Gaussianity bounds for quantum mixed states with a positive Wigner function

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Abstract. According to Hudson’s theorem, the only quantum pure states with a positive Wigner function are Gaussian states. We summarize and compare some recent attempts at extending this theorem to the space of quantum mixed states, and complement them with new results obtained from numerical observations. Specifically, we look for upper bounds on the admissible non-Gaussianity of mixed states with a positive Wigner function.

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1. Introduction
The Wigner representation of quantum states [1], which is realized by joint quasi-probability distributions of canonically conjugate variables such as $x$ and $p$, has a specific property that differentiates it from a true probability distribution: it can attain negative values. The existence of negative domains in the range of Wigner functions is usually interpreted as a signature of the non-classicality of the corresponding state. Several works have tried to establish theoretically a connection between this feature and other purely quantum effects such as entanglement [2], non-locality [3], and Schrödinger cats. In practice, the occurrence of negative areas in the range of the Wigner function of a state can be a requirement for the success of quantum information protocols since it guarantees that the probability distribution resulting from any quadrature measurement can not be “mimicked” by a classical local model [4, 5].

It was proven by Hudson [6] that, among pure states, the only ones with a non-negative everywhere Wigner function are Gaussian states [7]. A question that arises naturally is whether Hudson’s theorem can be extended to mixed states, among which not only Gaussian states may possess a positive Wigner function. The first formulation and solution to this problem in the space of mixed states is due to Bröcker and Werner [9]. Working with the Fourier-Weyl transform of density matrices, they suggested a classification of mixed states according to their Wigner spectrum. They proved that states with a positive Wigner function are the states which include 0 and 1 in their Wigner spectrum, and they further classified this set of these states. They showed, in particular, that the set of convex mixtures of Gaussian pure states is strictly included in the set of states with a positive Wigner function. However, even though this extension of Hudson’s theorem is mathematically accurate, calculating the Wigner spectrum of a state is a rather complicated procedure, rarely achievable, so these results are not operational.
In a recent work, we have suggested a different, more practical, formulation of the problem, focusing on Gaussianity [10]. Given that for pure states, Gaussianity dictates the positivity of Wigner functions, we have asked the question of how much a mixed state with positive Wigner function is allowed to deviate from a Gaussian state. We have followed two different approaches to this problem [10, 11], which we compare hereafter. Similarly as in these works, we restrict our consideration to the single-particle (single-mode) case. We then complement the results that we had obtained in [11] with a numerical search, and derive a simple criterion for the identification of mixed states possessing a Wigner function with negative areas in its range.

2. Review of our previous approaches
The first issue that arises with our suggested formulation of the extension of Hudson’s theorem is the definition of non-Gaussianity. The problem of characterizing the non-Gaussianity of a state strongly resembles an older one, namely that of quantifying the non-classical character of a state [12]. In analogy with the common definitions of non-classicality [13, 14, 15], the non-Gaussianity of a pure state is to be defined as the minimum of the distance from the given state to all Gaussian states. The used measure of distance can be any construction that satisfies the usual requirements of a distance [16] and, in addition, that is invariant under symplectic (Gaussian) transformations. However, when looking at a computable measure of non-Gaussianity, this definition, even if correct, is not easily applicable.

In our previous works, we have chosen a recently suggested, easily evaluable, measure of non-Gaussianity [17], namely the normalized Hilbert-Schmidt distance [18] of a given state from a reference Gaussian (in general mixed) state of the same covariance matrix \( \gamma \). According to this measure, the degree of non-Gaussianity \( \delta \) of a state \( \hat{\rho} \) from the reference Gaussian state \( \hat{\rho}_G \) is quantified as,

\[
\delta = \frac{1}{2\mu} \text{Tr} \left( (\hat{\rho} - \hat{\rho}_G)^2 \right) = \frac{\mu_G + \mu - 2\text{Tr} (\hat{\rho}\hat{\rho}_G)}{2\mu},
\]  

