Extending Hudson's theorem to mixed quantum states

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According to Hudson's theorem, any pure quantum state with a positive Wigner function is necessarily a Gaussian state. Here, we make a step toward the extension of this theorem to mixed quantum states by finding upper and lower bounds on the degree of non-Gaussianity of states with positive Wigner functions. The bounds are expressed in the form of parametric functions relating the degree of non-Gaussianity of a state, its purity, and the purity of the Gaussian state characterized by the same covariance matrix. Although our bounds are not tight, they permit us to visualize the set of states with positive Wigner functions.

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The Wigner representation of quantum states [1], which is realized by joint quasiprobability distributions of canonically conjugate variables in phase space, has a specific property which differentiates it from a true probability distribution: it can attain negative values. Among pure states, it was proven by Hudson [2] (and later generalized to multimode quantum systems by Soto and Claverie [3]) that the only states which have non-negative Wigner functions are Gaussian states [4]. The question that naturally arises [2] is whether this theorem can be extended to mixed states, among which not only Gaussian states may possess a positive Wigner function. A logical extension of the theorem would be a complete characterization of the convex set of states with positive Wigner function. Although this question can be approached by using the notion of Wigner spectrum [5], a simple and operational extension of Hudson's theorem has not yet been achieved due to the mathematical complications which emerge when dealing with states with positive Wigner functions [5].

Motivated by the increasing interest for non-Gaussian states in continuous-variable quantum information theory (see, e.g., [6]) and the need for a better understanding of the de-Gaussification procedures for mixed states (see, e.g., [7]), we attempt here an exploration of the set of states with positive Wigner functions using Gaussian states as a reference. More precisely, we consider the subset of such states that have the same covariance matrix as a reference Gaussian state. We obtain a partial solution to the problem by analytically deriving necessary conditions (bounds) on a measure of non-Gaussianity for a state to have a positive Wigner function. This set of conditions bounds a region in a three-dimensional space with coordinates being the purity of the state, the purity of the corresponding Gaussian state, and the non-Gaussianity. As intuitively expected, the maximum degree of non-Gaussianity increases with a decrease in the purity of both the state and its Gaussian corresponding state.

Before deriving the main results of this paper, let us recall a convenient representation of the trace of the product of two one-mode quantum states, ρ and ρ', in terms of the Wigner representation [8],

$$\mathrm{Tr}(\rho\rho') = 2\pi\int\int dx\, dp W_\rho(x,p)W_{\rho'}(x,p), \qquad (1)$$

where W_ρ is the *Wigner function* of the state ρ. For example, the *purity* of a state, $\mu[\rho]=\mathrm{Tr}(\rho^2)$, may be calculated with the help of this formula. For a state with a *Gaussian* Wigner function determined by the covariance matrix γ and displacement vector $\mathbf{d}$, the purity is simply $\mu[\rho_G]=(\det\gamma)^{-1/2}$. The matrix elements of the covariance matrix of state ρ are defined as

$$\gamma_{ij} = \mathrm{Tr}(\{(\hat{r}_i - d_i),(\hat{r}_j - d_j)\}\rho), \qquad (2)$$

where $\hat{\mathbf{r}}$ is the vector of quadrature operators $\hat{\mathbf{r}}=(\hat{x},\hat{p})^T$, $\mathbf{d}=\mathrm{Tr}(\hat{\mathbf{r}}\rho)$, and $\{\cdot,\cdot\}$ is the anticommutator. Note that we can put the displacement vector to zero with no loss of generality since the purity (and all quantities we will be interested in) does not depend on $\mathbf{d}$. We will thus consider states centered on the origin in this paper.

Our aim is to derive bounds on the non-Gaussianity, i.e., on the "distance" between a state ρ of purity $\mu[\rho]$ possessing a positive Wigner function and the Gaussian state ρ_G determined by the same covariance matrix. While there are different measures in the literature for quantifying the distance between two mixed states, we have chosen to use a recently proposed one [9],

$$\delta[\rho,\rho_G] = \frac{\mu[\rho]+\mu[\rho_G]-2\,\mathrm{Tr}(\rho\rho_G)}{2\mu[\rho]}. \qquad (3)$$

Although the quantity $\delta[\rho,\rho_G]$ is obviously not symmetric under the permutation of the two states, it is convenient for quantifying the non-Gaussian character of ρ in the sense that $\delta\in[0,\varepsilon]$, with $\varepsilon<1$, and $\delta=0$ is attained if and only if $\rho\equiv\rho_G$. For one-mode states, it is conjectured in Ref. [9] that $\varepsilon=1/2$.

