hat{q}$, which satisfies the commutation relations $[\hat{q}, \hat{r}] = [\hat{r}, \hat{p}] = \hbar / i$, one obtains a bound on the product of the variances of three pairwise canonical observables,

$$\Delta^2 p \, \Delta^2 q \, \Delta^2 r \geq \left(\tau \frac{\hbar}{2} \right)^3 , \qquad \tau = \csc\left(\frac{2\pi}{3} \right) \equiv \sqrt{\frac{4}{3}} \,. \tag{4}$$

This *triple product uncertainty relation* has been found only recently [13]. Ignoring phase-space translations, only one state exists which achieves the minimum. Since the variance of $\hat{r}$ is given by

$$\Delta^2 r = \Delta^2 p + \Delta^2 q + 2C_{pq} \,, \tag{5}$$

the left-hand-side of (4) can also be considered as a function of the three second moments.

The inequalities (1) to (4) and the search for their minima arise from one single mathematical problem:

> *Does a given smooth function of the second moments have a lower bound*?
> *If so, which states will saturate the inequality if a minimum exists*?

In this paper, we answer these questions for a quantum particle with a single spatial degree of freedom by presenting a systematic approach to studying uncertainty relations derived from smooth functions $f(\Delta^2 p, \Delta^2 q, C_{pq})$. Proceeding in three steps we

1. identify a *universal* set of states $\mathscr{E}$ which can possibly minimize a given functional $f(\Delta^2 p, \Delta^2 q, C_{pq})$;

2. spell out conditions which determine the *extrema* of the functional f as a subset of the universal set, $\mathscr{E}(f) \subseteq \mathscr{E}$; if no admissible extrema exist, the functional has no lower bound;

3. determine the set of states $\mathscr{M}(f) \subseteq \mathscr{E}(f)$ which *minimize* the functional f, leading to an uncertainty relation in terms of the second moments.

The inequalities studied here will be *preparational* in spirit: they apply to scenarios in which the quantum state of the particle $|\psi\rangle$ is fixed during the three separate runs of the measurements required to determine the numerical values of the second moments. These inequalities do not describe the limitations of measuring non-commuting observables *simultaneously*.

The paper is divided into two major sections. In Sec. 2 we introduce uncertainty functionals and explain how to determine their extrema and minima. The impatient reader may jump directly to Sec. 3 where we derive new families of uncertainty relations and determine the states minimizing them. We conclude the paper with a summary and discuss further applications.

2 Minimising uncertainty

To begin, we introduce the *uncertainty functional* [11]

$$J[\psi] = f\left(\Delta^2 p, \Delta^2 q, C_{pq}\right) - \lambda\left(\langle\psi|\psi\rangle - 1\right), \tag{6}$$

which sends each element $|\psi\rangle$ of the one-particle Hilbert space $\mathscr{H}$ to a real number determined by the real differentiable function $f(x_1, x_2, x_3)$ of three variables. The Lagrange multiplier λ ensures the normalization of the states. The variances of position and momentum are defined by

$$\Delta^2 p = \langle\psi|\hat{p}^2|\psi\rangle - \langle\psi|\hat{p}|\psi\rangle^2, \tag{7}$$

etc., and the covariance of position and momentum reads

$$C_{pq} = \frac{1}{2}\langle\psi|\left(\hat{p}\hat{q} + \hat{q}\hat{p}\right)|\psi\rangle - \langle\psi|\hat{p}|\psi\rangle\langle\psi|\hat{q}|\psi\rangle\,. \tag{8}$$

The second moments form the real, symmetric *covariance matrix*

$$\mathbf{C} = \begin{pmatrix} \Delta^2 p & C_{pq} \\ C_{pq} & \Delta^2 q \end{pmatrix} \equiv \begin{pmatrix} x & w \\ w & y \end{pmatrix}, \tag{9}$$

with state-dependent matrix elements $x \equiv x(\psi)$ etc. The covariance may take any finite real value, $w \in \mathbb{R}$, while the variances of position and momentum take (finite) *positive* values only, $x, y > 0$. States of a quantum particle with *vanishing* position (or momentum) variance and *diverging* momentum (or position) variance are not taken into account since they only arise for non-normalizable states which cannot be prepared experimentally. Nevertheless, position (or momentum) eigenstates can be approximated arbitrarily well by states within the set we consider.

It will be convenient to work with states in which the expectation values of both momentum and position vanish, $\langle\psi|\hat{q}|\psi\rangle = \langle\psi|\hat{p}|\psi\rangle = 0$. This can be achieved by rigidly displacing the observables using the unitary operator

$$\hat{T}_\alpha = \exp\left[i\left(p_0\hat{q} - q_0\hat{p}\right)/\hbar\right], \qquad \alpha = \frac{1}{\sqrt{2\hbar}}\left(q_0 + ip_0\right), \tag{10}$$

where $p_0 = \langle\psi|\hat{p}|\psi\rangle$, etc. This transformation leaves invariant the values of the second moments (7) and (8) and has thus no impact on the minimization of the functional $J[\psi]$.

A lower bound of a functional $J[\psi]$ of the form (6) will result in an uncertainty relation associated with the function $f(x_1, x_2, x_3)$. To determine such a bound, we apply a method used in [11, 12, 13] (see also [14, 15, 16]). First, we derive an eigenvalue equation for the extrema of the functional $J[\psi]$ which also need to satisfy a set of consistency conditions given in Sec. 2.3. Then, we introduce a "space of moments" to visualize these results (Sec. 2.4) and, finally, we determine the minimizing states whenever the functional is guaranteed to be bounded from below (see Sec. 2.5 and Sec. 3).

2.1 Extrema of uncertainty functionals

When comparing the values of the functional J at the points $|\psi\rangle$ and $|\psi+\varepsilon\rangle \equiv |\psi\rangle + \varepsilon|e\rangle$, for any unit vector $|e\rangle$ and a small parameter ε, we find to first order that

$$J[\psi+\varepsilon] - J[\psi] = \varepsilon D_\varepsilon J[\psi] + O\left(\varepsilon^2\right), \tag{11}$$

where the expression

$$D_\varepsilon = \langle e|\frac{\delta}{\delta\langle\psi|} + \frac{\delta}{\delta|\psi\rangle}|e\rangle, \tag{12}$$

denotes a Gâteaux derivative. If the functional $J[\psi]$ does not change under this variation,

$$D_\varepsilon J[\psi] = \langle e|\left(\frac{\delta}{\delta\langle\psi|} f\left(x,y,w\right) - \lambda|\psi\rangle\right) + \text{c.c.} = 0, \tag{13}$$

it has an extremum at the state $|\psi\rangle$. More explicitly, this condition reads

$$\langle e|\left(\frac{\partial f}{\partial x}\frac{\delta x}{\delta\langle\psi|} + \frac{\partial f}{\partial y}\frac{\delta y}{\delta\langle\psi|} + \frac{\partial f}{\partial w}\frac{\delta w}{\delta\langle\psi|} - \lambda|\psi\rangle\right) + \text{c.c.} = 0\,, \tag{14}$$

which should hold for arbitrary variations. Since the vectors $|e\rangle$ and $\langle e|$ can be varied independently (just consider their position representations $e^*(x)$ and $e(x)$), the expression in round brackets must vanish identically which implies that the complex conjugate term will also vanish. Using

$$\frac{\delta x}{\delta\langle\psi|} \equiv \frac{\delta\Delta^2 p}{\delta\langle\psi|} = \frac{\delta\langle\psi|\hat{p}^2|\psi\rangle}{\delta\langle\psi|} = \hat{p}^2|\psi\rangle\,, \tag{15}$$

a similar relation for $\delta y/\delta\langle\psi|$, and the identity

$$\frac{\delta w}{\delta\langle\psi|} \equiv \frac{1}{2}\left(\hat{q}\hat{p} + \hat{p}\hat{q}\right)|\psi\rangle\,, \tag{16}$$

we arrive at an *Euler-Lagrange*-type equation,

$$\left(\frac{\partial f}{\partial x}\hat{p}^2 + \frac{\partial f}{\partial y}\hat{q}^2 + \frac{1}{2}\frac{\partial f}{\partial w}\left(\hat{q}\hat{p} + \hat{p}\hat{q}\right) - \lambda\right)|\psi\rangle = 0. \tag{17}$$

The parameter λ can be eliminated by multiplying this equation with the bra $\langle\psi|$ from the left and solving for λ; substituting the value obtained back into Eq. (17), one finds a nonlinear eigenvector-eigenvalue equation,

$$\left(f_x\hat{p}^2 + f_y\hat{q}^2 + \frac{f_w}{2}\left(\hat{q}\hat{p} + \hat{p}\hat{q}\right)\right)|\psi\rangle = \left(f_x x + f_y y + f_w w\right)|\psi\rangle\,, \tag{18}$$

using the standard shorthand for partial derivatives.