where \( \mu = \text{Tr} (\hat{\rho}^2) \) is the purity of the state \( \hat{\rho} \) and \( \mu_G = \text{Tr} (\hat{\rho}_G^2) \) is the purity of the corresponding Gaussian state \( \hat{\rho}_G \) (having the same covariance matrix \( \gamma \) as the state \( \hat{\rho} \)). Note that the purity of the Gaussian state \( \hat{\rho}_G \) can be simply expressed as \( \mu_G = 1/\sqrt{\text{det} \gamma} \). Observing that the non-Gaussianity \( \delta \) is expressed in terms of purities \( \mu \) and \( \mu_G \), we choose hereafter to use \( \mu \) and \( \mu_G \) as measures of mixedness and uncertainty, respectively. We have \( 0 \leq \mu \leq 1 \) and \( \mu = 1 \) for pure states, while we have \( \mu_G = 1/(\Delta x \Delta p) \) in the case of phase-invariant states, which makes the bridge with the Heisenberg uncertainty principle. We have \( 0 \leq \mu_G \leq 1 \) and \( \mu_G = 1 \) for (pure Gaussian) states saturating the uncertainty principle.

Now, having chosen the measures of non-Gaussianity \( \delta \), purity \( \mu \), and uncertainty \( \mu_G \), we can formulate our problem: given the purity \( \mu \) and covariance matrix \( \gamma \) (and therefore \( \mu_G \)), what is the maximum degree of non-Gaussianity \( \delta \) that a state may achieve provided that it possesses a positive Wigner function? In view of Equation (1), the search for a maximum non-Gaussianity can be replaced with the search for a minimum overlap \( \text{Tr} (\hat{\rho}\hat{\rho}_G) \) with the Gaussian reference state \( \hat{\rho}_G \). In this work, we mostly employ the second option. Such a formulation of the problem implies the need for an extremization procedure. The latter may work either in the space of density matrices, or with Wigner functions, or with characteristic functions (similarly as in the work [9]). Although all these representations are equivalent, as we will see each one has its own advantages and limits.

In our first attempt [10], we have worked in Wigner phase-space representation. There, we have employed the method of Lagrange multipliers in order to identify the positive Wigner functions that achieve the maximum degree of non-Gaussianity \( \delta \) given the constraints of \( \mu \) and \( \mu_G \). Together with these constraints, which are rather simple to account for in phase-space representation, one should also require that the solution to the extremization problem is a valid Wigner function corresponding to a physical quantum state. This last condition is
Unfortunately hard to express in phase-space representation. In the lack of such an applicable criterion in phase space [19], we have proceeded without it. Naturally, what we have obtained then is the maximum non-Gaussianity that a classical continuous distribution in phase-space may achieve. This provides an upper bound on the maximum non-Gaussianity of quantum states with a positive Wigner function and given $\mu$ and $\mu_G$. However, this upper bound was proven by our later results to be loose, that is, not attainable by any quantum state.

In our second attempt [11], we have worked in the state representation, that is, using density matrices. First, we have proven that among the states that achieve the minimum permitted value of $\mu$ for given values of $\text{Tr}(\hat{\rho}\hat{\rho}_G)$ and $\mu_G$, there necessarily are phase-invariant states, i.e., states which can be expressed as mixtures of number states (Fock states). This observation implies that a part of the lower bound on $\text{Tr}(\hat{\rho}\hat{\rho}_G)$ (or upper bound on the non-Gaussianity $\delta$) as a function of $\mu_G$ and $\mu$ is realized by phase-invariant states. Then, we have identified these extremal phase-invariant states with the method of Lagrange multipliers. In this way, we were able to find the maximally non-Gaussian states in some areas of the parametric space $\{\mu_G, \mu\}$. This is what we call the region-I lower bound on $\text{Tr}(\hat{\rho}\hat{\rho}_G)$ (or upper bound on the non-Gaussianity $\delta$) in Fig. 1 ([11]). In the rest of the parametric space $\{\mu_G, \mu\}$, the lower bound on $\text{Tr}(\hat{\rho}\hat{\rho}_G)$ corresponds to the upper bound on the purity $\mu$ when $\text{Tr}(\hat{\rho}\hat{\rho}_G)$ and $\mu_G$ are given.

