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Purity- and entropy-bounded uncertainty relations for mixed quantum states

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Abstract
We give a review of different forms of uncertainty relations for mixed quantum states obtained over the last two decades and present many new results. The nonclassical properties of mixed states minimizing the purity-bounded uncertainty relations (a possibility of sub-Poissonian statistics, squeezing etc) are considered. The normalized Hilbert–Schmidt distance between the minimizing states and the 'most classical' thermal states is used as a 'measure of nonclassicality' together with the Mandel parameter. For highly mixed minimizing states (whose 'purities' are very small), the normalized Hilbert–Schmidt distance tends to a finite limit, which depends on the nature of the state (15% of the maximal possible distance if the deviation from pure states is characterized by the 'standard purity' Tr $\hat{\rho}^2$ and 37% if the 'superpurity' $\lim_{r\to 0}[\mathrm{Tr}(\hat{\rho}^{1+1/r})]^r$ is chosen as a measure of deviation).

Keywords: Uncertainty relations, mixed quantum states, canonical transformations, invariant uncertainty product, generalized purities, quantum entropies, squeezing, nonclassical states, sub-Poissonian statistics, Hilbert–Schmidt distance, ambiguity function

1. Introduction

The Heisenberg uncertainty principle [1] was strictly formulated in the form of the inequality for variances of the canonically conjugated observables $\sigma_{pp} \equiv \langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2$ and $\sigma_{xx} \equiv \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2$

$$\sigma_{pp}\sigma_{xx} \geqslant \hbar^2/4 \tag{1}$$

by Kennard [2] and Weyl [3] for *pure* quantum states, which can be described in terms of wavefunctions. The validity of (1) for *mixed* quantum states, described by means of the statistical operator (density matrix) $\hat{\rho}$, was established for the first time in the paper by Mandelstam and Tamm [4] (see also, e.g., [5–10]). It is known that the equality in relation (1) occurs only for pure coherent states, whereas for mixed states we always have a strong inequality. For example, in the case of an equilibrium state of a harmonic oscillator with frequency ω at temperature T, the uncertainty product is given by (k_B is the Boltzmann constant)

$$\sigma_{pp}\sigma_{xx} = \left[\frac{\hbar}{2}\coth\left(\frac{\hbar\omega}{2k_B T}\right)\right]^2. \tag{2}$$

In the high-temperature case $k_B T \gg \hbar\omega$, the right-hand side of (2) is so large that inequality (1), despite being absolutely correct, becomes practically useless. Therefore, the following problem arises naturally—to find generalizations of inequality (1) which would contain some extra dependence on parameters characterizing the 'degree of purity' of a quantum state, in such a way that generalized relations could turn into an equality (perhaps approximate) even for highly mixed states. Although this problem has been considered by several authors over the past two decades, it seems that the achievements in this field are still unknown to a wide community. It is the goal of this paper to give a review of various known forms of the uncertainty relations for mixed states, bringing together old and new results. We confine ourselves to the inequalities for coordinate and momentum 'uncertainties' in one space

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dimension, leaving aside the case of finite-dimensional Hilbert spaces.

The plan of the exposition is as follows. In section 2 we consider generalizations of the Heisenberg–Weyl inequality (1) containing in the right-hand side certain functions of the 'quantum purity' $\mu \equiv \mathrm{Tr}(\hat{\rho}^2)$. The inequalities containing the 'generalized purities' $\mu^{(r)} \equiv [\mathrm{Tr}(\hat{\rho}^{1+1/r})]^r$ are considered in section 3, with a detailed study of the limit case $r = 0$. Another limit case, $r \to \infty$, results in the 'entropy-bounded' uncertainty relations, which are considered in section 4, where a brief discussion of other 'entropic' uncertainty relations is given. Section 5 is devoted to the 'nonclassical' properties of the states minimizing the inequalities considered in sections 2–4. Other approaches to the problem, in particular those based on modifications of the definition of 'uncertainties' for mixed states, are discussed in section 6. The concluding section 7 contains a discussion and a short list of unsolved problems.

2. Inequalities containing the 'second-order purity'

The simplest parameter characterizing the 'purity' of a quantum state is [11]

$$\mu = \mathrm{Tr}\,\hat{\rho}^2 \tag{3}$$

because for pure states $\hat{\rho}^2 = \hat{\rho}$ and $\mu = 1$ due to the normalization condition $\mathrm{Tr}\,\hat{\rho} = 1$, whereas for mixed states $\hat{\rho}^2 \neq \hat{\rho}$ and $0 < \mu < 1$. It is known that for any quantum state described by means of a *Gaussian* density matrix or Wigner function (or some other quasiprobability distribution), the following equality holds for systems with one degree of freedom (see, e.g., [12]):

$$\sigma_{pp}\sigma_{xx} - \sigma_{xp}^2 = \frac{\hbar^2}{4\mu}, \tag{4}$$

where

$$\sigma_{xp} \equiv \tfrac{1}{2}\langle \hat{p}\hat{x} + \hat{x}\hat{p}\rangle - \langle \hat{p}\rangle\langle \hat{x}\rangle \equiv \sigma_{px}$$

is the quantum covariance. Consequently, the generalized inequality can be of the form

$$\sqrt{\sigma_{pp}\sigma_{xx} - \sigma_{xp}^2} \geqslant \frac{\hbar}{2}\Phi(\mu), \tag{5}$$

where $\Phi(\mu)$ is a monotonic function of μ satisfying the relations

$$\Phi(1) = 1 \leqslant \Phi(\mu) \leqslant \mu^{-1} \qquad \text{for} \quad 0 < \mu \leqslant 1.$$

(Inequality (5) with unity instead of $\Phi(\mu)$ was proved for the first time in [13, 14] and later, e.g., in [5, 15]; nowadays it is known under the name Schrödinger–Robertson uncertainty relation [8, 16, 17].) It is reasonable to expect that $\Phi(\mu)$ must go to infinity when μ tends to zero (and this conjecture will be confirmed). We call inequality (5) the 'purity-bounded uncertainty relation'.

As a matter of fact, it is sufficient to find function $\Phi(\mu)$ considering a subfamily of states with zero covariance, taking into account that the quantity

$$\mathcal{D} \equiv \sigma_{pp}\sigma_{xx} - \sigma_{xp}^2 \tag{6}$$

is invariant with respect to arbitrary linear canonical transformations of operators $\hat{x}$ and $\hat{p}$ [12, 18, 19].

The first explicit expression for the function $\Phi(\mu)$ in the form $\Phi_{\mathrm{B}}(\mu) = 8/(9\,\mu)$ was found by Bastiaans [20] in the context of the problem of partially coherent light beams, where parameter μ had the meaning of the degree of space coherence. However, function $\Phi_{\mathrm{B}}(\mu)$ does not satisfy the condition $\Phi(1) = 1$; i.e., using this function one arrives at an inequality which is weaker than (1) for pure quantum states. Besides, the lower limit of the uncertainty product $4\hbar/(9\mu)$ cannot be achieved for any quantum state. Actually, $\Phi_{\mathrm{B}}(\mu)$ is an *asymptotical form* of the exact expression found for the first time in [16, 21, 22].