In a first step, we are going to derive bounds on the trace overlap $\mathrm{Tr}(\rho\rho_G)$ for fixed values of $\mu[\rho_G]$ and $\mu[\rho]$. It will then be straightforward to express bounds on the non-Gaussianity $\delta[\rho,\rho_G]$ in terms of $\mu[\rho_G]$ and $\mu[\rho]$ by using Eq. (3).

We use Eq. (1) in order to reformulate the problem as an optimization problem that can be tackled with the method of Lagrange multipliers. More specifically, we need to extremize the functional $I[W_\rho]=\mathrm{Tr}(\rho\rho_G)$ represented by Eq. (1) with the constraint that the Gaussian Wigner function W_{ρ_G}

and the positive function W_ρ possess the same second order moments. In order to simplify our derivation, we apply a symplectic transformation S on the states ρ and ρ_G, giving $S\rho S^\dagger$ and $S\rho_G S^\dagger$, respectively, in such a way that the Gaussian state becomes invariant under rotation in the x-p plane (i.e., becomes a thermal state). In this way the problem is reduced to a simpler but equivalent one since the functional $I[W_\rho]$ and the purities of the states remain invariant under S and since the positivity of W_ρ is preserved. This last statement can be justified by the fact that the time evolution of a Wigner function under a quadratic Hamiltonian can always be viewed as an affine transformation on the variables x and p [8]. Furthermore, we claim that the function W_ρ^{ex} which extremizes the functional $I[W_\rho]$ is invariant as well under rotation in the x-p plane, and we will justify this assumption at the end of the derivation.

After application of the symplectic transformation and under the assumption of rotation-invariant solutions, the functions $W_\rho(r)$ and $W_{\rho_G}(r)=\frac{1}{2\pi C}e^{-r/2C}$ only depend on the squared radius $r=x^2+p^2$, and the functional $I[W_\rho]$ is written in a simpler form as

$$I[W_\rho]=\mathrm{Tr}(\rho\rho_G)=2\pi^2\int_0^\infty W_\rho(r)W_{\rho_G}(r)dr. \tag{4}$$

The constrains that we impose on the function W_ρ can be summarized as follows:

(1) It is positive for the values of r belonging to some set $\mathfrak{s}$ and zero elsewhere.

(2) It is normalized, $\pi\int_{\mathfrak{s}}W_\rho(r)dr=1$.

(3) It has the same variance as the corresponding Gaussian state, ρ_G,

$$\pi\int_{\mathfrak{s}}W_\rho(r)rdr=2C=1/\mu[\rho_G]. \tag{5}$$

(4) It is such that the state ρ has purity $\mu[\rho]$,

$$2\pi^2\int_{\mathfrak{s}}W_\rho^2(r)dr=\mu[\rho]. \tag{6}$$

(5) It is square integrable and continuous.

This last requirement follows directly from the general property of Wigner functions,

$$\int_{-\infty}^\infty W(x,p)dp=\langle x|\rho|x\rangle, \tag{7}$$

$$\int_{-\infty}^\infty W(x,p)dx=\langle p|\rho|p\rangle. \tag{8}$$

Recall that a state can always be diagonalized in a basis of pure states, namely, $\rho=\Sigma_i\lambda_i|\psi_i\rangle\langle\psi_i|$. Since wave functions must satisfy the conditions of continuity and integrability in both position and momentum representation, one concludes that a Wigner function of variables x and p and more generally of any variable that is a continuous function of these, e.g., $r=x^2+p^2$, has to satisfy the same requirements.

Finally, let us stress that without the requirement of positive definiteness of the operator ρ, the set of conditions listed above is *not sufficient* to constrain the solutions $W_\rho(r)$ to eligible Wigner functions. To our knowledge, there exists no operational criterion on phase-space functions ensuring that the operator ρ is physical (see [10] for an extensive discussion). On the other hand, one can verify whether a quasiprobability distribution is unphysical by using a theorem which states that a square integrable and normalized function is an eligible Wigner function if its overlap with the Wigner function of *every* pure state is positive [11].