Eq. (18) is our first result following from the approach conceived in [11]: the extrema of arbitrary smooth functions of the second moments are encoded in an eigenvalue equation for a Hermitean operator quadratic in position and momentum. However, the equation is not linear in the state $|\psi\rangle$ because the quantities $x, y, \ldots, f_w$ are functions of expectation values taken in the yet unknown state. Previously, similar results had only been found for specific uncertainty functionals such as the product of the standard deviations or position and momentum.

Let us briefly illustrate the crucial features of Eq. (18) in a simple case before systematically investigating its solutions. For a function linear in x, y, and w, the derivatives f_x, f_y, and f_w will be fixed constant numbers. In this case, the operator on the left-hand-side of (18) represents a quadratic form in the position and momentum operators, falling into one of three possible categories [17]. Up to a multiplicative constant, the operator will be unitarily equivalent to the Hamiltonian of (i) a harmonic oscillator with unit mass and frequency, $\hat{p}^2 + \hat{q}^2$, (ii) a free particle, $\hat{p}^2$, or (iii) an inverted harmonic oscillator, $\hat{p}^2 - \hat{q}^2$. In the first case, the spectrum of the operator will be discrete and bounded from below (or above); the spectra of the operators in the other two cases are continuous which is tantamount to the absence of normalizable eigenstates. Thus, a linear function $f(x, y, w)$ possesses a non-trivial bound only if it gives rise to an operator in (18) which is unitarily equivalent to the Hamiltonian of a harmonic oscillator. Generally, our method will signal the absence of lower bounds corresponding to the cases (ii) and (iii).

2.2 Universality

To find a lower bound of the functional $J[\psi]$, we will determine all its extrema and then pick those where $J[\psi]$ assumes its smallest value. However, Eq. (18) is not a standard eigenvalue equation: even for a linear function f, the right-hand-side of (18) depends non-linearly on the as yet unknown state $|\psi\rangle$, and if the function f is non-linear, the operators on the left-hand-side of the equation acquire state-dependent coefficients given by its partial derivatives.

Nevertheless, the eigenvalue problem can be solved systematically, in a *self-consistent* way. Initially, we treat the expectations x, y, w, and f_x, f_y, f_w in (18) as parameters with given values, i.e. we ignore their dependence on the state $|\psi\rangle$. The solutions $|\psi(x, y, w)\rangle$ will depend on these parameters which means that the solutions must be checked for consistency since the relations (7) now require that $x = \langle\psi(x, y, w)|\hat{p}^2|\psi(x, y, w)\rangle$, etc. It may or may not be possible to satisfy these restrictions on the parameters.

To begin, we write the operator on the left-hand side of (18) in matrix form,

$$(\hat{p}\,,\hat{q}) \begin{pmatrix} f_x & f_w/2 \\ f_w/2 & f_y \end{pmatrix} \begin{pmatrix} \hat{p} \\ \hat{q} \end{pmatrix} \equiv \hat{\mathbf{z}}^\top \cdot \mathbf{F} \cdot \hat{\mathbf{z}} \,. \tag{19}$$

Williamson's theorem [18] ensures that any positive or negative definite matrix can be mapped to a diagonal matrix by conjugation with a symplectic matrix $\boldsymbol{\Sigma}$. We will assume from now on that the matrix $\mathbf{F}$ is *positive* definite. The negative definite case is easily dealt with by considering $-f(x, y, w)$ instead of $f(x, y, w)$. Applied to the 2×2 matrix $\mathbf{F}$, Williamson's result states that we can write

$$\boldsymbol{\Sigma}^\top \cdot \mathbf{F} \cdot \boldsymbol{\Sigma} = c\,\mathbf{I}\,, \qquad \boldsymbol{\Sigma} \in \mathrm{Sp}(2, \mathbb{R})\,, \quad c > 0\,, \tag{20}$$

where $\mathbf{I}$ is the identity matrix, whenever $\mathbf{F} > 0$ holds. This requires both

$$\det \mathbf{F} \equiv f_x f_y - f_w^2/4 > 0 \quad \text{and} \quad f_x > 0\,, \tag{21}$$

implying that $f_y > 0$ will hold, too. These requirements clearly agree with the observations made for linear uncertainty functionals $f(x, y, w)$: since the operators $\hat{p}^2$ and $\hat{p}^2 - \hat{q}^2$ result in matrices $\mathbf{F}$ with zero or negative determinant, the left-hand-side of (18) cannot be mapped to an oscillator Hamiltonian by means of a symplectic transformation.

A direct calculation shows that the matrix $\mathbf{F}$ is diagonalized by the symplectic matrix $\Sigma = (\mathbf{S}_\gamma \mathbf{G}_b)^{-1}$, where

$$\mathbf{G}_b = \begin{pmatrix} 1 & 0 \\ b & 1 \end{pmatrix}, \quad \text{and} \quad \mathbf{S}_\gamma = \begin{pmatrix} e^{-\gamma} & 0 \\ 0 & e^{\gamma} \end{pmatrix}, \tag{22}$$

with real parameters

$$b = \frac{f_w}{2f_y} \in \mathbb{R} \quad \text{and} \quad \gamma = \frac{1}{2}\ln\left(\frac{f_y}{\sqrt{\det \mathbf{F}}}\right) \in \mathbb{R}, \tag{23}$$

leading to $c = \sqrt{\det \mathbf{F}}$ in Eq. (20). The symplectic matrices $\mathbf{S}_\gamma$ and $\mathbf{G}_b$ give rise to the Iwasawa (or $\mathscr{K}\mathscr{A}\mathscr{N}$) decomposition of the matrix $\mathbf{\Sigma}^{-1} \in \mathrm{Sp}(2,\mathbb{R})$ (cf. [19], for example) if they are written in opposite order and the parameter b is replaced by be^{γ}; the third factor happens to be the identity.

Next, we observe that the linear action of the matrices $\mathbf{G}$ and $\mathbf{S}$ on the canonical pair of operators $(\hat{p}, \hat{q})^\top$ can be implemented by conjugation with suitable unitary operators, known as *metaplectic* operators [19]. We have, for example,

$$\begin{pmatrix} 1 & 0 \\ b & 1 \end{pmatrix} \begin{pmatrix} \hat{p} \\ \hat{q} \end{pmatrix} = e^{ib\hat{p}^2/2\hbar} \begin{pmatrix} \hat{p} \\ \hat{q} \end{pmatrix} e^{-ib\hat{p}^2/2\hbar}, \tag{24}$$

or, in matrix notation,

$$\mathbf{G}_b \cdot \hat{\mathbf{z}} = \hat{G}_b \, \hat{\mathbf{z}} \, \hat{G}_b^\dagger \tag{25}$$

where the unitary operator

$$\hat{G}_b = e^{ib\hat{p}^2/2\hbar} \tag{26}$$

describes a *momentum gauge transformation*. Similarly, the squeeze operator

$$\hat{S}_\gamma = e^{i\gamma(\hat{q}\hat{p}+\hat{p}\hat{q})/2\hbar}, \tag{27}$$

symplectically *scales* position and momentum according to

$$\mathbf{S}_\gamma \cdot \hat{\mathbf{z}} = \hat{S}_\gamma \, \hat{\mathbf{z}} \, \hat{S}_\gamma^\dagger. \tag{28}$$

With $\mathbf{\Sigma}^{-1} = \mathbf{S}_\gamma \mathbf{G}_b$ in (20), we rewrite (19) as

$$\hat{\mathbf{z}}^\top \cdot \mathbf{F} \cdot \hat{\mathbf{z}} = \sqrt{\det \mathbf{F}} \, (\mathbf{S}_\gamma \cdot \mathbf{G}_b \cdot \hat{\mathbf{z}})^\top \cdot (\mathbf{S}_\gamma \cdot \mathbf{G}_b \cdot \hat{\mathbf{z}}). \tag{29}$$

Finally, using the identities (25) and (28) and multiplying Eq. (18) with the unitary $\hat{S}_\gamma^\dagger \hat{G}_b^\dagger$ from the left, the condition for the existence of extrema of the functional $J[\psi]$ takes on the desired form,

$$\frac{1}{2}\left(\hat{p}^2 + \hat{q}^2\right) |\psi(b,\gamma)\rangle = \left(\frac{x f_x + y f_y + w f_w}{2\sqrt{\det \mathbf{F}}}\right) |\psi(b,\gamma)\rangle. \tag{30}$$

Thus, the solutions

$$|\psi(b,\gamma)\rangle \equiv \hat{S}_\gamma^\dagger \hat{G}_b^\dagger |\psi\rangle \tag{31}$$

must be proportional to the eigenstates $|n\rangle, n \in \mathbb{N}_0$, of a *unit oscillator*, i.e. a quantum mechanical oscillator with unit mass and unit frequency. Equivalently, the candidates for states extremizing the functional $J[\psi]$ are given by the family of states,

$$|n(b,\gamma)\rangle = \hat{G}_b \hat{S}_\gamma |n\rangle, \qquad b,\gamma \in \mathbb{R}, \quad n \in \mathbb{N}_0. \tag{32}$$