To obtain this exact expression, we use the property of any statistical operator $\hat{\rho}$ to possess a diagonal expansion over some complete orthogonal set of pure states labelled by an integral index m:

$$\hat{\rho} = \sum_m \rho_m |m\rangle\langle m|, \qquad \sum \rho_m = 1, \qquad \langle m|n\rangle = \delta_{mn}. \tag{7}$$

Let us order this set in accordance with the inequalities

$$1 \geqslant \rho_0 \geqslant \rho_1 \geqslant \cdots \geqslant \rho_m \geqslant \rho_{m+1} \geqslant \cdots \geqslant 0, \tag{8}$$

and introduce an auxiliary function

$$E(\xi) = \frac{\sigma_{pp}}{\xi} + \xi\sigma_{xx}, \tag{9}$$

which can be considered as twice the mean energy of some harmonic oscillator with a unit frequency. The eigenstates $|\tilde{n}\rangle$ of this auxiliary oscillator also form a complete orthonormalized set of states. The coefficients of the expansion

$$|m\rangle = \sum_n a_{mn}(\xi)|\tilde{n}\rangle$$

form a unitary matrix

$$\sum_n a_{mn}a_{kn}^* = \delta_{mk}. \tag{10}$$

Bastiaans [20] proved the relations

$$\frac{E(\xi)}{\hbar} = \sum_{mn} \rho_m |a_{mn}(\xi)|^2(2n+1) \geqslant \sum_m \rho_m(2m+1), \tag{11}$$

where the last inequality is essentially based on the orthogonality condition (10) and the ordering condition (8) (see the appendix). Since the right-hand side of (11) no longer depends on parameter ξ, the minimization of $E(\xi)$ with respect to ξ results in the inequality

$$\sqrt{\sigma_{pp}\sigma_{xx}} \geqslant \frac{\hbar}{2}\sum_{m=0}^{\infty} \rho_m(2m+1). \tag{12}$$

Consequently, one has to find a minimum of the function

$$f(\rho_0, \rho_1, \ldots) = \sum_m \rho_m(2m+1) \tag{13}$$

under the additional constraints

$$\sum \rho_m = 1, \qquad \sum \rho_m^2 = \mu. \tag{14}$$

Introducing the Lagrange multipliers, let us consider the function

$$\tilde{f} = f + \sum(\lambda_2\rho_m^2 - \lambda_1\rho_m).$$

Its minimum is achieved for values linearly decreasing with index m

$$\rho_m = \frac{\lambda_1 - 1 - 2m}{2\lambda_2}$$

(notice that the ordering condition (8) is satisfied). The values of the Lagrange multipliers λ_1 and λ_2 can be easily found from equations (14). Finally, it appears convenient to parametrize the optimal set of coefficients as

$$\rho_m = \frac{2(M+\gamma-m)}{(M+1)(M+2\gamma)}, \tag{15}$$

where M is the maximal integer until which the summations should be performed in equations (13) and (14), and γ is confined in the interval $0 \leqslant \gamma \leqslant 1$. The relations between parameters M, γ and purity μ are as follows:

$$2\gamma = \left\{\frac{M(M+2)}{3[\mu(M+1)-1]}\right\}^{1/2} - M, \tag{16}$$

$$\mu = \frac{2M(2M+1) + 12\gamma(M+\gamma)}{3(M+1)(M+2\gamma)^2}. \tag{17}$$

For a given value of the purity coeffient μ, the integer M must satisfy two constraints. First, it follows from (16) that γ is real provided

$$1 + M \geqslant \mu^{-1}. \tag{18}$$

The meaning of this inequality is simple—in order to obtain a highly mixed state with $\mu \ll 1$, the number of terms in the expansion (7) must be large enough. The second limitation follows from the condition $\gamma \geqslant 0$; it results in the inequality

$$M \leqslant \frac{4 - 3\mu + \sqrt{16+9\mu^2}}{6\mu}. \tag{19}$$

Inequalities (18) and (19) are compatible for any value $\mu \leqslant 1$. For given M and μ, the minimal value of function (13) is given by

$$f_*(\mu; M) = 1 + M - \left\{\frac{M}{3}(M+1)(M+2)\left[\mu - \frac{1}{M+1}\right]\right\}^{1/2}. \tag{20}$$

Now, the function $\Phi(\mu)$ can be obtained from (20), if one chooses the appropriate value of integer M. For example, if $1-\mu \ll 1$ (a slightly mixed state), then the only possible value of M is $M = 1$. Consequently, for values of μ close to unity, function $\Phi(\mu)$ takes the form

$$\Phi_1(\mu) = 2 - \sqrt{2\mu - 1}. \tag{21}$$

If $\varepsilon \equiv 1-\mu \ll 1$, then $\Phi_1(1-\varepsilon) = 1+\varepsilon+\varepsilon^2/2+\cdots$, which is obviously less than $\mu^{-1} = 1+\varepsilon+\varepsilon^2+\cdots$ (although the relative difference does not exceed 10% in the interval $0.5 < \mu < 1$ and is equal to zero at the ends of this interval).

Function (21) is well defined for $\mu > 1/2$. However, as a matter of fact, expression (21) gives the minimal possible value of the product $\sqrt{\sigma_{pp}\sigma_{xx}}$ only in the interval $1 \geqslant \mu \geqslant 5/9$, because at the point $\mu_2 = 5/9$ the value $M = 2$ becomes admissible in accordance with (19), and the new expression for $\Phi(\mu)$ emerges:

$$\Phi_2(\mu) = 3 - \sqrt{8(\mu - 1/3)}. \tag{22}$$

At the point μ_2, the functions (21) and (22) coincide:

$$\Phi_1(5/9) = \Phi_2(5/9) = 5/3.$$

Moreover, their first derivatives with respect to μ coincide at this point, too. However, for $\mu < 5/9$ we have $\Phi_1(\mu) > \Phi_2(\mu)$. It is easy to verify that for the given value of purity μ, the minimal value of function (20) is achieved for the maximal admissible value of integer M, because the derivative of function (20) with respect to M is equal to $-\infty$ at $M = \mu^{-1}-1$, which means that this function decreases with increasing M.

Thus we find a set of functions $\Phi_k(\mu) \equiv f_*(\mu; M = k)$ representing the minimizing function $\Phi(\mu)$ in the intervals $\mu_k \geqslant \mu \geqslant \mu_{k+1}$, where the boundary points μ_k are determined from the condition that (19) becomes an equality for $M = k$

$$\mu_k = \frac{2(2k+1)}{3k(k+1)}. \tag{23}$$

In particular,

$$\mu_3 = \tfrac{7}{18}, \qquad \mu_4 = \tfrac{3}{10}, \qquad \mu_5 = \tfrac{11}{45}, \qquad \mu_6 = \tfrac{13}{63}.$$

For large values of k it is convenient to use the formula

$$\mu_k = \frac{4}{3k}\left[1 - \frac{1}{2(k+1)}\right].$$

The first functions $\Phi_k(\mu)$ are as follows:

$$\Phi_3(\mu) = 4 - \sqrt{20(\mu - 1/4)},$$

$$\Phi_4(\mu) = 5 - \sqrt{40(\mu - 1/5)},$$

$$\Phi_5(\mu) = 6 - \sqrt{70(\mu - 1/6)}.$$

For $\mu = \mu_k$, these functions assume the same values

$$\Phi(\mu_k) = \frac{1+2k}{3} = \frac{4+\sqrt{16+9\mu_k^2}}{9\mu_k}. \tag{24}$$

The first derivatives of functions $\Phi_k(\mu)$ and $\Phi_{k+1}(\mu)$ also coincide at the boundary points μ_{k+1}, but their derivatives of the second and higher orders are different at these points.