After having applied the method of Lagrange multipliers, we obtain the extremal solution

$$W_\rho^{ex}(r)=A_1+A_2\frac{1}{2\pi C}e^{-r/2C}+A_3 r, \tag{9}$$

with the A's being determined by conditions 2–4. Square integrability, condition 5, limits the class of possible functions $W_\rho^{ex}(r)$ in Eq. (9) to those that have zero, one, or two positive roots denoted as r_B (in the one- and two-root cases) and r_A (in the two-root case). Furthermore the condition of continuity dictates that $\mathfrak{s}=[r_A,r_B]$ in the two-root case, $\mathfrak{s}=[0,r_B]$ in the one-root case, and $\mathfrak{s}=[0,\infty]$ in the zero-root case. The latter case is the trivial one, where $W_\rho^{ex}(r)$ coincides with $W_{\rho_G}(r)$ and thus $\delta[\rho,\rho_G]$ vanishes. We treat the other two cases separately and obtain two continuously connected branches of solutions for W_ρ^{ex}. The expressions that we obtain for $\mathrm{Tr}(\rho\rho_G)^{ex}$ and $\mu[\rho]^{ex}$ are highly nonlinear, so that it is not possible to derive an analytic expression that directly connects the two quantities. Nevertheless, we are able to express the extremal solutions in the form of parametric functions.

(I) Two roots: $W_\rho^{ex}(r_A)=W_\rho^{ex}(r_B)=0$. We express the extremum purity $\mu[\rho]^{ex}$ and overlap $\mathrm{Tr}(\rho\rho_G)^{ex}$ in terms of the purity of the corresponding Gaussian state $\mu[\rho_G]$ and parameter $\alpha=(r_B-r_A)\mu[\rho_G]$,

$$\mu[\rho]^{ex}=\mu[\rho_G]\frac{2[\alpha^2-9\,\sinh(\alpha)\alpha+2(\alpha^2+6)\cosh(\alpha)-12]}{3\alpha\left[\alpha\,\cosh\left(\frac{\alpha}{2}\right)-2\,\sinh\left(\frac{\alpha}{2}\right)\right]^2}, \tag{10}$$

$$\mathrm{Tr}(\rho\rho_G)^{ex}=\mu[\rho_G]2\,\exp\left\{-\frac{\alpha[\alpha+e^\alpha(2\alpha-3)+3]}{3[e^\alpha(\alpha-2)+\alpha+2]}\right\}\times(e^\alpha-1)/\alpha, \tag{11}$$

where $0<\mu[\rho_G]\le 1$. By imposing the condition $r_A>0$, we obtain the bound $0<\alpha\le x_r$, with x_r being the root of equation,

$$e^x(x-3)+2x+3=0. \tag{12}$$

(II) One root: $W_\rho^{ex}(r_B)=0$. The extremal solution is defined by the following pair of parametric functions,

$$\mu[\rho]^{ex} = \mu[\rho_G]\frac{4\{e^{2\beta}(\beta-3)^2 + 8e^{\beta}\beta(\beta-3) + \beta[\beta(2\beta+9)+12]-9\}}{[2e^{\beta}(\beta-3)+\beta(\beta+4)+6]^2}, \tag{13}$$

$$\mathrm{Tr}(\rho\rho_G)^{ex} = \mu[\rho_G]\frac{4\{\beta[\cosh(\beta)+2]-3\sinh(\beta)\}}{2e^{\beta}(\beta-3)+\beta(\beta+4)+6}, \tag{14}$$

where $0<\mu[\rho_G]\leq 1$ and $\beta = r_B\mu[\rho_G]$. The range of the latter parameter is $\beta \geq x_r$.