Upon rewriting the operator $\hat{S}^\dagger_\gamma \hat{G}^\dagger_b$ these states are seen to coincide with the *squeezed number states* [6]. As shown in in Appendix A, the product of a squeeze transformation $\hat{S}_\gamma$ (with real parameter γ) and a momentum gauge transformation $\hat{G}_b$ equals

$$\hat{G}_b \hat{S}_\gamma = \hat{S}(\xi)\hat{R}(\chi)\,, \tag{33}$$

i.e. the product of a rotation in phase space,

$$\hat{R}(\chi) = e^{i\chi \hat{a}^\dagger \hat{a}} \qquad \chi \in [0, 2\pi)\,, \tag{34}$$

and a squeeze transformation (with complex ξ) along a line with inclination θ,

$$\hat{S}(\xi) = e^{\frac{1}{2}\left(\xi \hat{a}^{\dagger 2} - \overline{\xi}\hat{a}^2\right)}\,, \qquad \xi = re^{i\theta} \in \mathbb{C}\,. \tag{35}$$

Summarizing our findings, we draw two conclusions:

1. The complete set of solutions of Eq. (30) coincides with the *squeezed number states*,

$$\mathscr{E} = \bigcup_{n=0}^{\infty} \mathscr{E}_n \equiv \bigcup_{n=0}^{\infty} \left\{ |n(\alpha,\xi)\rangle = \hat{T}_\alpha \hat{S}(\xi)|n\rangle\,, \alpha, \xi \in \mathbb{C} \right\}\,, \tag{36}$$

   where non-zero expectation values of position and momentum have been reintroduced via the translation operator $\hat{T}_\alpha$ (see Eq. (10)) and irrelevant constant phases have been suppressed.

2. The value of the right-hand-side of Eq. (30) can take only specific values,

$$\frac{x f_x + y f_y + w f_w}{2\sqrt{\det \mathbf{F}}} = \left(n + \frac{1}{2}\right)\hbar\,, \qquad n \in \mathbb{N}_0\,, \tag{37}$$

   given by the eigenvalues of the unit oscillator. This relation constrains the state-dependent quantities of the left-hand-side which needs to be checked for consistency, just as Eq. (21) does.

We have thus obtained our second main result. The extrema $\mathscr{E}$ of an arbitrary functional $J[\psi]$ characterized by a function $f(x,y,w)$ are necessarily *squeezed number states*, a set which is *independent* of the function at hand. In other words, the set $\mathscr{E}$ containing all the states which may arise as minima of an uncertainty functional $J[\psi]$, is *universal*. The minima of any functional must be a subset $\mathscr{E}(f) \subseteq \mathscr{E}$ which will depend explicitly on the function $f(x,y,w)$, determined by the consistency conditions to be studied next.

2.3 Consistency conditions

We now spell out the conditions which must be satisfied by the states $|n(b,\gamma)\rangle$ in (32) – or, equivalently, the states $|n(\alpha,\xi)\rangle$ in (36) – to qualify as extrema for a specific functional $J[\psi]$:

1. Recalling that $x \equiv \Delta^2 p$, etc., the relations

$$x = \langle n(b,\gamma)|\hat{p}^2|n(b,\gamma)\rangle\,, \qquad y = \langle n(b,\gamma)|\hat{q}^2|n(b,\gamma)\rangle\,, \tag{38}$$

   and

$$w = \frac{1}{2}\langle n(b,\gamma)|\left(\hat{p}\hat{q} + \hat{q}\hat{p}\right)|n(b,\gamma)\rangle\,, \tag{39}$$

   represent three, generally nonlinear *consistency equations* between the second moments since the parameters b and γ are functions of x, y and w (cf. Eq. (23)).

2. The values of the moments x, y and w must satisfy Eq. (37).

3. The matrix $\mathbf{F}$ of the first derivatives must be positive definite.

Using (32), (25) and (28), the first consistency condition in (38) leads to

$$x = \langle n(b,\gamma)|\hat{p}^2|n(b,\gamma)\rangle = e^{2\gamma}\langle n|\hat{p}^2|n\rangle = e^{2\gamma}\left(n+\frac{1}{2}\right)\hbar\,, \quad n \in \mathbb{N}_0\,, \tag{40}$$

or, recalling the definition of γ in (23),

$$x\sqrt{\det \mathbf{F}} = \left(n+\frac{1}{2}\right)\hbar f_y\,, \qquad n \in \mathbb{N}_0\,. \tag{41}$$

Similar calculations result in

$$y\sqrt{\det \mathbf{F}} = \left(n+\frac{1}{2}\right)\hbar f_x\,, \qquad n \in \mathbb{N}_0\,, \tag{42}$$

and

$$-2w\sqrt{\det \mathbf{F}} = \left(n+\frac{1}{2}\right)\hbar f_w\,, \qquad n \in \mathbb{N}_0\,, \tag{43}$$

respectively. These conditions may be expressed in matrix form,

$$\frac{\mathbf{F}\cdot\mathbf{C}}{\sqrt{\det \mathbf{F}}} = \left(n+\frac{1}{2}\right)\hbar\,\mathbf{I}, \qquad n \in \mathbb{N}_0\,, \tag{44}$$

involving both the covariance matrix $\mathbf{C}$ and $\mathbf{F}$.

Taking the trace of the last relation shows that Eq. (37) is satisfied automatically. Without specifying a function $f(x,y,w)$, no conclusions can be drawn about the validity of Eqs. (41-43) or the positive definiteness of the matrix $\mathbf{F}$.

2.4 Geometry of extremal states

We visualize the interplay of the consistency conditions by expressing them in the form

$$xf_x = yf_y\,, \qquad xf_w = -2wf_y\,, \tag{45}$$

and

$$xy - w^2 = \left(n+\frac{1}{2}\right)^2\hbar^2\,, \qquad n \in \mathbb{N}_0\,, \tag{46}$$

following easily from either (41-43) or (44). The third constraint is *universal* since it does not depend on the function $f(x,y,w)$. Using the variables

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

we define the three-dimensional *space of (second) moments,* with coordinates (u,v,w). For each non-negative integer, the third condition

$$u^2 - v^2 - w^2 = e_n^2\,, \qquad e_n = \left(n+\frac{1}{2}\right)\hbar\,, \quad n \in \mathbb{N}_0\,, \tag{47}$$

determines one sheet of a two-sheeted hyperboloid, located in the "upper" half of the space of moments, i.e. $u > 0$ and $v, w \in \mathbb{R}$ (cf. Fig. 1). The points on the n-th sheet, which

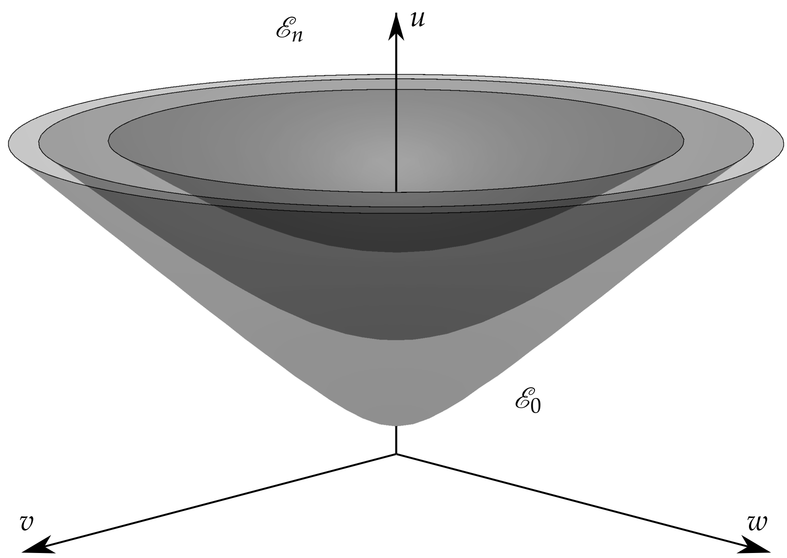

Figure 1: Space of (second) moments, with points (u, v, w): the extremal states of smooth functionals $J[\psi]$ are located on a discrete set of nested hyperboloids $\mathscr{E} = \bigcup_{n=0}^{\infty} \mathscr{E}_n$ the first three of which are shown, using light ($n = 0$), medium ($n = 1$) and dark shading ($n = 2$), respectively. The accessible *uncertainty region* for a quantum particle is given by the points on and inside of the convex surface $\mathscr{E}_0 : u^2 - v^2 - w^2 = \hbar^2/4$ which coincides with the minima $\mathscr{M}(f^{RS})$ of the RS inequality, i.e. squeezed states with minimal uncertainty.

intersects the u-axis at $u = +e_n$, are in one-to-one correspondence with the squeezed states originating from the number state $|n\rangle$, forming the set $\mathscr{E}_n$ in (36).