We see that the explicit analytical form of function $\Phi(\mu)$ turns out different for different segments of the interval $0 < \mu \leqslant 1$. Therefore, sometimes it could be convenient to use a simple interpolation expression, which is obtained by means of replacing an integer M in (20) by its maximal admissible value (19) (even if this value is not integral)

$$\tilde{\Phi}(\mu) = \frac{4+\sqrt{16+9\mu^2}}{9\mu}. \tag{25}$$

The functions $\tilde{\Phi}(\mu)$ and $\Phi(\mu)$ coincide at points μ_k; in some interval immediately to the right of these points, one has $\tilde{\Phi}(\mu) > \Phi(\mu)$, whereas immediately to the left of these points $\tilde{\Phi}(\mu) < \Phi(\mu)$. However, the difference between the exact and approximate values does not exceed 0.02 even for the values of μ close to unity. Moreover, for $\mu \to 0$ this difference becomes less than $\mu^2/64$. For $\mu \ll 1$, the following asymptotical formula holds:

$$\tilde{\Phi}(\mu) = \frac{8}{9\mu}\left(1 + \frac{9}{64}\mu^2 + \cdots\right), \tag{26}$$

and $|\Phi(\mu) - 8/(9\mu)| < 0,01$ for $\mu \leqslant 0,25 \approx \mu_5$.

3. Inequalities containing 'purities' of arbitrary orders

The 'degree of purity' of a quantum state can be characterized by means of many other quantities different from $\mu = \mathrm{Tr}\,\hat{\rho}^2$. Bastiaans [23] proposed (looking for quantitative measures of spatial coherence of optical beams) to use the traces of arbitrary powers of operator $\hat{\rho}$. It is convenient to define the 'generalized purities' as follows (our definition coincides with that proposed by Bastiaans in [24], provided his index p is replaced by $1+1/r$; in [23] he used a slightly different definition):

$$\mu^{(r)} = \left[\mathrm{Tr}\left(\hat{\rho}^{1+1/r}\right)\right]^r, \qquad r > 0, \tag{27}$$

so that $\mu^{(1)} = \mu$, where μ is the 'usual' purity parameter μ used in the preceding section. Equivalently, one can use 'generalized' [25–27] or 'nonextensive' entropies [28]

$$S_q = \frac{1 - \mathrm{Tr}(\hat{\rho}^q)}{q-1}, \qquad q > 1 \tag{28}$$

($S_2 \equiv 1 - \mu$ is usually called 'linear entropy'), but formulae look simpler for the definition (27).

Using the same scheme as in the preceding section, one can easily find that the optimal weights of states $|m\rangle\langle m|$ in quantum mixtures minimizing the uncertainty product for the fixed value of parameter $\mu^{(r)}$ have the form

$$\rho_m = A(M + \gamma - m)^r, \qquad m = 0, 1, \ldots, M, \qquad 0 \leqslant \gamma \leqslant 1, \tag{29}$$

where coefficients A and γ must be determined from the constraints

$$\sum_{m=0}^{M} \rho_m = 1, \qquad \left(\sum_{m=0}^{M} \rho_m^{1+1/r}\right)^r = \mu^{(r)}.$$

The 'generalized purity-bounded uncertainty relation' has the form (5), where the minimizing function $\Phi^{(r)}(\mu^{(r)})$ possesses different analytical expressions in different subintervals of the total interval $0 < \mu^{(r)} \leqslant 1$

$$\Phi_M^{(r)}(\mu^{(r)}) = 1 + 2(M+\gamma) - 2\,\frac{\sum_{m=0}^{M}(M+\gamma-m)^{r+1}}{\sum_{m=0}^{M}(M+\gamma-m)^r} \tag{30}$$

and the dependence on $\mu^{(r)}$ is 'hidden' in parameters γ and M, which should be found from the equation

$$\frac{\left[\sum_{m=0}^{M}(M+\gamma-m)^{1+r}\right]^r}{\left[\sum_{m=0}^{M}(M+\gamma-m)^r\right]^{r+1}} = \mu^{(r)}. \tag{31}$$

The 'critical points' $\mu_M^{(r)}$ (where integer M changes by unity) correspond to zero values of γ in (31).

The sum in (30) can be calculated explicitly for integral values of $r = 1, 2, \ldots$ in terms of the Bernoulli polynomials $B_n(x)$ [29]. In particular,

$$\Phi_M^{(r)} = 1 + 2(M+\gamma) - 2\,\frac{r+1}{r+2}\,\frac{B_{r+2}(M+1+\gamma) - B_{r+2}(\gamma)}{B_{r+1}(M+1+\gamma) - B_{r+1}(\gamma)}. \tag{32}$$

However, even in this case it is impossible to resolve explicitly the algebraic equation of the order $r(r+1)$ which connects parameter γ with purity $\mu^{(r)}$ (except for the case of $r = 1$ studied in the preceding section)

$$\mu^{(r)} = \frac{(r+1)^{r+1}}{(r+2)^r}\,\frac{[B_{r+2}(M+1+\gamma) - B_{r+2}(\gamma)]^r}{[B_{r+1}(M+1+\gamma) - B_{r+1}(\gamma)]^{r+1}}. \tag{33}$$

For example, for $r = 2$ and $\gamma = 0$ we have

$$\Phi_M^{(2)} = \frac{M^2 + M + 1}{2M+1}, \qquad \mu^{(2)} = \frac{27M(M+1)}{2(2M+1)^3}.$$

Explicit expressions can be obtained either for slightly mixed ($1 - \mu^{(r)} \ll 1$) or highly mixed ($\mu^{(r)} \ll 1$) states, or in the limit cases $r = 0$ or ∞.

3.1. Slightly mixed states

For slightly mixed states, the optimal quantum mixtures have only two terms in the diagonal decomposition; i.e., $M = 1$. Then

$$\Phi_1^{(r)} = 1 + \frac{2\xi^r}{1+\xi^r}, \tag{34}$$

where $\xi = \gamma/(1+\gamma)$ must be found from the equation

$$\mu^{(r)} = \frac{(1+\xi^{r+1})^r}{(1+\xi^r)^{r+1}} \tag{35}$$

which cannot be solved explicitly for $r \neq 1$ (if $0 < r < \infty$).

Function (34) minimizes the uncertainty product in the interval $\mu_2^{(r)} \leqslant \mu^{(r)} \leqslant 1$, where $\mu_2^{(r)}$ corresponds to $\gamma = 1$ (or $\xi = 1/2$) in (35):

$$\mu_2^{(r)} = \frac{(2^{r+1}+1)^r}{(2^r+1)^{r+1}}, \qquad \mu_2^{(0)} = \tfrac{1}{2}, \qquad \mu_2^{(\infty)} = 1. \tag{36}$$

At the left-hand end of this interval, we have

$$\Phi_1^{(r)}(\mu_2^{(r)}) = \frac{3+2^r}{1+2^r}. \tag{37}$$

For small values of the difference $1 - \mu^{(r)}$, we obtain

$$\Phi_1^{(r)}(\mu^{(r)}) = 1 + \frac{2}{r+1}(1 - \mu^{(r)}) + \cdots. \tag{38}$$

3.2. Inequalities for 'superpurity' (r = 0)

Explicit expressions for all functions $\Phi_M^{(r)}(\mu^{(r)})$ in the whole interval $0 < \mu^{(r)} \leqslant 1$ can be found in the case $r = 0$. It is easy to verify that the limit of $\mu^{(r)}$ for $r \to 0$ is nothing but the *maximal of coefficients* ρ_{m} in the diagonal decomposition (7) [23, 24]. Moreover, it can be shown [24] that $\mu^{(r)}$ is a continuous nonincreasing function of r for $r > 0$, i.e. $\mu^{(0)} \geqslant \mu^{(r)} \geqslant \mu^{(p)}$ for $0 \leqslant r \leqslant p < \infty$ (at the same time, coefficients $[\mu^{(r)}]^{1/(1+r)}$ are *nondecreasing* functions of r [23]). For this reason, we use the name 'superpurity' for $\mu_s \equiv \mu^{(0)}$ (thus our μ_s coincides with μ_∞ of Bastiaans [23]).