We now need to show that, although we have only considered solutions W_ρ^{ex} with no angular dependence, our result is general. If we waive this assumption and consider the most general case, we arrive to

$$W_\rho^{ex}(x,p) = A_1 + A_2\frac{1}{2\pi C}e^{-(x^2+p^2)/2C} + A_3x^2 + A_4p^2 + A_5xp, \tag{15}$$

which is the analog of Eq. (9) but allowing for an angular dependence. We can then apply a phase rotation on states ρ and ρ_G in order to eliminate the term A_5xp in Eq. (15). Such a rotation does not affect the corresponding Gaussian state (since it is thermal) nor the trace overlap, so that the resulting extremal function becomes symmetric by reflection with respect to the x or p axis in phase space. The condition $\langle x^2\rangle = \langle p^2\rangle = C$ for the function in Eq. (15) is satisfied if $A_3 = A_4$. Thus, the most general solution reduces to the rotation-invariant one, namely, Eq. (9).

By using the derived bounds on the trace overlap [Eqs. (10)–(14)], we plot in Fig. 1(a) the corresponding (upper) bounds on the non-Gaussianity $\delta[\rho,\rho_G]^{ex}$. By direct inspection, we conclude that the intersection of the plotted surface with the plane of pure states $\mu[\rho]=1$ provides us with an upper bound on the non-Gaussianity of any state with a positive Wigner function and fixed covariance matrix (or, equivalently, fixed $\mu[\rho_G]$) which is independent of its purity $\mu[\rho]$. We denote it as the *ultimate upper bound* $\delta^{u.ult}(\mu[\rho_G])$ and its parametric expression can be directly derived by setting $\mu^{ex}[\rho]=1$ in Eqs. (10)–(14). In Fig. 2 we plot $\delta^{u.ult}$ together with a lower estimation on this, $\delta^{l.ult}$, obtained by the convex combination of two symmetrically displaced coherent states. The tight ultimate upper bound on $\delta[\rho,\rho_G]$ must be located between these two curves.

The bounds derived by using the Lagrange multiplier method confine δ only from above. In order to obtain a lower bound on δ, we need to find an upper bound on the trace overlap. We achieve this by applying the Cauchy-Schwarz inequality on the Wigner representation of the trace overlap [Eq. (1)]. By using the definition of the purity, we arrive at

$$\mathrm{Tr}(\rho\rho_G) \leq \sqrt{\mu[\rho_G]\mu[\rho]} \equiv \mathrm{Tr}(\rho\rho_G)_{\mathrm{CS}} \tag{16}$$

where CS stands for "Cauchy-Schwarz." This bound, displayed in Fig. 1(b), delimits together with the upper bound of Fig. 1(a), the region accessible for states with positive Wigner function in this 3D representation. Let us note that this lower bound holds for states with both positive and negative Wigner functions.

Let us now address the question of the physicality of the upper bound, namely, the extremal solution W_ρ^{ex}. By resorting to Hudson's theorem, we can conclude that the intersections of the surface with the planes $\mu[\rho]=1$ and $\mu[\rho_G]=1$ [see dotted and double thick blue lines in Fig. 1(a)] cannot correspond to physical states where $\delta \neq 0$. The only physical solution belonging to these lines is thus one point, namely, $\mu[\rho]=1$, $\mu[\rho_G]=1$, and $\delta=0$. In order to test the physicality of the rest of the surface, we applied the theorem mentioned