The consistency conditions (45) clearly depend on the function $f(x, y, w)$ at hand. The constraints will only be satisfied for specific subsets $\mathscr{E}_n(f)$ of points on the hyperboloids $\mathscr{E}_n$, resulting in the f-dependent set of states

$$\mathscr{E}(f) = \bigcup_{n=0}^{\infty} \mathscr{E}_n(f)$$

which contains all the candidates possibly minimizing the functional $J[\psi]$. The candidate sets $\mathscr{E}(f)$ may depend on one or two parameters, or contain isolated points only. If the consistency conditions cannot be satisfied, then the functional $J[\psi]$ has no lower bound. Furthermore, if the matrix $\mathbf{F}$ is not positive definite for any of the states in $\mathscr{E}(f)$, the method makes no predictions about the minima of the functional $J[\psi]$. We have, however, not found any non-trivial cases of this behaviour.

Finally, we need to evaluate the functional $J[\psi]$ for all candidate states $\mathscr{E}(f)$ and pick the smallest possible value. The states achieving this minimum value constitute the solutions $\mathscr{M}(f) \subseteq \mathscr{E}(f)$ of the minimization problem. In their entirety, the minima $\mathscr{M}(f)$ may consist of isolated states or of sets depending on one or two parameters. Usually, the states saturating the bound are located on the sheet $\mathscr{E}_0$.

Let us briefly introduce the concept of a *space of moments*, defined by the triples of numbers $(u, v, w)^\top \in \mathbb{R}^3$. For $n = 0$, Eq. (47) is equivalent to (3) which implies that not all points of this set can arise as moment triples. The accessible part of the space, bounded by the extremal hyperboloid $\mathscr{E}_0$ defined in Eq. (47), is called the *uncertainty region* (cf.

Fig. 1). The boundary of an analogously defined uncertainty region for a quantum spin s [20] is not convex. The relation between moment triples and the underlying pure or mixed states of quantum particles is discussed elsewhere [21].

2.5 Known uncertainty relations

To illustrate our approach we re-derive three of the four bounds mentioned in the introduction: the uncertainty relations by *Robertson-Schrödinger*, by *Heisenberg-Kennard*, and the *triple-product* inequality.

Robertson-Schrödinger uncertainty relation. Defining

$$f^{RS}(x,y,w) = xy - w^2 \,, \tag{48}$$

the matrix of first-order derivatives associated with the quadratic form (19) is given by

$$\mathbf{F} = \begin{pmatrix} y & -w \\ -w & x \end{pmatrix} , \tag{49}$$

and, interestingly, its determinant

$$\det \mathbf{F} = xy - w^2 \equiv f^{RS}(x,y,w) \tag{50}$$

coincides with the original functional. At this point of the derivation, it is not yet known whether the matrix $\mathbf{F}$ is strictly positive.

The relations Eq. (45) do not constraint the parameters x, y, and w, since they are satisfied automatically, leaving Eq. (46) as the only restriction. Since the left-hand-side of (46) coincides with the function $f^{RS}(x,y,w)$, all squeezed states are candidates to minimize the RS functional,

$$\mathscr{E}(f^{RS}) = \mathscr{E} \,. \tag{51}$$

Therefore, the function f^{RS} comes with the largest possible set of candidates to minimize it, given by the union of the sets $\mathscr{E}_n$ in Fig. 1. The lower bound on f^{RS} now follows directly from combining (46) with (48),

$$f^{RS}(x,y,w) = \left(n + \frac{1}{2}\right)^2 \hbar^2 \geq \frac{\hbar^2}{4} \,, \tag{52}$$

reproducing the RS inequality. Eqs. (50) and (52) imply that the determinant of $\mathbf{F}$ is positive everywhere in the uncertainty region.

The hyperboloid closest to the origin of the (u,v,w)-space provides the states minimizing the function f^{RS},

$$\mathscr{M}(f^{RS}) = \mathscr{E}_0 \,, \tag{53}$$

i.e. the set of squeezed states based on the ground state $|0\rangle$ of a unit oscillator. This is, of course, a two-parameter family since the relations (23) take the form

$$b = -\frac{z}{x} \,, \quad \text{and} \quad \gamma = \frac{1}{2} \ln{(2x)} \,, \tag{54}$$

meaning that, with $x > 0$ and $z \in \mathbb{R}$, both b and γ take indeed arbitrary real values. Thus, each squeezed state can be reached and, when adding phase-space translations, we obtain the four-parameter family of *all* squeezed states as minima of f^{RS}:

$$\mathscr{M}_\alpha(f^{RS}) = \hat{T}_\alpha \mathscr{M}(f^{RS}) \,. \tag{55}$$

This property singles out the RS functional among all uncertainty functionals.

If an uncertainty functional associated to a function f, is different from the RS functional, the first two consistency relations will, in general, *not* be satisfied automatically but impose non-trivial constraints on the second moments. Therefore, the extrema of the functional must be a proper subset of those of the RS functional, i.e. $\mathscr{E}(f) \subset \mathscr{E}$, as the following example shows.

Heisenberg's uncertainty relation. Let us determine the minimum of the product of the standard deviations Δp and Δq by considering the function

$$f^H(x,y,w) = \sqrt{xy}\,. \tag{56}$$

Its partial derivatives satisfy

$$2f_x^H = \sqrt{\frac{y}{x}}\,, \qquad 2f_y^H = \sqrt{\frac{x}{y}}\,, \qquad f_w^H = 0\,, \tag{57}$$

resulting in a positive definite diagonal matrix $\mathbf{F}$, namely,

$$\mathbf{F} = \frac{1}{2}\begin{pmatrix} \sqrt{y/x} & 0 \\ 0 & \sqrt{x/y} \end{pmatrix}\,, \quad \det\mathbf{F} = \frac{1}{4} > 0\,. \tag{58}$$

Eqs. (41) and (42) collapse into the conditions

$$\sqrt{xy} = \left(n + \frac{1}{2}\right)\hbar \equiv e_n\,, \quad n \in \mathbb{N}_0\,, \tag{59}$$

which determine the value of the product of the standard deviations at the extrema of $f^H(x,y,w)$, labeled by the positive integers. In the (u,v,w)-space, the intersections of the surfaces defined by (59) and the hyperboloids (47) consist of hyperbolas in the (u,v)-plane containing the points $(e_n,0)$, $n \in \mathbb{N}_0$. The union of these hyperbolas define the set $\mathscr{E}(f^H)$, corresponding to the potential minima of the function $f^H(x,y)$ (cf. Fig. 2). The third condition, Eq. (43), implies that $w = 0$. Combining (59) with (56), we obtain the bound

$$f^H(x,y,w) = \left(n + \frac{1}{2}\right)\hbar \geq \frac{\hbar}{2}\,, \tag{60}$$

reproducing Heisenberg's uncertainty relation (1).

The family of states minimizing Heisenberg's uncertainty relation is found by using the identity (59) for $n = 0$ in the definition of the parameter γ in (23), leading to $f_y = x/\hbar$. Since the consistency conditions do not impose any other condition on the variance x, it may take any positive value implying that $\gamma \in \mathbb{R}$. Since $\mathrm{f}_w = 0$ leads to $b = 0$, the set of states minimizing the Heisenberg's uncertainty relation is given by squeezed states with real squeezing parameter,

$$\mathscr{M}_\alpha(f^H) = \hat{T}_\alpha \mathscr{E}(f^H) \equiv \left\{ \hat{T}_\alpha \hat{S}_\gamma |0\rangle\,, \alpha \in \mathbb{C}, \gamma \in \mathbb{R} \right\}\,, \tag{61}$$

where we have re-introduced arbitrary phase-space displacements.