Functions $\Phi_M^{(0)}(\mu_s)$ change their analytical form at the points $\mu_{sM} = 1/M$. In each interval $M^{-1} \geqslant \mu_s \geqslant (M+1)^{-1}$, we have the sets of optimal coefficients

$$\rho_m = \begin{cases} \mu_s, & m = 0, 1, \ldots, M-1, \\ 1 - M\mu_s, & M = m, \end{cases} \tag{39}$$

which result in the linear dependences

$$\Phi_M^{(0)}(\mu_s) = 1 + 2M - M(M+1)\mu_s. \tag{40}$$

The total function $\Phi^{(0)}(\mu_s)$ is continuous:

$$\Phi^{(0)}(\mu_{sM}) = \Phi_M^{(0)}(\mu_{sM}) = \Phi_{M-1}^{(0)}(\mu_{sM}) = M = \mu_{sM}^{-1},$$

although its derivatives have jumps at the critical points μ_{sM}. Comparing formulae (39) and (40) with general expressions (29)–(38), one should take into account that in the limit $r \to 0$ parameters γ and ξ also tend to zero in such a way that $\gamma^r \sim \xi^r$ remains nonzero (actually, $\lim_{r\to 0} \gamma^r = \mu_s^{-1} - M$).

The hyperbola

$$\tilde{\Phi}^{(0)}(\mu_s) = \mu_s^{-1} \tag{41}$$

passing through all critical points μ_{sM} gives a good approximation of $\Phi^{(0)}(\mu_s)$ (the accuracy is about 10% even in the middle of the interval $1/2 < \mu_s < 1$, and it is much better for $\mu_s \ll 1$). Between the critical points, we have a strict inequality $\tilde{\Phi}^{(0)}(\mu_s) < \Phi^{(0)}(\mu_s)$. Note that the value μ_s^{-1} was interpreted in [30] as 'effective number of degrees of freedom' of partially coherent optical beams.

3.3. Asymptotics for highly mixed states

One can obtain an approximate (asymptotical) expression for the function $\Phi^{(r)}(\mu^{(r)})$ for *highly mixed states* with $\mu^{(r)} \ll 1$. In this case, the number of terms M in the sums of (30) and (31) is so large that one can replace these sums by integrals over dm from 0 to M (using the simplest variant of the Poisson summation formula) and neglect $\gamma \ll M$. Then

$$A \approx \frac{r+1}{M^{r+1}}, \qquad \mu^{(r)} \approx \frac{(r+1)^{r+1}}{M(r+2)^r}, \qquad \Phi^{(r)} \approx \frac{2M}{2+r}.$$

Expressing M in terms of $\mu^{(r)}$ we obtain an approximate dependence

$$\tilde{\Phi}^{(r)}(\mu^{(r)}) = \frac{2}{\mu^{(r)}}\left(\frac{r+1}{r+2}\right)^{r+1}, \qquad \mu^{(r)} \ll 1. \tag{42}$$

Using another approach, Bastiaans [23] proved that the uncertainty product is always greater than $\hbar\tilde{\Phi}^{(r)}(\mu^{(r)})/2$ for any $r > 0$, and the equality occurs in the limit case $r = 0$ for $\mu_s = \mu_{sM}$ (in our notation). The approximation (42) is weaker than the usual uncertainty relation (1) for slightly mixed states with $\mu^{(r)}$ close to unity, because the coefficient at $[\mu^{(r)}]^{-1}$ in (42) is less than unity for $r > 0$.

4. 'Entropy-bounded' versus 'entropic' uncertainty relations

Since the 'second critical point' $\mu_2^{(r)}$ (36) tends to unity for $r \to \infty$, one may hope to obtain a unique analytical expression for $\Phi^{(\infty)}(\mu^{(\infty)})$ in the whole interval $0 < \mu^{(\infty)} \leqslant 1$. On the other hand, the limit case $r = \infty$ in (27) is equivalent to the limit $q \to 1$ in the nonextensive entropy (28), when this entropy becomes the usual von Neumann entropy

$$S = -\operatorname{Tr}(\hat{\rho}\ln\hat{\rho}) = -\sum \rho_m \ln \rho_m. \tag{43}$$

Therefore it is not surprising that parameter $\mu^{(\infty)}$ is connected with the entropy (43). Bastiaans [24] showed that this connection is very simple

$$\mu^{(\infty)} \equiv \mu_S = \exp(-S). \tag{44}$$

The following useful inequalities hold:

$$\mu_s \equiv \mu^{(0)} \geqslant \mu^{(1)} \equiv \mu \geqslant \mu^{(\infty)} \equiv \mu_S.$$

Looking for the minimum of the function

$$\sum_{m=0}^{\infty} \rho_m(2m + 1 - \lambda_1 + \lambda_2 \ln \rho_m),$$

one obtains an *infinite* set of optimal coefficients in the form

$$\rho_m = (1 - e^{-\beta})e^{-\beta m}, \tag{45}$$

where parameter β is determined by the condition

$$\beta(e^{\beta} - 1)^{-1} - \ln(1 - e^{-\beta}) = S. \tag{46}$$

Therefore the invariant uncertainty product for mixed states with the given entropy S is bounded by the function which has a form of an effective Planck distribution [16, 21, 22]:

$$\sqrt{\sigma_{pp}\sigma_{xx} - \sigma_{px}^2} \geqslant \frac{\hbar}{2}\left[1 + \frac{2}{e^{\beta(S)} - 1}\right]. \tag{47}$$

This relation can be called the 'entropy-bounded uncertainty relation'. It was also obtained (for $\sigma_{px} = 0$ and in a different explicit form, which is, nonetheless, completely equivalent to (47)) in [24].

For $S \gg 1$ equation (46) has an approximate analytical solution $\beta \approx \exp(1 - S)$. Putting this into (47) we find a simplified inequality

$$\sqrt{\sigma_{pp}\sigma_{xx} - \sigma_{px}^2} > \hbar e^{S-1} = \frac{\hbar}{e\mu_S}, \qquad S \gg 1, \tag{48}$$

in full accordance with the limit $r \to \infty$ in (42).

It is worth emphasizing that inequalities (47) and (48) contain 'true' von Neumann's entropy, in contrast to a large family of 'entropic uncertainty relations' [16, 31–37], which are based on more specific 'entropies' defined in terms of distributions of canonically conjugated variables in some distinguished representations. The coordinate–momentum entropic uncertainty relation for *pure states* reads

$$S_x + S_k \geqslant \ln(e\pi), \tag{49}$$

where

$$S_x = -\int |\psi(x)|^2 \ln(|\psi(x)|^2)\,\mathrm{d}x, \tag{50}$$

$$S_k = -\int |\varphi(k)|^2 \ln(|\varphi(k)|^2)\,\mathrm{d}k \tag{51}$$

and

$$\varphi(k) = \int \psi(x)\exp(-\mathrm{i}kx)\,\mathrm{d}x/\sqrt{2\pi}. \tag{52}$$

Inequality (49) has many advantages over the Heisenberg–Weyl inequality (1). In particular, the Heisenberg–Weyl inequality (1) can be derived from (49) (but not *vice versa*). This is a consequence of the inequality (valid for arbitrary distributions and turning into an equality for Gaussian distributions)

$$S_x \geqslant \tfrac{1}{2}\ln(2\pi e\sigma_x). \tag{53}$$

A disadvantage of inequality (49) is that it is intimately connected with the notion of a wavefunction, being valid, therefore, only for *pure* quantum states (which have zero 'true' entropy). Trying to stay in the realm of pure (even if not completely physical) states, Abe and Suzuki [38] used the thermofield formalism, enlarging the Hilbert space by means of introducing extra artificial degrees of freedom. Then the 'entropies' can be defined as in (50), provided $\psi(x)$ is replaced by $\psi(x,\tilde{x})$ and the integration is performed over $\mathrm{d}x\,\mathrm{d}\tilde{x}$, where $\tilde{x}$ is an additional fictitious coordinate. In this way, Abe and Suzuki obtained (in the special case of zero covariance) a 'thermal Heisenberg uncertainty relation', which can be transformed (after simple algebra) exactly to the form (47) (with $\sigma_{xp} = 0$). An obvious disadvantage of the Abe–Suzuki inequality was a lack of clear physical meaning of the parameter β—it could be interpreted as an inverse temperature of the artificial enlarged system, but it has no direct relation to the entropy or other characteristics of the real system under study.