This is the region-II lower bound on $\text{Tr}(\hat{\rho}\hat{\rho}_G)$ (or upper bound on the non-Gaussianity $\delta$) as exhibited in Fig. 3 in [11].

Similarly as with the extremization procedure in phase space, this procedure in density matrix representation cannot be used to account for all constraints of the problem. Indeed, we find here the maximum degree of non-Gaussianity for all mixed states and not just for states with a positive Wigner function. In fact, we could not just repeat the same procedure with the additional requirement of positivity of the Wigner function because there is no obvious way how to incorporate this constraint into the extremization problem formulated in terms of density matrices. We have proceeded numerically and have identified a part of the global bound on $\delta$ that is realized by states with positive Wigner function. Our simulation showed that the fraction of the bound where the maximum degree of non-Gaussianity for all states coincides with the maximum degree of non-Gaussianity for states with positive Wigner function is rather small, and it is mostly confined to the low-purity area (see Fig. 5 in [11]). However, for the rest, big part, of the parametric space $\{\mu_G, \mu\}$ we could not draw any conclusion.

3. Numerical search

In the present work, we pursue the search for a tight upper bound on the non-Gaussianity of states with a positive Wigner function, following a numerical approach. For reasons which become obvious below, we choose to work with the overlap $\text{Tr}(\hat{\rho}\hat{\rho}_G)$ instead of the non-Gaussianity $\delta$. As before, we start by dividing the lower bound on $\text{Tr}(\hat{\rho}\hat{\rho}_G)$ into two parts, namely, region-I where the purity $\mu$ is minimized and region-II where the purity $\mu$ is maximized for given values of $\text{Tr}(\hat{\rho}\hat{\rho}_G)$ and $\mu_G$. In Fig. 1, region-I and region-II correspond, respectively, to segment $G-M_1$ and $M_1-P_1$.

According to our previous work [11], we observe that the region-I of the bound for all states (segment $G-M_2$ in Fig. 1) can be achieved by the states with a phase-invariant Wigner function (regardless of the positivity of this Wigner function). The main step of the proof of this property is based on the Cauchy-Schwarz inequality, which holds for any pair of functions and does not depend on their positivity. Thus, this result is valid for all states, and it necessarily also holds for the subset of states with a positive Wigner function. Therefore, we can conclude that region-I of the bound for states with a positive Wigner function (segment $G-M_1$) can be realized by states with phase-invariant Wigner function, i.e., states that can be expressed as statistical mixtures of number states.

The numerical method to obtain the region-I of the bound for states with positive Wigner
Figure 1. An explanatory depiction of the bounds on the parametric space \( \{ \mu_G, \mu, \text{Tr}(\hat{\rho}\hat{\rho}_G) \} \) for all states (index 2) and for states with positive Wigner function (index 1) employing an indicative plane of fixed \( \mu_G \). Segment G-C: upper bound on \( \text{Tr}(\hat{\rho}\hat{\rho}_G) \) for all states. Segments G-P\(_{2(1)}\): lower bounds on \( \text{Tr}(\hat{\rho}\hat{\rho}_G) \). Segments G-A-M\(_{2(1)}\): region-I of the bounds. In this part the purity \( \mu \) is minimized for given values of \( \text{Tr}(\hat{\rho}\hat{\rho}_G) \) and \( \mu_G \). Segment M\(_{2(1)}\)-P\(_{2(1)}\): region-II. It stands for the part of the bound where the purity is maximized. Point G: Gaussian states.