Triple product inequality. Using Eq. (5), we see that we need to find the minimum of the expression

$$f^T(x,y,w) = xy\,(x + y + 2w) \tag{62}$$

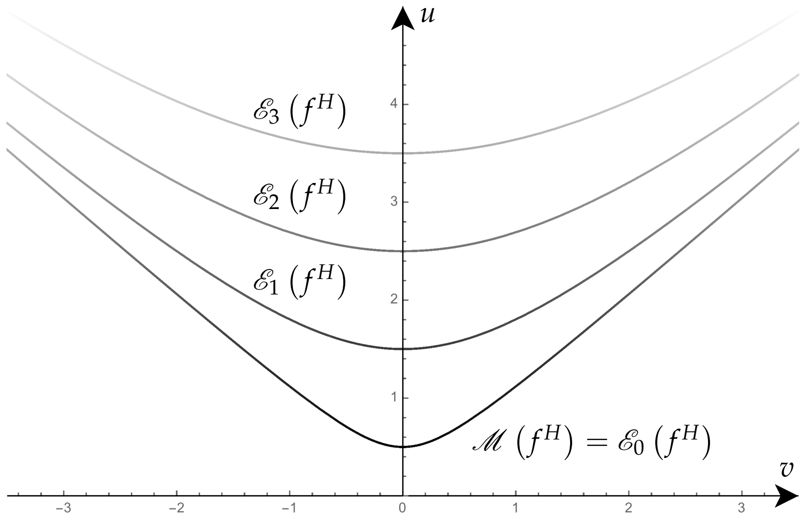

Figure 2: Hyperbolas in the (u, v)-plane through the points $(e_n, 0)$, $n \in \mathbb{N}_0$, stemming from intersections of the hyperboloids (47) and the surfaces defined by (59). The union of the hyperbolas defines the set $\mathscr{E}(f^H)$ which represents the location of all possible minima of the function $f^H(x, y)$; the points on the "lowest" (darkest) hyperbola $\mathscr{E}_0(f^H)$ correspond to the set of states $\mathscr{M}(f^H)$ which saturate Heisenberg's uncertainty relation.

in order to reproduce the triple product uncertainty relation (4). The first consistency condition in Eq. (45) implies that $x = y$; using this identity in the second condition, one finds

$$x(w + x)(w + \frac{x}{2}) = 0 . \tag{63}$$

Recalling that variances are always non-zero for normalizable states, $x > 0$, the correlation w must equal either $-x$ or $-x/2$. According to (5), the first case would imply $\Delta^2 r \equiv 0$, which is impossible since the operator $\hat{r}$ has no normalizable eigenstates. Therefore, using the solution $w = -x/2$ of (63) and $x = y$ in the third consistency condition, one finds that

$$x^2 = \frac{4}{3}\left(n + \frac{1}{2}\right)^2 \hbar^2 , \quad n \in \mathbb{N}_0 , \tag{64}$$

must hold. It is now straightforward to evaluate $f^T(x, y, w)$ at its extrema to find its global minimum,

$$f^T(x, y, w) = x^3 = \left(\sqrt{\frac{4}{3}}\left(n + \frac{1}{2}\right)\hbar\right)^3 \geq \left(\tau\frac{\hbar}{2}\right)^3 ,$$

which reproduces (4). It is easy to confirm that the matrix $\mathbf{F}$ is positive definite with determinant $\det \mathbf{F} = \hbar^4/3$. Since the minimum occurs for $n = 0$, the values of the second moments are given by

$$x = y = -2w = \frac{\hbar}{\sqrt{3}} \equiv \tau\frac{\hbar}{2} . \tag{65}$$

These relations fix the values of the parameters in (23),

$$b = \frac{1}{2} \quad \text{and} \quad \gamma = \frac{1}{4} \ln \tau . \tag{66}$$

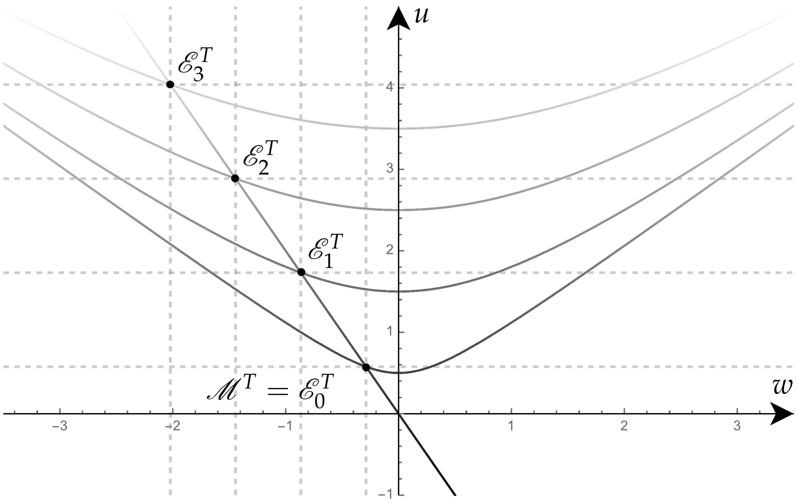

Figure 3: Candidate states $\mathscr{E}(f^T) \equiv \mathscr{E}^T$ possibly minimizing the product of three variances $f^T(u,v,w)$, represented by dots located on the intersections of the hyperboloids (47) and the planes defined by the consistency conditions (69); the point closest to the origin, $\mathscr{M}(f^T) \equiv \mathscr{M}^T$, represents the state $|\Xi_0\rangle$ achieving the minimum of the triple product uncertainty relation (4) (and of any other S_3-invariant inequality associated with a functional $f_N^{(3)}$ in (93)).

Using (32) or (36) we obtain one single state which saturates the triple uncertainty, namely

$$|\Xi_0\rangle \equiv \hat{G}_{\frac{1}{2}} \hat{S}_{\frac{1}{2}\ln\tau} |0\rangle = \hat{S}_{\frac{i}{2}\ln 3} |0\rangle \,. \tag{67}$$

If one includes rigid phase-space translations, the set of states minimizing the triple uncertainty is finally given by the two-parameter family

$$\mathscr{M}_\alpha(f^T) = \left\{ \hat{T}_\alpha |\Xi_0\rangle \,,\, \alpha \in \mathbb{C} \right\} \,, \tag{68}$$

in agreement with [13].

Geometrically, the state $|\Xi_0\rangle$ arises from the intersection of the sequence of hyperboloids with the surfaces defined by

$$u = \tau e_n \,, \quad v = 0 \,, \quad w = -\frac{1}{2}\tau e_n \,, \quad n \in \mathbb{N}_0 \,. \tag{69}$$

The planes defined by constant values of u have concentric circles in common with the hyperboloids, and the vertical uw-plane (given by $v = 0$) intersects with each of the circles in two points only. Finally, the condition on the variable w selects a single one of the points with the same value of u. According to (69), the candidate states in (u,v,w)-space are located on a straight line,

$$\mathscr{E}(f^T) = \left\{ \tau e_n \begin{pmatrix} 1 \\ 0 \\ -1/2 \end{pmatrix}, n \in \mathbb{N}_0 \right\} \,, \tag{70}$$

and the state $|\Xi_0\rangle$ corresponds to the point closest to the origin (see Fig. (3)).

3 New uncertainty relations

3.1 Generalizing known relations

The *linear combination* of second moments

$$f^L(x,y,w) = \mu x + \nu y + 2\lambda w\,, \qquad \mu,\nu,\lambda,\in \mathbb{R}\,, \tag{71}$$

leads to the uncertainty relation

$$\mu\Delta^2 p + \nu\Delta^2 q + 2\lambda C_{pq} \geq \hbar\sqrt{\mu\nu - \lambda^2}, \qquad \mu,\nu > 0\,, \quad \mu\nu > \lambda^2\,. \tag{72}$$

The constraints on the parameters follow from the matrix $\mathbf{F}$ in (19) being strictly positive definite. The consistency conditions (45) associated with f^L relate both y and w to x according to

$$y = \frac{\mu}{\nu}x\,, \qquad w = -\frac{\lambda}{\nu}x\,. \tag{73}$$

Then, Eq. (46) simplifies to

$$\frac{(\mu\nu - \lambda^2)}{\nu^2}x^2 = \left(n + \frac{1}{2}\right)^2 \hbar^2 = e_n^2\hbar^2\,, \tag{74}$$

which is consistent due to $\det \mathbf{F} = \mu\nu - \lambda^2 > 0$. Expressing the functional $f^L(x,y,w)$ in terms of x only, we obtain the bound given in (72),

$$f^L(x,y,w) = \frac{2\left(\mu\nu - \lambda^2\right)}{\nu}x = 2e_n\hbar\sqrt{\mu\nu - \lambda^2} \geq \hbar\sqrt{\mu\nu - \lambda^2}\,. \tag{75}$$

Up to phase-space translations $\hat{T}_\alpha$, a single squeezed state saturates the bound, namely

$$\mathscr{M}(f^L) = \left\{ |\mu,\nu,\lambda\rangle = \hat{G}_{\frac{\lambda}{\nu}}\hat{S}_{\frac{1}{2}\ln\left(\frac{\nu}{\sqrt{\mu\nu-\lambda^2}}\right)}|0\rangle \right\}. \tag{76}$$

When expressing the correlation term C_{pq} in terms of the variance $\Delta^2 r$ according to Eq. (5), we obtain, for $\mu = \nu = 2\lambda = 1$ in (72), the *triple sum* uncertainty relation

$$\Delta^2 p + \Delta^2 q + \Delta^2 r \geq \sqrt{3}\hbar\,, \tag{77}$$

derived in [13], and the minimum is achieved for the state $|1,1,1/2\rangle \equiv |\Xi_0\rangle$ which also minimizes the triple product uncertainty (cf. Eq. (67) and Fig. 3).