Hall [39] generalized the definition of 'coordinate' and 'momentum' uncertainties to the case of mixed states, using the corresponding probability distributions (such as $\rho(x,x)$ instead of $|\psi(x)|^2$) in (50) and (51). He considered the 'noise-dependent' states defined as follows:

$$\Gamma(\hat{\rho}) = \iint \mathrm{d}x\,\mathrm{d}p\; p_\gamma(x,p;n_\gamma)\hat{D}_{xp}\hat{\rho}\hat{D}_{xp}^{\dagger},$$

$$p_\gamma(x,p;n_\gamma) = (2\pi n_\gamma)^{-1}\exp\left(-\frac{x^2+p^2}{2n_\gamma}\right),$$

$$\hat{D}_{xp} = \exp(\mathrm{i}p\hat{X} - \mathrm{i}x\hat{P}).$$

For these states, he proved the inequalities (here $\hbar = 1$)

$$S_X + S_P \geqslant \ln(e\pi) + \ln(2n_\gamma + 1), \tag{54}$$

$$\Delta X\Delta P \geqslant \tfrac{1}{2} + n_\gamma \tag{55}$$

(relation (55) is a consequence of inequality (54)). Evidently, (55) has the same form as (47). However, it was not shown in [39] how to extract parameter n_γ ('mean number of added noise photons') from an *arbitrary given* statistical operator $\hat{\rho}$.

Anastopoulos and Halliwell [40] used the so-called Wehrl entropy [41]

$$I = \int \frac{\mathrm{d}p\,\mathrm{d}q}{2\pi\hbar}\rho(p,q)\ln\rho(p,q), \tag{56}$$

where $\rho(p,q) = \langle z|\hat{\rho}|z\rangle$ is a non-negative quasiprobability distribution (Husimi function [42]), defined by means of coherent states $|z\rangle$ of some oscillator with an arbitrary frequency ω, so that $z = (\omega q + \mathrm{i}p)/\sqrt{2\hbar\omega}$. Taking into account the properties of the Wehrl entropy

$$S \leqslant I \leqslant \ln\left[(e/\hbar)\sqrt{\det\mathcal{M}}\right] \tag{57}$$

(where $\mathcal{M}$ is the covariance matrix of the distribution $\rho(p,q)$) and the arbitrariness of parameter ω, they have obtained inequality (48) (including the covariance term).

5. Nonclassical properties of minimizing states

Let us discuss now properties of the states which minimize the uncertainty relations for mixed states. Evidently, the equality in the entropy-bounded relation (47) is achieved for the 'thermal' (Gaussian) states constructed from the harmonic oscillator eigenfunctions with the aid of equations (7) and (45). These states can be considered as the 'most classical' mixed quantum states, in the same sense as coherent states are considered frequently as the 'most classical' pure states.

In contrast, the equality sign in the generalized purity bounded uncertainty relation (5) is attained for the *finite* mixtures of the oscillator's m-quantum states $|m\rangle\langle m|$ (7), where coefficients ρ_m are given by equation (29), so these minimizing states are 'nonclassical'. In [43] it was proposed to use the *minimal Hilbert–Schmidt distance* between $\hat{\rho}$ and all operators describing *displaced thermal states* with the same degree of purity μ as a quantitative measure of 'nonclassicality' of any state described by the statistical operator $\hat{\rho}$ (a long list of references to studies devoted to the problems of 'nonclassicality' and distances between quantum states can be found in [44]). For mixtures of unshifted Fock states, the minimum of the distance is achieved for the unshifted thermal state

$$\hat{\rho}_{\mathrm{th}} = \frac{2\mu}{1+\mu}\sum_{m=0}^{\infty}\left(\frac{1-\mu}{1+\mu}\right)^m |m\rangle\langle m|. \tag{58}$$

Since the distances between any states with the same value of purity go to zero when $\mu \to 0$, we introduce the *normalized Hilbert–Schmidt distance* as

$$d^2 \equiv \frac{\mathrm{Tr}\left(\hat{\rho} - \hat{\rho}_{\mathrm{th}}\right)^2}{2\mu} = 1 - 2\sum_m \frac{(1-\mu)^m}{(1+\mu)^{m+1}}\rho_m. \tag{59}$$

We consider two sets of states, for which all explicit expressions are known. The first set consists of the states minimizing the uncertainty product for the given value of the usual purity μ

$$\hat{\rho}^{(1)}_{M\gamma} = \sum_{m=0}^{M}\frac{2(M+\gamma-m)}{(M+2\gamma)(M+1)}|m\rangle\langle m|. \tag{60}$$

In the particular case $\gamma = 0$, these states were also studied in [45]. The minimal distance between the state (60) and the family of displaced thermal states with the same purity μ is given by

$$d_1^2 = 1 - \frac{(1+\mu)[(1-x)(M+\gamma-\gamma x^{M+1}) - x(1-x^M)]}{\mu^2(M+1)(M+2\gamma)},$$

where $x = (1-\mu)/(1+\mu)$. For $M = 1$, this distance increases as

$$d_1(\gamma) = \gamma^2[1 + 3\gamma(1+\gamma)]^{-1},$$

reaching the value $d_1(1) = 1/7$ at the point $\mu_2 = 5/9$. For $M \geqslant 2$, the distance practically does not depend on M and γ (i.e. on μ), remaining at approximately the same level $d \approx 1/7$. The asymptotical value of the normalized distance for $\mu \to 0$ is given by

$$d_1(\mu \to 0) = \tfrac{1}{4}\sqrt{1 - 9\exp(-8/3)} \approx 0.15 \qquad (61)$$

(one should take into account that $M \approx 4/(3\mu)$ when $\mu \ll 1$, therefore $(1-2\mu)^M \to \exp(-8/3)$ as $\mu \to 0$).

The values of distance found above show that the minimizing mixed states (60) (MMS) are not 'extremely far' from the thermal ones, in accordance with the fact that the exact function $\Phi(\mu)$ is also not very far from the dependence μ^{-1} characterizing Gaussian states. The same is true for the mean number of photons,

$$\overline{n}^{(1)} = \frac{M(M-1+3\gamma)}{3(M+2\gamma)}, \qquad \overline{n}_{\rm th} = \frac{1-\mu}{2\mu}, \qquad (62)$$

so we have $\overline{n}^{(1)} \approx 4/(9\mu)$ and $\overline{n}_{\rm th} \approx 1/(2\mu)$ for $\mu \to 0$ (note that the coefficients at μ^{-1} turn out to be the same as in the asymptotical bounds for uncertainty products).