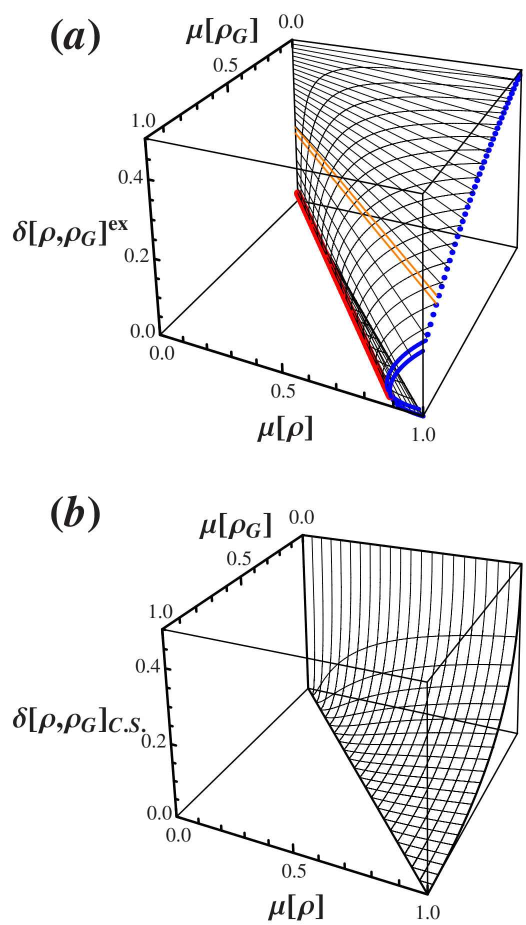

FIG. 1. (Color online) (a) Upper bound on non-Gaussianity $\delta[\rho,\rho_G]^{ex}$ derived with the Lagrange multiplier method. The double thin orange line marks the boundary between the two branches of solutions. The dotted blue line indicates the intersection with the plane $\mu[\rho]=1$ (also noted $\delta^{u.ult}$ in Fig. 2) while the double thick blue line shows the intersection with the plane $\mu[\rho_G]=1$. The red thick straight line denotes the "left" extremity of the surface. (b) Lower bound on non-Gaussianity $\delta[\rho,\rho_G]_{\mathrm{CS}}$ implied by the Cauchy-Schwarz inequality. We plot this lower bound only up to the intersecting line of $\delta[\rho,\rho_G]_{\mathrm{CS}}$ and $\delta[\rho,\rho_G]^{ex}$ ($\mu[\rho_G]=\mu[\rho]$ and $\delta[\rho,\rho_G]=0$).

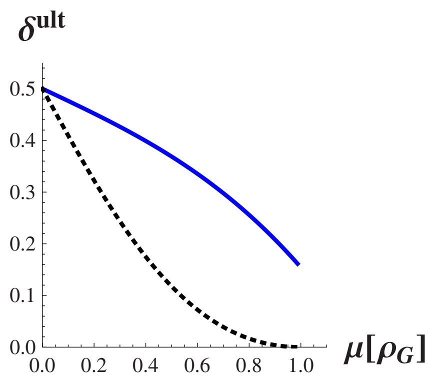

FIG. 2. (Color online) Ultimate upper bound $\delta^{u.ult}$ (blue solid line) on the non-Gaussianity of states with positive Wigner function as a function of the purity of corresponding Gaussian state $\mu[\rho_G]$. A lower estimate $\delta^{l.ult}$ (black dashed line) on the ultimate upper bound that was obtained for a mixture of coherent states. The two curves limit the region where the tight ultimate upper bound on non-Gaussianity must be located.

above employing the eigenstates of the quantum harmonic oscillator as test pure states. From our analytical results on the first 40 number states, we infer that the only functions W_ρ^{ex} giving a positive overlap with every number state as $n \to \infty$ are the states with $\mu[\rho_G]=0$, that is, infinitely mixed states. Therefore, we conclude that the extremal solution of the form of Eq. (9) is unfortunately unphysical; hence, *our bound is not tight*.

Finally, one may notice in Fig. 1(a) that the left extremity of the bound (red thick straight line) is on the left of the plane $\mu[\rho_G]=\mu[\rho]$. The equation for this line can be easily derived,

$$\mu[\rho] = \tfrac{8}{9}\mu[\rho_G] \tag{17}$$

and thus sets a lower bound on the purity of a mixed state given the purity of the corresponding Gaussian state. This bound has been derived in another context by Bastiaans [12] and has been proven to be the asymptotic form of an exact expression derived later by Dodonov and Man'ko [13] in the context of purity bounded uncertainty relation. The exact bound is more strict than the bound in Eq. (17), and it is realized by positive Wigner functions [14]. This fact confirms again that our bound is unphysical but it also gives some evidence about the underlying link between Hudson's theorem and the Heisenberg uncertainty principle.

In conclusion, we have found both upper and lower bounds on the non-Gaussianity of mixed states with positive Wigner function. These bounds only depend on the purity and covariance matrix of these states, and an ultimate upper bound can be derived that does not even depend on the purity, making it experimentally accessible. An open question remains to derive tighter bounds for the non-Gaussianity. All our results apply to one single mode, so another natural question would be to investigate the case of several modes.

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