Sums of powers of position and momentum variances are bounded from below according to the inequality

$$\mu\left(\Delta^2 p\right)^m + \nu\left(\Delta^2 q\right)^{m'} \geq \left(\frac{\hbar}{2}\right)^{\frac{2mn}{m+m'}} \left(\mu\left(\frac{\nu}{\mu}\frac{m'}{m}\right)^{\frac{m}{m+m'}} + \nu\left(\frac{\mu}{\nu}\frac{m}{n}\right)^{\frac{n}{m+m'}}\right), \qquad m,m' \in \mathbb{N}\,, \tag{78}$$

reducing to the *pair sum* uncertainty relation (2) in the simplest case ($\mu = \nu = m = m' = 1$).

Next, we study a *generalized RS-uncertainty functional* (48),

$$f^{RS}_{m,m'}(x,y,w) = (xy)^m - \mu w^{m'}\,, \qquad \mu > 0\,, \quad m,m' \in \mathbb{N}\,. \tag{79}$$

For arbitrary integers m and n, the consistency conditions cannot be solved in closed form. Setting $m' = 2m$ and assuming that both $m > 1$ and $\mu > 1$ hold, we obtain the explicit bound

$$\left(\Delta^2 p \cdot \Delta^2 q\right)^m - \mu \left(C_{qp}\right)^{2m} \geq \left(\frac{\hbar}{2}\right)^{2m} \frac{\mu}{\left(\mu^{\frac{1}{m-1}} - 1\right)^m} . \tag{80}$$

An interesting special case of $f^{RS}_{m,2m}$ occurs for $m = 1/2$ and $0 < \mu < 1$,

$$\Delta p \Delta q - \mu \left|C_{pq}\right| \geq \frac{\hbar}{2}\sqrt{1-\mu^2} , \tag{81}$$

which can be treated in spite of the presence of the non-differentiable term. The extremal states depend on one free parameter,

$$\mathscr{E}_\alpha(f^{RS}_{1,1/2}) = \left\{ |\alpha, n\rangle = \hat{T}_\alpha \hat{G}_{\pm \frac{\mu e_n \hbar}{2x\sqrt{1-\mu^2}}} \hat{S}_{\frac{1}{2}\ln\left(\frac{x}{e_n \hbar}\right)} |n\rangle \right\} , \qquad x > 0 ; \tag{82}$$

in the absence of the covariance term, $\mu = 0$, they reduce to the squeezed number states with a real parameter known to extremize Heisenberg's inequality.

*Rational function*s of the variances lead to another class of uncertainty relations. For example, defining

$$f^r_{\mu,\nu}(x,y) = \frac{x^m y^m}{\mu x^{m'} + \nu y^{m'}} , \quad \mu, \nu > 0 , \tag{83}$$

we find, if the numerator dominates, the inequality

$$\frac{\Delta^{2m} p \Delta^{2m} q}{\mu \Delta^{2m'} p + \nu \Delta^{2m'} q} \geq \left(\frac{h}{2}\right)^{2m-m'} \frac{1}{2\sqrt{\mu\nu}} , \quad 2m > m' > 0 . \tag{84}$$

Using $m = m' = 1/2$ in (83), this relation reduces to a simple uncertainty relation involving the standard deviations only,

$$\frac{\Delta p \Delta q}{\mu \Delta p + \nu \Delta q} \geq \frac{1}{2}\sqrt{\frac{\hbar}{2\mu\nu}} , \tag{85}$$

with minimal states given by the set

$$\mathscr{M}_\alpha(f^r_{1/2,1/2}) = \left\{ |\alpha, 0\rangle = \hat{T}_\alpha \hat{S}_{\frac{1}{2}\ln\left(\frac{\nu}{\mu}\right)} |0\rangle \right\} . \tag{86}$$

If $m' > 2m$, the expression $f^r_{\mu,\nu}(x,y)$ has an *upper* bound since the denominator is bounded from below and grows faster than the numerator for increasing variances. In general, functions of the second moments with upper bounds are easily constructed from inverting inequalities such as (1) which implies $1/\Delta p \Delta q \leq 2/\hbar$, for example. If $2m = m'$, the functional $f^r_{\mu,\nu}(x,y)$ is neither bounded from below nor from above: the fact that its determinant is negative, $\det \mathbf{F} = f_x f_y < 0$, signals that no solutions of the consistency equations will exist.

Next, we present an example of an uncertainty relation which seems to be entirely out of reach of traditional derivations. Defining the functional

$$f^e(x,y) = x + \mu e^{y/\nu} , \quad \mu, \nu > 0 , \tag{87}$$

we obtain the inequality

$$\Delta^2 p + \mu e^{\Delta^2 q/\nu} \geq \left(1 + 2W(\hbar/4\sqrt{\mu\nu})\right) e^{2W(\hbar/4\sqrt{\mu\nu})}\,, \tag{88}$$

using the fact that Lambert's W-function $W(s)$, defined as the inverse of $s(W) = W \exp W$, is a strictly increasing function. In the limit of $\mu \to \infty$ and assuming $\mu = \nu$, the left-hand-side of (88) turns into $(\mu + \Delta^2 p + \Delta^2 q + \mathcal{O}(1/\mu))$ while the expansion of its right-hand-side produces the correct bound $(\mu + \hbar + \mathcal{O}(1/\mu))$, since $W(s) = s + \mathcal{O}(s^2)$.

The position and momentum variances at the extremum with label $n \in \mathbb{N}_0$ are given by

$$x = 2\mu W\left(\frac{e_n\hbar}{2\sqrt{\mu\nu}}\right) e^{W\left(\frac{e_n\hbar}{2\sqrt{\mu\nu}}\right)} \tag{89}$$

and

$$y = 2\nu W\left(\frac{e_n\hbar}{2\sqrt{\mu\nu}}\right), \tag{90}$$

respectively. Using Eqs. (23) with $\det \mathbf{F} = (\mu/\nu)e^{y/\nu}$, one finds

$$b = 0\,, \qquad \gamma = \frac{1}{4}\ln\left(\frac{\mu}{\nu}\right) + \frac{1}{2}W\left(\frac{e_n\hbar}{2\sqrt{\mu\nu}}\right), \tag{91}$$

which means that only a single state (and its rigid displacements) will saturate the inequality (88). If $\mu = \nu$, we recover $x = y = \hbar^2/4$ as well as $b = \gamma = 0$, i.e. the ground state of a unit oscillator since $W(0) = 0$.

Finally, we point out that some general statements can be made about functionals of the form $f = f(xy, w)$ and $f = f(\mu x^m + \nu y^{m'}, w)$, i.e. generalizations of the expressions in (78) and (79), respectively. By examining the consistency conditions one can show that the extrema of the first expression come as a one-parameter set, while they are isolated or a one-parameter family in the second case. However, without knowing the explicit form of the functions no further conclusions can be drawn.

3.2 Uncertainty functionals with permutation symmetries

The triple product uncertainty relation and the one derived by Heisenberg possess discrete symmetries. Here we investigate more general uncertainty functionals which are invariant under the exchange of three and two variances.

S_3-invariant functionals

Consider a function of three variables which is invariant under the exchange of any pair,

$$f^{(3)}(x, y, z) = f^{(3)}(y, x, z) = f^{(3)}(x, z, y)\,. \tag{92}$$

We now derive the lower bound of a large class of S_3-invariant uncertainty functionals $J[\psi]$ and show that their minima coincide with the state $|\Xi_0\rangle$ minimizing the triple product inequality. The variables x, y and z will denote the variances of the operators $\hat{p}, \hat{q}$ and $\hat{r}$, respectively.

More specifically, we study the minima of sums of completely homogeneous polynomials of degree n, with arbitrary *non-negative* coefficients,

$$f_N^{(3)}(x,y,z) = \sum_{n=1}^{N} \sum_{j+k+\ell=n} a_{jk\ell} x^j y^k z^\ell \,, \quad a_{jk\ell} \geq 0 \,, \tag{93}$$

dropping the unimportant constant term a_{000}. The determinant of the associated $\mathbf{F}$-matrix,

$$\det \mathbf{F} \equiv f_x f_y + f_y f_z + f_z f_x \,, \tag{94}$$

is positive definite since $x, y, z > 0$ and the partial derivatives are just positive polynomials.