Nonetheless, the photon statistics in the MMS is essentially different from the super-Poissonian statistics of thermal states, characterized by the Mandel parameter

$$Q_{\rm th} = \frac{1+\mu}{2\mu^2}, \qquad Q \equiv \frac{\overline{n^2} - (\overline{n})^2 - \overline{n}}{\overline{n}}. \qquad (63)$$

The complete expression for $Q^{(1)}(M,\gamma)$ in the MMS is rather cumbersome, but its special cases for $\gamma = 0$ and $M \geqslant 2$ or for any γ and $M = 1$ are very simple

$$Q^{(1)}(M,0) = \frac{M-4}{6}, \qquad M \geqslant 2, \qquad (64)$$

$$Q^{(1)}(1,\gamma) = -\frac{\gamma}{1+2\gamma} = \frac{1}{2}\left(\sqrt{2\mu-1} - 1\right). \qquad (65)$$

Consequently, the statistics in MMS is *sub-Poissonian* for $M < 4$ (i.e. for $\mu > 3/10$). Moreover, although $Q^{(1)} \geqslant 0$ for $\mu \leqslant 3/10$, the statistics in MMS turns out to be 'much less' super-Poissonian than in the thermal states—this is clearly seen from the relationships which hold for $\mu \to 0$

$$Q^{(1)} \approx \frac{2}{9\mu}, \qquad Q_{\rm th} \approx \frac{1}{2\mu^2}. \qquad (66)$$

The second set consists of the states minimizing the uncertainty product for the given value of the 'superpurity' $\mu_{\rm s}$

$$\hat{\rho}_M^{(0)} = \mu_{\rm s}\sum_{m=0}^{M-1}|m\rangle\langle m| + (1 - M\mu_{\rm s})|M\rangle\langle M|. \qquad (67)$$

The usual purity of the state (67) is given by

$$\mu = \mu_{\rm s} + [1 - M\mu_{\rm s}][1 - (M+1)\mu_{\rm s}], \qquad (68)$$

so $\mu = \mu_{\rm s} = \mu^{(r)}$ for $\mu_{{\rm s}M} = 1/M$, $0 \leqslant r \leqslant \infty$, and the (non-negative) difference $\mu_{\rm s} - \mu$ decreases as $\mu_{\rm s}^2$ when $\mu_{\rm s} \to 0$.

The distance between the state (67) with $M = 1$ and the thermal state with the same purity is given by

$$d_0 = \frac{2(1-\mu_{\rm s})^2}{1+\mu_{\rm s}}, \qquad \tfrac{1}{2} \leqslant \mu_{\rm s} \leqslant 1. \qquad (69)$$

For $\mu_{\rm s} \leqslant 1/2$, simple expressions can be written for the critical values $\mu_{{\rm s}M} = 1/M$ (when $\mu = \mu_{\rm s}$)

$$d_0 = \left(\frac{M-1}{M+1}\right)^{M/2}, \qquad (70)$$

so that $d_0 = 1/3$ for $M = 2$ and $d_0 \to 1/e \approx 0.37$ when $M \to \infty$ (i.e. $\mu_{\rm s} \to 0$). Since $d_0 > d_1$ for the same values of purity μ, one may conclude that state (67) is 'more nonclassical' than state (60). This is confirmed by the analysis of the photon statistics. The mean number of photons is given by

$$\overline{n}^{(0)} = \frac{M-1}{2}M\mu_{\rm s} + M(1 - M\mu_{\rm s}). \qquad (71)$$

Simple expressions for the Mandel parameter are obtained for $1/2 \leqslant \mu_{\rm s} \leqslant 1$ and for $\mu_{{\rm s}M} = 1/M$:

$$Q^{(0)} = \mu_{\rm s} - 1, \qquad \tfrac{1}{2} \leqslant \mu_{\rm s} \leqslant 1, \qquad Q_M^{(0)} = \frac{M-5}{6}. \qquad (72)$$

The statistic is sub-Poissonian in a wider interval $1 \geqslant \mu_{\rm s} > 1/5$, and the absolute values of the Q-factor are larger in this interval than in the case of states (60). For small values of the 'asymptotical purity', we have $Q^{(0)} \approx [6\mu_{\rm s}]^{-1}$, which is less than $Q^{(1)}$ for the same value of purity.

The *Wigner functions* of the MMS can be easily obtained from the statistical operator decomposition (7) with coefficients (29), if one uses the known expression for the Wigner function of the Fock states in terms of the Laguerre polynomials [46–48]. Using dimensionless variables, corresponding formally to a harmonic oscillator with unit mass, frequency and Planck's constant, we can write the Wigner functions of the MMS as

$$W_{M\gamma}^{(r)} = A{\rm e}^{-y}\sum_{m=0}^{M}(M+\gamma-m)^r(-1)^m L_m(2y), \qquad (73)$$

where $y \equiv x^2 + p^2$.

It is remarkable that *all* functions of the form (73) are *non-negative* in the whole phase plane (x, p), although they describe nonclassical states. It was shown by Bastiaans [45] that

$$\sum_{m=0}^{\infty}\rho_m(-1)^m L_m(y) \geqslant 0$$

for any $y \geqslant 0$, provided coefficients ρ_m are ordered as in (8). It is known that the only non-negative Wigner function of *pure* quantum states is the Gaussian one. However, functions (73) are related to the *mixed* states. Bastiaans [45] gave also an interesting asymptotical form for the function $W_{M0}^{(1)}$ for highly mixed states with $\mu \ll 1$ (i.e. $M \gg 1$). In the normalized form, it reads

$$W_{M0}^{(1)}(y) \approx \frac{4}{(2M+1)^2} \begin{cases} (2M+1-y), & y < 2M+1, \\ 0, & y \geqslant 2M+1. \end{cases}$$

5.1. Squeezing and whole families of minimizing states

The minimizing states in the form (7) (with $|m\rangle$ meaning the Fock state) are obviously unsqueezed, since they possess equal variances of the quadrature components

$$\sigma_{pp} = \sigma_{xx} = \sigma_* \equiv \tfrac{1}{2} + \overline{n}.$$

However, these states form only a small subfamily of a much larger family of states minimizing inequality (5). The members of this large family have the form

$$\hat{R}_M = \hat{U}\hat{\rho}_M\hat{U}^\dagger, \qquad \hat{U} = \exp\left[-\mathrm{i}\left(\tfrac{1}{2}\hat{\boldsymbol{q}}B\hat{\boldsymbol{q}} + \boldsymbol{c}\hat{\boldsymbol{q}}\right)\right], \quad (74)$$

where $\hat{\boldsymbol{q}} = (\hat{p}, \hat{x})$ is the two-dimensional vector operator, $\boldsymbol{c}$ is an arbitrary vector with real components and B is an arbitrary 2×2 *symmetrical* real matrix. Since $\hat{U}$ is the unitary operator, the state $\hat{R}_M$ has the same (usual or generalized) purity as the initial state $\hat{\rho}_M$. On the other hand, $\hat{U}$ is a generator of a *linear canonical transformation* [49–51]

$$\hat{U}\hat{\boldsymbol{q}}\hat{U}^{-1} = \Lambda\hat{\boldsymbol{q}} + \boldsymbol{\delta}_c, \quad (75)$$

which preserves the commutators $[\hat{q}_j, \hat{q}_k] = -\mathrm{i}\hbar\Sigma_{jk}$ due to the symplecticity of matrix Λ (hereafter tilde means matrix transposition and E means the unit matrix)

$$\Lambda\Sigma\tilde{\Lambda} = \Sigma, \qquad \Sigma = \|\Sigma_{jk}\| = -\tilde{\Sigma}, \quad (76)$$

$$\Lambda = \exp(\Sigma B), \qquad \boldsymbol{\delta}_c = [\exp(\Sigma B) - E]B^{-1}\boldsymbol{c}. \quad (77)$$

Since the combination of variances (6) is invariant with respect to arbitrary linear canonical transformations [12, 18, 19], any state (74) minimizes the generalized uncertainty relation (5). Therefore, choosing matrix B in an appropriate way, one can construct minimizing mixed states with any desired degree of squeezing. Using the terminology accepted for some years, one may say that the family (74) consists of the special finite mixtures of the *displaced and squeezed Fock states* $\hat{U}|m\rangle\langle m|\hat{U}^\dagger$ with the same transformation operator $\hat{U}$ for each member of the mixture (the states $\hat{U}|m\rangle$ were introduced, as a matter of fact, by Plebański [52, 53]).