function is straightforward. Among the convex combinations of number states

\[
\hat{\rho} = \sum_{n=0}^{N} p_n |n\rangle \langle n|
\]

with \( 0 \leq p_n \leq 1 \) and \( \sum_n p_n = 1 \), we identify the states which possess a positive Wigner function. Then, we pick the ones which achieve the minimum purity \( \mu \) given \( \text{Tr}(\hat{\rho}\hat{\rho}_G) \) and \( \mu_G \). We test states with \( N \) up to 50 and ensure that we sample over all possible combinations by choosing the mixing amplitudes \( \sqrt{p_n} \) uniformly over the Haar measure (actually over the positive part of the \( N \)-dimensional sphere). Overall, we test \( 2.5 \times 10^6 \) states and, among these, we identify \( \sim 5 \times 10^4 \) states with positive Wigner function. The selected states make region-I of the bound for states with a positive Wigner function. The latter, in turn, is composed of two parts, namely the one already identified in [11] which coincides with the global bound for all states (segment G-A in Fig. 1), and a new part which deviates from it (segment A-M\(_1\) in Fig. 1), though the deviation in terms of \( \text{Tr}(\hat{\rho}\hat{\rho}_G) \) does not exceed 0.2\%.

In Fig. 2, we present the region-I of the bounds for states with positive Wigner function and for all states projected on the planes \( \{ \mu_G, \delta \} \) and \( \{ \mu_G, \mu \} \). There, we also mark the area of coincidence for the two bounds.

Now, let us study in more details the states which belong the region-I of the bounds and which achieve the lowest values of \( \text{Tr}(\hat{\rho}\hat{\rho}_G) \) (points \( M_1 \) and \( M_2 \) in Fig. 1). Such states realize the boundary between region-I and region-II of the bound, and thus provide us with an ultimate (independent of the purity \( \mu \)) lower bound on \( \text{Tr}(\hat{\rho}\hat{\rho}_G) \). In the case of the states with positive Wigner function, we identify this lower bound from our numerical data and represent it in Fig. 3 (thin solid line) using a polynomial function

\[
M_1 (\mu_G) = 0.0095 + 0.620 \mu_G + 0.711 \mu_G^2 - 0.333 \mu_G^3,
\]

fitting the numerical data in very good approximation. In Fig. 3, we also present (lower bold line) the minimum \( \text{Tr}(\hat{\rho}\hat{\rho}_G) \) for all states which, as was proven in [11], is realized by mixtures
**Figure 2.** Region-I of the non-Gaussianity bound. In (a), the bound for all states projected on the plane \{\(\mu_G, \delta\)\} for different values of \(\mu\) covers the region between the line \(\delta = 0\) and the blue solid line. The allowed states lie below the surface generated by this bound for varying values of \(\mu\). The case of states with a positive Wigner function is similar, except that the blue solid line is replaced by the black dotted line. In (b) the bound for all states projected on the plane \{\(\mu_G, \mu\)\} for different values of \(\delta\) mostly covers the area between the line \(\mu_G = \mu\) and the blue solid line, while it even goes slightly below \(\mu_G = \mu\) as a careful inspection reveals. Note that for states below \(\mu_G = \mu\), the non-Gaussianity is bounded both from below and above and a double-valued projection appears in (b). Again, the case of states with a positive Wigner function is similar, except that the blue solid line is replaced by the black dotted line. Finally, we observe in (a) and (b) that a part of the bound for all states coincides with that for states with a positive Wigner function. This coinciding part of the two bounds is marked with a red grid.

\[ M_2(\mu_G) = \frac{4\mu_G^2(\mu_G - 1)^n}{(\mu_G + 1)^{n+2}} (1 + n), \]  

where \(n = 0, 1, \ldots\) and \(p = (1 - 4(1 + n)\mu_G + (5 + 8n + 4n^2)\mu_G^2) / 2\mu_G^2 \in [0, 1]\). From Fig. 3, one can see that in a certain region of \(\mu_G\), the two ultimate lower bounds, Eqs. (3) and (4), do not coincide. This clear difference suggests a sufficient condition for the existence of negative parts in the range of the Wigner function of a mixed state: if a state characterized by a given uncertainty (i.e., a purity of the corresponding Gaussian states equal to \(\mu_G\)) achieves a value of \(\text{Tr}(\hat{\rho}\hat{\rho}_G)\) lower than function \(M_1(\mu_G)\), then its Wigner function cannot be everywhere non-negative. In other words, if the non-Gaussianity \(\delta\) of the state exceeds a given threshold, then the state must have areas of negative values in its Wigner function.