The symmetry under S_3-permutations (92) implies that the coefficients must satisfy the conditions

$$a_{jk\ell} = a_{kj\ell} = a_{j\ell k} \,, \quad 0 \leq j, k, \ell \leq n \,, \tag{95}$$

so that the first terms of the polynomials are given by

$$\begin{aligned} f_N^{(3)}(x,y,z) \;=\; & a_{100}(x+y+z) \\ & + a_{200}\left(x^2+y^2+z^2\right) + a_{110}\left(xy+yz+zx\right) \\ & + a_{300}\left(x^3+y^3+z^3\right) + a_{210}\left(x^2(y+z)+y^2(z+x)+z^2(x+y)\right) \\ & + a_{111}xyz + \ldots \end{aligned} \tag{96}$$

If the only nonzero coefficients are $a_{100} = 1$ or $a_{111} = 1$, we recover the functionals associated with the triple sum (77) or the triple product inequality (4), respectively. In general, a completely homogeneous S_3-symmetric polynomial in three variables of degree $n \geq 1$ consists of $\kappa_n = \left\lfloor \frac{(n+3)^2+6}{12} \right\rfloor$ terms where the floor function $\lfloor s \rfloor$ denotes the integer part of the number s: each term arises from one way to partition $j + k + \ell = n$ objects into three sets with j, k and ℓ elements, respectively [23]. Thus, a symmetric polynomial of degree up to N depends on $\left(\sum_{n=1}^{N} \kappa_n\right)$ independent coefficients if one ignores the constant term.

The main result of this section follows from rewriting the consistency conditions (45) and (46) in terms of the variables x, y and z,

$$x f_x - y f_y + (x-y) f_z = 0 \,, \tag{97}$$

$$z f_z - x f_x + (z-x) f_y = 0 \,, \tag{98}$$

$$2\left(xy+yz+zx\right) - x^2 - y^2 - z^2 = (2n+1)^2 \hbar^2 \,, \tag{99}$$

where we have used the identity $z = x + y + 2w$ given in (5). The conditions (97) and (98) imply that the extrema of any symmetric polynomial $f_N^{(3)}(x,y,z)$ occur whenever the three variances take the same value,

$$x = y = z \,. \tag{100}$$

To show that $x = y$ holds we pick any nonzero term $a_{jk\ell} x^j y^k z^\ell$ in the expansion (93) and assume that the powers of x and y are different, i.e. $j \neq k$; the case $j = k$ will be considered later. Due to the symmetry under the exchange $x \leftrightarrow y$, the sum also must contain the term $a_{kj\ell}x^k y^j z^\ell$, with $a_{kj\ell} \equiv a_{jk\ell}$. Defining $t(x,y,z) = a_{jk\ell}\left(x^j y^k + x^k y^j\right) z^\ell$, the first two terms of (98) take the form

$$x t_x - y t_y = (j-k) a_{jkl} \left(x^j y^k - x^k y^j\right) z^\ell . \tag{101}$$

Assuming that $j = k + \delta$, with $\delta > 0$, we find

$$\begin{aligned} x t_x - y t_y &= a_{k+\delta\, kl}\,\delta\left(x^\mu - y^\mu\right) x^k y^k z^\ell & (102)\\ &= (x-y)\delta a_{k+\delta\, k\ell}\left(x^{\delta-1} + x^{\delta-2}y + \ldots + xy^{\delta-2} + y^{\delta-1}\right) z^\ell & (103)\\ &\equiv (x-y) g_+(x,y,z)\,, & (104) \end{aligned}$$

where $g_+(x,y,z) > 0$. Using this expression in (98), the consistency condition takes the form

$$(x-y)\left(g_+(x,y,z) + t_z\right) = 0\,, \tag{105}$$

with another positive function $t_z(x,y,z)$. If $\delta < 0$ we write $k = j - \delta \equiv j + |\delta|$ and eliminate k instead of j from (101), only to find that its left-hand-side again turns into $(x-y)$ multiplied with a positive function. If the powers of x and y of the term $a_{kj\ell}x^k y^j z^\ell$ are equal, $j = k$, one immediately finds that $(x\partial_x - y\partial_y) a_{jkl} x^j y^j z^\ell = 0$, also reducing Eq. 97 to $(x-y)\partial_z a_{jkl} x^j y^j z^\ell = 0$.

The argument just given covers *all* terms in the sum (93), and the positivity of the coefficients $a_{jk\ell}$ implies that the first consistency condition can only be satisfied for $x = y$. Using the symmetry of $f_N^{(3)}(x,y,z)$ under the exchange $y \leftrightarrow z$, an identical argument leads to the identity $y = z$.

Using (100) to evaluate the left-hand-side of Eq. (99) results in

$$x = y = z = \tau e_n \hbar\,, \qquad n \in \mathbb{N}_0\,, \tag{106}$$

where $\tau = \sqrt{4/3}$, so that we obtain an uncertainty relation for any S_3-invariant function

$$f_N^{(3)}(x,y,z) \geq f_N^{(3)}(x,y,z)\Big|_{x=y=z=\hbar/\sqrt{3}} . \tag{107}$$

This result correctly reproduces the special cases of Eqs. (4) and (77), and there is only one state which saturates the inequality, namely $|\Xi_0\rangle$ given in Eq. (67). Letting $N \to \infty$ in Eq. (93), we conclude that the main result of this section, Eq. (107), also applies to any S_3-symmetric function $f_\infty^{(3)}(x,y,z)$ with a Taylor expansion with positive coefficients and infinite radius of convergence, as long as its first partial derivatives exist.

S_2-invariant functionals

Assume now that, in analogy to Eq. (92), we have a functional depending on just two variances in a symmetric way,

$$f^{(2)}(x,y) = f^{(2)}(y,x)\,. \tag{108}$$

An argument similar to the one given for the function $f^{(3)}(x,y,z)$ results in the uncertainty relation

$$f_N^{(2)}(x,y) \geq f_N^{(2)}(x,y)\Big|_{x=y=\hbar/2}\,, \tag{109}$$

which covers the cases of Heisenberg's relation (1) and the pair sum inequality (2). Thus, the actual form of the function at hand determines whether the set of minima $\mathscr{M}(f_N^{(2)})$

will depend on a continuous parameter or not. If the functional is invariant under scaling transformation $x \to \lambda x$, $y \to y/\lambda$, in addition to the permutation symmetry, there is a one-parameter family of solutions and the right-hand-side of Eq. (109) achieves its minimum on the set of points with $xy = (\hbar/2)^2$, not just those with $x = y = \hbar/2$.

To derive (109), we suppose that the function $f_N^{(2)}(x,y)$ has an expansion in analogy to $f_N^{(3)}(x,y,z)$ in Eq. (93) but without the variable z. Adapting the reasoning applied to $f_N^{(3)}(x,y,z)$, the consistency equations (45) are found to imply $x = y$ and $w = 0$. Using this result in (46), the bound $x \geq \hbar^2/4$ follows immediately, so that the inequality (109) must hold for S_2-invariant functionals.

Interestingly, the inequality (84) also reproduces the case of $\mu = \nu = 1$ in Eq. (84) although the functional $f^{(r)}(x,y)$ has an expansion which contains negative coefficients, too. We thus suspect that the inequalities (109) and (107) should hold for S_2- and S_3-invariant functions more general than those considered here.

4 Summary and discussion

This paper responds to the fact that, without exception, the states minimizing the known preparational uncertainty relations for a quantum particle in one dimension are given by (sets of) squeezed states. To explain this fact we systematically study lower bounds for smooth functions $f(\Delta^2 p, \Delta^2 q, C_{pq})$ of second moments. The resulting theory explains the universal role of squeezed states for preparational uncertainty relations depending on second moments only, and it completely charts the landscape of inequalities of this type.

The chain of inclusions

$$\mathscr{E} \supseteq \mathscr{E}(f) \supseteq M(f) \tag{110}$$

concisely summarizes the general structure of our findings. First, we have shown that only squeezed number states of a quantum mechanical harmonic oscillator with unit frequency and mass occur as extrema of an uncertainty functional $J[\psi]$ depending on second moments. We denote this *universal* set of states by $\mathscr{E}$. Second, the extrema of a *specific* functional $J_f[\psi]$, associated with a function $f(\Delta^2 p, \Delta^2 q, C_{pq})$, form the subset $\mathscr{E}(f)$ of the universal set $\mathscr{E}$. Third, the functional will assume its minimum for one or more of the extrema $\mathscr{E}(f)$, a subset which we denote by $\mathscr{M}(f)$. The set of minima may be empty, $\mathscr{M}(f) = \varnothing$. If it is not empty, a lower bound on the functional $J_f[\psi]$ has been found, and it represents a preparational uncertainty relation in terms of the second moments.

Strictly speaking, we obtained the relations $\mathscr{E}_\alpha \supseteq \mathscr{E}_\alpha(f) \supseteq \mathscr{M}_\alpha(f)$ instead of Eq. (110) as it is possible to move quantum states in phase space without affecting the values of the second moments. The four-parameter set $\mathscr{E}_\alpha \equiv \hat{T}_\alpha \mathscr{E}$, for example, consists of the squeezed states $\mathscr{E}$ plus those obtained from them by means of the translation operator $\hat{T}_\alpha$ defined in Eq. (10). Thus, each state saturating a specific inequality with vanishing expectation values gives rise to a two-parameter family of minima.