The kernel of the operator $\hat{U}$ is a Gaussian exponential for most representations usually used (coordinate, momentum, coherent states) [49–51]. In all these representations, the density matrices related to the state (74) can be written as some involved finite sums of two-dimensional Hermite polynomials [51] (the connection between these polynomials and the states, which are known nowadays as displaced squeezed number states, was established in another context in [54, 55]).

A remarkable exception is the Wigner representation, where the kernel of the operator $\hat{U}$ is reduced to the *delta-function* [47, 56]

$$G_U(\boldsymbol{q}, \boldsymbol{q}') = \delta(\boldsymbol{q}' - \Lambda\boldsymbol{q} - \boldsymbol{\delta}_c).$$

Therefore, the Wigner function describing the state (74) is given by the same expression (73), with the only difference that the argument y is now given by

$$y = \boldsymbol{q}\tilde{\Lambda}\Lambda\boldsymbol{q} + 2\boldsymbol{\delta}_c\Lambda\boldsymbol{q} + \boldsymbol{\delta}_c^2. \quad (78)$$

The variance matrix in the generic state (74) is

$$\mathcal{M} \equiv \left\| \begin{matrix} \sigma_{pp} & \sigma_{px} \\ \sigma_{xp} & \sigma_{xx} \end{matrix} \right\| = \sigma_*\tilde{\Sigma}\tilde{\Lambda}\Lambda\Sigma. \quad (79)$$

6. Inequalities for modified 'uncertainties'

From the mathematical point of view, both 'variance' and 'entropic' uncertainty relations for coordinate and momentum in the case of pure quantum states are consequences of some mutual properties of the Fourier pairs $\psi(x)$ and $\varphi(k)$, where $\psi(x)$ is a *complex* wavefunction describing the state in the coordinate representation and $\varphi(k)$ (52) is its counterpart in the momentum representation [16, 34, 35]. On the other hand, mixed states are described in terms of density matrices $\rho(x, x')$ or Wigner functions $W(x, p)$, which have twice as many arguments and obey certain constraints, such as $\rho(x, x') = [\rho(x', x)]^*$ or $\mathrm{Im}\, W = 0$. Besides, the normalization rules and the relations with average values of operators are different for $\rho(x, x')$ or $W(x, p)$ and $\psi(x)$. Therefore, it is impossible to transfer literally to mixed states the same approaches that work for pure states, considering $\rho(x, x')$ or $W(x, p)$ simply as 'effective two-dimensional wavefunctions'. Some modifications are necessary, including, in particular, a redefinition of 'uncertainties' and, in general, 'mean values'.

Usually, the mean values entering the definition of quantum variances are calculated with the aid of the statistical operator $\hat{\rho}$ as

$$\langle\hat{A}\rangle = \mathrm{Tr}(\hat{A}\hat{\rho}). \quad (80)$$

Remembering that $\hat{\rho}^n = \hat{\rho}$ for pure states, but $\hat{\rho}^n \neq \hat{\rho}$ for mixed ones, there is a possibility to change the definition (80), replacing operator $\hat{\rho}$ in (80) by $\hat{\rho}^n$ or, in the simplest case, by $\hat{\rho}^2$. This idea was formulated in connection with another problem in [12, 57].

Chountasis and Vourdas [58] used a similar idea to find a generalization of uncertainty relations for mixed states. Considering the Wigner function

$$W(x, p) = \int \rho(x + X/2, x - X/2)\exp(-\mathrm{i}Xp)\,\mathrm{d}X$$

and its Fourier transform (known as the Weyl function or ambiguity function [59])

$$\tilde{W}(X, P) = \int W(x, p)\exp[-\mathrm{i}(Px - Xp)]\frac{\mathrm{d}x\,\mathrm{d}p}{2\pi}$$
$$= \int \rho(x + X/2, x - X/2)\exp(-\mathrm{i}xP)\,\mathrm{d}x,$$

they have introduced two kinds of 'uncertainty'

$$\delta x \equiv [\langle\langle x^2\rangle\rangle - \langle\langle x\rangle\rangle^2]^{1/2}, \qquad \delta X \equiv \langle\langle X^2\rangle\rangle^{1/2}, \quad (81)$$

where

$$\langle\langle x\rangle\rangle \equiv \int x[W(x, p)]^2\frac{\mathrm{d}x\,\mathrm{d}p}{2\pi} = \mathrm{Tr}[\hat{x}\hat{\rho}^2], \quad (82)$$

$$\langle\langle x^2\rangle\rangle \equiv \int x^2[W(x,p)]^2 \frac{\mathrm{d}x\,\mathrm{d}p}{2\pi} = \tfrac{1}{2}\mathrm{Tr}[\hat{x}^2\hat{\rho}^2] + \tfrac{1}{2}\mathrm{Tr}[\hat{x}\hat{\rho}\hat{x}\hat{\rho}], \tag{83}$$

$$\langle\langle X^2\rangle\rangle \equiv \int X^2|\tilde{W}(X,P)|^2 \frac{\mathrm{d}X\,\mathrm{d}P}{2\pi} = 2\,\mathrm{Tr}[\hat{x}^2\hat{\rho}^2] - 2\,\mathrm{Tr}[\hat{x}\hat{\rho}\hat{x}\hat{\rho}] \tag{84}$$

(and similar definitions for p and P; note that $\langle\langle X\rangle\rangle = \langle\langle P\rangle\rangle = 0$ identically).

The generalized relations found in [58] read

$$\delta X\delta p \geqslant \tfrac{1}{2}\,\mathrm{Tr}\,\hat{\rho}^2, \qquad \delta x\delta P \geqslant \tfrac{1}{2}\,\mathrm{Tr}\,\hat{\rho}^2 \tag{85}$$

with

$$\mathrm{Tr}\,\hat{\rho}^2 = \int [W(x,p)]^2 \frac{\mathrm{d}x\,\mathrm{d}p}{2\pi}.$$

The equality sign in (85) is achieved for Gaussian thermal states.

Ponomarenko and Wolf [60] have defined two complementary 'generalized variances' of any operator $\hat{A}$ in the following way:

$$\langle(\Delta\hat{A})^2\rangle_\pm \equiv \pm\,\mathrm{Tr}([\Delta\hat{A},\hat{\rho}]_\pm^2), \tag{86}$$

where $\Delta\hat{A} = \hat{A} - \mathrm{Tr}(\hat{A}\hat{\rho})$ and $[,]_+$ stands for the anticommutator. In the basis of eigenstates of operator $\hat{A}$, the generalized variances can be expressed as [60]

$$\langle(\Delta\hat{A})^2\rangle_\pm = \sum_{a,a'}(a \pm a')^2|\langle a|\hat{\rho}|a'\rangle|^2. \tag{87}$$

The authors of [60] derived the inequality

$$\langle(\Delta\hat{A})^2\rangle_-\langle(\Delta\hat{B})^2\rangle_+ \geqslant |\,\mathrm{Tr}([\hat{A},\hat{B}]_-\,\hat{\rho}^2)|^2 \tag{88}$$

and proved that it is minimized on Gaussian (squeezed thermal) states. However, using (87) one can check that for Gaussian states (without covariance, for simplicity) the generalized variances are related to the standard ones as follows (here $\mu \equiv \mathrm{Tr}\,\hat{\rho}^2$):

$$\langle(\Delta\hat{x})^2\rangle_+ = 2\sigma_x\mu, \qquad \langle(\Delta\hat{x})^2\rangle_- = 2\sigma_x\mu^3$$

(and similar relations for the momentum), so relation (88) is reduced to the known identity (4).