A second question that we face, of course, is the identification of the region-II (segment \(M_1-P_1\) in Fig. 1) of the bound for states with positive Wigner function. Contrary to the case of
region-II for all states [11], we have no information about the structure of the states which realize the bound. However, for states with a positive Wigner function, one can infer the position of the bound in the limit of pure states \( \mu \to 1 \) (point \( P_1 \) in Fig. 1) in the following way. From Hudson’s theorem, it is known that the only pure states with positive Wigner function are Gaussian states \( \mu_G = 1 \). Therefore, one can show that the mixed states with positive Wigner function which may approach the limit of \( \mu \to 1 \) (keeping \( \mu_G < 1 \)) must be a mixture of a pure Gaussian state with some other state possessing a positive Wigner function with the mixing amplitude of the Gaussian state tending to 1. When considering the approach to the limit of pure states, one should simultaneously increase the distance (in phase space) between the two states in order to cover the whole range of values \( \mu_G \) that quantifies the “spreading” of the Wigner function, otherwise we would have \( \mu_G \to 1 \) as \( \mu \to 1 \).

All the states we have tested numerically give the same result for Tr \( (\hat{\rho} \hat{\rho}_G) \) in the limit of pure states. The simplest one, which we choose to present here, is a mixture of two displaced and squeezed states expressed in the Wigner phase space as

\[
W(x, p, q, s, \alpha) = \frac{\alpha}{\pi} e^{-\frac{(x-q)^2}{2s^2}} + \frac{(1-\alpha)}{\pi} e^{-\frac{(x+q)^2}{2s^2}}.
\]  

(5)

The limit of pure states \( \mu \to 1 \) is achieved, for example, when \( \alpha \to 0 \) while \( \alpha sq^2 \) is kept equal to some constant in order to have a fixed value of \( \mu_G < 1 \). For the state of Eq. (5), we have analytically derived the limiting value of Tr \( (\hat{\rho} \hat{\rho}_G) \) as a function of \( \mu_G \), namely

\[
P_1(\mu_G) = \sqrt{2\mu_G}/\sqrt{1+\mu_G^2}.
\]  

(6)

We present this limiting case in Fig. 3 as a dotted line. In comparison with the ultimate lower bound, Eq. (3), this value of Tr \( (\hat{\rho} \hat{\rho}_G) \) is much higher. We note here that this limit \( \mu \to 1 \) is rather singular, as we can find states with a positive Wigner function which are almost pure, while their non-Gaussianity is far from zero (hence, they are far from saturating the uncertainty principle). Physically, these states correspond to the mixture of a Gaussian state with an infinitesimal fraction of another one, whose distance in phase space is increasingly large to keep a fixed value of the uncertainty \( \mu_G \).

Finally, for completeness, we present in Fig. 3 the ultimate upper bound on Tr \( (\hat{\rho} \hat{\rho}_G) \) for all states, given by \( \sqrt{\mu_G} \) as that we derived in [10] employing the Cauchy-Schwartz inequality.
4. Conclusions

In conclusion, we have presented analytical and numerical estimates of the upper bound on the non-Gaussianity $\delta$ of mixed states with positive Wigner functions. From Hudson’s theorem, we know that such an upper bound vanishes for pure states, but the question of estimating the highest achievable non-Gaussianity remains open in the case of mixed states, which are the states most often encountered in realistic situations. We have considered the division of the upper bound on $\delta$ into two parts, one that minimizes the purity (region-I) and one that maximizes the purity (region-II) for fixed $\mu_G$ and $\text{Tr}(\rho \rho_G)$. We have numerically identified region-I of the bound, and have shown that this part deviates slightly from the corresponding bound for all states derived in [11]. In a second time, we have numerically investigated region-II of the bound, and have found an indication that it moves further away from the corresponding bound for all states as the purity increases. Finally, we have numerically identified the lower bound on $\text{Tr}(\hat{\rho} \hat{\rho}_G)$ that a state with positive Wigner function may attain given $\mu_G$. For some interval of values of $\mu_G$, this bound is distinct from the one for all states [11], and can be used as a sufficient criterion for the existence of negative parts in a Wigner function of a state.

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