Our results have a useful geometric representation in the real three-dimensional space of moments. The uncertainty region, consisting of all triples of moments which can arise from (pure or mixed) states of a quantum particle, turns out to be a convex set bounded by a one-sheeted hyperboloid. The boundary is invariant under the elliptic rotations, hyperbolic boosts and parabolic transformations which generate the group $\mathrm{SO}(1,2)$. This observation squares with the importance of the group $\mathrm{SO}(1,2)$ in quantum optics where coherent and squeezed states are ubiquitous.

The invariance of the bounding hyperboloid can, in turn, also be understood as an invariance of the functional $J[\psi]$ defining the surface. Each point on this hyperboloid is

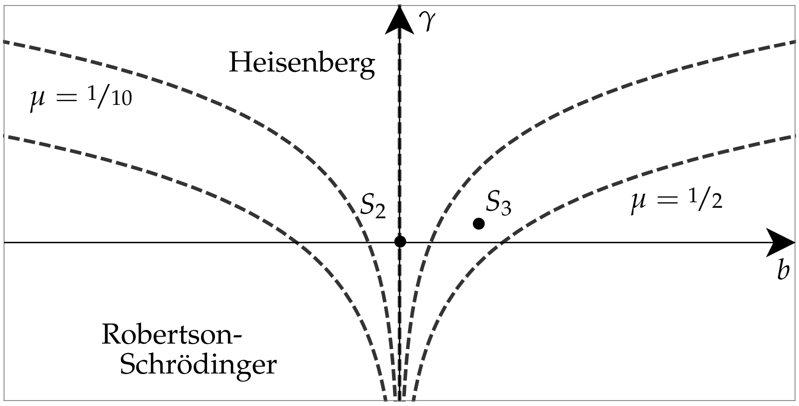

Figure 4: States on the boundary of the uncertainty region minimizing known and new uncertainty relations parameterized by the real numbers (b, γ), with $\hbar = 1$; each point of the plane corresponds to a squeezed state saturating the RS-inequality (3); points on the vertical dashed line represent minima of Heisenberg's uncertainty relation (1); the two curved dashed lines indicate the minima of the modified RS-inequality (81) with $m = 1/2$ and values $\mu = 1/2$ (bottom) and $\mu = 1/10$ (top); the full dots correspond to minima of S_2-invariant functionals (109) such as the pair sum (2) and S_3-invariant functionals (107) such as the triple product (4).

associated with a unique Gaussian state saturating the Robertson-Schrödinger inequality. Changing from an active view of transformations (i.e. mapping one state with minimal uncertainty to another one) to a passive view, we see that the RS-functional (or a suitable smooth function thereof) is invariant under the elements of the group $\mathrm{Sp}(2, \mathbb{R})$ applied to the canonical pair $(\hat{p}, \hat{q})$. The allowed symplectic transformations include rotations, scalings and linear gauge transformations, or shears.

Repeatedly, we have encountered subsets of the maximal possible symmetry group $\mathrm{Sp}(2, \mathbb{R})$ (cf. [7]). The Heisenberg functional $f^H(x, y, z)$ in Eq. 56, for example, is invariant under a scaling transformation $\hat{p} \to \lambda \hat{p}$, $\hat{q} \to \hat{q}/\lambda$, with $\lambda > 0$, resulting in a one-parameter set of states with minimal uncertainty depicted in Fig. 2. Similarly, uncertainty functionals invariant under permutations of order two or three are minimized by states with corresponding symmetry properties. Examples are the triple product uncertainty relation (4) and, more generally, the functionals with discrete symmetries discussed in Sec. 3.2.

We also derived new and explicit uncertainty relations. Fig. 4 uses the (b, γ)-plane to illustrate the sets of states which minimize (some of) the uncertainty relations discussed in this paper. The sets of minima $\mathscr{M}$ may depend on *two* parameters (all squeezed states minimizing the RS-inequality), on *one* parameter (such as the real squeezed states saturating Heisenberg's uncertainty relation) or consist of a *single point* only (associated with S_3-invariant inequalities such as the triple product inequality, for example). We have not been able to backward-engineer functionals which would be minimized by prescribed subsets of the plane such as a circle or a disk. The minimizing states we found were all pure, located on the *boundary* of the uncertainty region. In principle, functionals could also take their minima *inside* this region although we have found only trivial examples with this property [21].

We currently investigate three conceptually interesting generalizations of our approach. First, there is no fundamental reason to restrict oneself to uncertainty functionals depending only on second moments in position and momentum [24]. On the contrary, higher order expectation values would enable us to move away from Gaussian quantum mechanics which is largely reproducible in terms of a classical model "with an epistemic restriction" of the allowed probability distributions [25]. Including fourth-order terms $\langle\psi|\hat{q}^4|\psi\rangle$, for example, will result in an eigenvalue equation (18) which is not related to a unit oscillator in a simple way. It is known that fourth-order moments for single-particle expectations can give rise to inequalities which cannot be reproduced by models based on classical probabilities [26, 27]. Thus, it might become possible to study truly non-classical behaviour in a systematic manner using suitable uncertainty functionals.

Secondly, our approach can be generalized to the case of two or more continuous variables. We expect that a systematic study of uncertainty functionals becomes possible, leading to criteria which would detect pure entangled states. For example, a generalization of the triple uncertainty relation (4) to bipartite systems has been shown to detect entangled states in a quantum optical setting [28]. Other scenarios are known which rely on intuitive choices of suitable bi-linear observables [29, 30].

Finally, the comprehensive study [20] of uncertainty relations for a single spin s has been limited to observables transforming covariantly under the group $\mathrm{SU}(2)$. The method proposed here is easily adapted to investigate functionals depending on arbitrary functions of moments.

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A A Baker-Campbell-Hausdorff identity

The relation $\hat{G}_b\hat{S}_\gamma = \hat{S}(\xi)\hat{R}(\chi)$ in Eq. (33) can be shown by requiring that both products map the annihilation operator $\hat{a} = (\hat{q} + i\hat{p})\,/\sqrt{2\hbar}$ to the same operator. We obtain

$$\hat{G}_b\hat{S}_\gamma\hat{a}\hat{S}_\gamma^\dagger\hat{G}_b^\dagger = \hat{a}\left(\cosh\gamma - i\frac{b}{2}e^\gamma\right) + \hat{a}^\dagger\left(\sinh\gamma + i\frac{b}{2}e^\gamma\right) \tag{111}$$

and

$$\hat{S}(\xi)\hat{R}(\chi)\hat{a}\hat{R}^\dagger(\chi)\hat{S}^\dagger(\xi) = \hat{a}e^{-i\chi}\cosh r - \hat{a}^\dagger e^{-i\chi}e^{i\theta}\sinh r\,, \tag{112}$$

respectively. Equating the coefficients of the operators $\hat{a}$ and $\hat{a}^\dagger$ leads to two equations

$$\cosh\gamma - i\frac{b}{2}e^\gamma = e^{-i\chi}\cosh r\,, \tag{113}$$

$$\sinh\gamma + i\frac{b}{2}e^\gamma = -e^{i(\theta-\chi)}\sinh r\,, \tag{114}$$

which we need to solve for the variables $\xi \equiv re^{i\theta}$ and χ. Separating the real and imaginary parts of the first equation, one finds that

$$\chi = \arctan\left(\frac{b}{1+e^{-2\gamma}}\right) \in (-\frac{\pi}{2}, \frac{\pi}{2})\,. \tag{115}$$

In a similar way, the second equation allows one to solve for the function $\tan(\theta - \chi)$ which, upon using (115), leads to

$$\theta = \arctan\left(\frac{b}{1 - e^{-2\gamma}}\right) + \arctan\left(\frac{b}{1 + e^{-2\gamma}}\right) \in (-\pi\,,\pi)\,. \tag{116}$$

The case of $\gamma = 0$ needs to be treated separately leading to the relation

$$\theta = \pm\frac{\pi}{2} + \arctan\left(\frac{b}{2}\right) \in (-\pi, \pi). \tag{117}$$

Finally, the condition $\cosh r\, \cos\chi = \cosh\gamma$ results in the expression

$$r = \operatorname{arcosh}\left(\cosh^2\gamma + \frac{b^2}{4}e^{2\gamma}\right)^{1/2} \in [0, \infty)\,, \tag{118}$$

which establishes the desired identity (33).

The number states $|n\rangle, n \in \mathbb{N}$, are eigenstates of phase-space rotations $\hat{R}(\chi)$. Therefore, the product $\hat{G}_b\hat{S}_\gamma$ acts on those states according to

$$\hat{G}_b\hat{S}_\gamma|n\rangle \cong \hat{S}(\xi)|n\rangle\,, \tag{119}$$

where an irrelevant phase has been suppressed. Thus, the operator $\hat{S}(\xi)$ generates all squeezed states from $|0\rangle$ when the parameter ξ runs through the points of the complex plane.

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