7. Discussion

We have obtained a family of exact inequalities in the form (5) which give (attainable) lower bounds for the invariant uncertainty product of mixed states with a given value of some generalized purity (27), labelled by a continuous non-negative index r and parametrized implicitly by equations (30) and (31). We have studied in detail various special cases where simple explicit expressions can be obtained (see, e.g., equations (20)–(22), (40) and (47)). In these special cases, the 'degree of mixture' of quantum states is characterized by the 'superpurity' (for $r = 0$), 'standard purity' (for $r = 1$) or von Neumann's entropy (for $r = \infty$). We have also found interpolation formulae for the limiting function $\Phi^{(r)}(\mu^{(r)})$ (5) in the cases of $r = 1$ (25) and 0 (41), as well as asymptotical formulae in the cases where $1 - \mu^{(r)} \ll 1$ (38) or $\mu^{(r)} \ll 1$ (42) with any value of r. Moreover, we have considered the nonclassical properties of mixed states minimizing the purity-bounded uncertainty relations, using as measures of 'nonclassicality' the Mandel parameter and the normalized Hilbert–Schmidt distance from ('classical') thermal states.

As a matter of fact, the problem discussed in this paper is a particular case of a more general problem formulated in [8]—to find stricter inequalities than the Heisenberg–Weyl inequality (1), if some additional information on the quantum system is known (such as, for instance, degrees of purity or internal entanglement for multidimensional systems, higher-order moments etc). Although some results in this direction have been obtained recently (e.g., corrections to (1) caused by some higher-order moments were considered in [61], but only for pure quantum states), a lot of work is still to be done. For example, lower bounds on the products of *higher-order statistical moments* for mixed states were the subject of paper [62], but only results of some numerical experiments were presented. It would also be interesting to try to generalize to the case of mixed states the concepts of the 'overall width' and the 'mean peak width' introduced by Hilgevoord and Uffink [63], as well as other different 'local' uncertainty relations discussed, for example, in the review [16].

Some generalizations of the purity-bounded uncertainty relations to the multidimensional case were found recently by Karelin and Lazaruk [64, 65]. They looked for inequalities for the product $\Delta\boldsymbol{x}\Delta\boldsymbol{p}$, where $\boldsymbol{x}, \boldsymbol{p}$ are s-dimensional vectors and (choosing a reference frame in which the first-order average values are equal to zero)

$$\Delta\boldsymbol{x} \equiv \frac{1}{s}\sum_{i=1}^{s}\mathrm{Tr}(\hat{x}_i^2\hat{\rho}), \qquad \Delta\boldsymbol{p} \equiv \frac{1}{s}\sum_{i=1}^{s}\mathrm{Tr}(\hat{p}_i^2\hat{\rho}).$$

In [64] Karelin and Lazaruk obtained an inequality which can be considered as a generalization of the asymptotical Bastiaans inequality (42) for $r = 1$ (i.e. for the standard purity $\mu = \mathrm{Tr}\;\hat{\rho}^2$)

$$(\Delta\boldsymbol{x}\Delta\boldsymbol{p})^s \geqslant \left(\frac{\hbar}{2}\right)^s\frac{C(s)}{\mu}, \qquad C(s) = \frac{2^{s+1}(s+1)!}{(s+2)^{s+1}},$$

$$C(1) = \tfrac{4}{9}, \qquad C(s\to\infty) \sim \left(\frac{2}{e}\right)^{s+2}\sqrt{\frac{\pi s}{2}}.$$

Stricter (and more complicated) inequalities, generalizing those considered in section 2, were considered in [65]. In particular, the following interpolating form was given:

$$\Delta\boldsymbol{x}\Delta\boldsymbol{p} \geqslant \frac{\hbar}{2}\,\frac{s + 2L(\mu)}{s+2},$$

where $L(\mu)$ is a root of the transcendental equation ($\Gamma(z)$ is Euler's gamma-function)

$$\mu = \frac{(s+2L)(s+1)!\,\Gamma(L)}{(s+2)\Gamma(L+s+1)}.$$

However, the story is not finished yet, because in the multi-dimensional case there are many different invariant combinations of variances for which inequalities generalizing (1) can be written [16, 17, 66]. It would be interesting to find stricter inequalities containing purities or entropies for these combinations, too.

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Appendix. Proof of inequality (11)

Due to the important role of inequality (11) in the derivation of the purity-bounded uncertainty relations, we reproduce here its proof given in [20][2].

Let the sequence of numbers b_m be defined by

$$b_m = \sum_{n=0}^{\infty} |a_{mn}|^2 \mu_n, \qquad m = 0, 1, \ldots,$$

where $\mu_0 \leqslant \mu_1 \leqslant \cdots \leqslant \mu_n \leqslant \cdots$ and coefficients a_{mn} satisfy the orthonormality condition

$$\sum_{n=0}^{\infty} a_{ln} a_{mn}^* = \delta_{lm}, \qquad l, m = 0, 1, \ldots.$$

One may consider the numbers b_m for $m = 0, 1, \ldots, M$ as the diagonal entries of an $(M+1)$-square Hermitian matrix $H = \|h_{ij}\|$ with

$$h_{ij} = \sum_{n=0}^{\infty} a_{in} a_{jn}^* \mu_n, \qquad i, j = 0, 1, \ldots, M.$$

Let the eigenvalues ν_m of H be ordered according to

$$\nu_0 \leqslant \nu_1 \leqslant \cdots \leqslant \nu_n \leqslant \cdots \leqslant \nu_M.$$

From Cauchy's inequalities for eigenvalues of a submatrix of a Hermitian matrix, we conclude that $\nu_m \geqslant \mu_m$ $(m = 0, 1, \ldots, M)$ and hence

$$\sum_{m=0}^{M} b_m = \sum_{m=0}^{M} h_{mm} = \sum_{m=0}^{M} \nu_m \geqslant \sum_{m=0}^{M} \mu_m.$$

Furthermore, with the numbers λ_m satisfying the property $\lambda_0 \geqslant \lambda_1 \geqslant \cdots \geqslant \lambda_m \geqslant \cdots$, we can formulate the chain of relations

$$\begin{aligned}
\sum_{m=0}^{M} \lambda_m b_m &= \lambda_0 b_0 + \sum_{m=1}^{M} \lambda_m b_m \\
&= \lambda_0 b_0 + \sum_{m=1}^{M} \lambda_m \left[\sum_{n=0}^{m} b_n - \sum_{n=0}^{m-1} b_n \right] \\
&= \lambda_0 b_0 + \sum_{m=1}^{M} \lambda_m \sum_{n=0}^{m} b_n - \sum_{m=0}^{M-1} \lambda_{m+1} \sum_{n=0}^{m} b_n \\
&= \sum_{m=0}^{M-1} \lambda_m \sum_{n=0}^{m} b_n + \lambda_M \sum_{n=0}^{M} b_n - \sum_{m=0}^{M-1} \lambda_{m+1} \sum_{n=0}^{m} b_n \\
&= \lambda_M \sum_{n=0}^{M} b_n + \sum_{m=0}^{M-1} (\lambda_m - \lambda_{m+1}) \sum_{n=0}^{m} b_n \\
&\geqslant \lambda_M \sum_{n=0}^{M} \mu_n + \sum_{m=0}^{M-1} (\lambda_m - \lambda_{m+1}) \sum_{n=0}^{m} \mu_n = \sum_{m=0}^{M} \lambda_m \mu_m.
\end{aligned}$$

[2] Where it was written that this proof was due to M L J Hautus.

On choosing $\mu_n = 2n + 1$ and taking the limit $M \to \infty$, we arrive at the inequality (11)

$$\sum_{m=0}^{\infty} \lambda_m \sum_{n=0}^{\infty} |a_{mn}|^2 (2n+1) \geqslant \sum_{m=0}^{\infty} \lambda_m (2m+1),$$

which becomes an equality if $|a_{mn}| = \delta_{mn}$.

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